

# PLENARY AND KEYNOTE / INVITED SPEAKERS

## CST AWARDEES 2023

## PLENARY SPEAKERS



**Alexander Kuhn**

2023 CNRS Silver Medal  
 Institute of Molecular Sciences,  
 University of Bordeaux

PL-01



**Andrew P. Dove**

2022 Corday-Morgan Prize  
 School of Chemistry,  
 University of Birmingham

PL-02



**Pimchai Chaiyen**

L'Oréal-UNESCO Woman  
 Science Crytal Award  
 School of Biomolecular Science  
 and Engineering, VISTEC

PL-03



**Javier García Martínez**

IUPAC President  
 Department of Inorganic Chemistry,  
 University of Alicante

PL-04

### Plenary Lectures:

Date : **January 26, 2024**

Room : **Bhiraj Halls II and III**

11:15 - 12:00 PL-01 : Unconventional approaches to energy conversion

15:15 - 16:00 PL-02 : Designing polymers with the end in mind:  
 Creating circular routes to polymers using light-based strategies

Date : **January 27, 2024**

Room : **Bhiraj Halls II and III**

09:00 - 09:45 PL-03 : Enzyme catalysis for green chemistry

16:15 - 17:00 PL-04 : Rethinking our relationship with the planet at molecular scale

## KEYNOTE / INVITED SPEAKERS

### AC : Analytical Chemistry



**Ryszard Lobinski**

IPREM - UMR5254, France



**Qiuquan Wang**

Xiamen University, China



**Shin-Ichi Ohira**

Kumamoto University, Japan



**Nadnudda Rodthongkum**

Chulalongkorn University, Thailand



**Takashi Kaneta**

Okayama University, Japan

## KEYNOTE / INVITED SPEAKERS

### CC : Catalytic Chemistry



**Günther Rupprechter**

Technische Universität Wien, Austria



**Hirotomo Nishihara**

Tohoku University, Japan



**Edman Tsang**

University of Oxford,  
United Kingdom



**Chularat Wattanakit**

Vidyasirimedhi Institute of Science  
and Technology (VISTEC), Thailand



**Pongtanawat Khemthong**

National Nanotechnology Center  
(NANOTEC), Thailand



**Thongthai Wittoon**

Kasetsart University, Thailand

## KEYNOTE / INVITED SPEAKERS

### CE : Chemical Education



**Saksri Supasorn**

Ubon Ratchathani University,  
Thailand



**Witawas Handee**

Silpakorn University, Thailand



**Pattamaporn Pimthong**

Kasetsart University, Thailand

## KEYNOTE / INVITED SPEAKERS

### EE : Environmental Chemistry and Renewable Energy



**Sandhya Babel**

Sirindhorn International Institute of  
Technology (SIIT), Thailand



**Joseph S. M. Samec**

Stockholm University, Sweden



**Tosapol Maluangnont**

King Mongkut's Institute of  
Technology, Thailand



**Pawin Iamprasertkun**

Sirindhorn International Institute of  
Technology (SIIT), Thailand



**Il-Kwon Oh**

Ajou University, Korea



**Wanida Jinsart**

Chulalongkorn University, Thailand

## KEYNOTE / INVITED SPEAKERS

### FA : Food, Agriculture and Cosmetics



**Kamolwan Israkarn**

National Metal and Materials  
Technology Center (MTEC), Thailand



**Naphatsorn Ditthawutthikul**

Mae Fah Luang University, Thailand



**Kunchit Judprasong**

Mahidol University, Thailand

## KEYNOTE / INVITED SPEAKERS

### IC : Inorganic Chemistry



**Christophe M. Thomas**

Chemie ParisTech, PSL University,  
France



**Jan J. Weigand**

Technical University Dresden,  
Germany



**Takumi Konno**

National Taiwan Normal University, Taiwan  
Osaka University, Japan



**Khamphree Phomphrai**

Vidyasirimedhi Institute of Science  
and Technology (VISTEC), Thailand



**Worawat Wattanathana**

Kasetsart University, Thailand



**Thanthapatra Bunchuay**

Mahidol University, Thailand

## KEYNOTE / INVITED SPEAKERS

### IE : Industrial and Engineering Chemistry



**Sineenuch Kokanutaporn**

Thai Eastern Group, Thailand



**Natthakorn Kraikul**

PTT Global Chemical Public  
Company Limited, Thailand



**Sasinotai Rochanutama**

Indorama Ventures PCL, Thailand



**Apichai Jomphoak**

National Electronics and  
Computer Technology Center  
(NECTEC), Thailand

## KEYNOTE / INVITED SPEAKERS

### MN : Material Chemistry and Nanotechnology



**Thuc-Quyen Nguyen**

University of California,  
Santa Barbara, USA



**T. Randall Lee**

University of Houston, USA



**Wisit Hirunpinyopas**

Kasetsart University, Thailand



**Il Won Kim**

Soongsil University, Korea

## KEYNOTE / INVITED SPEAKERS

### MN : Material Chemistry and Nanotechnology



**Jeng-Yu Lin**

Tunghai University, Taiwan



**Chen-Yu Yeh**

National Chung Hsing University,  
Taiwan



**Kanokwan Kongpatpanich**

Vidyasirimedhi Institute of Science  
and Technology (VISTEC), Thailand

## KEYNOTE / INVITED SPEAKERS

NP : Natural Products, Biological Chemistry and Chemical Biology



**Masaki Kuse**

Kobe University, Japan



**Shuangjun Lin**

Shanghai Jiao Tong University, China



**Prasat Kittakoop**

Chulabhorn Graduate Institute,  
Thailand



**Kowit Hengphasatporn**

University of Tsukuba, Japan



**Mylene Uy**

Mindanao State University-Iligan Institute  
of Technology, Philippines

## KEYNOTE / INVITED SPEAKERS

OM : Organic Synthesis and Medicinal Chemistry



**Karol Grela**

University of Warsaw, Poland



**Roderick W. Bates**

Nanyang Technological University,  
Singapore



**Sunisa Akkarasamiyo**

Kasetsart University, Thailand



**Mihaiela Stuparu**

Nanyang Technological University,  
Singapore



**Anna Kajetanowicz**

University of Warsaw, Poland

## KEYNOTE / INVITED SPEAKERS

PC : Polymer Chemistry and Bio-Based Materials



**Nikos Hadjichristidis**

King Abdullah University of Science and  
Technology (KAUST), Saudi Arabia



**Voravee P. Hoven**

Chulalongkorn University, Thailand



**Pakorn Opaprakasit**

Sirindhorn International Institute of  
Technology (SIIT), Thailand



**Panya Sunintaboon**

Mahidol University, Thailand



**Yasuhiro Morisaki**

Kwansei Gakuin University, Japan

## KEYNOTE / INVITED SPEAKERS

### PT : Physical and Theoretical Chemistry



**Seiji Mori**

Ibaraki University, Japan



**Toshifumi Mori**

Kyushu University, Japan



**Deanpen Japrunng**

National Nanotechnology Center  
(NANOTEC), Thailand



**Cheng-Chau Chiu**

National Sun Yat-sen University,  
Taiwan



**Siriporn Jungsuttiwong**

Ubon Ratchathani University,  
Thailand

## CST AWARDEES 2023



**CST Distinguished Chemist Award 2023  
(Analytical Chemistry)**

**Duangjai Nacapricha**

Mahidol University, Thailand



**CST Distinguished Young Chemist  
Award 2023 (Inorganic Chemistry)**

**Jaursup Boonmak**

Khon Kaen University, Thailand



**ACES-CST Early Career Award for  
Contribution to Green Chemistry 2023**

**Thanyaporn Wongnate**

Vidyasirimedhi Institute of Science and  
Technology (VISTEC), Thailand



**Shimadzu CST  
Young Chemist Award 2023**

**Thanit Praneenarat**

Chulalongkorn University, Thailand



**Merck CST  
Distinguished Dissertation Award 2023**

**Sopon Butcha**

Vidyasirimedhi Institute of Science and  
Technology (VISTEC), Thailand



**Metrohm-CST  
Young Chemist Award 2023**

**Panwad Chavalekvirat**

Thammasat University, Thailand

## CST AWARDEES 2023



**Merck CST-TYCN for  
Sustainable Future Award 2023**

**Thanthapatra Bunchuay**  
Mahidol University, Thailand



**Dow CST Award for  
Distinguished School Science Teacher 2023  
Lower Secondary Education**

**Pongsaton Panyanukit**  
Hatyaiwittayalai 2 School



**Dow CST Award for  
Distinguished School Science Teacher 2023  
Upper Secondary Education**

**Nuttarikan Khamchu**  
Prachinratsadornamroong School

**BILATERAL SYMPOSIUM  
BETWEEN THAILAND AND JAPAN  
ON RECENT PROGRESS OF PHOTOPHYSICAL CHEMISTRY**



**Kazuo Akagi**

Ritsumeikan University, Japan



**Nawee Kungwan**

Chiang Mai University, Thailand



**Shigeyuki Yagi**

Osaka Metropolitan University, Japan



**Suwat Nanan**

Khon Kaen University, Thailand



**Ken-ichi Sugiura**

Tokyo Metropolitan University, Japan



**Kontad Ounnunkad**

Chiang Mai University, Thailand

**BILATERAL SYMPOSIUM  
BETWEEN THAILAND AND JAPAN  
ON RECENT PROGRESS OF PHOTOPHYSICAL CHEMISTRY**



**Masashi Hasegawa**  
Kitasato University, Japan



**Jaroon Jakmunee**  
Chiang Mai University, Thailand



**Satoko Suzuki**  
JASCO Corporation, Japan



**Anawat Ajavakom**  
Chulalongkorn University, Thailand



**Hiroyuki Nishikawa**  
Ibaraki University, Japan



**Songwut Suramitr**  
Kasetsart University, Thailand

## SMALL-SCALE CHEMISTRY TEACHERS NETWORKING SPEAKER



**Metodija Najdoski**

Ss. Cyril and Methodius University  
Republic of North Macedonia

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## Committees

### Conference Organizers

1. Chemical Society of Thailand under the Patronage of Professor Dr. Her Royal Highness Princess Chulabhorn Krom Phra Srisavangavadhana
2. Kasetsart University

### Conference Chair

Paiboon Ngermmeesri

Kasetsart University

### International Advisory Committee

Javier García Martínez	IUPAC President, Spain
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Supa Hannongbua	CST Past-President, Kasetsart University, Thailand
Vudhichai Parasuk	CST President, Chulalongkorn University, Thailand

### Scientific Committee

Günther Rupprechter	Technische Universität Wien, Austria
Shuangjun Lin	Shanghai Jiao Tong University, China
Qiuquan Wang	Xiamen University, China
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Kowit Hengphasatporn	University of Tsukuba, Japan
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Chatree Faikhamta	Kasetsart University, Thailand
Pimpa Hormnirun	Kasetsart University, Thailand
Sirirat Jitkarnka	Chulalongkorn University, Thailand
Wirunya Keawwattana	Kasetsart University, Thailand
Sutasinee Kityakarn	Kasetsart University, Thailand
Utai Klinkesorn	Kasetsart University, Thailand
Patraporn Luksirikul	Kasetsart University, Thailand
Supawadee Namuangruk	National Nanotechnology Center, Thailand
Thitaphat Ngernsutivorakul	Kasetsart University, Thailand
Wanchai Pluempanupat	Kasetsart University, Thailand
Prapasiri Pongprayoon	Kasetsart University, Thailand
Chaiya Prasittichai	Kasetsart University, Thailand
Vinich Promarak	VISTEC, Thailand
Vatcharin Rukachaisirikul	Prince of Songkla University, Thailand
Atitaya Siripinyanond	Mahidol University, Thailand



Weekit Sirisaksoontorn	Kasetsart University, Thailand
Ekasith Somsook	Mahidol University, Thailand
Thawatchai Tuntulani	Chulalongkorn University, Thailand
Tirayut Vilaivan	Chulalongkorn University, Thailand
Pinsuda Viravathana	Kasetsart University, Thailand
Pakorn Wattana-Amorn	Kasetsart University, Thailand
Edman Tsang	University of Oxford, United Kingdom
T. Randall Lee	University of Houston, United States of America

### Organizing Committee

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Khongkhwan Akkarachaneeeyakorn	Kasetsart University, Thailand
Sunisa Akkarasamiyo	Kasetsart University, Thailand
Orapin Chienthavorn	Kasetsart University, Thailand
Natthawat Chuanopparat	Kasetsart University, Thailand
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Tanwawan Duangthongyou	Kasetsart University, Thailand
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Pimpa Hormnirun	Kasetsart University, Thailand
Witcha Imaram	Kasetsart University, Thailand
Junya Jattanasen	Kasetsart University, Thailand
Kannika Jeamjumnunja	Kasetsart University, Thailand
Thitinun Karpkird	Kasetsart University, Thailand
Wirunya Keawwattana	Kasetsart University, Thailand
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Patraporn Luksirikul	Kasetsart University, Thailand

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Tanin Nanok	Kasetsart University, Thailand
Paiboon Ngernmeesri	Kasetsart University, Thailand
Thitaphat Ngernsutivorakul	Kasetsart University, Thailand
Somkiat Nokbin	Kasetsart University, Thailand
Piboon Pantu	Kasetsart University, Thailand
Waraporn Parasuk	Kasetsart University, Thailand
Wanchai Pluemanupat	Kasetsart University, Thailand
Prapasiri Pongprayoon	Kasetsart University, Thailand
Chaiya Prasittichai	Kasetsart University, Thailand
Chadchalem Raksakoon	Kasetsart University, Thailand
Montida Raoarun	Kasetsart University, Thailand
Ramida Rattanakam	Kasetsart University, Thailand
Tharinee Saleepoch	Kasetsart University, Thailand
Patchreenart Saparpakorn	Kasetsart University, Thailand
Jakkapan Sirijaraensre	Kasetsart University, Thailand
Weekit Sirisaksoontorn	Kasetsart University, Thailand
Wilai Siriwatcharapiboon	Kasetsart University, Thailand
Apisit Songsasen	Kasetsart University, Thailand
Bunyarithi Sookcharoenpinyo	Kasetsart University, Thailand
Pannaree Srinoi	Kasetsart University, Thailand
Wannisa Sukjee	Kasetsart University, Thailand
Songwut Suramitr	Kasetsart University, Thailand
Potjanart Suwanruji	Kasetsart University, Thailand
Siree Tangbunsuk	Kasetsart University, Thailand
Pinsuda Viravathana	Kasetsart University, Thailand
Boontana Wannalerse	Kasetsart University, Thailand
Chompunuch Warakulwit	Kasetsart University, Thailand
Pakorn Wattana-Amorn	Kasetsart University, Thailand
Kuntawit Witthayolankowit	Kasetsart University, Thailand
Peerada Yingyuad	Kasetsart University, Thailand
Wanlapa Aeungmaitrepirom	Chemical Society of Thailand



Chanat Aonbangkhen	Chemical Society of Thailand
Supakorn Boonyean	Chemical Society of Thailand
Suchada Chatrapromma	Chemical Society of Thailand
Ekarat Detsri	Chemical Society of Thailand
Narumol Kreua-ngarjnucool	Chemical Society of Thailand
Phoosak Hirunyatrakul	Chemical Society of Thailand
Surin Laosooksathit	Chemical Society of Thailand
Ladda Meesuk	Chemical Society of Thailand
Thanuttkhul Mongkolaussavarat	Chemical Society of Thailand
Orasa Onjun	Chemical Society of Thailand
Vudhichai Parasuk	Chemical Society of Thailand
Waraporn Parasuk	Chemical Society of Thailand
Buncha Pulpoka	Chemical Society of Thailand
Pumidech Puthongkham	Chemical Society of Thailand
Singto Sakulkhaemaruehai	Chemical Society of Thailand
Montip Srirattana	Chemical Society of Thailand
Boonnak Sukhummek	Chemical Society of Thailand
Supawan Tantayanon	Chemical Society of Thailand
Prapaipit C. Terni	Chemical Society of Thailand
Boonsom Watcharachanchai	Chemical Society of Thailand
Kanda Wongwailikhit	Chemical Society of Thailand

## General Information

### Registration Desk

Registration desk is located in front of EH 100 Event Hall on the first floor (See the 1st floor plan)

### Registration Hours

Friday, 26 January 06.30 – 17.00

Saturday, 27 January 08.00 – 12.00

**Note 1:** Participants planning to attend the opening ceremony and the special keynote lecture by Professor Dr. Her Royal Highness Princess Chulabhorn Krom Phra Srisavangavadhana must finish registration before 8:00 a.m. on 26 January to guarantee access to the ceremony hall.

**Note 2:** The opening ceremony and the special keynote lecture by Professor Dr. Her Royal Highness Princess Chulabhorn Krom Phra Srisavangavadhana will be broadcast in real-time within the designated waiting area for participants who complete registration after 8.00 a.m. on 26 January.

### Poster Session and Exhibitions by Sponsors

The poster session and sponsors' exhibition booths are in Bhiraj Hall I

### Lunch and Coffee Break

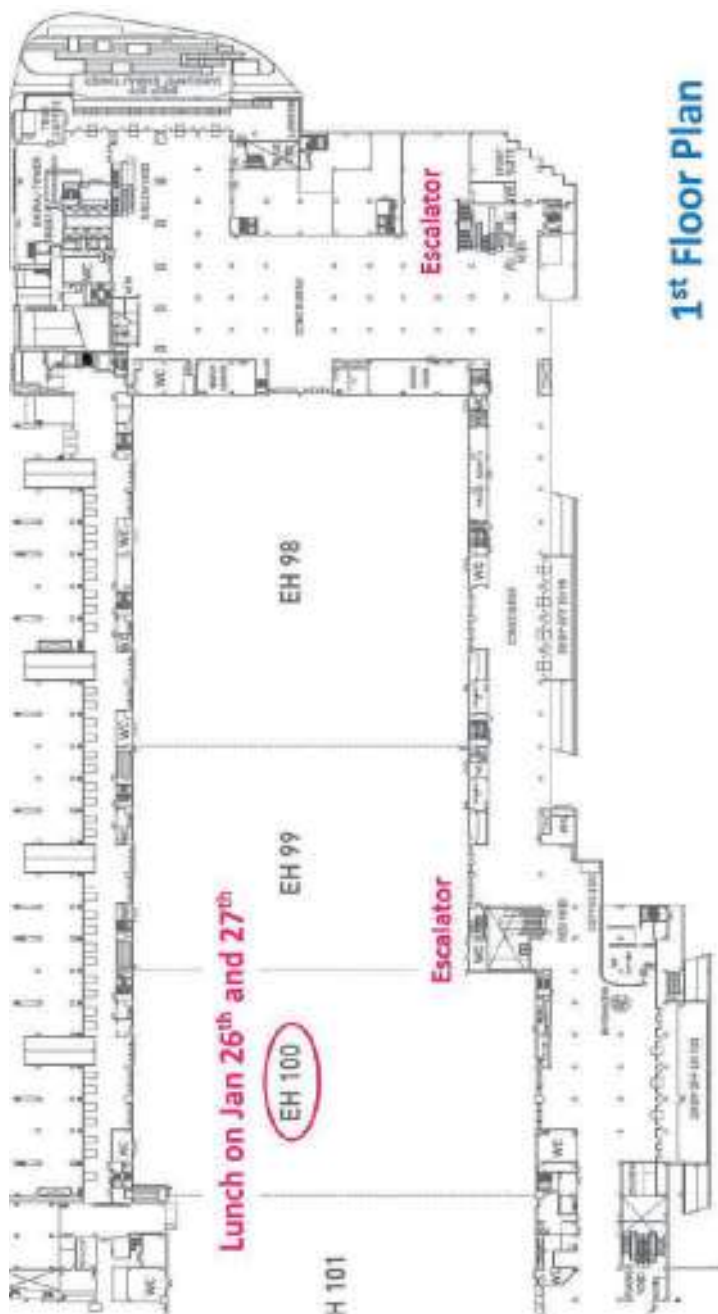
Lunch is served in the EH 100 Event Hall, which is located on the first floor.

Coffee break is served in front of the Convention Hall and the Conference Room.

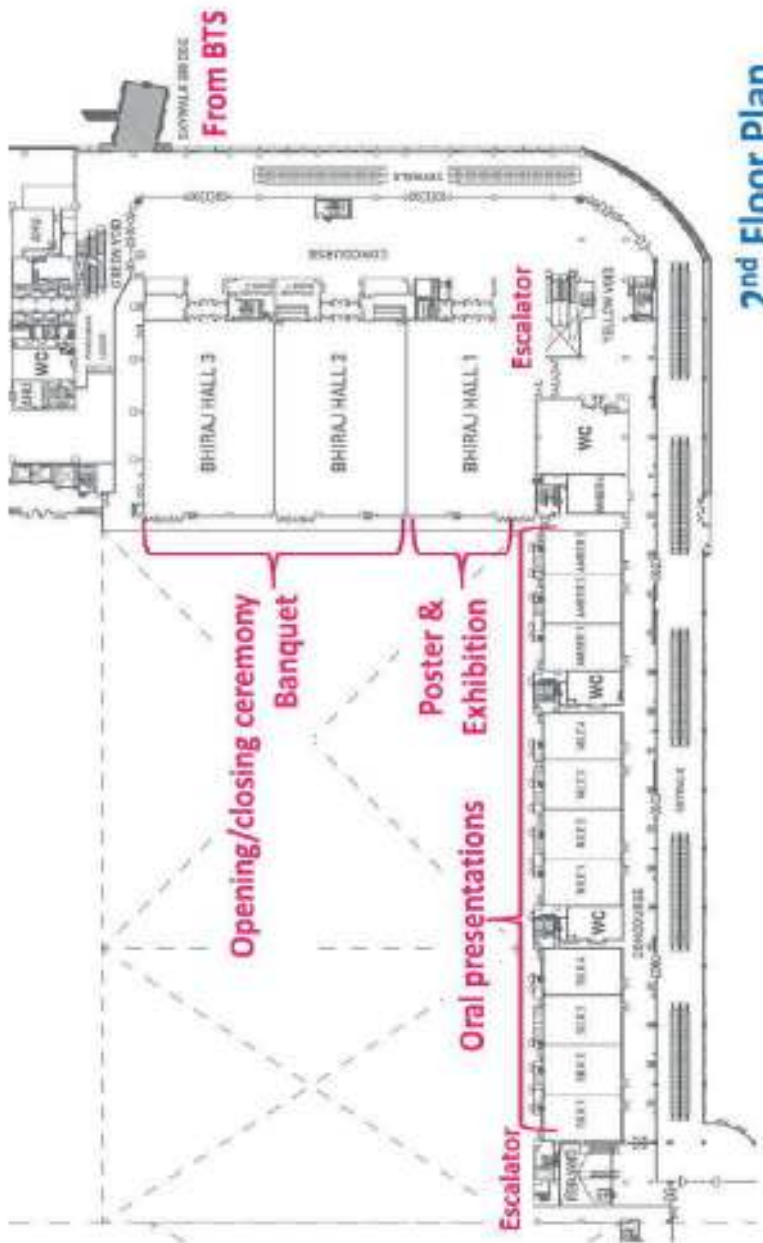
### Conference Banquet

The conference banquet will be held in Bhiraj Halls II and III on Friday, 26 January, from 18:15 - 21:00

## 1<sup>st</sup> Floor Plan



## 2<sup>nd</sup> Floor Plan





## Information for Presenters and Authors

### Presentation Code

Presentation codes are assigned for each presentation as

**PL-00** for **P**lenary speaker presentation

**XX-K-00** for **K**eynote speaker presentation

**XX-I-00** for **I**nvited speaker presentation

**XX-O-00** for **O**ral presentation

**XX-P-00** for **P**oster presentation

where XX is a session code and 00 is an identification number for each presentation.

### Instruction for Oral Presentation

#### *Presentation Upload Time*

You are requested to upload your presentation file in the conference room where you will be delivering your presentation.

Date	Session	Time for uploading the presentation file
26 Jan	Afternoon	12.00 – 12.45
27 Jan	Morning	08.30 – 09.30
27 Jan	Afternoon	12.00 – 12.45

Please contact our staff upon your registration for the presenting conference room.

#### *Presentation time*

The presentation time for general oral presentation is 15 minutes (12 minutes presentation + 3 minutes for Q&A). The time for keynote/invited presentation is 30 minutes (25 minutes presentation + 5 minutes for Q&A). Please check for the latest updates on the conference website and in front of the presenting room. There will be warning signals for the end of your presentation. Please strictly follow the schedule.

## Audio-Visual Aids

The rooms used for the presentation are equipped with

- A laptop PC with Power Point for presentation and a screen for single projection
- An LCD projector with VGA and HDMI connections
- A laser pointer

Due to a very tight schedule, we strongly encourage uploading your presentation files in the computer provided in the conference room where you will be delivering your presentation. The files will be completely removed after the session is ended. For those who wish to use your own laptop, please contact our staff at the conference room in advance to check the compatibility with our audio-visual instruments. Make sure that you carry appropriate adaptor or connector with you.

## Instruction for Poster Presentation

### *Time for Poster Attachment & Location*

The poster session will be at Bhiraj Hall I and the location for poster attachment will be specified according to Abstract ID which can be found in the Program Book. Accessories (like adhesive tape) for setting up the poster will be provided by the organizers and can be collected at the Poster Registration Desk.

### *Poster Sessions:*

There will be two poster sessions according to the schedule below.

Date	Session*	Setting up time	Presentation time	Poster removal time
26 Jan	I	12.00 – 13.00	17.15 – 18.15	18.15 – 18.30
27 Jan	II	08.30 – 09.30	11.00 – 12.00	16.00 – 16.15

\*Session I: Posters with presentation IDs ending in odd numbers  
 Session II: Posters with presentation IDs ending in even numbers

Participants are expected to be present in front of their posters during their scheduled sessions. Please note that there will be judges to interview the presenters during all sessions to evaluate for the Poster Presentation Awards, which will be announced during the Closing Ceremony on Saturday, January 27, 2024.

Note: The organizer will not be responsible for the posters that are left behind after the day of poster presentation.



## Plenary Lectures

**PL-01:** Alexander Kuhn

Institute of Molecular Sciences, University of Bordeaux

**PL-02:** Andrew P. Dove

School of Chemistry, University of Birmingham

**PL-03:** Pimchai Chaiken

School of Biomolecular Science and Engineering, VISTEC

**PL-04:** Javier García Martínez

Department of Inorganic Chemistry, University of Alicante

## Scientific Sessions

### AC-Analytical Chemistry

Chair: Atitaya Siripinyanond

Co-Chair: Thitaphat Ngernsutivorakul

### CC-Catalytic Chemistry

Chair: Metta Charoenpanich

Co-Chair: Patraporn Luksirikul

### CE-Chemical Education

Chair: Chatree Faikhamta

Co-Chair: Sutasinee Kityakarn

### EE-Environmental Chemistry and Renewable Energy

Chair: Ekasith Somsook

Co-Chair: Weekit Sirisaksoontorn

### FA-Food, Agriculture and Cosmetics

Chair: Utai Klinkesorn

Co-Chair: Wanchai Pluempunupat

### IC-Inorganic Chemistry

Chair: Thawatchai Tuntulani

Co-Chair: Pimpa Hormnirun

## **IE-Industrial and Engineering Chemistry**

Chair: Sirirat Jitkarnka

Co-Chair: Pinsuda Viravathana

## **MN-Material Chemistry and Nanotechnology**

Chair: Vinich Promarak

Co-Chair: Chaiya Prasittichai

## **NP-Natural Products, Biological Chemistry and Chemical Biology**

Chair: Vatcharin Rukachaisirikul

Co-Chair: Pakorn Wattana-Amorn

## **OM- Organic Synthesis and Medicinal Chemistry**

Chair: Tirayut Vilaivan

Co-Chair: Natthawat Chuanopparat

## **PC-Polymer Chemistry and Bio-Based Materials**

Chair: Kanoktip Boonkerd

Co-Chair: Wirunya Keawattana

## **PT-Physical and Theoretical Chemistry**

Chair: Supawadee Namuangruk

Co-Chair: Prapasiri Pongprayoon

## **BSTJ-Bilateral symposium between Thailand and Japan on recent progress of photophysical chemistry**

Chairs: Hiroyuki Nishikawa, Shigeyuki Yagi and Nawee Kungwan

## **Small-Scale Chemistry Teachers Networking**

## **Merck-CST-TYCN Symposium**

## **Special Session (Elsevier, Bruker, and Thai Carbon)**

## Overall Program

Time	26 January 2024	Time	27 January 2024
06.30	Registration Open*	08.00	Registration Open
09.00 – 10.00	<b>Opening Ceremony</b>	09.00 – 09.45	<b>Plenary Talk: PL-03</b>
10.00 – 11.00		09.45 – 10.45	<b>Oral Presentation</b>
11.00 – 11.15	<i>Coffee Break</i>	10.45 – 11.00	<i>Coffee Break</i>
11.15 – 12.00	<b>Plenary Talk: PL-01</b>	11.00 – 12.00	<b>Poster Session II</b>
12.00 – 13.00	<i>Lunch</i>	12.00 – 13.00	<i>Lunch</i>
13.00 – 15.00	<b>Oral Presentation</b>	13.00 – 15.00	<b>Oral Presentation</b>
15.00 – 15.15	<i>Coffee Break</i>	15.00 – 15.15	<i>Coffee Break</i>
15.15 – 16.00	<b>Plenary Talk: PL-02</b>	15.15 – 16.15	<b>Oral Presentation</b>
16.00 – 17.15	<b>Oral Presentation</b>	16.15 – 17.00	<b>Plenary Talk: PL-04</b>
17.15 – 18.15	<b>Poster Session I</b>	17.00 – 18.00	<b>Award Announcement &amp; Closing Ceremony</b>
18.15 – 21.00	<b>Conference Banquet</b>	19.00 – 22.00	<b>Appreciation Dinner</b>

### Note\*

1. Participants planning to attend the opening ceremony and the special keynote lecture by Professor Dr. Her Royal Highness Princess Chulabhorn Krom Phra Srisavangavadhana must finish registration before 8:00 a.m. on 26 January to guarantee access to the ceremony hall.
2. The opening ceremony and the special keynote lecture by Professor Dr. Her Royal Highness Princess Chulabhorn Krom Phra Srisavangavadhana will be broadcast in real-time within the designated waiting area for participants who complete registration after 8.00 a.m. on 26 January.

# Program at a Glance

26 January 2024

Time	Silk 1	Silk 2	Silk 3	Silk 4	Nile 1	Nile 2	Nile 3	Nile 4	Amber 1	Amber 2	Amber 3	Amber 4	
06.30	Registration Open												
09.00-11.00	Opening Ceremony at Bhiraj Halls II and III												
11.00-11.15	Coffee Break												
11.15.12.00	PL-01: Unconventional Approaches to Energy Conversion by Professor Alexander Kuhn at Bhiraj Halls II and III												
12.00-13.00	Small Scale Chemistry Teachers Networking	Lunch at EH100											
13.00-13.15		AC-I-01	CC-K-01	EE-K-01	Chemical Society of Thailand (CST) and Head of Chemistry Department meeting	IC-I-01	IE-K-01	MN-K-01	NP-I-01	OM-I-01	PC-K-01	PT-I-01	
13.15-13.30													
13.30-13.45		Lunch at EH100	AC-I-02	CC-K-02		EE-I-01	IC-I-02	IE-K-02	MN-I-01	NP-I-02	OM-I-02	PC-I-01	PT-I-02
13.45-14.00													
14.00-14.15	Small Scale Chemistry Teachers Networking	AC-O-01	CC-I-01	EE-O-01		IC-I-03	IE-K-03	MN-O-01	NP-I-03	OM-O-01	PC-I-02	PT-O-01	
14.15-14.30		AC-O-02		EE-O-02				MN-O-02		OM-O-02		PT-O-02	
14.30-14.45		AC-O-03	CC-O-01	EE-O-03		IC-O-01	IE-O-01	MN-O-03	NP-O-01	OM-O-03	PC-O-01	PT-O-03	
14.45-15.00		AC-O-04	CC-O-02	EE-O-04		IC-O-02	IE-O-02			OM-O-04		PT-O-04	
15.00-15.15	Coffee Break												
15.15-16.00	PL-02: Designing Polymers with the End in Mind: Creating Circular Routes to Polymers using Light-Based Strategies by Professor Andrew P. Dove at Bhiraj Halls II and III												
16.00-16.15	CE-I-01	AC-I-03	CC-I-02	EE-I-02	Chemical Society of Thailand (CST) and Head of Chemistry Department meeting	IC-I-04	IE-K-04	MN-I-02	NP-I-04	OM-I-03	PC-I-03	PT-I-05	
16.15-16.30													
16.30-16.45	CE-I-02	AC-O-05	CC-O-03	EE-O-05		IC-O-03	IE-O-03	MN-O-04	NP-O-02	OM-O-05	PC-O-02	PT-O-05	
16.45-17.00		AC-O-06	CC-O-04	EE-O-06		IC-O-04	IE-O-04	MN-O-05	NP-O-03	OM-O-06	PC-O-03	PT-O-06	
17.00-17.15	CE-O-01	AC-O-07	CC-O-05	EE-O-07				MN-O-06		OM-O-07		PT-O-07	
17.15-18.15	Poster Session I at Bhiraj Hall I												
18.15-21.00	Conference Banquet at Bhiraj Halls II and III												

# Program at a Glance

27 January 2024

Time	Silk 1	Silk 2	Silk 3	Silk 4	Nile 1	Nile 2	Nile 3	Nile 4	Amber 1	Amber 2	Amber 3	Amber 4							
09.00-09.45	PL-03: Enzyme Catalysis for Green Chemistry by Professor Pimchai Chaiven at Bhiraj Hall II and III																		
09.45-10.00	CST-01	AC-I-04	CC-K-03	EE-K-02	Opening remarks	IC-I-05	MN-I-05	MN-I-03	NP-I-05	OM-I-04	PC-I-04	PT-I-04							
10.00-10.15					BSTJ-I-01														
10.15-10.30					BSTJ-I-02														
10.30-10.45	AC-O-17	AC-O-08	CC-O-06	EE-O-08	BSTJ-I-03	IC-O-05	MN-O-17	MN-O-07	NP-O-04	OM-O-08	PC-O-04	PT-O-08							
10.45-11.00	AC-O-18	AC-O-09	CC-O-07	EE-O-09		IC-O-06	MN-O-18	MN-O-08	NP-O-05	OM-O-09	PC-O-05	PT-O-09							
11.00-12.00	Coffee Break																		
12.00-13.00	Poster Session II at Bhiraj Hall I																		
13.00-13.15	Lunch at EH100																		
13.15-13.30	CST-06	AC-I-05	CC-I-03	EE-I-03	BSTJ-I-04 BSTJ-I-05 BSTJ-I-06 BSTJ-I-07 BSTJ-I-08 BSTJ-I-09	IC-I-06	MN-I-06	MN-I-04	FA-I-01	OM-I-05	CST-05	PT-I-03							
13.30-13.45													CST-02	CST-07	MN-O-09 MN-O-10	FA-I-02	OM-O-10 OM-O-11	CST-08	PT-O-10
13.45-14.00																			
14.00-14.15	AC-O-19	AC-O-10	CC-O-08	EE-I-04		IC-O-07	MN-O-19	MN-O-11	FA-O-01	SS-01	EE-O-14	CE-I-03							
14.15-14.30	AC-O-20	AC-O-11	CC-O-09	EE-O-10		IC-O-08	MN-O-20	MN-O-12	FA-O-02		EE-O-15								
14.30-14.45	AC-O-21	AC-O-12	CC-O-10	EE-O-11			MN-O-21	MN-O-13	FA-O-03		SS-02		EE-O-16	CE-O-02					
14.45-15.00	AC-O-22	AC-O-13		EE-O-12			MN-O-22	MN-O-14	FA-O-04	SS-03			CE-O-03						
15.00-15.15	AC-O-23	AC-O-14		EE-O-13															
15.15-15.30	AC-O-24	AC-O-15																	
15.30-15.45	AC-O-25	AC-O-16	Coffee Break				MN-O-23	Coffee Break					Coffee Break						
15.45-16.00	Coffee Break				BSTJ-I-10		Coffee Break	MN-O-15	FA-I-03		Coffee Break	CE-O-04							
16.00-16.15					BSTJ-I-11			MN-O-16				CE-O-05							
16.15-17.00					BSTJ-I-12					FA-O-05									
17.00-18.00					Closing Remarks				FA-O-06										
18.00-19.00	PL-04: Rethinking our Relationship with the Planet at Molecular Scale by Professor Javier García Martínez at Bhiraj Halls II and III																		
19.00-20.00	Award Announcement & Closing Ceremony at Bhiraj Halls II and III																		
20.00-22.00	Appreciation Dinner for Plenary/Keynote/Invited Speakers and Committees																		

# Small-Scale Chemistry Teachers Networking

January 26, 2024

## Background of Implementation of Small-Scale Chemistry in Asia.

The essential features of Small-Scale Chemistry are:

- A scaling down of chemical reagents to volumes and masses one thousand times smaller than those used in traditional labs.
- A shift from glassware to modern polymer or plastic materials in transfer, storage, and reaction devices.
- The use of multi-sample observational tools allows rapid, intuitive preparation, variation, and comparison of chemical systems in all phases: gases, liquids, and solids.

Small-Scale Chemistry is a new teaching approach to engage students in experimental chemistry. It provides a solution to most of the problems associated with laboratory instruction. Small-scale Chemistry has been introduced to Thailand since 2000. In 2013, Dow Thailand Group joined forces with the Chemical Society of Thailand (CST) to enhance educational equality for Thai students and encourage them to acquire good attitudes toward science studies through practical, hands-on experience, called the “Dow Chemistry Classroom” project.

In May 2022, CST and Dow Thailand signed an agreement with the Office of the Basic Education Commission (OBEC) to expand the small-scale chemistry laboratory to schools across Thailand. Moreover, the CST has extended this new approach of teaching small-scale chemistry laboratories to 5 ASEAN countries under financial support from Bangkok Bank Public Company Limited (BBL), beginning in 2017. In 2022, the CST extended further to emerging countries, in which Nepal is the first one, under the auspice of the International Union of Pure and Applied Chemistry (IUPAC), and in 2023 to Sri Lanka. Then 10 teachers, who attended the small-scale chemistry workshop in their own countries, are selected from each country to attend the Small Scale Chemistry Teachers Networking in PACCON every year.

## Networking Program

**26 January 2024**

Participants: outstanding teachers from Sri Lanka (10), Philippines (10), and Thailand (40)

- |               |  |
|---------------|--|
| 12:00 – 13.30 | Demonstration of the designed experiments by outstanding teachers  |
| 13:30 – 14.00 | Lunch  |
| 14:00 – 15.00 | Lecture on “Microscale/Small scale chemistry experiments from Macedonia” (online) by Metodija Najdoski from Faculty of Natural Sciences and Mathematics, Ss. Cyril and Methodius University, Republic of North Macedonia               |
| 15.00 – 16.00 | Speed Networking <ul style="list-style-type: none"><li>- Build new connections among the outstanding teachers</li><li>- Share and gain knowledge on small-scale chemistry experiment (5 small-scale experiments by rotation)</li></ul> |
| 18:15 – 21.00 | Conference Banquet   |



Networking of the outstanding teachers from Cambodia (15), Indonesia(14), Nepal(10), Thailand(30) and Vietnam(11) on 21 January 2023

# Merck-CST-TYCN Symposium

## Chemistry Horizons: Exploring Diverse Paths in Early Careers



**Location:** Bhiraj halls II and III

**27 January 2024**

- |               |  |
|---------------|--|
| 10.00 – 10.30 | <b>Merck-CST-TYCN for Sustainable Future Award Talk</b><br>(20-min talk, 10-min Q&A)     |
| 10.30 – 11.15 | <b>TYCN symposium: Rapid-fire talks</b><br>(3-min talks, 8 speakers)                     |
| 11:15 – 12:15 | <b>Panel Discussion:</b><br>Chemistry Horizons: Exploring Diverse Paths in Early Careers |
| 12:15 – 13:00 | Networking (lunch)   |



# ORAL PRESENTATION PROGRAM

## AC-Analytical Chemistry

**Friday, 26 January 2024, Room: Silk 2**

**Chairs:** 1) Takashi Kaneta, Okayama University  
2) Jaroon Jakmunee, Chiang Mai University

Time	Code	Title	Presenter
13.00 – 13.30	AC-I-01	High resolution accurate mass mass spectrometry (HRAM MS) for a better understanding of the health and the resilience of ecosystems	Ryszard Lobinski
13.30 – 14.00	AC-I-02	Single-cell analysis using ICP-qMS	Qiuquan Wang
14.00 – 14.15	AC-O-01	Absolute quantification of phenyl-butanoids in <i>Zingiber cassumunar</i> Roxb. rhizome by quantitative <sup>1</sup> H NMR	Chatkamon Lekwongphaiboon
14.15 – 14.30	AC-O-02	Production and certification of certified reference material of andrographolide in <i>Andrographis paniculata</i> powder by a network of competent laboratories approach	Ponhatai Kankaew
14.30 – 14.45	AC-O-03	Gold nanoparticle-based dip strip immunoassay with silver enhancement method for cardiac troponin I detection	Napakporn Poosinuntakul
14.45 – 15.00	AC-O-04	Synthesis of platinum on manganese (IV) oxide nanowires in chitosan scaffold as a catalyst in prostate immunosensor	Suphaporn Chenkhuruthum
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		

## AC-Analytical Chemistry

**Friday, 26 January 2024, Room: Silk 2**

**Chairs:** 1) Ryszard Lobinski, IPREM - UMR5254

2) Maliwan Amatatongchai, Ubon Ratchathani University

Time	Code	Title	Presenter
16.00 – 16.30	AC-I-03	Electrodialytic ionic solutes handling for matrix isolation, purification, and separation	Shin-Ichi Ohira
16.30 – 16.45	AC-O-05	Surfactant-free air bubble flotation for the rapid purification of basic dyes and drugs	Tohru Saitoh
16.45 – 17.00	AC-O-06	Electrical field-flow fractionation for separation and characterization of metal nanoparticles	Takdanai Techarang
17.00 – 17.15	AC-O-07	An efficient method of tyramine detection in food and beverage products by capillary electrophoresis using silica-nanolayer coated capillary with UV detection	Apinya Obma
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		



## AC-Analytical Chemistry *Saturday*,

**27 January 2024, Room: Silk 2**

**Chairs:** 1) Qiuquan Wang, Xiamen University

2) Atitaya Siripinyanond, Mahidol University

Time	Code	Title	Presenter
09.45 – 10.15	AC-I-04	Wearable sweat glucose sensor connected with a smartphone readout	Nadnudda Rodthongkum
10.15 – 10.30	AC-O-08	Development of an electrochemical DNA super-sandwich assay for porcine adulteration detection via one-step immobilization using a polyadenine oligonucleotide approach	Vasita Lapee-e
10.30 – 10.45	AC-O-09	Non-transferrin-bound iron (NTBI) quantification in human plasma using BODIPY-pyridylhydrazone (BODIPY-PH) entrapped in a thin green film coupled with a portable fluorescence-based device	Puttaraksa Naksen
10.45 – 11.00	Coffee Break		
11.00 – 12.00	Poster Session II at Bhiraj Hall I		
12.00 – 13.00	Lunch at EH100		
Chairs: 1) Shin-Ichi Ohira, Kumamoto University 2) Nadnudda Rodthongkum, Chulalongkorn University			
13.00 – 13.30	AC-I-05	Toward user-friendly paper-based analytical devices	Takashi Kaneta
13.30 – 13.45	AC-O-10	Mickey mouse-shaped laminated paper-based analytical device in simultaneous total cholesterol and glucose determination in whole blood	Akarapong Prakobkij
13.45 – 14.00	AC-O-11	Vanadium-doped porous cobalt oxide for its superior peroxidase mimic in simultaneous total cholesterol and glucose testing in whole blood on a 2D paper-based device	Nattasa Kitchawengkul

## AC-Analytical Chemistry

**Saturday, 27 January 2024, Room: Silk 2**

Time	Code	Title	Presenter
14.15 – 14.30	AC-O-13	Enhanced detection of favipiravir using a $\text{Cu}_2\text{O}@\text{MnO}_2$ modified glassy carbon electrode	Nuenghathai Chaiya
14.30 – 14.45	AC-O-14	Development of aptamer-based detection kit by electrochemistry for rapid assessment of vitamin D levels	Sattawat Boonchaleaw
14.45 – 15.00	AC-O-15	Ecological risk assessment of heavy metals in sediment from Klong Luang Reservoir, Chonburi, Thailand	Sophit Buth
15.00 – 15.15	AC-O-16	Effect of some short chain and long chain fatty acids on KOH number of concentrate natural rubber latex	Najmee Hemmad
15.15 – 15.30	<b>Coffee Break</b>		

## AC-Analytical Chemistry

**Saturday, 27 January 2024, Room: Silk 1**

**Chairs:** 1) Orapin Chienthavorn, Kasetsart University  
2) Nuanlaor Ratanawimarnwong, Srinakharinwirot University

Time	Code	Title	Presenter
09.45 – 10.15	CST-01	From liquid to gas to unconventional detections	Duangjai Nacapricha
10.15 – 10.30	AC-O-17	Sensitive and selective 3D-ePAD for dual simultaneous analysis of VMA and 5-HIAA tumor markers using graphene screen printed electrode modified with molecularly imprinted polymers for point-of-care application	Kanpitcha Somnet
10.30 – 10.45	AC-O-18	Electrochemical sensor based on amine-functionalized magnetite magnetic nanoparticles and reduced graphene oxide nanocomposites for determination of chloramphenicol	Wasukamol Numphud
10.45 – 11.00	<b>Coffee Break</b>		
11.00 – 12.00	<b>Poster Session II at Bhiraj Hall I</b>		
12.00 – 13.00	<b>Lunch at EH100</b>		



## AC-Analytical Chemistry

**Saturday, 27 January 2024, Room: Silk 1**

**Chairs:** 1) Duangjai Nacapricha, Mahidol University

2) Thitaphat Ngernsutivorakul, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	CST-06	Origin classification of Thai agricultural products using chemical tools: towards sustainable use of geographical indication	Thanit Praneenararat
13.30 – 13.45	AC-O-19	Development of a paper-based analytical device for simultaneous detection of organophosphate pesticides and heavy metal in fruit and vegetable samples	Supattra Arsawiset
13.45 – 14.00	AC-O-20	Microfluidic paper-based analytical devices for total amino acid detection in processed food	Jaruwan Mettakoonpitak
14.00 – 14.15	AC-O-21	A thread-based analytical device for nitrite detection in food samples	David Ajayi
14.15 – 14.30	AC-O-22	Development of a simple method for measuring nitrate ions in natural water samples	Mika Umeda
14.30 – 14.45	AC-O-23	A novel immunosensor based on cobalt oxide nanocomposite modified single walled carbon nanohorns for the selective detection of aflatoxin B1	Chulalak Damphathik
14.45 – 15.00	AC-O-24	Effect of extraction solvent ratio in biosynthesis of silver nanoparticles, determination of phytochemicals, and investigation of antioxidant activity using <i>Artabotrys suaveolens</i> (Blume) Blume leaves	Fode Toure
15.00 – 15.15	AC-O-25	Effect of Mg compound on KOH number of concentrated natural rubber latex ( <i>Hevea brasiliensis</i> )	Nadeeya Samae
15.15 – 15.30	<b>Coffee Break</b>		

## CC-Catalytic Chemistry

**Friday, 26 January 2024, Room: Silk 3**

**Chairs:** 1) Paisan Kongkachuichay, Kasetsart University

2) Khanin Nueangnoraj, Sirindhorn International Institute of Technology

**Co-Chair:** Metta Chareonpanich, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	CC-K-01	From averaging over an entire catalyst to single particle catalysis: black box vs. atomic views	Günther Rupprechter
13.30 – 14.00	CC-K-02	Catalytic chemistry using carbon-based materials	Hiroto Nishihara
14.00 – 14.30	CC-I-01	Advanced catalytic upgrading of bioethanol to chemicals and carbon materials	Chularat Wattanakit
14.30 – 14.45	CC-O-01	Uncovering insights in data-driven catalyst design: A case study in oxidative coupling of methane	Shun Nishimura
14.45 – 15.00	CC-O-02	Ethanol steam reforming using Ni catalyst supported on ZrO <sub>2</sub> -doped Al <sub>2</sub> O <sub>3</sub> with magnetic inducement	Marucheth Thongthepairoj
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		

## CC-Catalytic Chemistry

**Friday, 26 January 2024, Room: Silk 3**

**Chair:** Chularat Wattanakit, Vidyasirimedhi Institute of Science and Technology

**Co-Chair:** Patraporn Luksirikul, Kasetsart University

Time	Code	Title	Presenter
16.00 – 16.30	CC-I-02	Selective conversion of xylose to lactic acid over Al-based catalysts: A comprehensive comparison between laboratory-scale and pilot-scale	Pongtanawat Khemthong
16.30 – 16.45	CC-O-03	Computational modeling of carbon monoxide oxidation on platinum supported on cerium dioxide	Georgi N. Vayssilov
16.45 – 17.00	CC-O-04	Chiral-induced spin selectivity effect at chiral-encoded Pt-Ir surfaces for enhanced Oxygen Reduction Reaction	Zikkawas Pasom
17.00 – 17.15	CC-O-05	I-doped $\text{Bi}_2\text{MoO}_6$ nanosheets for enhanced pollutant photodegradation and hydrogen evolution	Theeranun Siritanon
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## CC-Catalytic Chemistry

**Saturday, 27 January 2024, Room: Silk 3**

**Chair:** Piboon Pantu, Kasetsart University

**Co-Chair:** Patraporn Luksirikul, Kasetsart University

Time	Code	Title	Presenter
09.45 – 10.15	CC-K-03	Induced catalytic active sites by substrate over nano-structures	Edman Tsang
10.15 – 10.30	CC-O-06	Role of incorporated metal/phosphorus acidity modification over low Si/Al ratio HZSM-5 catalysts in methanol-to-olefins procesS	Chotika Yoocham
10.30 – 10.45	CC-O-07	Effect of manganese and magnesium promoter on catalytic hydrogenation of CO <sub>2</sub> over cobalt-based catalyst	Saowaluk Intarasiri
10.45 – 11.00	Coffee Break		
11.00 – 12.00	Poster Session II at Bhiraj Hall I		
12.00 – 13.00	Lunch at EH100		
<p><b>Chairs:</b> Metta Chareonpanich, Kasetsart University</p> <p><b>Co-Chair:</b> Thongthai Witoon, Kasetsart University</p> <p><b>Chair:</b> Thongthai Witoon, Kasetsart University</p> <p><b>Co-Chair:</b> Waleeporn Donphai, Kasetsart University</p>			
13.00 – 13.30	CC-I-03	Syngas conversion to light olefins: Influence of SiO <sub>2</sub> , Al <sub>2</sub> O <sub>3</sub> , and TiO <sub>2</sub> supports using Fe-Co-K catalysts	Thongthai Witoon
13.30 – 13.45	CC-O-08	Production of sustainable aviation fuel and green diesel from biodiesel via metathesis-deoxygenation over tungsten oxide based catalysts	Mochamad Solehudin
13.45 – 14.00	CC-O-09	Sol-gel preparation of copper cobaltite spinel for ciprofloxacin degradation via peroxymonosulfate activation	Hieu Trung Dinh
14.00 – 14.15	CC-O-10	Cd <sub>0.5</sub> Zn <sub>0.5</sub> S/Bi <sub>2</sub> MoO <sub>6</sub> heterostructure for rhodamine B photodegradation under visible light	Thitipong Choklap



## CE-Chemical Education

**Friday, 26 January 2024, Room: Silk 1**

**Chair:** Chatree Faikhamta, Kasetsart University

**Co-Chair:** Pattamaporn Pimthong, Silpakorn University

Time	Code	Title	Presenter
16.00 – 16.30	CE-I-01	Design and development of simple microfluidic paper- and thread-based devices for high school chemistry experiments	Saksri Supasorn
16.30 – 17.00	CE-I-02	Metacognitive calibration: Can students judge their abilities?	Witawas Handee
17.00 – 17.15	CE-O-01	Diagnosis of fundamental concepts of Chemical Basis of Life among high school students	Pongprapan Pongsophon
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## CE-Chemical Education

**Saturday, 27 January 2024, Room: Amber 4**

**Chair:** Saksri Supasorn, Ubon Ratchathani University

**Co-Chair:** Witawas Handee, Silpakorn University

Time	Code	Title	Presenter
14.00 – 14.30	CE-I-03	The power of STEM Partnership for promoting STEM Skills	Pattamaporn Pimthong
14.30 – 14.45	CE-O-02	Promoting students' scientific explanation through the 6E STEM for BCG model on the topic of rate of reaction	Parinya Mutchua
14.45 – 15.00	CE-O-03	Entrepreneurial STEAM-BCG in a Cup: The Development of High School Student's Sensemaking Practices through Dialogical Argumentation with Chemistry Concepts	Tharuesean Prasoplarb
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 15.30	CE-O-04	Using an esterification activity to enhance advanced placement (AP) chemistry students' competency in higher-order thinking (HOT)	Sonthi Phonchaiya
15.30 – 15.45	CE-O-05	The effect of STEAM BCG through natural tie dye activities	Tanchanok Poonsin

## EE-Environmental Chemistry and Renewable Energy

**Friday, 26 January 2024, Room: Silk 4**

**Chair:** Tosapol Maluangnont, King Mongkut's Institute of Technology Ladkrabang

**Co-Chair:** Weekit Sirisaksoontorn, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	EE-K-01	Microplastics contamination in Chao Phraya estuary and Bang Pu mangrove forest in Thailand	Sandhya Babel
13.30 – 14.00	EE-I-01	Metal oxides nanosheets/cellulose composites for energy harvesting via triboelectricS	Tosapol Maluangnont
14.00 – 14.15	EE-O-01	Microplastics and plastic additives in open dumping site soil from Thailand	Shinnosuke Yamahara
14.15 – 14.30	EE-O-02	Preparation of porous biochar derived from avocado peel and its application on ciprofloxacin removal	Thi Tuong Vi Tran
14.30 – 14.45	EE-O-03	Minimize residual formaldehyde content in melamine-formaldehyde PCM microcapsules	Nichakorn Wangkajai
14.45 – 15.00	EE-O-04	Conversion of fat and oil contaminant waste produced by stationary wastewater treatment plant into calcium soap for ruminant feed	Aung Thae Oo
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		



## EE-Environmental Chemistry and Renewable Energy

**Friday, 26 January 2024, Room: Silk 4**

**Chair:** Pawin Iamprasertkun, Thammasart University

**Co-Chair:** Weekit Sirisaksoontorn, Kasetsart University

Time	Code	Title	Presenter
16.00 – 16.30	EE-I-02	The rise of sustainable electrochemical intelligent of 2D materials	Pawin Iamprasertkun
16.30 – 16.45	EE-O-05	Exploring interphase instability in the LiTFSI-LiCl aqueous biphasic system through optical microscopy	Chalarat Chaemchamrat
16.45 – 17.00	EE-O-06	Nanostructured MoO <sub>2</sub> /MoS <sub>2</sub> /MoP heterojunction and N, S dual-doped reduced graphene oxide as high performance electrode for supercapacitors	Kasira Kaewplod
17.00 – 17.15	EE-O-07	The Fabrication of Ru <sub>2</sub> P nanoparticle decorated P-doped vegetable root-derived hierarchical porous carbon for supercapacitors with ultrahigh capacitance	Sudarat Laihang
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## EE-Environmental Chemistry and Renewable Energy

**Saturday, 27 January 2024, Room: Silk 4**

**Chair:** Weekit Sirisaksoontorn, Kasetsart University

Time	Code	Title	Presenter
09.45 – 10.15	EE-K-02	Holistic valorization of residual biomass	Joseph S. M. Samec
10.15 – 10.30	EE-O-08	Unveiling the potential of oxidative catalytic fractionation in spruce bark valorization	Suthawan Muangmeesri
10.30 – 10.45	EE-O-09	Conversion of food waste to a valuable soil resource in a day	Apichat Junsod
10.45 – 11.00	<b>Coffee Break</b>		
11.00 – 12.00	<b>Poster Session II at Bhiraj Hall I</b>		
12.00 – 13.00	<b>Lunch at EH100</b>		
13.00 – 13.30	EE-I-03	Surface chemistry in atomic layer deposition and selective deposition	IL-Kwon Oh
13.30 – 14.00	EE-I-04	Occupational health risk of workers exposed to hazardous air pollutants: case study in Thai Industries	Wanida Jinsart
14.00 – 14.15	EE-O-10	Comparative study of torrefaction and pyrolysis behavior on rice straw using Thermogravimetry-Mass Spectrometry (TG-MS) technique	Chakrya Theap
14.15 – 14.30	EE-O-11	Copper calcium hydroxide nitrate derived from chicken eggshell and their catalytic activity in the removal of aqueous methyl orange	Yiping Han
14.30 – 14.45	EE-O-12	Photocatalytic degradation of organic dye and antibiotic by ZnO-based photocatalyst under natural solar light	Suwat Nanan
14.45 – 15.00	EE-O-13	Performance evaluation of Phase Change Materials (PCMs) to improve energy saving potential of building	Kanyamon Ausaman
15.00 - 15.15	EE-O-17	Efficient wastewater dye degradation using $\text{Fe}_3\text{O}_4\text{-CuS@SiO}_2$ photocatalyst: Mechanism and performance	Fatemeh Sadegh
15.15 – 15.30	<b>Coffee Break</b>		



## EE-Environmental Chemistry and Renewable Energy

**Saturday, 27 January 2024, Room: Amber 3**

**Chair:** Wisit Hirunpinyopas, Kasetsart University

**Co-Chair:** Pawin Iamprasertkun, Thammasart University

Time	Code	Title	Presenter
13.00 – 13.30	CST-05	Pioneering sustainable futures: From enzyme-driven biocatalysis to revolutionary waste management in Thailand	Thanyaporn Wongnate
13.30 – 14.00	CST-08	Tuning surface energy to enhance MoS <sub>2</sub> nanosheet production via liquid-phase exfoliation: understanding the electrochemical adsorption of cesium chloride	Panwad Chavalekvirat
14.00 – 14.15	EE-O-14	One-dimensional simulation of an alkaline-acid direct glycerol fuel cell	Papitchaya Chaloeypanit
14.15 – 14.30	EE-O-15	Simulation of hydrogen production from water-hyacinth with equilibrium reactors	Sirikul Boonterm
14.30 – 14.45	EE-O-16	Unveiling novel mechanisms in energy storage materials with mimic battery technique	Kulika Pithaksinsakul

## FA-Food, Agriculture and Cosmetics

**Saturday, 27 January 2024, Room: Amber 1**

**Chair:** Utai Klinkesorn, Kasetsart University

**Co-Chair:** Wanchai Pluempanupat, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	FA-I-01	Science behind plant-based foods	Kamolwan Israkarn
13.30 – 14.00	FA-I-02	Toward sustainability in cosmetic industry: trends and case studies	Naphatsorn Ditthawutthikul
14.00 – 14.15	FA-O-01	Development of coffee silver skin into food beverage and testing antioxidant activity	Kimsuy Vang
14.15 – 14.30	FA-O-02	Characteristics of pomelo cellulopectin and its application in plant-based chicken nugget	Rattana Yooberg
14.30 – 14.45	FA-O-03	The application of coffee silver skin extract in pomegranate juice and study for its bioactivities	Thavy Kit
14.45 – 15.00	FA-O-04	Construction and application of digital platform for predicting metabolism and toxicity of pesticides	Jianhua Yao
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 15.45	FA-I-03	Vitamin D analysis in fish and mushrooms by Liquid Chromatography-Tandem Mass Spectrometry (LC-MS/MS)	Kunchit Judprasong
15.45 – 16.00	FA-O-05	The effect of ion exchange of clinoptilolite as a soil on the physiological response of radish	Yuri Kalvachev
16.00 – 16.15	FA-O-06	Extracting bioactive protein from fish head using enzymatic hydrolysis	Photawan Chaodee

## IC-Inorganic Chemistry

**Friday, 26 January 2024, Room: Nile 2**

**Chair:** Thawatchai Tuntulani, Chulalongkorn University

**Co-Chair:** Pimpa Hormnirun, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	IC-I-01	One-Pot Catalysis: A Privileged Approach for Sustainable Polymers	Christophe M. Thomas
13.30 – 14.00	IC-I-02	Tailoring 4-phosphoryl pyrazolones: Insights into lithium ion recognition and sustainable separation	Jan J. Weigand
14.00 – 14.30	IC-I-03	Creation of new conceptual ionic solids based on coordination chemistry	Takumi Konno
14.30 – 14.45	IC-O-01	Highly dispersed and stable palladium (II) species anchoring on ethylenediamine-grafted-MIL-101 (Cr) for styrene oxidation	Kittisak Choojun
14.45 – 15.00	IC-O-02	Biodegradable polyester composites, containing various metal oxide particles: a model study as shelf-life extendable packaging for bananas	Nattawut Yuntawattana
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		
16.00 – 16.30	IC-I-04	Highly active Cr, Al, and Sn metal complexes for CO <sub>2</sub> utilization and polyester synthesis	Khamphee Phomphrai
16.30 – 16.45	IC-O-03	A low-cost SFX-based hole transporting material for highly stable perovskite solar cells	Jeeranun Manit
16.45 – 17.00	IC-O-04	Switchable metal-ion selectivity in sulfur-functionalised pillar[5]arenes and their host-guest complexes	Bunyaporn Todee
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## IC-Inorganic Chemistry

**Saturday, 27 January 2024, Room: Nile 2**

**Chair:** Khamphree Phomphrai, Vidyasirimedhi Institute of Science and Technology

**Co-Chair:** Pimpa Hormnirun, Kasetsart University

Time	Code	Title	Presenter
09.45 – 10.15	IC-I-05	Benzoxazines and polybenzoxazines: Crystal structures, properties and applications	Worawat Wattanathana
10.15 – 10.30	IC-O-05	Pillararene supramolecular assembly in supramolecular organic frameworks (SOFs) and mechanically interlocked molecules (MIMs)	Pipatpong Laoviwat
10.30 – 10.45	IC-O-06	Synthetic studies and the applications of BINOL coordinated metalloporphyrins	Shafikul Islam
10.45 – 11.00	<b>Coffee Break</b>		
11.00 – 12.00	<b>Poster Session II at Bhiraj Hall I</b>		
12.00 – 13.00	<b>Lunch at EH100</b>		
13.00 – 13.30	IC-I-06	Strategic synthesis of supramolecular host molecules for recognition and sensing of charged species	Thanthapatra Bunchuay
13.30 – 14.00	CST-02	Multi-responsive chromism and luminescence in heteroatom-functionalized complexes	Jaursup Boonmak
14.00 – 14.15	IC-O-07	Neutral isocyanide-templated assembly of pillar[5]arene [2] and [3] pseudorotaxanes	Korawit Khamphaijun
14.15 – 14.30	IC-O-08	Development of chiral metal complexes coordinated by axial chiral ligands exhibiting circularly polarized luminescence	Daiki Tauchi



## IE-Industrial and Engineering Chemistry

**Friday, 26 January 2024, Room: Nile 3**

**Chair:** Sirirat Jitkarnka, Chulalongkorn University

**Co-Chair:** Pinsuda Viravathana, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	IE-K-01	TBA	Sineenuch Kokanutaporn
13.30 – 14.00	IE-K-02	TBA	Natthakorn Kraikul
14.00 – 14.30	IE-K-03	Journey on exploring advanced recycling technologies by Indorama Ventures Plc.	Sasinotai Rochanutama
14.30 – 14.45	IE-O-01	Synthesis of silicon carbide by using rice husk ash from power plant wastes	Benchanee Singrattanaphan
14.45 – 15.00	IE-O-02	Development of neural network architectures for prediction of energy consumption and carbon dioxide emission in natural gas separation process	Bhiranat Pongsri
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		
16.00 – 16.30	IE-K-04	The circularity of tire industry: recovered carbon black/graphene composite materials and applications	Apichai Jomphoak
16.30 – 16.45	IE-O-03	Heat transfer analysis of a microwave reactor using computational fluid dynamics for polymer recycling	Aung Khant Zaw
16.45 – 17.00	IE-O-04	Beyond the extraction limit–molecular cages as membranes for chemical separations	Jiratheep Pruchyathamkorn
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## MN-Material Chemistry and Nanotechnology

**Friday, 26 January 2024, Room: Nile 4**

**Chair:** Vinich Promarak, Vidyasirimedhi Institute of Science and Technology

**Co-Chair:** Wisit Hirunpinoyopas, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	MN-K-01	The role of organic photovoltaics in renewable energy to overcome climate change	Thuc-Quyen Nguyen
13.30 – 14.00	MN-I-01	TBA	T. Randall Lee
14.00 – 14.15	MN-O-01	Asymmetric D-A-D' type hybridized local and charge transfer fluorophores as deep-red/near-infrared emitters for efficient non-doped OLEDs	Teerapat Itsoponpan
14.15 – 14.30	MN-O-02	Boosting OLEDs performance via hot exciton mechanism: The study of heteroatom and different the number of donor unit effects on D- $\pi$ -A type emitters	Takdanai Unjarern
14.30 – 14.45	MN-O-03	Development of near-infrared phosphorescent organoiridium (III) complexes bearing 2-arylquinoxaline-based cyclometalated ligands	Ryuta Shikura
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		



## MN-Material Chemistry and Nanotechnology

**Friday, 26 January 2024, Room: Nile 4**

**Chair:** Chaia Prasittichai, Kasetsart University

**Co-Chair:** Vinich Promarak, Vidyasirimedhi Institute of Science and Technology

Time	Code	Title	Presenter
16.00 – 16.30	MN-I-02	Electrochemical applications of two dimensional (2D) materials for sustainable uses	Wisit Hirunpinyopas
16.30 – 16.45	MN-O-04	Facile synthesis of highly active and durable carbon composite as a non-precious metal oxygen reduction reaction electrocatalyst in alkaline media	Kittimaporn Nernprom
16.45 – 17.00	MN-O-05	Preparation and characterization of MoS <sub>2</sub> /lignin-based carbon nano-composite fibers for supercapacitor electrodes	Kamonluk Sirikarint
17.00 – 17.15	MN-O-06	Solution plasma-assisted integration of MXene nanosheets with iron and nitrogen-doped carbons as electrocatalysts for oxygen reduction reaction	Kasidit Janbooranapinij
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## MN-Material Chemistry and Nanotechnology

**Saturday, 27 January 2024, Room: Nile 4**

**Chair:** Jeng-Yu Lin, Tunghai University

**Co-Chair:** Chaiya Prasittichai, Kasetsart University

Time	Code	Title	Presenter
09.45 – 10.15	MN-I-03	Crystallization of pharmaceutical compounds	Il Won Kim
10.15 – 10.30	MN-O-07	Parameter optimization for the synthesis of hybrid gold nanoparticle-carbon dot colloids and their luminescent properties alteration	Thammika Srisaman
10.30 – 10.45	MN-O-08	Development of colloidal cellulose nanocrystal suspensions as a sprayable PM2.5 remover	Benyapha Kheawmancee
10.45 – 11.00	Coffee Break		
11.00 – 12.00	Poster Session II at Bhiraj Hall I		
12.00 – 13.00	Lunch at EH100		
Chair: Il-Won Kim, Soongsil University Co-Chair: Vinich Promarak, Vidyasirimedhi Institute of Science and Technology			
13.00 – 13.30	MN-I-04	δ-MnO <sub>2</sub> -based nanocomposite cathodes for aqueous Mg-ion electro-chemical energy storage devices	Jeng-Yu Lin
13.30 – 13.45	MN-O-09	Colorimetric sensing of polymers by using polydiacetylene/zinc(II)/zinc oxide nanocomposites: Effect of solvents and cationic surfactant	Sasiwan Boonmak
13.45 – 14.00	MN-O-10	Polydiacetylene-based materials for colorimetric sensing of fatty acids	Nannapat Kaewnukulkit
14.00 – 14.15	MN-O-11	Quercetin mediated Ag@Au core-shell nanoparticles: Synthesis, characterization and applications	Amtul Qayoom

## MN-Material Chemistry and Nanotechnology

*Saturday, 27 January 2024, Room: Nile 4*

Time	Code	Title	Presenter
14.15 – 14.30	MN-O-12	Synthesis of gold nanoparticles supported on carbon nanomaterials via solution plasma sputtering as electrochemical sensors for mercury(II) ion detection	Jidapa Chantaramethakul
14.30 – 14.45	MN-O-13	Synthesis and characterization of nitrogen-doped carbon dots from bird's nest for heavy metal detection	Teeraphat Prachayanipon
14.45 – 15.00	MN-O-14	Voltammetry of paraquat-based bismuth nanoparticles screen-printed electrodes for environmental surveillance	Patima Phumsathan
15.00 – 15.15	<i>Coffee Break</i>		
15.15 – 15.30	MN-O-15	pH-Responsive polymer as a new stable solid electrolyte interphase for water-in-salt battery	Rossukon Jommongkol
15.30 – 15.45	MN-O-16	Preparation and characterization of silver nanowires/cellulose nanofibrils-based conductive paper	Noppamas Thongsiri
15.45 - 16.15	MN-I-07	Novel electronic materials using metal precursors and TADF host materials for high performance DRAM and OLED applications	Jongwook Park

# MN-Material Chemistry and Nanotechnology

**Saturday, 27 January 2024, Room: Nile 3**

**Chair:** Joon-Wook Park, Kyung Hee University

**Co-Chair:** Kanokwan Kongpatpanich, Vidyasirimedhi Institute of Science and Technology

Time	Code	Title	Presenter
09.45 – 10.15	MN-I-05	Porphyrins for Energy Conversion	Chen-Yu Yeh
10.15 – 10.30	MN-O-17	Plasmon enhancement of photodetectors based on CsPbBr <sub>3</sub> quantum dots	Zar Ni Thein Htay
10.30 – 10.45	MN-O-18	Influence of chemical surface-treatment agent on mechanical and neutron-shielding properties of recycled high-density polyethylene (r-HDPE)/ gadolinium oxide (Gd <sub>2</sub> O <sub>3</sub> ) composites	Donruedee Toyen
10.45 – 11.00	Coffee Break		
11.00 – 12.00	Poster Session II at Bhiraj Hall I		
12.00 – 13.00	Lunch at EH100		
Chair: Chen-Yu Yeh, National Chung Hsing University Co-Chair: Vinich Promarak, Vidyasirimedhi Institute of Science and Technology			
13.00 – 13.30	MN-I-06	Development of metal-organic frame-works for energy and environmental applications	Kanokwan Kongpatpanich
13.30 – 14.00	CST-07	Highly enantioselective synthesis of chiral molecules at modified mesoporous metal electrodes	Sopon Butcha
14.00 – 14.15	MN-O-23	Synthesis of achiral fluorene derivatives exhibiting circularly polarized luminescence induced in chiral nematic liquid crystal medium	Yuki Fujita
14.15 – 14.30	MN-O-20	Bio-CaCO <sub>3</sub> from <i>Perna viridis</i> shells for plant coating	Orakanya Kumphon
14.30 – 14.45	MN-O-21	Microstructural modification of nickel aluminium bronze against erosion corrosion	Methawat Keereerak-wattana
14.45 – 15.00	MN-O-22	Synthesis of RGB fluorescent helical network polymers in chiral liquid crystals and evaluation of their circularly polarized luminescence	Hiromasa Yamamoto
15.00 – 15.15	MN-O-19	Metal-organic chalcogenolates – An emerging family of low-dimensional hybrid semi-conductors	Watcharaphol Paritmongkol
15.15 – 15.30	Coffee Break		



## NP-Natural Products, Biological Chemistry and Chemical Biology

**Friday, 26 January 2024, Room: Amber 1**

**Chair:** Wanchai Pluempunupat, Kasetsart University

**Co-Chair:** Pakorn Wattana-Amorn, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	NP-I-01	From darkness to light: investigating the chemical basis of Pholasin’s bioluminescent mechanism	Masaki Kuse
13.30 – 14.00	NP-I-02	Biosynthesis of antitumor alkaloid streptonigrin	Shuangjun Lin
14.00 – 14.30	NP-I-03	Deuterated drugs, new challenging molecules as drug candidates: Deuteration of natural products	Prasat Kittakoop
14.30 – 14.45	NP-O-01	NMR-based stability evaluation of ( <i>E</i> )-1-(3,4-dimethoxyphenyl) butadiene (DMPBD) from <i>Zingiber cassumunar</i> Roxb. Rhizome	Boonwiset Seaho
15.00 – 15.15	Coffee Break		
15.15 – 16.00	PL-02 at Bhiraj Halls II and III		
Chair: Prasat Kittakoop, Chulabhorn Graduate Institute Co-Chair: Pakorn Wattana-Amorn, Kasetsart University			
16.00 – 16.30	NP-I-04	Optimizing natural products as promising antiviral agents through computation-aided drug design	Kowit Hengphasatporn
16.30 – 16.45	NP-O-02	Molecular docking simulation tool CB-Dock2 confirmed high binding affinity between curcuminoids and IκBα/p50/p65 protein complex	Sompot Jantarawong
16.45 – 17.00	NP-O-03	in silico and in vitro studies on nucleoside-based inhibitors for pan-antiviral drug repurposing	Pitchayathida Mee-udorn
17.15 – 18.15	Poster Session I at Bhiraj Hall 1		
18.15 – 21.00	Conference Banquet at Bhiraj Halls II and III		

## NP-Natural Products, Biological Chemistry and Chemical Biology

**Saturday, 27 January 2024, Room: Amber 1**

**Chair:** Masaki Kuse, Kobe University

**Co-Chair:** Pakorn Wattana-Amorn, Kasetsart University

Time	Code	Title	Presenter
09.45 – 10.15	NP-I-05	Southern Philippines as a rich source of natural products	Mylene Uy
10.15 – 10.30	NP-O-04	Chemical constituents and their biological activities from the rhizomes and leaves of <i>Curculigo orchioides</i>	Phornnapa Saentao
10.30 – 10.45	NP-O-05	Immobilized chitinase as an effective biocatalytic platform for producing bioactive chitobiose from biomass-derived chitin	Ailada Charoenpol
10.45 – 11.00	<b>Coffee Break</b>		
11.00 – 12.00	<b>Poster Session II at Bhiraj Hall I</b>		
12.00 – 13.00	<b>Lunch at EH100</b>		



## OM- Organic Synthesis and Medicinal Chemistry

**Friday, 26 January 2024, Room: Amber 2**

**Chair:** Mihaiela Stuparu, Nanyang Technological University

**Co-Chair:** Anna Kajetanowicz, University of Warsaw

Time	Code	Title	Presenter
13.00 – 13.30	OM-I-01	Olefin metathesis catalysts specialised in bio-mass valorization: ethenolysis of fatty oils and musk production	Karol Grela
13.30 – 14.00	OM-I-02	Synthesis, computers and natural product mistakes	Roderick W. Bates
14.00 – 14.15	OM-O-01	Stannylation as the key strategy for the synthesis of C2-substituted cordycepin derivatives for antiviral drug development	Aticha Thiraporn
14.15 – 14.30	OM-O-02	Synthetic study of natural antimalarial, (+)-febrifugine, from D-glucose and D-serine: Development of new pathways via azide and azide free approaches	Suwanan Uipanit
14.30 – 14.45	OM-O-03	Amination of 1,2,4-oxadiazol-5(4H)-ones with tertiary amines	Muh Alfiadhi
14.45 – 15.00	OM-O-04	Comparison synthesis of picric acid from phenol and salicylic acid for crystallization of mitragynine as picrate salt at difference percent purity	Suntisuk Sinthunakorn
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		

## OM- Organic Synthesis and Medicinal Chemistry

**Friday, 26 January 2024, Room: Amber 2**

**Chair:** Tirayut Vilaivan, Chulalongkorn University

**Co-Chairs:** 1) Roderick W. Bates, Nanyang Technological University  
2) Nutthawat Chuanopparat, Kasetsart University

Time	Code	Title	Presenter
16.00 – 16.30	OM-I-03	Catalytic deoxygenation of epoxides to alkenes	Sunisa Akkarasamiyo
16.30 – 16.45	OM-O-05	Synthesis and evaluation of chrysin derivatives as histone deacetylase inhibitors	Thitiporn Kamloon
16.45 – 17.00	OM-O-06	Structural simplification of maytansine and synthesis efficiency for antitumor activity	Tomomi Uchida
17.00 – 17.15	OM-O-07	Syntheses and mechanistic investigations of formamides, formamidines, and formimidates	Chhorvy Kong
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## OM- Organic Synthesis and Medicinal Chemistry

**Saturday, 27 January 2024, Room: Amber 2**

**Chair:** Roderick W. Bates, Nanyang Technological University

**Co-Chair:** Karol Grela, Institute of Organic Chemistry, Polish Academy of Sciences

Time	Code	Title	Presenter
09.45 – 10.15	OM-I-04	Synthesis of curved nanographenes	Mihaiela Stuparu
10.15 – 10.30	OM-O-08	Synthetic and chiroptical studies on novel fluorophores based on chiral bipyrenyl platform	Reichi Kobayashi
10.30 – 10.45	OM-O-09	Gallic acid encapsulated pamam dendrimers: A promising antioxidant delivery system for controlled release and reduced toxicity	Aorada Sripunya
10.45 – 11.00	Coffee Break		
11.00 – 12.00	Poster Session II at Bhiraj Hall I		
12.00 – 13.00	Lunch at EH100		
<b>Chair:</b> Tirayut Vilaivan, Chulalongkorn University <b>Co-Chairs:</b> 1) Chanat Aon-Bangkhen, Chulalongkorn University 2) Nutthawat Chuanopparat, Kasetsart University			
13.00 – 13.30	OM-I-05	Olefin metathesis-sustainable methodology for synthesis of valuable compounds	Anna Kajetanowicz
13.30 – 13.45	OM-O-10	Synthesis of azanorbornadienes as building blocks to complex aryl products	Thomas Whatton
13.45 – 14.00	OM-O-11	Synthesis and properties of helical oligothiophenes anchored to binaphthyl	Hikari Kawashima

## PC-Polymer Chemistry and Bio-Based Materials

**Friday, 26 January 2024, Room: Amber 3**

**Chair:** Kanoktip Boonkerd, Chulalongkorn University

**Co-Chair:** Wirunya Keawwattana, Kasetsart University

Time	Code	Title	Presenter
13.00 – 13.30	PC-K-01	Macromolecular engineering: Well-defined model pentacrystalline pentablock quintopolymer	Nikos Hadjichristidis
13.30 – 14.00	PC-I-01	Bacterial cellulose as renewable polymeric platform for biosensing and biomedical applications	Voravee P. Hoven
14.00 – 14.30	PC-I-02	Functional polymeric nanomaterials for controlled release systems in biomedical and cosmetic applications	Pakorn Opaprakasit
14.30 – 14.45	PC-O-01	A study of pre-vulcanization time affected on the nano-porous structure preservation in silica aerogel/natural rubber composite	Chayanon Boonrawd
15.00 – 15.15	Coffee Break		
15.15 – 16.00	PL-02 at Bhiraj Hall II and III		
Chair: Panya Sunintaboon, Mahidol University Co-Chair: Kanoktip Boonkerd, Chulalongkorn University			
16.00 – 16.30	PC-I-03	Green synthesis multi-stimuli responsive trimethyl chitosan-based nanogel and its promising application as nanocarrier for cancer photothermal chemotherapy	Panya Sunintaboon
16.30 – 16.45	PC-O-02	Production and characterization of cellulose powders from brewery's spent grain	Kawalee Kumpangnil
16.45 – 17.00	PC-O-03	Development and characterization of amidated pectin-PVA hydrogels for enhanced drug delivery and antimicrobial properties	Supatcha Suankhem



## PC-Polymer Chemistry and Bio-Based Materials

**Saturday, 27 January 2024, Room: Amber 3**

**Chair:** Wirunya Keawwattana, Kasetsart University

**Co-Chair:** Nopparat Plucktaveesak, Thammasart University

Time	Code	Title	Presenter
09.45 – 10.15	PC-I-04	Synthesis of chiral cyclic oligomers and cyclic molecules based on planar chiral [2.2] paracyclophanes	Yasuhiro Morisaki
10.15 – 10.30	PC-O-04	Comparison properties of hybrid carbon-based nanocomposites between engineering-thermoplastic Acrylonitrile-Butadiene-Styrene and commodity-thermoplastic polypropylene for electrical and thermal application	Sorawit Duangsripat
10.30 – 10.45	PC-O-05	Apatite growth of bioactive glass containing elephant dung cellulose	Phimmada Nithipongwarodom
10.45 – 11.00	<i>Coffee Break</i>		
11.00 – 12.00	<i>Poster Session II at Bhiraj Hall I</i>		
12.00 – 13.00	<i>Lunch at EH100</i>		

## PT-Physical and Theoretical Chemistry

**Friday, 26 January 2024, Room: Amber 4**

**Chair:** Kaito Takahashi, Academia Sinica

**Co-Chair:** Siriporn Jungsuttiwong, Ubon Ratchathani University

Time	Code	Title	Presenter
13.00 – 13.30	PT-I-01	Importance of noncovalent interactions in homogeneous and enzymatic catalysis	Seiji Mori
13.30 – 14.00	PT-I-02	Theoretical study on the role of dynamics during enzyme catalysis	Toshifumi Mori
14.00 – 14.15	PT-O-01	The development of a new hypothetical MOF database for high-efficiency MOFs targeted for CO <sub>2</sub> utilization	Poobodin Mano
14.15 – 14.30	PT-O-02	Computational investigation of double-atoms catalysts decorated on defective boron nitride for catalyzing CO oxidation: A DFT study	Ratchadaree Intayot
14.30 – 14.45	PT-O-03	Enhanced formic acid production through catalytic CO <sub>2</sub> hydrogenation on frustrated Lewis pair functionalized UiO-67	Pimjai Pimbaotham
14.45 – 15.00	PT-O-04	A DFT study on a single transition metal doped C <sub>3</sub> N for CO oxidation reaction	Suparada Kamchompoo
15.00 – 15.15	<b>Coffee Break</b>		
15.15 – 16.00	<b>PL-02 at Bhiraj Halls II and III</b>		



## PT-Physical and Theoretical Chemistry

**Friday, 26 January 2024, Room: Amber 4**

**Chair:** Seiji Mori, Ibaraki University

**Co-Chair:** Cheng-Chau Chiu, National Sun Yat-sen University

Time	Code	Title	Presenter
16.00 – 16.30	PT-I-05	A net zero climate-resilient future: A computational chemistry approach for energy solutions	Siriporn Jungsuttiwong
16.30 – 16.45	PT-O-05	The effect of non-metal doped graphitic carbon nitride for carbon dioxide reduction reaction: A DFT study	Wassana Mongkonkan
16.45 – 17.00	PT-O-06	Enhancing carbon dioxide reduction through single and dual heteroatoms doped diamond: A DFT study	Yuwanda Injongkol
17.00 – 17.15	PT-O-07	How many water molecules react with simplest Criegee intermediates at atmospheric conditions?	Kaito Takahashi
17.15 – 18.15	<b>Poster Session I at Bhiraj Hall 1</b>		
18.15 – 21.00	<b>Conference Banquet at Bhiraj Halls II and III</b>		

## PT-Physical and Theoretical Chemistry

**Saturday, 27 January 2024, Room: Amber 4**

**Chair:** Supawadee Namuangruk, NANOTEC

**Co-Chair:** Luckhana Lawtrakul, Thammasart University

Time	Code	Title	Presenter
09.45 – 10.15	PT-I-04	Modeling the defective structure of MoS <sub>2</sub> : A first-principles kinetic Monte Carlo study	Cheng-chau Chiu
10.15 – 10.30	PT-O-08	Enhancing V <sub>2</sub> O <sub>5</sub> cathodes in magnesium-Ion batteries through aqueous electrolyte-induced hydrogen insertion: A first-principles approach	Suwit Suthirakun
10.30 – 10.45	PT-O-09	Roles of reactants for Suzuki C-C cross-coupling reaction using molecular volcano plots	Kwanchanok Kaewkwan
10.45 – 11.00	Coffee Break		
11.00 – 12.00	Poster Session II at Bhiraj Hall I		
12.00 – 13.00	Lunch at EH100		
Chair: Suwit Suthirakun, Suranaree University of Technology Co-Chair: Prapasiri Pongprayoon, Kasetsart University			
13.00 – 13.30	PT-I-03	Exploring human serum albumin modifications: Advancing screening and monitoring for non-communicable diseases	Deanpen Japrungr
13.30 – 13.45	PT-O-10	Molecular docking and dynamic simulations of anti-apoptotic Bcl-2 proteins as targets for bioactive compounds in <i>Durio zibethinus</i> for anti-cancer activity	Luckhana Lawtrakul

## SS-Special Session

*Saturday, 27 January 2024, Room: Amber 2*

Time	Code	Title	Presenter
14.00 – 14.30	SS-01	Driving chemistry for sustainable change	Mandar Bodas
14.30 – 15.00	SS-02	NMR experiments for small molecule analysis and structure elucidation – quick update	Teh Chin Hoe
15.00 – 15.15	<i>Coffee Break</i>		

## SS-Special Session

*Saturday, 27 January 2024, Room: Amber 3*

Time	Code	Title	Presenter
14.45 – 15.15	SS-03	Biocarbon value chain development from agricultural waste: A key driver in Thailand's Bio-Circular-Green economy	Kent Goeking
15.15 – 15.30	<i>Coffee Break</i>		

## BSTJ-Bilateral symposium between Thailand and Japan on recent progress of photophysical chemistry

*Saturday, 27 January 2024, Room: Nile 1*

**Chair: Hiroyuki Nishikawa**

Time	Code	Title	Presenter
09.50 – 10.10	Opening remarks by Hiroyuki Nishikawa		
09.50 – 10.10	BSTJ-I-01	Chiroptical properties of helical conjugated polymers synthesized in chiral liquid crystals	Kazuo Akagi
10.10 – 10.30	BSTJ-I-02	Excited-state intramolecular proton transfer (ESIPT) molecules for optoelectronic materials, fluorescent sensors, and imaging agents	Nawee Kungwan
10.30 – 10.50	BSTJ-I-03	Generation of circularly polarized electroluminescence from organic light-emitting diodes with optically inactive phosphorescent emitters under an external magnetic field	Shigeyuki Yagi
10.50 – 11.00	<i>Coffee Break</i>		
11.00 – 12.00	<i>Poster Session II at Bhiraj Hall I</i>		
12.00 – 13.00	<i>Lunch at EH100</i>		
13.00 – 13.20	BSTJ-I-04	Sunlight-responsive photocatalysts for detoxification of organic dyes and antibiotics in natural water	Suwat Nanan
13.20 – 13.40	BSTJ-I-05	Visualization of electronic and magnetic transition moments aiming at the design of CPL chromophore having enhanced chiroptical properties	Ken-ichi Sugiura

Time	Code	Title	Presenter
13.40 – 14.00	BSTJ-I-06	New electrochemical detection strategies for clinical diagnosis	Kontad Ounnunkad
14.00 – 14.20	BSTJ-I-07	Synthesis and chiroptical properties of strained paraphenylene anchoring chiral binaphthyl	Masashi Hasegawa
14.20 – 14.40	BSTJ-I-08	Advancements in nanomaterials for augmenting electrochemical and photometric sensor performance	Jaroon Jakmunee
14.40 – 15.00	BSTJ-I-09	Newly developed systems for advanced CD and CPL measurements and their measurement methods and applications	Satoko Suzuki
15.00 – 15.10	<i>Coffee Break</i>		
15.10 – 15.30	BSTJ-I-10	The synthesis and development of novel fluorescence compounds as heavy metal ion sensors	Anawat Ajavakom
15.30 – 15.50	BSTJ-I-11	Development of aggregation-induced emissive materials exhibiting circularly polarized luminescence	Hiroyuki Nishikawa
15.50 – 16.10	BSTJ-I-12	Photophysical properties for excited-state intramolecular proton transfer (ESIPT) reaction of N-salicylidene-o-aminophenol: DFT based approaches	Songwut Suramitr
16.10 – 16.15	Closing remarks by Nawee Kungwan		

# PLENARY SPEAKER ABSTRACTS

## Unconventional approaches to energy conversion

Alexander Kuhn

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Humanity harnesses several types of primary energies. A primary energy represents untransformed versions of energy (chemical, nuclear, solar...). These energies must be converted in order to be used in the form of final energy (heating, movement, lighting, etc.). Therefore, the transformation of energy is the keystone of our existence and plays a central role in circular and/or green economy. We are going to discuss several types of energy conversion, very important for our daily life, and compare for each example the conventional approaches with more exotic transformation schemes, involving chemical,<sup>1,2</sup> physical<sup>3</sup> and biological concepts,<sup>4,5</sup> or a synergetic combination thereof.<sup>6-8</sup>

**Keywords:** Energy; Motion; CO<sub>2</sub> conversion; Green hydrogen; Biofuel

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### ■ Professional Biography

Alexander Kuhn is Professor at the Institute of Molecular Science (University Bordeaux, CNRS, Bordeaux INP, France), as well as Adjunct Professor at VISTEC (Thailand) and Henan University (China). After studying chemistry at the TU München, University of Oxford and University Bordeaux, he obtained his Master in Chemistry from the TU München in 1991 and his Ph.D. in 1994 from the University Bordeaux. Following his post-doctoral studies at Caltech (1995/1996 he obtained an Assistant Professor (1996) and later a Full Professor (2000) position in Bordeaux. He is a senior member of the Institut Universitaire de France, distinguished senior member of the French Chemical Society and Fellow of the International Society of Electrochemistry. His current main research interests are modified electrodes with a special focus on applications in electroanalysis, bioelectrochemistry and electrocatalysis; nanomaterials; micro- and nanomotors; Janus particles; bipolar electrochemistry; chirality.

PL

## Designing polymers with the end in mind: Creating circular routes to polymers using light-based strategies

Thiago M. Ouriques,<sup>1</sup> Joshua C. Worch,<sup>1,2</sup> Connor J. Stubbs,<sup>1</sup> Alexis Perrot,<sup>1</sup> Arianna Brandolese,<sup>1</sup> Richard Grainger<sup>1</sup>, and Andrew P. Dove<sup>1\*</sup>

<sup>1</sup>*School of Chemistry, The University of Birmingham, Edgbaston, Birmingham, UK, B15 2TT*

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One of the unresolved consequences of the massive global production of plastic is the lack of proper waste management. As a consequence of technological limitations as well as inefficient collection and sorting methods, current recycling schemes are underperforming. In part this is a result of the inherent linear design of our polymer systems, and lack of consideration of waste management and environmental impact of the waste that does escape into the environment, at the polymer design stage. We, among others, are focussing on creating tools that could be applied to design polymers ‘with the end in mind’ – i.e. to incorporate chemical bonding that can be easily processed to make polymers but readily reversed either ‘on demand’ for recycling, or upon exposure to environmental triggers. To this end, we have focussed on two different aspects of this challenge: (1) to design photosest materials that can be processed by advanced methods such as additive manufacturing that are sustainably sourced but can be readily circularised in a closed loop process and (2) to apply efficient click chemistries for the synthesis of polymers that not only have useful properties and inherent recyclability but also degrade to specific and predictable, non toxic by products upon exposure to light.

**Keywords:** Photopolymerisation; Circular economy; 3D printing; Depolymerization; Polymer degradation.



## ■ Professional Biography

Andrew graduated from the University of York with an MChem degree in 1999. His subsequent Ph.D. studies were conducted under the supervision of Prof. Vernon C. Gibson FRS at Imperial College, London, focused on metal catalysed co-ordination insertion polymerisation. Andrew undertook post-doctoral research under the guidance of Prof. Robert M. Waymouth and Dr James L. Hedrick at Stanford University and at IBM, San Jose, California. Andrew returned to the UK to take up a RCUK Fellowship in Nanotechnology in September 2005 before being appointed as an Assistant Professor in September 2006 and subsequently as an Associate Professor in September 2009 before being appointed as a Full Professor in June 2014. In January 2018, Andrew joined the School of Chemistry at the University of Birmingham as Professor of Chemistry. His research is focused on sustainable polymers and degradable biomaterials.

PL



## Enzyme catalysis for green chemistry

Pimchai Chauiyen\*, Kridsakorn Prakinee, Aisaraphon Phintha, Chalermroj Sutthaphirom, Pattarawan Intasian, Juthamas Jaroensuk, and Pratchaya Watthaisong

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Our group interests are in the broad areas of enzyme catalysis, enzyme engineering, systems biocatalysis, metabolic engineering and synthetic biology. In this talk, I will highlight our recent and current work on engineering of enzymes and cofactor enhancing systems for creation of robust biocatalysts. We used mechanistic understanding and rational-engineering to improve performance of flavin-dependent halogenase and dehalogenase to improve their biocatalytic applications. We have created two types of *in vivo* enhancing systems to increase intermediates and cofactors which are common for product synthesis in metabolically engineered cells. One of the systems uses xylose reductase and lactose (XR/lactose), to increase levels of a pool of sugar-phosphates which are connected to the biosynthesis of NAD(P)H, FAD, FMN and ATP in *Escherichia coli*. The XR/lactose system could increase the amounts of the precursors of these cofactors and was tested with three different metabolically engineered cell systems (fatty alcohol biosynthesis, bioluminescence light generation and alkane biosynthesis) with different cofactor demands. Productivities of these cells were increased 2-4-fold by the XR/lactose system. Untargeted metabolomic analysis revealed different metabolite patterns among these cells; demonstrating that only metabolites involved in relevant cofactor biosynthesis were altered. We propose that the approach of increasing cellular sugar phosphates can be a generic tool to increase *in vivo* cofactor generation upon cellular demand for synthetic biology. We also developed of an enzymatic cascade and engineering of a flavin-dependent monooxygenase, HadA, which catalyzes the dehalogenation and denitration of the toxicants, nitro- and halogenated phenols, to benzoquinone. The HadA reaction was applied in one-pot reactions towards the de novo synthesis of D-luciferin. Currently, this technology allows us to develop a new method for synthesizing various D-luciferin analogues. As nitro- and halogenated phenols are key indicators of human overexposure to pesticides commonly used worldwide and indicators of pesticide contamination, the technology provides a sensitive and convenient tool for biomedical and environmental detection at ppb sensitivity in biological samples without the requirement for any pre-treatment.

**Keywords:** Enzyme catalysis; Enzyme engineering; Biocatalysis; Synthetic biology; Metabolic engineering



### ■ Professional Biography

Professor Pimchai Chaiyen is one of the most accomplished biochemists in Thailand. She has received numerous awards including the L'Oréal-UNESCO Fellowship, Taguchi Prize for Outstanding Research Achievement in Biotechnology, TRF-CHE-Scopus Researcher Award from Thailand Research Fund, and Outstanding Scientist of Thailand, the country's highest honour in science. She is an editorial board member and referee for many international journals, and a reviewer in many national and international granting agencies. She also gave a TEDx talk in 2015.

PL

## Rethinking our relationship with the planet at molecular scale

J. García Martínez

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Chemistry is usually defined, conceived, and taught as the science of transformation. To adapt to the circular economy, chemistry must evolve towards being the science (and industry) of reuse. We cannot continue to extract, emit, and dispose at the levels we are doing now without compromising our climate, the environment, and our health. If we want to have a viable industry and a healthy planet, the circular economy cannot be just an aspiration but the key objective of chemistry.<sup>1</sup>

Rethinking chemistry for a circular economy involves profound changes, from the way molecules are conceived to how processes are designed to ensure traceability, recyclability, and reuse<sup>2</sup>. Circularity at the molecular level means turning chemistry toward the reuse of atoms, molecules, monomers, polymers, etc—and represents an opportunity to place chemistry at the center of the new circular economy.<sup>3</sup>

Figure 1 captures how chemistry can adapt from a linear (transformation) to a circular process (reuse) and how this involves designing molecules in a way that they can be disassembled and reconstructed to minimize the production of waste and ensure recyclability.

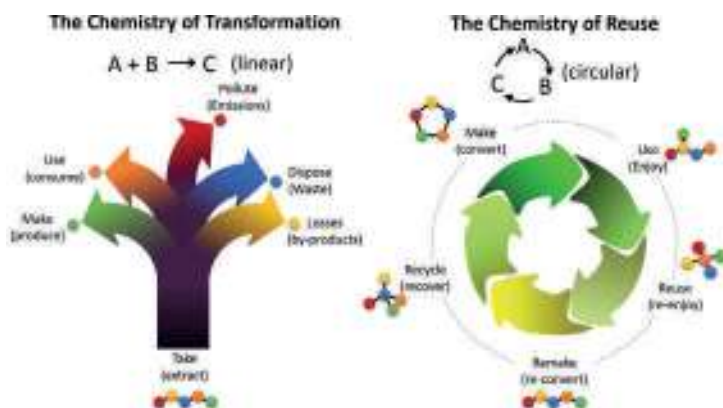


Figure 1. Schematic representation of the two models of chemistry: (left) the old linear concept based on the transformation of raw materials into products and waste and (right) the new chemistry of reuse that involves a close loop system where resources are continuously used and the production of waste is minimized.<sup>2</sup>

Several examples of circular economy will be presented, including the design of a new generation of plastics with break-points<sup>4</sup> or dynamic bonds<sup>5</sup> that allow for their disassembly into their monomers and their reconstruction. This process can be done at ca. 100 % yield and multiple times. These and other examples of circular chemistry will be described in detail and an outlook of the area will be provided.

During my presentation, I will also describe some of the activities that we are carrying out at IUPAC to foster sustainable chemistry education, research, and industry while we accelerate the achievement of the Sustainable Development Goals, as we are celebrating the International Year of Basic Sciences for Sustainable Development.



## ■ Professional Biography

Professor of Inorganic Chemistry and Director of the Molecular Nanotechnology Lab, a world-leading research centre working on the synthesis and application of nanostructured materials for the sustainable production of chemicals and energy at the University of Alicante, Spain.

Founder of Rive Technology, a technology-based company commercialising nanostructured catalysts that reduce millions of tonnes of CO<sub>2</sub> per year while increasing energy efficiency. Since 2012, Shell has been using this technology in several of its plants and in 2019, W. R. Grace acquired this technology and is now commercialising it globally.

President of the International Union of Pure and Applied Chemistry (IUPAC), where he introduced major changes such as the establishment of the Scientific and Executive Boards, the integration of the International Younger Chemists Network (IYCN) and the creation of the Presidents' Forum.

His contributions to catalysis, energy and chemistry have been recognised with some of the most prestigious awards, including 1) Young Global Leader, 2009 - World Economic Forum, 2) Innovator of the Year, 2007 - MIT, 3) Member of the Round Table of Top Entrepreneurs, 2008 - European Commission, 4) Emerging Researcher Award, 2015 and Kathryn C. Hach Award for Entrepreneurial Success, 2018 - American Chemical Society, 5) Premio Rey Jaime I, 2014, 6) Fellow of the Royal Society of Chemistry, 2007 and the American Chemical Society, 2021, and 7) Member of the Council of Emerging Technologies - World Economic Forum.

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# KEYNOTE \ INVITED SPEAKER ABSTRACTS

## High resolution accurate mass mass spectrometry (HRAM MS) for a better understanding of the health and the resilience of ecosystems

Ryszard Lobinski

AC

*French National Centre for Scientific Research (CNRS), Institute of Analytical and Physical Chemistry for the Environment and Materials (IPREM - UMR5254), Hélioparc, 2, av. Pr. Angot, 64053 Pau, France*

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Biological organisms have learned to synthesize metal-complexing molecules (metallophores) responsible for the capacity of resilience of plants and bacterial communities facing an excess of a toxic metal or a deficit of an essential micronutrient. The discovery and characterization of these molecules are the first step and a fundamental challenge to the understanding of the adaptation mechanisms involved on the molecular level.

Much research has been conducted to evaluate the effects of metals on plants and microorganisms in metal contaminated and metal deficient ecosystems. Most of it was based on the correlation of the total metal concentration with environmental or physiological factors, ignoring the real actors of the metal trafficking process, i.e. the metal complexes with the ligands in charge of the metal acquisition and transport. The advent of electrospray mass spectrometry and its implementation in genomics, proteomics and metabolomics have also opened new avenues for biological metal-related research, globally referred to as metallomics.

High resolution mass spectrometry offers the possibility of large-scale untargeted screening for metal-complexes in microvolumes of plant xylem and extracellular bacterial exudate. The high mass accuracy (down to 0.1 ppm) allows the unambiguous assignment of empirical formula to the detected compounds. Candidate parent ion fragmentation and multistage mass spectrometry permits to elucidate the formula.

The lecture discusses the fundamentals of HRAM for large scale metal speciation and illustrates its potential for understanding the metal acquisition and transport in hyperaccumulating plants in post-mining areas and acquisition of iron in a peatland ecosystem.

**Keywords:** Metals; Metallophores; Mass spectrometry; Phytoremediation; -Omics



## ■ Professional Biography

Ryszard Lobinski is professor of chemistry, research director at the National Research Center of France (CNRS) and director of the Institute of Analytical and Physical Chemistry in Pau, France.

He graduated as chemical engineer from the Warsaw University of Technology, Poland, from which he obtained his Ph.D. He was post-doctoral fellow of the Max-Planck Society in Germany, Dortmund and then research assistant at the University of Antwerp in Belgium. In 2006-2008 he was President of the Analytical Chemistry Division of the IUPAC. In 2006 he was awarded a CNRS Silver Medal and, in 2007, was admitted fellow of the Royal Society of Chemistry (UK).

His research interests concern the development of analytical methods for the identification and the determination of chemical forms of elements in the biological environment (speciation and metallomics) and the description of the mechanisms of uptake, metabolism, accumulation and excretion of trace elements by living organisms.

AC



## Single-cell analysis using ICP-*q*MS

Qiuquan Wang

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Single cell is the basic unit of life. Comprehensively physical, chemical and biological profiling of a single-cell is essential to understand its behavior, especially its biofunctions in the life process. During which, scientists have been trying to characterize a single-cell from different aspects covering morphology, genomics, proteomics and metabolomics via developing methods and using different tools. Even though great progresses have been achieved, there are many gaps remained for fully recognize and understand the behavior of a single cell due to the cell-to-cell heterogeneity existing between different cell lines even in the same type of cells. Here, I will talk about single-cell analysis using inductively coupled plasma quadrupole mass spectrometry (ICP-*q*MS). I will briefly introduce the element-tagging strategies towards the biomolecules expressed on the cell surface at first, which are responsibly participating in the behavior of a cell. Considering a single-cell analysis using the hard-ionization and scanning-type ICP-*q*MS, we designed and fabricated a microfluidic chip for manipulating the cells with an appropriate interval time before they entered into ICP-*q*MS one by one to realize a real single-cell analysis, on the other hand, we used methane as a collision gas to stretch the ion-plume of the transient single-cell event in the collision-reaction-cell equipped in ICP-*q*MS for a single-cell multiplex analysis. Moreover, an element-tagged macrophage MS2 nanoparticle was developed for signal-multiplication to guarantee the quantification of the element-tagged biomolecules on the surface of a single-cell. Single-cell analysis can thus be unambiguously performed regarding the cell surface biomolecules using ICP-*q*MS.

**Keywords:** ICP-*q*MS; Single-cell analysis; Element-tag; Microfluidic chip; Viruslike nanoparticle signal-multiplication



### ■ Professional Biography

Qiuquan Wang is a full professor at College of Chemistry and Chemical Engineering of Xiamen University. He is the deputy director of the Key Laboratory of Spectrochemical Analysis and Instrumentation of the Ministry of Education of China located at Xiamen University.

He got his PhD in 1998 under the supervision of Prof. Hideo Akaiwa and Prof. Kin-ichi Tsunoda from Gunma University Japan. He worked as a Postdoc fellow with Prof. Benli Huang at Xiamen University from 1998 to 2000. His research interests include new atomization and ionization methods of atomic optical and mass spectrometry, element/isotope-tagging strategy based ICP-qMS bioanalysis, design of novel monolithic stationary phases for chromatography, metallomics and reactive proteomics for understanding the molecular mechanisms of toxicity of metals and organic pollutants. He has published more than 100 peer-reviewed scientific papers and owns more than 10 patents. He serves currently as co editor of Analytical and Bioanalytical Chemistry (Springer Nature).

AC

## Electrodialytic ionic solutes handling for matrix isolation, purification, and separation

Shin-Ichi Ohira

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Ionic solutes are important chemical forms and widely measured. However, the analysis is required sample pretreatment purposed to isolate matrices, and adjust the concentrations suited to the analyzer. Even though sample pretreatment is the one of the key processes, there is no universal methods. Electrodialytic ion handling was developed and applied to matrices isolation, purification, and separation for chemical analysis. Flow based electrodialytic ion handling device was successfully applied to pretreatment for the analysis of common cation/anion with ion chromatography, organic acids in drinks, heavy metals in serum samples. Furthermore, the developed method can enrich the ionic solutes continuously. Conventional enrichment method, such as solid phase extraction, and evaporation dryness cannot enrich continuously. The developed continuous enrichment method was applied to determine chloroacetates in tap water with conventional HPLC-UV, and ultra-trace metals in ultra-pure water. The separation for speciation analysis was also succeeded. Chromium in environment is mainly Cr(III) and Cr(VI). Cr(III) is essential but Cr(VI) is strongly toxic. Because Cr(III) and Cr(VI) are respectively cation and anion, these can simply be separated with electrodialytic ion handling. This separation can simultaneously be achieved with matrices isolation and enrichment. The separation was further expanded to chiral separation. The electrodialytic chiral separation was successfully achieved with molecularly imprinted membranes. Also, purification of particulates are recently achieved for metal nano particles analysis. In the presentation, the basic theory and performance of developed ion handling method and the application of the methods will be shown.

**Keywords:** Electrodialysis; Chiral separation; Chromium oxidation states; Particles purifications



### ■ Professional Biography

Shin-Ichi Ohira is a professor of Analytical Chemistry at Kumamoto University, Japan. He received his Bachelor (2000), Master (2002), and Doctor (2005) of Science degrees from Kumamoto University. He served as Research Fellow for Young Scientists of the Japan Society for the Promotion of Science (JSPS) at Kumamoto University (2005 – 2006), Postdoctoral Fellow for Research Abroad of JSPS at Texas Tech University (2006) and The University of Texas at Arlington (UTA) (2007-2008), and Postdoctoral Research Fellow at UTA(2008-2009). He was promoted to associate professor at Kumamoto University in 2009 and professor in 2021. He received Award for Researchers from the Japan Association for Flow Injection Analysis (2022), Ion Chromatography Discussion Group of the Japan Society for Analytical Chemistry (JSAC) (2021). His current work focuses specifically on the electrodialytic ionic solutes handling, universal detection for high performance liquid chromatography, and gas sensing systems.

AC

## Wearable sweat glucose sensor connected with a smartphone readout

Nadtinan Promphet<sup>1</sup>, Chusak Thanawattano<sup>2</sup>, Thidarut Laochai<sup>1</sup>, Panlop Lormaneenopparat<sup>1</sup>, Pranee Rattanawaleedirojn<sup>1,3</sup>, Pranut Potiyaraj<sup>1,3</sup>, Krisana Siralertmukul<sup>1,3</sup>, and  
Nadnudda Rodthongkum<sup>1,3\*</sup>

<sup>1</sup>*Metallurgy and Materials Science Research Institute, Chulalongkorn University, Soi Chula 12, Phayathai Road, Pathumwan, Bangkok 10330, Thailand;* <sup>2</sup>*National Science and Technology Development Agency, Pathumthani 12120, Thailand;* <sup>3</sup>*Center of Excellence in Responsive Wearable Materials, Chulalongkorn University, Soi Chula 12, Phayathai Road, Pathumwan, Bangkok, 10330, Thailand*

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Diabetes is a chronic, non-communicable disease that affects people of all ages, leading to an increased mortality rate worldwide. Glucose is a key biomarker for diabetes.<sup>1</sup> Nowadays, glucose levels are commonly measured through blood drawing requiring a painful sample collection. Alternatively, glucose can be detected in other biofluids such as tears, saliva and sweat.<sup>2</sup> Herein, a wearable electrochemical is fabricated for real-time sweat glucose detection. The flexible working electrode surface is chemically modified with Prussian blue (PB)/carbon nanotube (CNTs)-cellulose nanofiber (CNF) and immobilized glucose oxidase (GOx) to enhance the overall sensor performances and specificity for sweat glucose detection. The modified electrode surfaces are systematically characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM) and fourier transform raman spectroscopy (FTIR). Amperometry is carried out on hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) detection for electrochemical characterization of the modified electrodes. A waist strap circuit and a smartphone readout of this sensor are customized designed to be directly connected with a bluetooth for real-time measurement of sweat glucose excreted from the wearer's waist area. This sensor provides a satisfactory linear range of 0 – 1.2 mM with a detection limit of 0.1 mM. It can effectively determine a cut-off glucose level (0.3 mM), which can effectively distinguish between a normal individual and the one with a diabetic condition. This platform opens a new avenue for smart phone based sensor for real-time detection of other sweat biomarkers in the future.

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Figure 1. Illustration of waist strap glucose sensor



### ■ Professional Biography

Dr. Nadnudda Rodthongkum (*h*-index: 30, Citations: 3,054) is a research professor and deputy director of Metallurgy and Materials Science Research Institute, Chulalongkorn University. She obtained her Ph.D. in Chemistry from University of Massachusetts, Amherst, USA. Her research interest focuses on design and synthesis of new materials for analytical applications.

AC

## Toward user-friendly paper-based analytical devices

Takashi Kaneta

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Paper-based analytical devices (PADs) are one of the technologies that will satisfy the ASSURED (affordable, sensitive, specific, user-friendly, rapid, equipment-free, delivered) criteria proposed by the World Health Organization. The PADs have achieved sensitive and specific detections, rapid measurements, equipment-free quantification, and improved portability by introducing several reactions and detection schemes. Conversely, to satisfy the requirement of user-friendly devices, one of the drawbacks is to use micropipettes for sample introduction because users, except for chemists, are unfamiliar with them. To overcome the issue, we tried to develop several types of PADs that employ a dip-and-readout method and a volume gauge to correct injection volume. The dip-and-readout method controls the injection volume by adjusting the dipping time of the PAD in a sample solution. The sample solutions flow into the channels of the PAD via capillary force spontaneously and are then transferred to a detection zone at a specific volume in a fixed time. Therefore, the dipping time keeps the injection volume constant. The PADs with volume gauges were also developed to achieve sample introduction without micropipettes. The PAD consists of a detection channel for the distance-based readout and a volume gauge located downstream of the detection channel. When introducing a sample solution with a dropper, the analyte forms a colored product in the detection channel. The sample solution without the analyte continuously flows to the volume gauge to determine the injected volume. Thus, we can correct the injected volume by measuring the length at the volume gauge in the PADs.

**Keywords:** Paper-based analytical device; ASSURED; Pipetteless sample introduction; Dip-and-readout; Volume gauge



### ■ Professional Biography

Takashi Kaneta is a professor at the Department of Chemistry, Okayama University, Japan. He has published more than 120 articles in peer-reviewed international journals in the analytical chemistry field and obtained more than 3,000 citations. His research interests include bioanalytical chemistry with laser-induced fluorescence and capillary electrophoresis, laser manipulation of biological particles and vesicles, and the development of paper-based analytical devices for environmental and food analyses. He received the FIA Award for Science from The Japanese Association for Flow Injection Analysis in 2021 and the Award of The Japan Society for Analytical Chemistry in 2022. He has been an associate editor of Microchemical Journal published by Elsevier since 2022.

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# KEYNOTE \ INVITED SPEAKER ABSTRACTS

## High resolution accurate mass mass spectrometry (HRAM MS) for a better understanding of the health and the resilience of ecosystems

Ryszard Lobinski

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Biological organisms have learned to synthesize metal-complexing molecules (metallophores) responsible for the capacity of resilience of plants and bacterial communities facing an excess of a toxic metal or a deficit of an essential micronutrient. The discovery and characterization of these molecules are the first step and a fundamental challenge to the understanding of the adaptation mechanisms involved on the molecular level.

Much research has been conducted to evaluate the effects of metals on plants and microorganisms in metal contaminated and metal deficient ecosystems. Most of it was based on the correlation of the total metal concentration with environmental or physiological factors, ignoring the real actors of the metal trafficking process, i.e. the metal complexes with the ligands in charge of the metal acquisition and transport. The advent of electrospray mass spectrometry and its implementation in genomics, proteomics and metabolomics have also opened new avenues for biological metal-related research, globally referred to as metallomics.

High resolution mass spectrometry offers the possibility of large-scale untargeted screening for metal-complexes in microvolumes of plant xylem and extracellular bacterial exudate. The high mass accuracy (down to 0.1 ppm) allows the unambiguous assignment of empirical formula to the detected compounds. Candidate parent ion fragmentation and multistage mass spectrometry permits to elucidate the formula.

The lecture discusses the fundamentals of HRAM for large scale metal speciation and illustrates its potential for understanding the metal acquisition and transport in hyperaccumulating plants in post-mining areas and acquisition of iron in a peatland ecosystem.

**Keywords:** Metals; Metallophores; Mass spectrometry; Phytoremediation; -Omics



## ■ Professional Biography

Ryszard Lobinski is professor of chemistry, research director at the National Research Center of France (CNRS) and director of the Institute of Analytical and Physical Chemistry in Pau, France.

He graduated as chemical engineer from the Warsaw University of Technology, Poland, from which he obtained his Ph.D. He was post-doctoral fellow of the Max-Planck Society in Germany, Dortmund and then research assistant at the University of Antwerp in Belgium. In 2006-2008 he was President of the Analytical Chemistry Division of the IUPAC. In 2006 he was awarded a CNRS Silver Medal and, in 2007, was admitted fellow of the Royal Society of Chemistry (UK).

His research interests concern the development of analytical methods for the identification and the determination of chemical forms of elements in the biological environment (speciation and metallomics) and the description of the mechanisms of uptake, metabolism, accumulation and excretion of trace elements by living organisms.

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## Single-cell analysis using ICP-*q*MS

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Single cell is the basic unit of life. Comprehensively physical, chemical and biological profiling of a single-cell is essential to understand its behavior, especially its biofunctions in the life process. During which, scientists have been trying to characterize a single-cell from different aspects covering morphology, genomics, proteomics and metabolomics via developing methods and using different tools. Even though great progresses have been achieved, there are many gaps remained for fully recognize and understand the behavior of a single cell due to the cell-to-cell heterogeneity existing between different cell lines even in the same type of cells. Here, I will talk about single-cell analysis using inductively coupled plasma quadrupole mass spectrometry (ICP-*q*MS). I will briefly introduce the element-tagging strategies towards the biomolecules expressed on the cell surface at first, which are responsibly participating in the behavior of a cell. Considering a single-cell analysis using the hard-ionization and scanning-type ICP-*q*MS, we designed and fabricated a microfluidic chip for manipulating the cells with an appropriate interval time before they entered into ICP-*q*MS one by one to realize a real single-cell analysis, on the other hand, we used methane as a collision gas to stretch the ion-plume of the transient single-cell event in the collision-reaction-cell equipped in ICP-*q*MS for a single-cell multiplex analysis. Moreover, an element-tagged macrophage MS2 nanoparticle was developed for signal-multiplication to guarantee the quantification of the element-tagged biomolecules on the surface of a single-cell. Single-cell analysis can thus be unambiguously performed regarding the cell surface biomolecules using ICP-*q*MS.

**Keywords:** ICP-*q*MS; Single-cell analysis; Element-tag; Microfluidic chip; Viruslike nanoparticle signal-multiplication



### ■ Professional Biography

Qiuquan Wang is a full professor at College of Chemistry and Chemical Engineering of Xiamen University. He is the deputy director of the Key Laboratory of Spectrochemical Analysis and Instrumentation of the Ministry of Education of China located at Xiamen University.

He got his PhD in 1998 under the supervision of Prof. Hideo Akaiwa and Prof. Kin-ichi Tsunoda from Gunma University Japan. He worked as a Postdoc fellow with Prof. Benli Huang at Xiamen University from 1998 to 2000. His research interests include new atomization and ionization methods of atomic optical and mass spectrometry, element/isotope-tagging strategy based ICP-qMS bioanalysis, design of novel monolithic stationary phases for chromatography, metallomics and reactive proteomics for understanding the molecular mechanisms of toxicity of metals and organic pollutants. He has published more than 100 peer-reviewed scientific papers and owns more than 10 patents. He serves currently as co editor of Analytical and Bioanalytical Chemistry (Springer Nature).

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## Electrodialytic ionic solutes handling for matrix isolation, purification, and separation

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Ionic solutes are important chemical forms and widely measured. However, the analysis is required sample pretreatment purposed to isolate matrices, and adjust the concentrations suited to the analyzer. Even though sample pretreatment is the one of the key processes, there is no universal methods. Electrodialytic ion handling was developed and applied to matrices isolation, purification, and separation for chemical analysis. Flow based electrodialytic ion handling device was successfully applied to pretreatment for the analysis of common cation/anion with ion chromatography, organic acids in drinks, heavy metals in serum samples. Furthermore, the developed method can enrich the ionic solutes continuously. Conventional enrichment method, such as solid phase extraction, and evaporation dryness cannot enrich continuously. The developed continuous enrichment method was applied to determine chloroacetates in tap water with conventional HPLC-UV, and ultra-trace metals in ultra-pure water. The separation for speciation analysis was also succeeded. Chromium in environment is mainly Cr(III) and Cr(VI). Cr(III) is essential but Cr(VI) is strongly toxic. Because Cr(III) and Cr(VI) are respectively cation and anion, these can simply be separated with electrodialytic ion handling. This separation can simultaneously be achieved with matrices isolation and enrichment. The separation was further expanded to chiral separation. The electrodialytic chiral separation was successfully achieved with molecularly imprinted membranes. Also, purification of particulates are recently achieved for metal nano particles analysis. In the presentation, the basic theory and performance of developed ion handling method and the application of the methods will be shown.

**Keywords:** Electrodialysis; Chiral separation; Chromium oxidation states; Particles purifications



### ■ Professional Biography

Shin-Ichi Ohira is a professor of Analytical Chemistry at Kumamoto University, Japan. He received his Bachelor (2000), Master (2002), and Doctor (2005) of Science degrees from Kumamoto University. He served as Research Fellow for Young Scientists of the Japan Society for the Promotion of Science (JSPS) at Kumamoto University (2005 – 2006), Postdoctoral Fellow for Research Abroad of JSPS at Texas Tech University (2006) and The University of Texas at Arlington (UTA) (2007-2008), and Postdoctoral Research Fellow at UTA(2008-2009). He was promoted to associate professor at Kumamoto University in 2009 and professor in 2021. He received Award for Researchers from the Japan Association for Flow Injection Analysis (2022), Ion Chromatography Discussion Group of the Japan Society for Analytical Chemistry (JSAC) (2021). His current work focuses specifically on the electrodialytic ionic solutes handling, universal detection for high performance liquid chromatography, and gas sensing systems.

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## Wearable sweat glucose sensor connected with a smartphone readout

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Diabetes is a chronic, non-communicable disease that affects people of all ages, leading to an increased mortality rate worldwide. Glucose is a key biomarker for diabetes.<sup>1</sup> Nowadays, glucose levels are commonly measured through blood drawing requiring a painful sample collection. Alternatively, glucose can be detected in other biofluids such as tears, saliva and sweat.<sup>2</sup> Herein, a wearable electrochemical is fabricated for real-time sweat glucose detection. The flexible working electrode surface is chemically modified with Prussian blue (PB)/carbon nanotube (CNTs)-cellulose nanofiber (CNF) and immobilized glucose oxidase (GOx) to enhance the overall sensor performances and specificity for sweat glucose detection. The modified electrode surfaces are systematically characterized using scanning electron microscopy (SEM), transmission electron microscopy (TEM) and fourier transform raman spectroscopy (FTIR). Amperometry is carried out on hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) detection for electrochemical characterization of the modified electrodes. A waist strap circuit and a smartphone readout of this sensor are customized designed to be directly connected with a bluetooth for real-time measurement of sweat glucose excreted from the wearer's waist area. This sensor provides a satisfactory linear range of 0 – 1.2 mM with a detection limit of 0.1 mM. It can effectively determine a cut-off glucose level (0.3 mM), which can effectively distinguish between a normal individual and the one with a diabetic condition. This platform opens a new avenue for smart phone based sensor for real-time detection of other sweat biomarkers in the future.

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Figure 1. Illustration of waist strap glucose sensor



### ■ Professional Biography

Dr. Nadnudda Rodthongkum (*h*-index: 30, Citations: 3,054) is a research professor and deputy director of Metallurgy and Materials Science Research Institute, Chulalongkorn University. She obtained her Ph.D. in Chemistry from University of Massachusetts, Amherst, USA. Her research interest focuses on design and synthesis of new materials for analytical applications.

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## Toward user-friendly paper-based analytical devices

Takashi Kaneta

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Paper-based analytical devices (PADs) are one of the technologies that will satisfy the ASSURED (affordable, sensitive, specific, user-friendly, rapid, equipment-free, delivered) criteria proposed by the World Health Organization. The PADs have achieved sensitive and specific detections, rapid measurements, equipment-free quantification, and improved portability by introducing several reactions and detection schemes. Conversely, to satisfy the requirement of user-friendly devices, one of the drawbacks is to use micropipettes for sample introduction because users, except for chemists, are unfamiliar with them. To overcome the issue, we tried to develop several types of PADs that employ a dip-and-readout method and a volume gauge to correct injection volume. The dip-and-readout method controls the injection volume by adjusting the dipping time of the PAD in a sample solution. The sample solutions flow into the channels of the PAD via capillary force spontaneously and are then transferred to a detection zone at a specific volume in a fixed time. Therefore, the dipping time keeps the injection volume constant. The PADs with volume gauges were also developed to achieve sample introduction without micropipettes. The PAD consists of a detection channel for the distance-based readout and a volume gauge located downstream of the detection channel. When introducing a sample solution with a dropper, the analyte forms a colored product in the detection channel. The sample solution without the analyte continuously flows to the volume gauge to determine the injected volume. Thus, we can correct the injected volume by measuring the length at the volume gauge in the PADs.

**Keywords:** Paper-based analytical device; ASSURED; Pipetteless sample introduction; Dip-and-readout; Volume gauge



### ■ Professional Biography

Takashi Kaneta is a professor at the Department of Chemistry, Okayama University, Japan. He has published more than 120 articles in peer-reviewed international journals in the analytical chemistry field and obtained more than 3,000 citations. His research interests include bioanalytical chemistry with laser-induced fluorescence and capillary electrophoresis, laser manipulation of biological particles and vesicles, and the development of paper-based analytical devices for environmental and food analyses. He received the FIA Award for Science from The Japanese Association for Flow Injection Analysis in 2021 and the Award of The Japan Society for Analytical Chemistry in 2022. He has been an associate editor of Microchemical Journal published by Elsevier since 2022.

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## From averaging over an entire catalyst to single particle catalysis: Black box vs. atomic views

Günther Rupprechter

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Operando spectroscopy of catalytic reactions has been very successful in mechanistic studies, especially when combined with computational modelling (DOI:10.1002/sml.202004289). An example will be presented for CuO/CeO<sub>2</sub> nanosphere catalysts applied to CO oxidation and preferential oxidation of CO (PROX), with the simulations probing various Cu and vacancy sites as reactive centers enabling selective pathways (DOI:10.1007/s11244-023-01848-x). However, as spectroscopy typically examines large areas/volumes, this averaging “smoothens out” local variations that may be critical to understand how a reaction proceeds on an atomic level. Furthermore, dynamics in catalyst structure, composition and adsorbate coverage may also go unnoticed by averaged spectral data.

A straightforward way overcoming these limitations is to use correlative surface microscopy to directly “watch” ongoing catalytic reactions, i.e. to apply several microscopic and spectro-microscopic techniques to the same catalyst locations under identical reaction conditions (DOI:10.1021/acscatal.2c03692). The methods presented not only image catalyst structure or composition, but also the adsorbed reactants, so that active and inactive states can be discerned, active regions identified and mechanisms elucidated (kinetics by imaging; DOI:10.1016/j.susc.2015.05.021). Examples of real-time in situ imaging of H<sub>2</sub> oxidation are presented, covering micrometre-sized supported Rh particles (DOI:10.1021/acscatal.3c00060) and catalysis by a single Rh nanoparticle (DOI:10.1038/s41467-023-43026-3).

**Keywords:** Operando; Modelling; Hydrogen oxidation; Field emission microscopy; Single particle catalysis

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## ■ Professional Biography

Günther Rupprechter is Professor of Surface and Interface Chemistry at TU Wien (Vienna, Austria). He has been Renowned Overseas Professor of Shanghai University of Engineering Science and Guest Professor at Kasetsart University Bangkok.

Rupprechter is Director of Research of the new Austrian Cluster of Excellence “Materials for Energy Conversion and Storage (MECS)” of the Austrian Science Fund (FWF), including 5 Austrian universities/institutions. He is member of the Austrian Academy of Sciences and the European Academy of Sciences, Vice-Chair of the Austrian Catalysis Society and Editorial Board Member of “Catalysis Letters” and “Topics in Catalysis”.

Research interests of Günther Rupprechter include heterogeneous catalysis and nanomaterials, particularly in situ (operando) spectroscopy/microscopy of technological and model catalysts, applied to processes relevant for energy and environment: hydrogen as clean fuel, methane reforming, CO<sub>2</sub> and olefin hydrogenation, automotive catalysis, sensing and waste remediation.

## Catalytic chemistry using carbon-based materials

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Carbon materials possess numerous intriguing advantages, and moreover, the carbon matrix can readily accommodate other species and elements through both non-covalent and covalent interactions. In this talk, recent progress in catalytic chemistry using carbon-based materials is introduced.

Supported catalysts, such as metal-loaded carbons, have been extensively employed. While carbon “defects” play a critical role in anchoring metal nanoparticles, they can also lead to corrosion of the carbon matrix, particularly in oxidizing environments. However, there are actually two distinct types of defects— edge sites and non-hexagon carbon rings known as topological defects. We have developed a novel mesoporous carbon, graphene mesosponge (GMS),<sup>1</sup> containing only the latter defects. Since GMS does not possess edge sites, it exhibits exceptional oxidation resistance, surpassing that of carbon nanotubes.<sup>2,3</sup> Additionally, GMS can anchor a large number of metal nanoparticles, such as Pt and Ru, for fuel cell<sup>4</sup> and lithium-oxygen battery applications,<sup>5</sup> respectively.

While the carbon basal plane, composed of carbon hexagonal rings, is chemically inert and lacks catalytic activity, the aforementioned defects endow carbon materials with unique catalysts. We have recently established a quantitative relationship between carbon radicals derived from edges and their catalytic activity in oxidation processes.<sup>6</sup> Also, topological defects exhibit distinctive catalysis when employed as a cathode in lithium-oxygen batteries.<sup>7</sup>

Carbon can host single-metal species within its basal plane. While many carbon-metal catalysts containing single-metal sites have been reported for various catalytic applications, we have pioneered a distinct category of materials known as “ordered carbonaceous frameworks (OCFs),<sup>8,9</sup> characterized by their ordered porous structures, originating from their parent organic crystals.

**Keywords:** Carbon catalysis; Edge site; Topological defects; Metal nanoparticles

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### ■ Professional Biography

Hiroto Nishihara is a professor at Tohoku University. He received his PhD degree in 2005 from Kyoto University and subsequently served as an assistant professor at Tohoku University. In 2011, he was promoted to associate professor and in 2020, he was promoted to full professor. He has published more than 150 papers thus far. He also serves as an editorial board member for several international journals, including Scientific Reports, Energy Storage Materials, Carbon Research, and Carbon Reports. His research interests encompass carbon materials, nanoporous materials, adsorption, and energy storage, particularly in the field of batteries.

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## Induced catalytic active sites by substrate over nano-structures

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As generally known, the elucidation of active sites' structure in solid nanocatalysts under real reaction conditions is one of the most important challenges facing the scientific community. There is an increasing amount of evidence by the in situ/operando characterization that active sites can be generated by the interaction of substrate molecules with the inorganic nanocatalysts as akin to enzyme-substrate interaction, which can result in the significant promotion of catalytic performance. In addition, surface rearrangement could occur under reaction conditions, which may cause dynamic changes in the active sites. Therefore, the real active sites under working conditions could be significantly different from those characterized under ex situ conditions. Yet, current limitations in state-of-the-art characterization techniques regarding spatial, temporal and temperature/pressure gaps are sometimes unable to provide the answers for the understanding. In-situ/operando characterization using modern designated synchrotron offers exciting possibilities. Hence, in this meeting, some examples how Frustrated Lewis Pair (FLP) sites on solid nanostructure will be given, which offer to catalyse a wide range of chemical reactions. It is hoped that this talk could stimulate new science/new instrumentation in catalysis and other disciplines in future.

**Keywords:** In situ; Operando active sites; Nanostructure characterization



### ■ Professional Biography

Edman Tsang is a Professor of Chemistry and Head of Wolfson Catalysis Centre at the University of Oxford, UK. His main research interests are on nanomaterials and catalysis concerning energy and environment which include developments of catalytic, photocatalytic and electrocatalytic technologies for fine chemicals, cleaner combustion, green chemistry, energy storages, processes and production, etc. Particular expertise is in design and architecture of nanocatalysts, which can lead to understanding of catalytic surfaces and interfaces. He has about 300 referred research publications including Nature, Science and Nature sister journals. He has delivered over 200 plenary and invited presentations at conferences, universities and companies. He has had extensively collaborations with chemical industries. He held a Distinguish Overseas Young Scientist Award from National Natural Science Foundation (NSFC-B award 2005) and Changjiang Scholar Award from Ministry of Education (B award 2007) and is a recipient of Global 1000 Talents visiting Award (B award 2014). He has won a number of international awards/recognitions including Royal Society University Fellowship (1995–2000); IChemE award on iAc innovation in catalysis (2005), IChemE NES Awards for Novel Engineering-shortlisted candidate (2008); Royal Society Kan Tong Po Professorship (2012); Royal Society Green Chemistry award (2012) and Royal Society Surfaces and Interfaces award (2013), etc. He serves as international panel members for a number of research councils and industries worldwide. He is an associate editor in Science Advances (Science sister journal); Editorial member of ChemCatChem (catalysis journal from VCH). Editorial member of Catalysis, Structure & Reactivity (CAT) from Maney (a new journal); IChemE: Catalysis Subject Group Committee and Member of the EPSRC College School. (<https://www.chem.ox.ac.uk/people/edman-tsang>).

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## Advanced catalytic upgrading of bioethanol to chemicals and carbon materials

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The bioethanol upgrading to high value-added chemicals and materials has become a promising pathway for biorefinery. In this contribution, we illustrate the design of zeolites and zeolite composites with hierarchical structures, which have been used as catalysts for bioethanol upgrading.<sup>1-7</sup> Interestingly, the designer catalysts show outstanding physicochemical properties in particular high surface area and porosity, suitable acidity, and thermal stability, eventually improving catalytic performances in bioethanol conversion to various chemicals and carbon materials. Apart from the isolated hierarchical zeolite, the binder-free hierarchical ZSM-5 monolith derived from zeolite@layered double hydroxides (LDH) composites obtained via traditional extrusion and 3D printing technologies significantly boosts ethylene yield up to 96% due to the synergistic effect of zeolites and LDHs. To further demonstrate the real industrial application, we also exemplify the application of the synthesized hierarchical zeolite in bioethanol dehydration to ethylene on a pilot-plant scale.

Apart from ethylene as a desired product from bioethanol, we also illustrate the fabrication of qualified carbon nanotubes (CNTs) over hierarchical zeolites from bioethanol via ethylene as an intermediate. Typically, by using the traditional process for CNTs production from the direct conversion of ethanol, a significantly lower quality and yield of CNTs was obtained.<sup>3-4</sup> Indeed, even without removal of a zeolite template, the obtained CNTs/zeolite composites can be utilized in a wide range of applications such as catalysis, electrocatalysis, and antibacterial agent.<sup>3-4</sup> These examples open up new perspectives on the bioethanol upgrading using various types of catalysts for the production of fine-chemicals and carbon materials.

**Keywords:** Hierarchical zeolites; Bioethanol; Ethylene; Zeolite@LDH composites; Carbon nanotubes (CNTs)

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### ■ Professional Biography

Chularat Wattanakit is currently an Associate Professor at VISTEC. She received a Ph.D. in Physical Chemistry under the joint program between Kasetsart University, and the University of Bordeaux in 2013. Then, she was a postdoctoral researcher at Nagoya University and worked as a researcher for SCG Chemicals Co., Ltd. Since 2015, she serves as a faculty member at VISTEC. She received the Thailand Young Scientist Award by the Foundation for the Promotion of Science and Technology under the Patronage of His Majesty the King, and the L'Oreal-UNESCO Fellowship for Women in Science in Physical Science 2018. In addition, she was also awarded with the Distinguished Lectureship 2020 by the Chemical Society of Japan and the Distinguished Young Chemist Award 2020 by the Chemical Society of Thailand (CST). Recently, she received the Tremplin prize 2023 for bilateral cooperation between French and ASEAN researchers. Her research interests relate to heterogeneous catalysis and electrocatalysis.

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## Selective conversion of xylose to lactic acid over Al-based catalysts: A comprehensive comparison between laboratory-scale and pilot-scale

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Efficient production of lactic acid from sugars represents a crucial pathway for the development of renewable chemicals because it can be employed as a feedstock for food, pharmaceutical, cosmeceutical, and chemical industries. This study explores the use of metal-based Lewis acids in the conversion of D-xylose to lactic acid in aqueous solutions, leveraging their abundance, cost-effectiveness, and ecological friendliness. The noteworthy performance in lactic acid yield is attributed to the catalyst's substantial specific surface area, rich Lewis acid sites, and hydroxy groups on its surface. Theoretical analysis employing Density Functional Theory (DFT) reveals that the activation of C–C bonds and the thermodynamic stability along the D-xylose to lactic acid pathway are influenced by reactive Lewis acid sites. Furthermore, DFT results indicate that H<sub>2</sub>O molecules undergo dissociative adsorption at the Al site, directing the reaction pathway toward lactic acid rather than furfural. Scaling up this catalytic system demonstrates its substantial potential as a prospective industrial application for lactic acid generation.

**Keywords:** Lactic acid; D-xylose; DFT; Laboratory-scale; Pilot-scale





### ■ Professional Biography

Dr. Pongtanawat Khemthong has holding the position of Principal Researcher, which is equivalent to that of a professor, He is a distinguished scientist and researcher from National Nanotechnology Center (NANOTEC), Thailand, who has made significant contributions to the fields of innovative nanomaterial synthesis and advanced synchrotron-based characterizations for catalysis, environmental, and medical applications. His professional journey has been marked by numerous achievements and notable research experiences as a visiting scientist at prestigious institutions, demonstrating his commitment to exploring global research opportunities.

Dr. Pongtanawat Khemthong has an impressive record of publications, contributing to the scientific community's knowledge base in various areas. Over the past five years, he has made a significant impact on the scientific community with his international publications. Notably, his work has encompassed a wide range of areas, including energy storage, catalysis, biofuel production, materials science, and environmental protection.

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## Syngas conversion to light olefins: Influence of $\text{SiO}_2$ , $\text{Al}_2\text{O}_3$ , and $\text{TiO}_2$ supports using Fe-Co-K catalysts

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Light olefins such as ethylene ( $\text{C}_2\text{H}_4$ ), propylene ( $\text{C}_3\text{H}_6$ ), and butylene ( $\text{C}_4\text{H}_8$ ) are crucial for manufacturing polymers, electronic components, automotive parts, and packaging within the petrochemical industry. The current production technologies for these olefins depend on nonrenewable fossil resources, leading to price volatility and environmental concerns. Syngas derived from biomass and natural gas via gasification or reforming offers an alternative, sustainable path. This study explores the conversion of syngas to light olefins using Fe-Co-K catalysts supported by  $\text{SiO}_2$ ,  $\text{TiO}_2$ , and  $\text{Al}_2\text{O}_3$ .  $\text{SiO}_2$  and  $\text{TiO}_2$  were found to strongly interact with Fe, inhibiting the active iron carbides phase formation and thus reducing olefin yields.  $\text{Al}_2\text{O}_3$  was the most effective support, promoting the formation of iron carbides and enabling a high space-time yield of light olefins ( $17.2 \text{ mmol g}_{\text{cat}}^{-1} \text{ h}^{-1}$  at  $360^\circ\text{C}$  and 20 bar). These results provide valuable insights for developing tailored catalysts for sustainable light olefin production, marking a significant step for industrial application and environmental sustainability.

**Keywords:** Syngas; Light olefins; Supports; Metal-support interaction



### ■ Professional Biography

Thongthai Witoon completed his Ph.D. in Chemical Engineering at Kasetsart University through the Thai government's Royal Golden Jubilee Ph.D. Programme, where he also serves as a Professor. His research focuses on synthesis of porous silica materials, separation, catalysis, and converting CO<sub>2</sub> or biomass into value-added chemicals. A prolific author, he has over 100 peer-reviewed publications, an H-index of 36, and more than 3,500 citations. He is an editorial board member of the Molecular Catalysis journal. His accolades include the National Young Scientist Award (2014), Thailand Frontier Researcher Award (2016), the PTIT Scholar Award (2017/2018), and the TRF-OHEC-Scopus Researcher Award (2018).

CC

## Design and development of simple microfluidic paper- and thread-based devices for high school chemistry experiments

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The microfluidic device is gaining popularity as an alternative experiment platform in chemistry since it is cost-effective as well as less chemical-consuming, time-consuming and waste-generation. We have developed and standardized both microfluidic paper-based and thread-based analytical devices ( $\mu$ PAD and  $\mu$ TAD) to be utilized as an alternative experiment platform for high school through undergraduate chemistry. Our outstanding  $\mu$ PADs experiments include the paper-based galvanic cells to investigate electrochemistry, the simple wax screen-printing paper-based analytical devices to demonstrate the limiting reagent concept, and the rubber latex screen-printing paper towel-based experimental device to demonstrate the factors affecting chemical equilibrium and chemical equilibrium constant determination. Our outstanding  $\mu$ TAD experiment is the silver-nanoparticle-loaded cotton thread to demonstrate the catalytic reduction of 4-nitrophenol. These  $\mu$ PAD and  $\mu$ TAD experiments were easily implemented as an alternative experiment to a conventional experiment for high school and undergraduate students. These microfluidic devices were effective to enhance students' experience in doing chemistry experiments as well as students' conceptual understanding of the corresponding concepts.

**Keywords:** Microfluidic paper-based device; Microfluidic thread-based device; Small-scale experiment; High school chemistry experiment

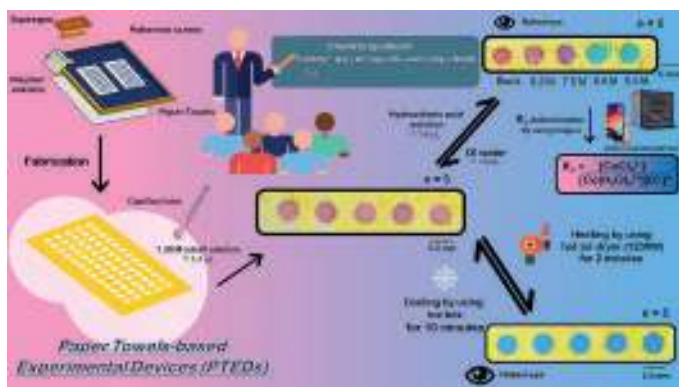


Figure 1. The rubber latex screen-printing paper towel-based experimental device to demonstrate the factors affecting chemical equilibrium

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### ■ Professional Biography

Saksri Supasorn is a Vice-Dean for Academic Affairs of Faculty of Science, Ubon Ratchathani University, Thailand. He is an associate professor who have been responsible for the graduate programs in science education. His research areas of interest include (1) development and evaluation of experimental kits for high school and undergraduate chemistry, (2) development and evaluation of multimedia learning tools (simulation, animation, web-based learning) in chemistry and science, (3) investigation effects of multimedia learning and/or experimental kits on student understanding and concepts. Supasorn and his colleagues is now working on the simple microfluidic paper- and thread-based devices to be used as experiment platforms for high school chemistry, which he will be sharing in the PACCON 2024.

CE

## Metacognitive calibration: Can students judge their abilities?

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Metacognitive calibration refers as the measurement of differences between students' metacognitive judgement and external criteria. Traditionally, the evaluation of learning involves assessing judgment of learning (JOL). However, other types of metacognitive calibration can also be considered, such as perspective versus retro-perspective or immediate versus delayed measurements. The JOL is simply described as "extent of congruence between students' estimates of their capabilities and their actual performance", which could provide many useful parameters, including metacognitive accuracy, reliability, and bias. These parameters are calculated via a variety of methods but Goodman–Kruskal Gamma correlations and contingency tables are frequently used. Here an example of multi-dimension measurements of metacognitive calibration of 260 Thai junior students in a biochemistry class is presented. The results demonstrated that metacognitive calibration was strongly connected with students' goal orientation, self-evaluation performance, and task management ability. Metacognitive calibration remains a powerful tool to diagnose the alignment of students' learning progress and expected learning outcomes.

**Keywords:** Metacognitive calibration; Judgement of learning; Biochemistry



### ■ Professional Biography

Witawas Handee, Ph.D., is a lecturer in bio-chemistry and related courses in the science education program in the Department of Chemistry, Faculty of Science, Silpakorn University. His research centers around studying students' metacognition, self-awareness, and misconception, primarily how metacognitive control plays a role in developing stages of cognition when learning chemistry and biochemistry. He is also interested in how to use metacognitive tools to prompt students' metacognition, including activities and games. He specializes in the development of science board games and how to use board games to increase cognition and metacognition.

CE

## The power of STEM partnership for promoting STEM skills

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### CE

The advancement of technology has increased the importance of supply chain employees possessing STEM skills in modern, complex supply chains. However, shortages in the STEM workforce are prevalent worldwide. Employers express concern about the readiness and quality of STEM graduates and often mention that they may lack the necessary work readiness skills. These graduates require cognitive knowledge of STEM and the specific working skills needed for their career paths. In the STEM field, professionals are expected to have the STEM skills that employers demand. A STEM partnership is a collaboration or alliance between individuals, organizations, or entities in science, technology, engineering, and mathematics (STEM) to promote STEM education. Partnerships with industries, universities, and organizations highly involved in STEM activities can provide students with authentic, high-quality, real-world experiences. STEM partnerships take various forms depending on the goals and the parties involved. By participating in STEM partnerships, students can understand how STEM education in schools relates to their future lives. These partnerships also equip students with the necessary STEM skills and knowledge. In addition, STEM partnerships are a successful strategy for raising awareness about further STEM education opportunities and careers.

**Keywords:** STEM partnership; STEM skills; STEM workforce; STEM career; STEM education



### ■ Professional Biography

Pattamaporn Pimthong is an Associate Professor of Science Education at the Faculty of Education, Kasetsart University, Thailand. She is responsible for teaching undergraduate Science and STEM methods courses and supervises graduate students in STEM education and related fields. Her research areas include Science Education, STEM Education, Project-Based Learning, and Conceptual Change. She has established a STEM partnership with a Mathematic Educator, a Scientist, a Science Teacher, and an Engineer to develop STEM research and enhance STEM partnerships in schools across Thailand. She has also authored several STEM education books promoting STEM understanding and a positive attitude towards STEM education for those interested in this field.

CE

## Microplastics contamination in Chao Phraya estuary and Bang Pu mangrove forest in Thailand

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Mangrove ecosystem is recognized as the potential receptacle of plastic waste and microplastics (MPs). The Bang Pu mangrove forest, one of the distinctive natural habitats in estuarine and coastal ecosystems in Thailand, has been invaded by tonnes of plastic waste for years. This study examines MPs contamination in Thai vinegar crabs (TVCs) (*Episesarma mederi*), giant mudskippers (GMs) (*Periophthalmodon schlosseri*), and their surrounding surface water from the upper and lower Bang Pu mangrove forests in the rainy season. Two-step digestion with 10% potassium hydroxide and Fenton's reagent was applied to animal samples. Fourier transform infrared spectroscopy was employed for polymer identification. Findings showed that MPs abundance was  $7.5 \pm 3.8$  to  $10.4 \pm 3.9$  items/individual in TVCs. For GMs, MPs found were  $6.3 \pm 2.3$  to  $10.6 \pm 2.6$  items/individual, and  $33 \pm 18$  to  $37 \pm 1$  items/L in surface water. MPs were detected in gastrointestinal tracts of both species including soft tissues of TVCs and fillets of GMs, which are used as food for human consumption. Detected MPs were mainly fibers ranging from 0.05 to 0.3 and 0.3 to 0.5 mm. Most MPs were transparent with polyethylene and polypropylene as predominant polymers. The results demonstrated the widespread distribution of MPs in the surrounding environment which is a significantly crucial habitat for native animals. The presence of MPs possibly harms the biodiversity of the ecosystem and also poses a threat to human health through consumption of TVCs and GMs.

**Keywords:** Microplastics; Mangrove; Mudskippers; Crabs; Surface water; Human health



### ■ Professional Biography

Dr. Sandhya Babel is a full professor at the School of Biochemical Engineering and Technology, Sirindhorn International Institute of Technology, Thammasat University, Thailand. Her research interests include microplastics pollution and uptake by biota, microbial fuel cells, adsorption, photocatalysis, phytoremediation, LCA and membrane technology. She also works on the development of low-cost technologies using for the protection of environment. Dr Sandhya has published over 150 scholarly articles in reputed international journals, three edited books (on microplastics), and several book chapters. Her h-index is 33 and the total number of citations as of November 2023 is more than 9,000. She has been listed in the top 2% scientists in the world by Stanford University and Elsevier BV for four consecutive years in the field of Environmental Sciences for whole career and single year.

EE

## Holistic valorization of residual biomass

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### EE

In less than 40 years from now, our population will have grown from today's 8 billion to 10 billion. At the same time, our main resource for transportation, but also materials and chemicals –crude oil– is predicted to be exhausted. To supply a future demand without negatively affecting climate change, land use, water scarcity or depleting resource could be this century's most difficult, yet important challenge.

Biomass will most likely play a decisive role as feedstock for future generations. However, care must be taken not to compete with food production but also issues of biodiversity and water use must be addressed. One strategy is to use side-streams from current industry that currently are burnt to a low value.

In this talk, examples of using low value streams from forestry will be disclosed. In this effort, all components of the raw material should be upgraded into high value products.

**Keywords:** Lignin; Forest residue; Sustainability; Green chemistry; Textiles; Biofuels

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### ■ Professional Biography

Joseph Samec is professor at Stockholm University, Sweden since 2017. He has published more than 100 articles and filed 25 patent applications. Current research interests involve Green and Sustainable transformations of low value residues. He has cofounded 4 spin-off companies.

EE

## Metal oxides nanosheets/cellulose composites for energy harvesting via triboelectrics

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### EE

Triboelectric effect originates from the contact electrification of two dissimilar materials, providing electrical outputs, which can be tuned by the characters of the two materials. It is an alternative from of energy harvesting and sensing alike. The works in our group on metal oxides nanosheets (filler)/cellulose(matrix) composites will be presented herein, including  $\text{Ti}_{0.8}\text{O}_2$ /cellulose,  $\text{Ti}_{0.8}\text{O}_2$ -Ag/cellulose, titanate nanotubes/cellulose, and  $\text{Ti}_2\text{NbO}_7$ /cellulose composites. These examples demonstrate the wide variation of nanosheets structure and composition, and also the type (microstructure) of cellulose either plant- or bacteria-derived. The presence and distributions of nanosheets onto/into the cellulose matrix were investigated by X-ray diffraction (XRD), energy dispersive analysis (EDX), synchrotron radiation X-ray tomography (SRXTM), and atomic force microscopy (AFM). Insights into the role of each component were obtained by examining various quantities as derived from impedance measurements, including dielectric permittivity and dielectric loss, conductivity, electric modulus, etc. Applications of these composites as an energy harvester (i.e., triboelectric nanogenerator, TENG) or as a motion sensor will be showcased.

**Keywords:** Nanosheets; TENG; Impedance; Composites



### ■ Professional Biography

Tosapol Maluangnont is at College of Materials Innovation and Technology, King Mongkut's Institute of Technology Ladkrabang. He obtained the PhD degree from Oregon State University in 2011, working with Prof. Michael Lerner on graphite intercalation compounds. Then in 2012, he was a postdoctoral researcher at National Institute for Materials Science, Japan, working with Dr. Takayoshi Sasaki on the exfoliation of layered metal oxides. He joined KMITL first as a lecturer (2013), which was followed by a promotion to an assistant professor (2016), prior to the current position as an associate professor (2020-present). His research focuses on chemical/physical properties of layered materials and nanosheets derived therefrom, for applications such as energy harvesting and catalysis.

EE

## The rise of sustainable electrochemical intelligent of 2D materials

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Understanding the characteristics, both physical and electrochemical, of two-dimensional (2D) materials is crucial for the advancement of various electrochemical devices such as energy storage systems, electrocatalysts, ions selective membranes, and wastewater treatment technologies. To achieve this goal, controlled synthesis of 2D materials plays a vital role. In this study, we focus on the structural control achieved through liquid phase exfoliation of bulk materials, specifically: (i) **graphite-graphene**, (ii) **transition metal dichalcogenides**, and (iii) **heterostructure formation**. This involves material handling techniques and recycling of waste generated during the synthesis process. Furthermore, the exfoliated materials were utilised in diverse applications including supercapacitors (including electrode materials and binders), electrocatalysts, and removal of ions for wastewater treatment. To delve deeper into the complex realm of materials science and electrochemistry, we incorporated data science methodologies such as machine learning and statistical tools. Through simple data analysis, valuable electrochemical insights were derived, paving the way for the design of machine learning algorithms—an innovative approach in this field. To the best of our knowledge, this integration of data science as well as the materials synthesis in the context of 2D materials holds great potential for their development and application in various fields.

**Keywords:** Electrochemistry; Machine Learning; 2D Materials; SDG-6, 7, 13; Data analysis



### ■ Professional Biography

Dr. Pawin Iamprasertkun is an accomplished scholar with a Ph.D. in Materials Chemistry from the University of Manchester, UK, and degrees in Chemical Engineering from Kasetsart University, Thailand. Recognized for academic excellence, he has received prestigious awards, including the Sheelagh Campbell Award from the Royal Society of Chemistry, and Anglo-Thai society, UK.

As a Lecturer at the School of Bio-Chemical Engineering and Technology, Sirindhorn International Institute of Technology, Thammasat University, Dr. Iamprasertkun contributes his expertise in fundamental electrochemistry, two-dimensional materials, large-scale devices, and machine learning in chemical and environmental domains. Actively engaged in professional committees, including the Radioactive Waste Management Committee in Thailand, and serving as a Guest Editor for Energies journal.

EE



## Surface Chemistry in Atomic Layer Deposition and Selective Deposition

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To date, atomic layer deposition (ALD) and area-selective ALD (AS-ALD) has been used to deposit a large selection of materials, including oxides, nitrides, sulfides, metals, and compounds with three or more elements. However, there are many materials that cannot yet be grown by ALD and AS-ALD. A main limitation for the availability of a material by ALD and AS-ALD is the restricted choice of effective reaction pathways that lead to material deposition by precursors and co-reactants, strongly dependent on the ALD chemistry used. The specific reactions that precursors undergo during ALD are also important because these reactions can affect the physicochemical properties of the deposited films. Thus, proper precursor selection is highly important to the development of ALD and AS-ALD.

In this work, I will present the effect of different ligands on the growth mechanisms of  $\text{Al}_2\text{O}_3$  for ALD and blocking mechanism for AS-ALD by comparing a series of metal precursors. We choose the series of Al precursors  $\text{Al}(\text{CH}_3)_x\text{Cl}_{3-x}$  and  $\text{Al}(\text{C}_y\text{H}_{2y+1})_3$  as a model due to their simple structures and also because  $\text{Al}(\text{CH}_3)_3$  is considered an excellent starting point for comparison. Changing both the number of methyl and chloride groups in  $\text{Al}(\text{CH}_3)_x\text{Cl}_{3-x}$  ( $x = 0, 1, 2$ , and  $3$ ) and the chain length of alkyl ligands in  $\text{Al}(\text{C}_y\text{H}_{2y+1})_3$  ( $y = 1$  and  $2$ ) provides key variables that can be used for precursor design. For instance, the series of  $\text{Al}(\text{CH}_3)_x\text{Cl}_{3-x}$  offers insights into the effect of Lewis acidity on precursor reactivity while keeping the precursor size almost constant. In contrast, the series of alkyl precursors,  $\text{Al}(\text{C}_y\text{H}_{2y+1})_3$ , has different sizes but similar reactivity, offering an analysis of steric hindrance effects on growth characteristics. This thorough study of precursor properties using both experimental and theoretical methods will allow us to determine the role of precursor selection in important ALD and AS-ALD parameters.

**Keywords:** Surface chemistry; Atomic layer deposition; Selective deposition; Precursor



### ■ Professional Biography

Dr. Il-Kwon Oh is an assistant professor in Department of Intelligence Semiconductor Engineering at Ajou University. 2016, he got the Ph.D degree in EE Department at Yonsei University and had a postdoc position in Chemical Engineering at Stanford University until 2021.

Prof. Oh's current research interests and topics are focused on fabricating emerging electronic devices based on surface chemistry and especially, cover wide range of semiconductor fields; 1) the fabrication and evaluation of electronic devices including in semiconductor/memory devices, 2) the fabrication and elucidating of new concepts of electronic devices with novel nanostructures by controlling surface chemical reaction.

EE



## Occupational health risk of workers exposed to hazardous air pollutants: case study in Thai industries

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This work is a review of occupational health research in Thai industries. The aim is to improve manufacturing operation concerning quality of work as well as quality of life of the workers. The exposure of hazardous air pollutants (HAPs) including volatile organic compounds, fine particulate matter PM<sub>2.5</sub> and heavy metals were investigated. Several HAPs sources in industrial areas were selected, the press factories, waste treatment plants and Al smelting plant. The concentrations of air pollutants were measured from the volunteer factories following the standard methods of USEPA and OSHA. Non-cancer risks were calculated from a standard HQ equation. The cancer risks were quantified by combining the exposure data with inhalation cancer potency factors. The workers in offset printings were at risk of VOCs exposure with Hazard quotient >1. Electronic waste treatment and Aluminum smelting plant were indicated high exposure concentrations of heavy metals. Health risk management was recommended to the factories such as the addition of air pollution control devices, the use of effective personal protection equipment and the change in production process.

**Keywords:** VOC; PM<sub>2.5</sub>; Occupational exposure; Health risk; Heavy metal



### ■ Professional Biography

Professor in air pollution and environmental health, at Department of Environmental science Chulalongkorn university. She had her Ph.D. in chemistry and biochemistry from La Trobe University in 1992 then continue worked as a research fellow in Molecular biology one year. She also had experiences in academic administration and research publications: Head, Department environmental science 2002-2006 and 2018-2020 Chair of the Toxicology industrial environment postgraduate program 2018-2020 President: Thai Society of Higher Education Institutes on Environment 2017-2023 Editor in Chief: Environment Asia, a scopus journal since 2017-2022 Board committee: The Science society of Thailand under the patronage of His Majesty the King 2022-2023.

EE



## Science behind plant-based foods

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### FA

Plant-based foods have been recognized as one of the sustainable alternatives to animal-based foods due to their reduced negative impact on environmental, animal welfare and human health. Nonetheless, plant-based proteins are largely different from animal proteins in terms of their molecular structures and physicochemical properties, leading to differences in their techno-functionality. Therefore, it is necessary to have a fundamental understanding of the properties and roles of plant-derived ingredients in order to create plant-based foods that mimic closely the appearance and organoleptic properties of those conventional animal-based products. In this talk, two key technologies, namely extrusion and mixing/blending, which can be used to produce plant-based products such as meat analogues and plant-based drinks, will be presented and discussed. Furthermore, to make plant-based foods truly sustainable, issues on digestibility and nutritional properties should also be considered.

**Keywords:** Plant-based foods; Meat analogue; Extrusion; Mixing technology; Phase separation



### ■ Professional Biography

Kamolwan Israkarn is a researcher of Food Materials Research Team (FOMT), National Metal and Materials Technology Center (MTEC), National Science and Technology Development Agency (NSTDA), Thailand. Ph.D. in Food Science from Kasetsart University under Royal Golden Jubilee Ph.D. Program and Fulbright-Thailand Research Fund Junior Research Scholarship Program. Her research interests include Food physical chemistry, food microstructure, digestibility of foods, plant-based products. Her current research focuses on Food structuring design of plant-based foods and effects of food structures on digestibility in vitro.

FA



## Toward sustainability in cosmetic industry: Trends and case studies

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FA

Far beyond the pandemic of COVID-19, green and eco-friendly trends are considered as a niched trend in the cosmetic industry, which targeted only small market. At that time, it focused on the usage of natural and organic ingredients. However, when the global warming issue has gained a lot of attention from the rise of social media usage, green trends were continuously evolved into many sub-trends and being accepted by more customer groups. The examples of new green trends are clean beauty and conscious beauty, which currently gain a lot of attention in the market. Sustainability is included as one among the sub-trend in the clean beauty. There are multiple components of sustainable cosmetic trend, for example, the raw material which used to produce the product. We already know that Thailand is a beautiful country which has high biodiversity. Many species of plants may be used as the valuable ingredients in cosmetic products. In fact, Thai government has supported the utilization of agricultural wastes for a long time. However, the outputs from those researches rarely reach to commercial level. Recently, many giant cosmetic raw material suppliers in the world have introduced many ingredients based on sustainable and upcycling concepts into the beauty world. This presentation will introduce the evolution of green beauty. The case studies of interesting commercially available cosmetic ingredients were also given with the hope to inspire the researchers to create a hidden gem for improving Thai cosmetic industry.

**Keywords:** Cosmetic; Cosmetic ingredient; Natural extract; Sustainability; Upcycling



### ■ Professional Biography

Naphatsorn Dittawutthikul received her Ph.D. in pharmacy from the Faculty of Pharmacy, Chiang Mai University. She is a licensed pharmacist who shows her passion to the formulation and evaluation of a cosmetic products since she was an undergraduate student. She is currently working as a full-time lecturer in School of Cosmetic Science at Mae Fah Luang University located in Chiang Rai, Thailand. She also working as a head of Cosmetics for Beauty and Wellness Research Unit in this University. She also interesting in cosmetic marketing trend research. As the cosmetic industry adapts and grows very fast, continuously monitoring the market trend is important. In this conference, she will give a detail about one among the most interesting trend in cosmetic industry, the sustainability. The case studies from the giant cosmetic suppliers will be also given as an inspiration for researcher to create valuable and unique raw materials from Thailand.

FA

## Vitamin D analysis in fish and mushrooms by liquid chromatography-tandem mass spectrometry (LC-MS/MS)

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FA

There are different forms of vitamin D in foods. The standard AOAC methods using high-performance liquid chromatography (HPLC) have been used to determine vitamin D<sub>2</sub> and D<sub>3</sub> in foods, however, their precursors and vitamin D<sub>4</sub> cannot be detected. This study aims to simultaneously determine seven forms of vitamin D including vitamin D<sub>2</sub>, vitamin D<sub>3</sub>, vitamin D<sub>4</sub>, ergosterol, 7-dehydrocholesterol, 25-OH D<sub>2</sub>, and 25-OH D<sub>3</sub> in foods by liquid chromatography-tandem mass spectrometry (LC-MS/MS). Ten fish and ten mushroom species were selected in this study. The edible portion of each sample was homogenized, freeze-dried, re-homogenized, and packed in aluminum foil bags. The samples were kept at -20 °C until analysis. Different forms of vitamin D were separated using ultra-pressure liquid chromatography (UPLC) and quantitated using LC-MS/MS. The results indicated that vitamin D<sub>3</sub> was the major form of vitamin D in fish. Common silver barb, red Nile tilapia, and Nile tilapia contained high vitamin D levels, with 48.5, 31.0, and 19.8 µg per 100g fresh weight (FW), respectively. Other fish contained low vitamin D levels, ranging from 2.4 to 5.7 µg per 100g FW. Vitamin D<sub>2</sub> was the major form of vitamin D in mushrooms. White Shimeji and Lung Oyster mushrooms contained high vitamin D levels, with 7.96 and 6.21 µg per 100g FW, respectively. Other mushrooms contained low vitamin D levels, ranging from 0.06 to 2.30 µg per 100g FW. The LC-MS/MS method is, therefore, the most suitable for studying different forms of vitamin D in foods with good sensitivity, precision, and accuracy.

**Keywords:** Vitamin D, Fish, Mushroom, LC-MS/MS





### ■ Professional Biography

Associate Professor Dr. Kunchit Judprasong is a lecturer at the Institute of Nutrition, Mahidol University (INMU), Thailand, and acts as ASEAN-FOODS Coordinator in the food composition database. He also acts as the head of the food chemistry unit and quality manager of ISO/IEC 17025 laboratories. He received his MSc in Food and Nutrition for Development from Mahidol University, Thailand, and his PhD in Analytical Chemistry from the same university in 2007. He has 36 years of working experience in food and nutrition research especially in the development of methodology for nutrient and non-nutrient analyses such as inulin, fructooligosaccharides, vitamin D, etc. Dr. Kunchit is one of the key persons in developing a food composition database for Thailand, studying nutritive values in different types of foods, developing food reference materials, and organizing proficiency testing for nutrition labeling. Today, he will present some part of his research work on vitamin D analysis using Liquid Chromatography Tandem Mass Spectrometry.

FA

## One-pot catalysis: A privileged approach for sustainable polymers

Kanokon Upitak and Christophe M. Thomas\*

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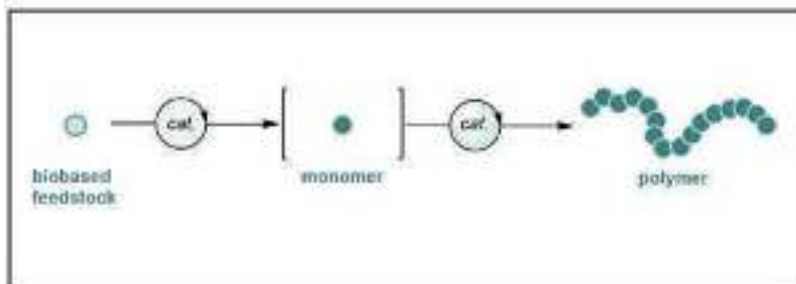
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IC

Polymer production is essentially based on finite feedstocks. These limitations force us to rethink the strategies for the synthesis of these materials. The development of new methods for transforming biomass into resources suitable for polymer production remains a crucial hurdle on the way to a more sustainable chemical economy. In this regard, the creation of renewable polymers through one-pot catalysis represents an important tool to support more sustainable plastics production.

We have used these synthetic schemes to investigate the formation of polyesters, polypeptides and poly(meth)acrylates. We will discuss their efficiency by highlighting their ability to perform multiple synthetic transformations, while bypassing several purification procedures at the same time. We will show that these one-pot procedures can enable the development of new polymers, and also contribute to reducing the environmental footprint.

**Keywords:** Biobased polymers; One-pot catalysis; Reaction mechanisms; Renewable monomers





### ■ Professional Biography

Christophe M. Thomas obtained his PhD in Switzerland, working under the supervision of Prof. Süss-Fink. He then joined Prof. Coates' group at Cornell University (USA) as a post-doctoral fellow supported by the Swiss National Science Foundation. After spending one year in Prof. Ward's laboratories, he was appointed as Assistant Professor at the University of Rennes (France) in 2004. In 2008, he was promoted to Professor at Chimie ParisTech (PSL University, France). His research interests are in homogeneous catalysis and polymer chemistry, with a focus on one-pot catalytic transformations, control of stereochemistry and synthesis of polymers obtained from bioresources.

IC

## Tailoring 4-phosphoryl pyrazolones: Insights into lithium ion recognition and sustainable separation

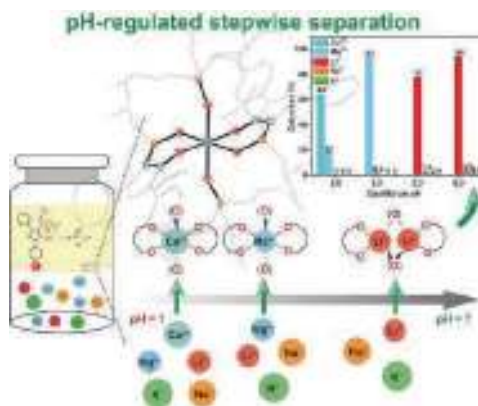
Jianfeng Zhang<sup>1</sup>, Narisara Tanjedrew<sup>2</sup>, Marco Wenzel<sup>1</sup>, Philipp Royla<sup>1</sup>, Hao Du<sup>3</sup>, Supavadee Kiatisevi<sup>2</sup>, and Jan J. Weigand<sup>1\*</sup>

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In addressing the challenge of efficiently separating lithium ions ( $\text{Li}^+$ ) from complex mixtures, particularly in the presence of other alkali metal ions, our research introduces a novel approach using 4-phosphoryl pyrazolones as receptors for  $\text{Li}^+$  recognition and extraction. This study reveals the unique capability of these ligands, especially when used in conjunction with industrial organophosphorus co-ligands such as tributylphosphine oxide (TBPO) or trioctylphosphine oxide (TOPO), to selectively recognize and extract  $\text{Li}^+$  ions from aqueous solutions. We present the first clear evidence of the formation of multinuclear  $\text{Li}^+$  complexes, highlighting the synergistic role of co-ligands in the extraction process. Our work further explores the development of new heteroditopic ligands capable of simultaneous cation and anion binding and extraction. Additionally, we introduce an efficient pH-controlled stepwise separation strategy using 4-phosphoryl pyrazolones. This strategy enables the selective separation of  $\text{Li}^+$  from other common ions such as  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$ ,  $\text{Na}^+$ , and  $\text{K}^+$ . Through a comprehensive investigation of factors influencing the liquid-liquid extraction process, including substitution patterns, diluent/water distribution, co-ligand usage, pH modulation, and metal complex speciation, we demonstrate the practicality and effectiveness of this method.

**Keywords:** Ca/Mg/Li Separation; 4-Phosphoryl Pyrazolone Ligands; pH-Regulated Receptors; SeparationScience





## ■ Professional Biography

Jan J. Weigand is a distinguished Professor at the TU University Dresden since 2013, with a robust academic background, including a diploma in chemistry (2002) and a Dr. rer nat. (2005) from LMU Munich. His postdoctoral endeavors at Dalhousie University, Canada, were supported by the AvH foundation's Lynen Scholarship, followed by a Lynen Return Fellowship in Germany.

Weigand's independent career, initiated with the FCI's Liebig scholarship, was further propelled by the DFG's Emmy Noether research program fellowship and the Wöhler research award for young scientists. In 2012, he received the ERC starting grant from the European Council.

Weigand's research focuses on molecular inorganic and phosphorus chemistry, with a special emphasis on developing sustainable methods for extraction and technical applications. This includes creating innovative catalyst systems for use in the petrochemical industry and transitioning resources to biogenic and fossil residues. In 2023, he received the Reinhardt Koselleck funding from the DFG for his project on modern sustainable phosphorus chemistry and joined the CTC-Expert Pool, showcasing his commitment to advancing chemical science towards sustainability.



## Creation of new conceptual ionic solids based on coordination chemistry

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In recent years, rational creation of polynuclear and supramolecular coordination compounds has attracted considerable attention not only in coordination chemistry but also in material science. In common, a self-assembly method that spontaneously affords molecular aggregates from organic building blocks and linking metal ions has been employed to construct this class of coordination compounds. On the other hand, our interest has been directed to a metalloligand approach, in which pre-designed metal complexes having several donor sites are stepwise treated with different kinds of metal ions.<sup>1</sup> For example, we have recently shown that digold(I)/trigold(I) complexes with mixed D-pen and phosphine ligands serve as functionalmetallo-ligands to construct fascinating metallosupramolecular architectures.<sup>2</sup> In this presentation, several metallosupramolecular ionic crystals created via metalloligand approach, which show new conceptual arrangements and properties of ionic species, will be presented.<sup>3</sup>

**Keywords:** Coordination chemistry; Metal complexes; Supramolecules; Metalloligands, Ionic solids

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### ■ Professional Biography

TK received a Ph.D. degree in 1985 from University of Tsukuba. After working at University of Tsukuba and University of Cincinnati as a post-doctoral fellow, he became an assistant professor at University of Tsukuba in 1987. In 1997, he moved to Gunma University as an associate professor and was promoted to a professor in 1998. He was appointed as a professor at Osaka University in 2000 and retired from Osaka University on March in 2022. After the retirement, he became a visiting professor at National Taiwan Normal University, as well as an emeritus professor at Osaka University. His research field is coordination chemistry, and his current interest is mainly directed to the rational, stepwise creation of novel polynuclear and supramolecular coordination compounds based on pre-designed thiol-containing metalloligands.

IC

# Highly active Cr, Al, and Sn metal complexes for CO<sub>2</sub> utilization and polyester synthesis

Jiraya Kiriratnikom, Nattiya Laiwattanapaisarn, Thasanaporn Ungpittagul,

Nattawat Jabprakon, and Khamphree Phomphrai\*

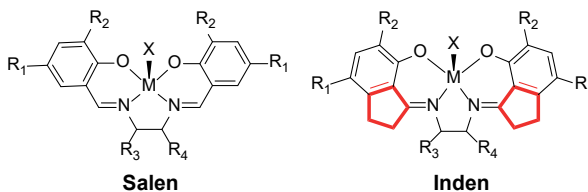
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IC

Single-site ligated metal complexes have been used extensively as efficient catalysts in several catalytic reactions such as metathesis, stereoselective epoxidation, ring-opening polymerization, olefin polymerization, and various organic transformations. The supporting ligands have played crucial roles to control the catalysts' activities and selectivities. Therefore, ligand optimizations and developments have been a vital process in catalytic science. In this work, we aim to develop the well-known tetradentate salen ligand framework derived from salicylaldehyde (sal) and ethylenediamine (en) for superior performance. By adding constraint on the ligand backbone around the aromatic ring and the imine bond (namely inden ligands), the catalysts can show superior performance. The constrained inden metal complexes based on Cr, Al, and Schiff-base Sn complexes were synthesized and shown to have excellent catalytic activities for the cycloaddition reactions of epoxides and carbon dioxide, and ring-opening copolymerization of epoxides and cyclic anhydrides.

**Keywords:** Carbon dioxide; Schiff-base ligands; Cyclic carbonate; Polyesters; Catalyst





### ■ Professional Biography

Dr. Khamphree Phomphrai received his BS in Chemistry from the University of Maryland at College Park (1998) and PhD in Inorganic Chemistry from the Ohio State University (2003), USA. After 2 years of postdoctoral work in olefin polymerization at Purdue University, he moved back to Thailand and joined the chemistry department at Mahidol University in 2005. In May 2015, he joined Vidyasirimedhi Institute of Science and Technology (VISTEC) as an Associate Professor conducting research in catalyst development for bioplastics, polyolefins, and carbon dioxide utilization. In addition to academia, he enjoys running and playing soccer with colleagues and playing the guitar to relax after work.

IC

## Benzoxazines and polybenzoxazines: Crystal structures, properties and applications

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IC

Dihydro-1,3,2*H*-benzoxazines (or benzoxazine monomers) are a class of compounds that have been widely utilized in many areas, such as the production of functional polybenzoxazines, optoelectronic materials, antimicrobial agents, and medicinal agents. Moreover, the benzoxazine monomers can be used to synthesize benzoxazine dimers, which are a group of compounds with a variety of properties, such as anticancer properties and good chelating behaviors. The structure variety of the benzoxazines plays a vital role in their desired properties. In order to gain a full understanding of the effects of the benzoxazine structures on their properties, the crystal structures of benzoxazines obtained from X-ray crystallography are required. Still, there have only been a few structures reported up to now. In this talk, we will demonstrate the relationship between the crystal structures of a set of benzoxazine derivatives and their properties, e.g., thermal, electronic, optical, and anti-corrosion properties. The coordination characteristics of the benzoxazines with different structures towards several metal ions are exemplified and discussed.

**Keywords:** Benzoxazine; Crystal structure; Thermal property; Optical property; Anticorrosion



### ■ Professional Biography

Worawat Wattanathana is an assistant professor at the Department of Materials Engineering, Faculty of Engineering, Kasetsart University. His research interests are X-ray crystallography, synchrotron X-ray absorption spectroscopy, and benzoxazine chemistry. He has conducted research in the field of the structure-property relationship of benzoxazines, polybenzoxazines, and their coordination compounds with the aid of X-ray techniques. Recently, he has been interested in developing novel benzoxazine-derived materials from natural and renewable resources.

IC

## Strategic synthesis of supramolecular host molecules for recognition and sensing of charged species

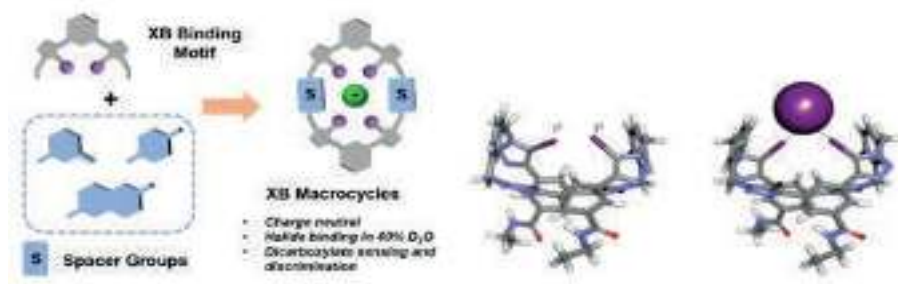
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IC

Nature has developed a number of hierarchical systems that function in highly specific and dynamic environments including enzyme—substrate interactions, selective transport of metal ions or molecules, and encoding of genetic information by DNA. The foundation of such processes is the reversible molecular recognition of chemical species by the assistance of concerted weak non-covalent intermolecular interactions. Taking inspiration from nature, our group has developed artificial receptors which have a unique geometrically restrained binding pocket and specific functional groups to selectively bind charged-guest species including cation, anion, and ion-pair particularly in aqueous media. In this presentation, the synthetic strategies to prepare a series of highly preorganised supramolecular hosts in the form of acyclic, macrocyclic, and mechanically interlocked molecules will be initially described, followed by discussion on the incorporation of reporting units to develop the electrochemical and optical sensing systems. Finally, the potential applications of these supramolecular hosts will be summarised.



**Keywords:** Anion; Cation; Ion-pair; Host-guest interactions; Supramolecular chemistry.



### ■ Professional Biography

Assoc. Prof. Dr. Thantapatra Bunchuay obtained a B.Sc (Hons) degree from Mahidol University where he did a senior project with Prof. Chutima Kuhakarn on iodine chemistry. After that, he carried on M.Sc degree in the field of MOFs materials under supervision of Assoc. Prof. Jonggol Tantirungrotechai. In 2014, he joined the group of Prof. Paul Beer at the University of Oxford, where he employed sigma-hole interactions incorporating into mechanically interlocked molecules for anion recognition in aqueous media. In 2019, he has established “The SupraValentine Research Lab” at Mahidol University. The prime research focus is the synthesis of novel macrocyclic molecules to study their unusual host-guest behaviour via advanced spectroscopic techniques. In addition, our synthetic macrocycles are used as the basis of functional materials for applications in sensing, extraction and recovery, delivery, and soft materials.

IC



## Transition towards low carbon society: A case study from chemical industry

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*PTT Global Chemical Public Company Limited, 555/1 Energy Complex, Building A,  
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### ■ Professional Biography

**NATTHAKORN KRAIKUL, Ph.D.**

Vice President, Decarbonization Center of Excellence

PTT Global Chemical Public Company Limited

Education:

- Ph.D. (Petrochemical Technology)

The Petroleum and Petrochemical College,  
Chulalongkorn University, Thailand (2004-2006)

- M.S. (Petrochemical Technology)

The Petroleum and Petrochemical College,  
Chulalongkorn University, Thailand (2002-2003)

- B.Sc. (Industrial Chemistry) – First Class Honor

King Mongkut's Institute of Technology North  
Bangkok, Thailand (1998-2001)

Experiences:

Circular Economy - GC

Corporate Sustainability Strategy - GC

Innovation Strategy and Technology Scouting - GC

Start-up Engineer, Sriracha Clean Fuel Project - Esso  
Sriracha Refinery, Esso (Thailand)

IE



## Journey on exploring advanced recycling technologies by Indorama Ventures Plc.

Sasinotai Rochanutama

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IE

Due to global challenges on plastic waste and sustainability trends in the circular economy as well as sustainable packaging, Indorama Ventures Plc., as a global chemical company with a head office in Bangkok, Thailand, is the No. 1 PET (polyethylene terephthalate) producer and recycler in the world. We commit to operating responsibly and incorporating sustainability into our operations. With the recycling business started in 2011 to recycle post-consumer PET bottles, our recycling targets are to recycle 50 million bottles per year by 2025 and 100 billion bottles per year by 2030. These targets are also committed to the Ellen McArthur Foundation. However, along our journey, there were limitations on mechanical recycling for colored PET bottles and textiles recycled in closed loops. Therefore, advanced recycling technologies are on-going researches and developed to overcome existing limitations and to go back to raw materials used for the production of PET. Indorama Ventures is currently exploring several promising technologies. Enzymatic Recycling, a technology from Cabrios, uses an enzyme capable of specifically depolymerizing the PET. Additionally, this technology allows the recycling of all types of PET waste as well as the production of 100% recycled PET products without loss of quality. Found to most fit with our business, it supports the circular economy concept, in which waste is now a precious raw material and plastic waste is eliminated at the same time.

**Keywords:** Recycling business; PET waste and textile recycling; Enzymatic recycling; Recycling commitment; Plastic waste and circular economy



### ■ Professional Biography

Miss Sasinotai Rochanutama graduated with a B.S. in Chemical Technology from the Faculty of Science and a M.S. in Petrochemical Technology from The Petroleum and Petrochemical College, both from Chulalongkorn University. From over 20 years of work in petroleum and petrochemical industries, she has been working for >10 years on sustainability in chemical industry. Currently, she serves as a Senior Manager–Sustainability in Indorama Ventures Plc. (IVL), responsible for the company’s reporting for various ratings, which has contributed various prestigious awards, granted by several world-class organizations, to the company. For instances, IVL was recognized as a winner of the Best Sustainable Product Award at the Chemical Week Sustainability Awards 2022, by S&P Global, as the winner of the “Top Sustainability Advocate in Asia” by Asia Corporate Excellence and Sustainability Awards (ACES) 2022, and as the Highly commended (2nd place) Responsible Business Awards of the “Circular Transition” in 2022 by the Reuters Events. Her current presentation topics relate to advanced recycling technologies and circular economy under the BCG concepts.

IE

## The circularity of tire industry: Recovered carbon black/graphene composite materials and applications

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IE

It is estimated that there are domestically about 800,000 tons of wasted tires per year. Recovered carbon black (rCB) is one of materials obtained from these wasted tires through a pyrolysis process. The properties of rCB can vary depending on the tire feedstock, pyrolysis conditions, and post-processing methods. Reduced graphene oxide (rGO) is a derivative of graphene oxide that has been reduced to graphene-like sheets. The properties of rGO depend on the degree of reduction, processing methods, and functionalization techniques. In this work, a composite of rCB and rGO fibers was synthesized by a wet spinning process. The combination of rCB and rGO has been shown to result in the production of fibers with enhanced properties, such as improved mechanical strength, capacitance, and electrical conductivity. The rCB-rGO fibers have potential applications in various fields, such as energy storage devices, sensors, and electronic textiles. Overall, rCB-rGO fibers are a promising material with enhanced properties that make them suitable for various applications. Further research is needed to optimize their production and to develop new applications for these fibers.

**Keywords:** Composite materials; Graphene; Recovered carbon black; Wasted tire



### ■ Professional Biography

Apichai Jomphoak received his Ph.D. degree in Information Technology from Japan Advanced Institute of Science and Technology (JAIST), Japan. His work was under the supervision of Prof. Dr. Ryo Maezono. He is now a researcher at opto-electrochemical sensing research team (OEC), spectroscopic and sensing devices research unit (SSDRG), National Electronics and Computer Technology Center (NECTEC), Thailand. His research interests focus mainly on the area of materials synthesis such as 2-dimensional materials (graphene, borophene, boron carbide ( $\text{BC}_3$ )) and graphene-based composite fibers synthesis. He has also applied computational simulations in materials informatics based on density functional theory (DFT), quantum Monte Carlo (QMC), and finite element method (FEM) for materials synthesis/fabrication, energy storages, and sensor applications.

IE



## The role of organic photovoltaics in renewable energy to overcome climate change

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MN

According to International Energy Outlook 2021 published by Energy Information Administration (EIA), global energy consumption will be double by 2050. Therefore, finding alternative energy sources is an urgent and pressing problem. Sunlight is by far the most abundant source of energy on Earth and, if harvested, can address the energy demands in the future. Organic photovoltaics (OPVs) potentially can offer low cost, large area, flexible, light-weight, clean, and quiet energy sources for indoor and outdoor applications such as energy-efficient buildings and greenhouses. OPVs are fabricated from organic semiconductors (OSCs), a class of carbon-based materials comprising of alternate single and double bonds (conjugated pi-bonds). OSCs can be synthesized to have band gaps from the UV to the near infrared regions of the electromagnetic spectrum. OSCs are attractive due to their unique properties: light weight, mechanical flexibility, low cost, low-temperature processing, and simple fabrication methods such as roll-to-roll coating, spray coating or ink-jet printing into desired size and shape. Such materials are expected to form the basis of new emerging technologies — called the Organic Electronics. OSCs have been implemented in commercial products such as displays and lightings and have potential applications in transistors, OPVs, photodetectors, thermoelectrics, ratchets, sensors, neuromorphic computing, and bioelectronics. In this talk, I will discuss the role of OPVs in transition to renewable energy to overcome the climate change.

**Keywords:** Solar energy; Organic photovoltaics; Organic semiconductors; Climate change; Energy efficient buildings



### ■ Professional Biography

Thuc-Quyen Nguyen is the Director of the Center for Polymers and Organic Solids and professor in the Department of Chemistry & Biochemistry, University of California, Santa Barbara. Her research interests are organic semiconductors for emerging technologies (bioelectronics, organic solar cells, LEDs, sensors, transistors, and photodetectors), renewable energy, and sustainability. She is a member of the *US National Academy of Engineering* and recipient of the *Wilhelm Exner Medal*, *De Gennes Prize*, and *Alexander von Humboldt Senior Research Award*. She is a Fellow of the Royal Society of Chemistry and of the American Association for the Advancement of Science (AAAS). Recognition for her research includes the 2015-2019 World's Most Influential Scientific Minds; Top 1% Highly Cited Researchers in Materials Science by Thomson Reuters and Clarivate Analytics and 2019 Hall of Fame - *Advanced Materials*. She co-authors over 300 publications and 3 book chapters that received over 36,500 citations (*h-index*: 98).

MN

## Electrochemical applications of two dimensional (2D) materials for sustainable uses

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The use of two-dimensional (2D) materials such as graphene for various applications, including energy storage and conversion has continued to gain great interest. There have been several papers that have investigated the properties of graphene oxide for carbon-based applications. However, these oxygen-rich carbon materials (>30%) suffer from poor stability in aqueous solutions due to the polar surface chemistry with low electronic conductivity. To overcome this, we used liquid phase exfoliation to produce graphene with size dependence possessing ultra-low oxygen content (<1%) for various graphene-based applications.

In this talk, we demonstrate three electrochemical applications. The first application, we described the optimum dimension of 2D nanosheets as a conductive binder for manufacturing porous carbon electrodes in energy storage applications. We found that 2D materials can replace the insulating polymer binders and provide flexible electrodes. The binding mechanism with charge storage performance of size-selected graphene binder was explored. Second, we used ultralow oxygen-containing graphene to form membrane laminates. The formation of stacked graphene nanosheets can provide nanocapillary channels for ionic and molecular nanofiltration. The membrane exhibited high stability in aqueous solutions with no observed swelling. Third, we investigated the optimum nanosheet size (length and thickness) for supporting gold nanoparticles (AuNPs) to enhance hydrogen evolution reaction. It was found that the decoration of AuNPs increased with increasing nanosheet size, counter to what is widely reported for smaller nanosheet size (high surface area). We believe that these could impact the world technology development for clean energy and water purification, following the 17 SDGs.

**Keywords:** Graphene; Electrode; Membrane; Electrocatalyst; Hydrogen evolution reaction





### ■ Professional Biography

Asst. Prof. Wisit Hirunpinyopas obtained his BSc in 2011 and MSc in 2013 in Chemistry from Kasetsart University, Bangkok, Thailand. He got a PhD scholarship from the Development and Promotion of Science and Technology Talents Project (DPST), supported by the Ministry of Education, Thailand. In 2019, he obtained a PhD in Chemistry from The University of Manchester, UK. He joined Kasetsart University in the Department of Chemistry as a lecturer in 2020 and was appointed as an Assistant Professor in Inorganic Chemistry in 2022. His research interests are related to material science, particularly two-dimensional (2D) materials such as graphene and transition metal dichalcogenides including synthesis, functionalization, characterization, and various applications. The applications are related to membrane-based filtration (2D material-based membrane), electrochemical energy storage (supercapacitors), and electrocatalyst (gas evolution).

MN

## Crystallization of pharmaceutical compounds

Il Won Kim

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Inadequate solubility of active pharmaceutical ingredients (APIs) is a lingering problem in many synthetic drugs, which translates into poor API bioavailability. Various strategies have been explored to alleviate the solubility problem of so-called class II APIs of the biopharmaceutical classification system. Selecting appropriate polymorphs, salts, and cocrystals of the APIs is a method to employ the thermodynamic aspect of solubility increase. Reducing the size of API particles or domains is another way to utilize the kinetic side by increasing the surface area available for dissolution. This presentation will highlight some of the efforts in our research group to control the crystallization of APIs to modulate their physical properties. It will primarily focus on the nanodrug formation and the cocrystallization of APIs.

**Keywords:** Active pharmaceutical ingredients; Crystallization; Dissolution



### ■ Professional Biography

Dr. Il Won Kim is a professor of Chemical Engineering at Soongsil University in Seoul, South Korea. He received bachelor's and master's degrees in Chemical Technology from Seoul National University and a Ph.D. in Macromolecular Science and Engineering from the University of Michigan at Ann Arbor (2004). Prof. Kim was also a postdoctoral fellow in Chemistry at New York University (2004-2007). He has been working on the biomineralization of calcium carbonate with an emphasis on the effect of organic components on inorganic crystallization. Currently, his research focus is pharmaceutical crystallization, where the physical properties of active compounds are modulated by controlling their crystallization behavior.

MN

## $\delta$ -MnO<sub>2</sub>-based nanocomposite cathodes for aqueous Mg-ion electrochemical energy storage devices

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The findings of this study are noteworthy, as it highlights the successful synthesis of two different types of nanocomposite cathode materials, namely  $\delta$ -MnO<sub>2</sub>/reduced graphene oxide (rGO) and K-doped MnO<sub>2</sub>/graphite nanofibers (GNF), both of which exhibit remarkable electrochemical properties. In particular, the  $\delta$ -MnO<sub>2</sub>/rGO nanocomposite cathode-based device demonstrated a high operating voltage of up to 2 V and a maximum energy density of 29.8 Wh kg<sup>-1</sup> at a power density of 823 W kg<sup>-1</sup>. More importantly, the device showed impressive discharge capacity and excellent cycling stability even at the low temperature of -20 °C. As for the K-doped MnO<sub>2</sub>/GNF electrode, it exhibited a high specific capacitance of 410.31 F g<sup>-1</sup> at a current density of 0.5 A g<sup>-1</sup> as well as superior cycle stability under high current density, retaining 57.0% of the charge/discharge efficiency at 4 A g<sup>-1</sup>. The device based on the K-doped MnO<sub>2</sub>/GNF electrode delivered a high specific capacitance of 32.51 F g<sup>-1</sup> at 0.5 A g<sup>-1</sup> and maintained 88.2% of the initial capacitance after 20000 cycles. Overall, this device has the potential to revolutionize the field and pave the way for more efficient energy storage solutions.

**Keywords:**  $\delta$ -MnO<sub>2</sub>; Nanocomposite; Mg-ion; Energy storage



### ■ Professional Biography

Prof. Jeng-Yu Lin is a distinguished professor at the Chemical and Materials Engineering Department of Tunghai University, Taiwan. He received his B.S. degree (2003) and Ph.D. degree (2008) from National Tsing-Hua University, Taiwan. He was awarded a visiting graduate fellow in Dr. Alan West's laboratory at the Chemical Engineering Department of Columbia University (2007-2008). He had postdoctoral research training (2009) at the Institute of Atomic and Molecular Sciences, Academia Sinica. He has published 140 peer-reviewed international journal papers (SCI) ( $h$ -index = 45) in semiconductor processing and energy conversion/storage technologies. He has obtained 20 projects from National Science and Technology Council (NSTC, Taiwan), including a three-year "Outstanding Young Researcher Award Project" in 2014, a three-year "Taiwan-Poland Joint Research Project" in 2017, a three-year "Taiwan-Russia Joint Research Project" in 2019, a three-year "Taiwan-Czech Joint Research Project" in 2020, a three-year "Taiwan- Slovak Joint Research Project" in 2022, and received an "**Academic Award for Young Researcher**" from Taiwan Institute of Chemical Engineers in 2014.

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## Porphyrins for energy conversion

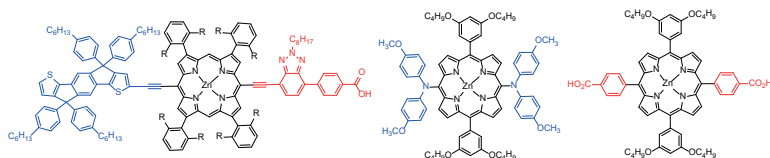
Chen-Yu Yeh\*, Chi-Lun Mai, Yu-Hsuan Chen, and Ching-Chin Chen

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Chlorophyll derivatives generally exhibited poor power conversion efficiency (PCE) when used as sensitizers in dye-sensitized solar cells (DSSCs), organic solar cells (OSCs) and perovskite solar cells (PSCs). In contrast, artificial chlorophylls, i.e., porphyrins, have been found to show high efficiency as used in DSSCs, OSCs, PSCs. Porphyrins with a push-pull framework for use in solar cells achieve high power conversion efficiency 10-13% under standard AM 1.5 sunlight. We also synthesized porphyrins for use in PSCs. Our studies show that porphyrins can be used as hole-transporting materials and defect passivators for high efficiency perovskite solar cells. In addition, porphyrins have been applied in perovskite solar cells as efficient hole-transporting materials. Perovskite solar cells (PSCs) using a porphyrin hole transporting materials (HTMs), defect passivators, or self-assembled monolayers (SAMs) achieves a PCE higher than 22%.

**Keywords:** Dye-sensitized solar cells; Hole-transporting; Passivation; Perovskite; Porphyrins



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2. Mai, C.-L.; Xiong, Q.; Li, X.; Chen, J.-Y.; Chen, C.-C.; Xu, J.; Liu, C.; Yeh, C.-Y.\*; Gao, P.\* “Thermally Stable D2h Symmetric Donor- $\pi$ -Donor Porphyrins as Hole-Transporting Materials for Perovskite Solar Cells”, *Angew. Chem. Int. Ed.* 2022, 61, e202209365.



### ■ Professional Biography

Chen-Yu Yeh was born in 1968. He received his BS in chemistry from National Chung Hsing University (NCHU) in 1990, his MS from National Taiwan University (NTU) in 1992, and his PhD from Michigan State University in 1999 under the guidance of professor Chi-Kwong Chang. After postdoctoral studies at MIT with Professor Daniel G. Nocera and at NTU with Professor Shie-Ming Peng, he joined NCHU in 2002, where he is currently a Professor in Chemistry. His research covers synthesis of porphyrins for energy conversion. He has been recognized with a number of awards, including the Bau Family Award, Academia Sinica Award for Junior Research Investigators, etc.

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## Development of metal-organic frameworks for energy and environmental applications

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Metal-organic frameworks (MOFs) are crystalline porous materials with several applications. However, the insoluble nature of MOFs limits their practical uses because it is difficult for material processing by solution-based techniques. Moreover, some properties that rely on the disordering systems including the charge mobility, conductivity, and polymeric/rheological properties are severely lacking from MOFs in the crystalline phase. Therefore, a study on the solid-to-liquid phase transition of MOFs would benefit the processability of MOFs for practical application as well as uncovering the new properties of MOFs for new applications. The talk will highlight the preparation of MOF aerogels and MOF nanofilm with sub-100 nm thickness. MOF aerogels have been customized on their chemical and porous properties to achieve strong chemical interactions with targeted heavy metals, resulting in high performance for heavy metal decontamination with a long lifetime. Moreover, the fabrication of MOF nanofilms with enhanced electrochemical properties will be discussed. The unique electrochemical properties in MOF nanofilms are further applied to the use of MOF materials as active layers in optoelectronic and electrochemical devices.

**Keywords:** Metal-organic framework; Coordination polymer; Porous materials; Material processing; Gel



### ■ Professional Biography

Kanokwan Kongpatpanich is an assistant professor at Vidyasirimedhi Institute of Science and Technology (VISTEC). She received B.S. (1<sup>st</sup> Class Hons) and M.S. degree in Chemistry from Kasetsart University, Thailand. She obtained Ph.D. in Engineering in 2015 from Kyoto University, Japan. In 2022, she is the recipient of a research fellowship from Thailand Toray Science Foundation and the L'Oréal-UNESCO For Women in Science award. She is honored with Young Technologist Awards in 2023. Her research interests include the development of metal-organic frameworks and other related porous materials.

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## From darkness to light: Investigating the chemical basis of pholasin's bioluminescent mechanism

Maiko Moriguchi<sup>1</sup> and Masaki Kuse<sup>2\*</sup>

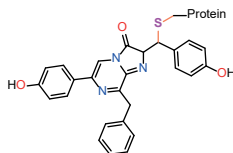
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<sup>2</sup>*Graduate School of Agricultural Science, Kobe University  
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Bioluminescence, an intricate biochemical process mediated by proteins like photoproteins, provides a luminescent output contingent on specific biological cues such as calcium ions. This study investigated the photoprotein pholasin, isolated from the bioluminescent marine bivalve *Pholas dactylus*. Pholasin utilizes dehydrocoelenterazine (DCL) as a chromophore and manifests luminescent activity in response to reactive oxygen species (ROS). The primary objective was to enhance pholasin's luminescent efficiency via structural modification of DCL. Employing cross-coupling reactions catalyzed by transition metals, a synthetic route to DCL analogs was established, commencing with commercially available aminopyrazine. To assess the luminescent activity of these DCL analogs, apopholasin—pholasin devoid of its natural chromophore—was essential. After extensive experimentation, the most productive approach for apopholasin production was realized through a baculovirus-silkworm multigene expression system. Subsequent incorporation of DCL analogs into apopholasin resulted in significant luminescence upon induction of ROS via a mixture of peroxidase and hydrogen peroxide. Notably, one DCL analog demonstrated a ten-fold increase in luminescent output compared to its natural counterpart. The enhanced luminescent system is currently optimized for high-sensitivity in vivo ROS detection. This study thus unveils the potential for engineering more efficient bioluminescent systems by manipulating chromophore structures.

**Keywords:** Bioluminescence; Photoprotein; Reactive oxygen species; Chromophore; Natural products



**Figure 1** Structure of the chromophore of Pholasin.



## ■ Professional Biography

Masaki Kuse

### 1. Professional Appointments:

Professor, Graduate School of Agricultural Science,  
Kobe University (Apr 2022-)

Associate Professor, Graduate School of Agricultural  
Science, Kobe University (Sep 2011-)

Assistant Professor, Research Center for Material  
Sciences, Nagoya University (Apr 2001-)

Research Associate, Graduate School of Bioagricultural  
Sciences, Nagoya University (Apr 2000-)

### 2. Education:

Ph.D., Nagoya University (2000) (Supervisor:  
Professor Minoru Isobe)

### 3. Research Interests:

Design and synthesis of biologically active compounds  
inspired by natural products.

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## Biosynthesis of antitumor alkaloid streptonigrin

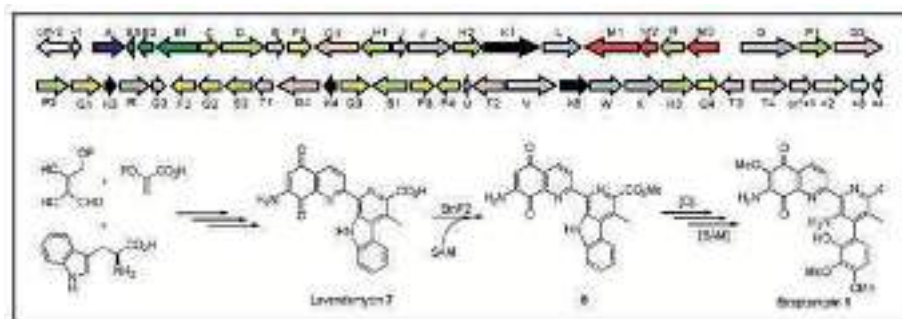
Fei Xu, Yi Zou, Dekun Kong, Xiaozheng Wang, Tingting Huang, and Shuangjun Lin\*

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Streptonigrin (STN) is a highly functionalized aminoquinone alkaloid containing four rings produced by *Streptomyces flocculus* ATCC13257. STN is highly active against a broad range of tumors, including breast, lung, head, and neck cancer, lymphomas and melanomas. In addition, STN also shows in vivo and in vitro antiviral properties and potent, broad spectrum antibacterial activities against bacteria and fungi. We cloned and sequenced the biosynthetic gene cluster of STN that consists of 48 genes. We biochemically demonstrated several novel enzymatic reactions including the stereoselective methylation of tryptophan, formation of  $\beta$ -carboline moiety. In addition, we characterized a potent promotor and created many new streptonigrinoid analogues as potential therapeutic agents using genetic and chemo-enzymatic methods.

**Keywords:** Natural product; Alkaloid; Streptonigrin; Biosynthesis





### ■ Professional Biography

Shuangjun Lin is a distinguished professor at Shanghai Jiao Tong University and Vice Dean of the School of Life Sciences and Biotechnology at Shanghai Jiao Tong University. After he obtained a Ph.D. in Chemistry from the Institute of Chemistry, Chinese Academy of Sciences in 2002, he conducted postdoctoral research at the University of Alberta in Canada and the University of Wisconsin-Madison in the United States. He joined the School of Life Sciences and Biotechnology at Shanghai Jiao Tong University as a professor in 2008. His research interest is focused on the discovery and biosynthesis of microbial natural products, the mechanisms and application of enzymatic reactions, and synthetic biology. So far, more than 100 SCI indexed papers have been published.

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## Deuterated drugs, new challenging molecules as drug candidates: Deuteration of natural products

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Ministry of Higher Education, Science, Research and Innovation, Thailand*

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Because of higher stability of the C-D bond relative to C-H, deuterated drug candidates have an improvement of pharmacokinetics and metabolic profiles with profound enhancement of half-lives without altering the potency. Two deuterated drugs were approved in 2017 and 2022 (*Nature Reviews Drug Discovery* **2023**, 22, 562-584); therefore, new deuteration techniques are of interest in drug discovery recently. This lecture covers a simple, clean and by-product-free, site-selective deuteration by acid-catalyzed reaction using deuterium halide (DX) generated from common and inexpensive reagents, i.e. prenyl-, allyl-, and propargyl halides. The deuterated products were obtained without chromatographic separation, and a gram-scale chromatography-free synthesis of some deuterated compounds was demonstrated in this work. This metal-free deuteration method covers a broad range of substrate including natural products, phenolic compounds (i.e. flavonoids and stilbenes), as well as indoles, pyrroles, carbonyl compounds, and steroids. Moreover, this deuteration technique was applied for commonly used drugs such as loxoprofen, haloperidol, stanolone, progesterone, androstenedione, donepezil, ketorolac, adrenosterone, cortisone, pregnenolone, and dexamethasone.

**Keywords:** Deuteration; Chromatography-free synthesis; Deuterated natural products; Acid-catalyzed reaction; Site-selective deuteration



### ■ Professional Biography

Prasat Kittakoop received B.Sc. (1st Class Honors, Chemistry) from Chiang Mai University, and Ph.D. (Biochemistry) from University of Wales, Swansea, U.K. His research interests are natural products chemistry, green chemistry, and medicinal chemistry. He published more than 145 papers, more than 5,270 total citations with h-index of 43 (Scopus database). Over the past 3 years (2020-2022), he was recognized as the World Top 2% Scientists in Medicinal & Biomolecular Chemistry (based on citations from Scopus database). He is a regular reviewer of more than 60 journals (1,114 reviews).

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## Optimizing natural products as promising antiviral agents through computation-aided drug design

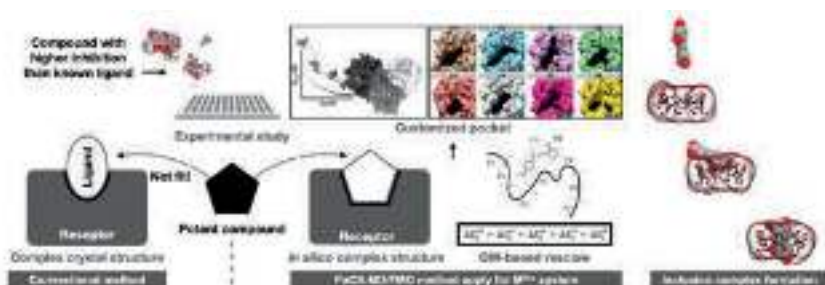
Kowit Hengphasatporn<sup>1\*</sup>, Tanatorn Khotavivattana<sup>2</sup>, Siwaporn Boonyasuppayakorn<sup>3</sup>, Thanyada Rungrotmongkol<sup>4</sup>, and Yasuteru Shigeta<sup>1</sup>

<sup>1</sup>Center for Computational Sciences, University of Tsukuba, 1-1-1 Tennodai, Tsukuba, Ibaraki, 305-8577, Japan; <sup>2</sup>Program in Bioinformatics and Computational Biology, Graduate School, Chulalongkorn University, Bangkok, 10330, Thailand; <sup>3</sup>Center of Excellence in Applied Medical Virology, Department of Microbiology, Faculty of Medicine, Chulalongkorn University, Bangkok, 10330, Thailand; <sup>4</sup>Center of Excellence in Natural Products Chemistry, Department of Chemistry, Faculty of Science, Chulalongkorn University, Bangkok, 10330, Thailand

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Employing a computational approach, we utilize molecular docking, molecular dynamics simulation, and the fragment molecular orbital method for virtual screening, identifying compounds with potential to optimize natural products as promising antiviral agents. These computational insights guide our synthesis team, streamlining the design and production of targeted compounds. Cell-based assays validate antiviral efficacy, despite challenges in aligning experimental suggestions with available protein structures. A key aspect of our methodology is an advanced technique simulating binding pockets, confirming compatibility with experimentally suggested compounds. Our study extends to observing inclusion complex formation in cyclodextrin for enhanced drug delivery. The synergy between cutting-edge computational methods and experimental validation underscores the significance of natural product optimization by computational study in advancing therapeutic interventions. This focused strategy highlights the potential impact of computation-aided drug design, emphasizing the pivotal role of natural products in the pursuit of effective antiviral solutions.

**Keywords:** Antivirus; Computational chemistry; Cyclodextrin; FMO; MD Simulation





## ■ Professional Biography

As a researcher in computational biology and chemistry, I've played a pivotal role in advancing the field, particularly in molecular modeling, drug discovery, and enzyme catalysis. My expertise lies in employing cutting-edge computational techniques, with a focus on the fragment molecular orbital (FMO) method and molecular dynamics (MD) simulations. I specialize in developing innovative platforms for the drug screening pipeline, integrating applied MD simulation, molecular mechanics (MM) calculation, ab initio quantum chemistry (QM) methods, and enhanced computational sampling techniques. This multifaceted approach is geared towards providing more realistic and highly accurate information, contributing to the precision and efficacy of computational methods in drug discovery and molecular research.

I earned my Ph.D. in Bioinformatics from Chulalongkorn University in Bangkok, Thailand, under the supervision of Assoc. Prof. Thanyada Rungrotmongkol. Currently, I hold the position of Assistant Professor at the Center for Computational Sciences, University of Tsukuba, under the Prof. Yasuteru Shigeta laboratory.

NP

## Southern Philippines as a rich source of natural products

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*Center for Natural Products and Drug Discovery, Premier Research Institute of Science and Mathematics,*

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The Philippines is considered one of the biodiversity hotspots and megadiverse countries in the world. Its rich terrestrial and marine ecosystems, particularly in Mindanao have remained under-tapped and under-explored.

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The importance of medicinal plants and traditional health systems in solving the health care problems of the world is gaining increasing attention. This interest in medicinal plants as a re-emerging health aid has been fueled by the rising costs of prescription drugs in the maintenance of personal health and well-being. Herbal medicines which have been in existence for years in most countries including the Philippines, play a major role in primary health care of approximately 80% of the world's inhabitants. The Philippines has about 1,500 medicinal plants from more than 13,500 plant species of which more than 3,500 are considered indigenous. However, majority of Philippine medicinal plants with centuries of ethnomedical history remains untapped and the potentials of these plants have not been fully investigated.

Moreover, the Philippines, with its long coastal lines, has drawn on its marine capital only to a small extent. Only a few marine organisms collected from various parts of the Philippines have been documented and investigated in terms of their potential as source of bioactive secondary metabolites, particularly anticancer compounds. Although majority of the marine organisms investigated were marine sponges, only a few of them were collected off the coasts in Mindanao.

This paper will present results obtained so far from the investigations made by the author's research team on some medicinal plants found in various parts of Mindanao including those that have been used traditionally by two Indigenous Peoples of the island. Results on the studies on marine sponges collected off the coasts of Mindanao will also be discussed.

**Keywords:** Southern Philippines; Biodiversity; Medicinal plants; Marine sponges; Natural products



### ■ Professional Biography

Dr. Mylene M. Uy, is a Professor and Researcher of the Chemistry Department of the Mindanao State University-Iligan Institute of Technology (MSU-IIT). She is the Director of the Center for Natural Products and Drug Discovery of the MSU-IIT Premier Research Institute of Science and Mathematics (PRISM), where she concurrently serves as its Executive Director.

She obtained her Doctor of Science degree from Hiroshima University, Japan in 2005 as a Monbukagakusho Scholar. She has been actively engaged in collaborative research in the field of bioorganic chemistry- natural products and has implemented several research programs funded by various government funding agencies. Her dedication and passion to natural products research has produced more than 70 international publications and a number of national and international presentations. Moreover, she has mentored more than 100 undergraduate and graduate students and discovered 11 new compounds.

She is a recipient of a number of Philippine awards, the latest of which is the Philippine Regulation Commission 2022 Outstanding Professional in the field of Chemistry.

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## Olefin metathesis catalysts specialised in bio-mass valorization: Ethenolysis of fatty oils and musk production

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Metathesis opened up potential opportunities to produce numerous fine chemicals from a biomass. From many types of olefin metathesis, the ethenolysis (cross metathesis with ethylene) can be used to convert many plant-derived raw materials into valuable fine chemicals. One of potential substrates are plant and algae oils, rich in oleic acid. Use of oleic acid esters in ethenolysis were however hampered by the lack of stable and productive catalysts for this reaction. During the lecture, some new and highly potent catalysts systems for ethenolysis of a biomass will be presented.

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On the other hand, using biomass-derived substrates, a number of valuable musk-macrocyclic lactones, ketones, and ethers can be obtained in Ring-Closing Metathesis (RCM) reaction in high yield and selectivity at concentrations 300 times higher than those typically used by organic chemists for similar macrocyclizations.



**Keywords:** Olefin metathesis; Ethenolysis; Palm oil; Biomass; Renewables



### ■ Professional Biography

Karol Grela received his PhD degree from the *Institute of Organic Chemistry, Polish Academy of Sciences*, in 1998. As *Alexander von Humboldt Scholar*, he spent one year in the *Max-Planck-Institut für Kohlenforschung*, Mülheim an der Ruhr, Germany, just in time to be present at the blooming of metathesis methodology in the laboratories of Professor Alois Fürstner. In 2008 he was promoted to Full Professor. Since 2008, he is a Director of a research laboratory at the *Biological and Chemical Research Centre of the Faculty of Chemistry, University of Warsaw*. His synthetic research focuses on improving synthetic efficiency of organic reactions, organometallic chemistry and catalysis. His work with metals involves the development of new catalysts and conditions for olefin metathesis. He cooperated with a number of companies, inc. Boehringer-Ingelheim Inc., Nalco Inc., Evonik AG, Umicore AG, Polpharma SA, Apeiron Synthesis SA.

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## Synthesis, computers and natural product mistakes

Roderick W. Bates,<sup>1\*</sup> Mikhail Elyashberg,<sup>2</sup> Andrei G. Kutateladze<sup>3</sup>, and Craig M. Williams<sup>4</sup>

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<sup>2</sup>*Advanced Chemistry Development Inc. (ACD/Labs), Toronto, ON, Canada.*

<sup>3</sup>*Department of Chemistry and Biochemistry*

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The use of natural products, chemicals produced by living organisms, has been extraordinarily beneficial to human health over millennia. The isolation of natural products from plants, fungi, bacteria and animals is an important scientific endeavor and must be accompanied by the determination of the molecular structure. Although this is now done by the use of a battery of sophisticated instrumental methods, mistakes in structure determination do happen and should be corrected. A number of such corrections, based upon intuition, organic synthesis, and computational methods, are presented in this talk. The importance of access to original data will be illustrated.

**Keywords:** Structure; Reassignment; Spectroscopy; Computational; Natural product



### ■ Professional Biography

Roderick Bates received his PhD at Imperial College, London with Professor Steven Ley, using organoiron complexes for organic synthesis. After a postdoctoral stint at Colorado State University with Professor L. S. Hegehus working on chromium carbenes, he moved to the University of North Texas as an Assistant Professor. After some years spent in Thailand at Chulalongkorn University and the Chulabhorn Research Institute and a short stay in the ill-fated Department of Chemistry at Exeter in England, he joined Nanyang Technological University as a pioneer member of the Division of Chemistry and Biological Chemistry. He is currently an Associate Professor, a Fellow of NTU's Teaching Excellence Academy and the University's Research Integrity Officer. He has research interests are in organic synthesis, and drug discovery. He is also a lecturer on Forensic Science for a Coursera MOOC.

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## Catalytic deoxygenation of epoxides to alkenes

Sunisa Akkarasamiyo

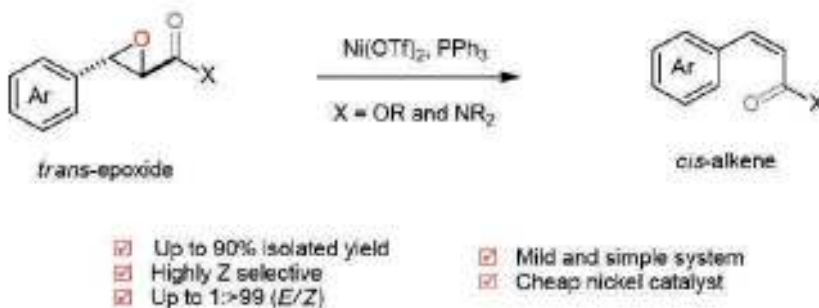
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Alkenes are versatile building blocks in organic synthesis. *cis*-Alkenes, less thermodynamically stable than *trans*-isomers, are less abundant in nature. Stereoselective methods for the synthesis of *cis*-alkenes have been challenging and less developed nowadays. A stereospecific deoxygenation of *trans*-epoxides to access *cis*-cinnamic acid derivatives using nickel (II) trifluoromethanesulfonate with triphenylphosphine will be presented. High functional group tolerance was observed where *cis*-cinnamate esters, *cis*-cinnamamides *cis*-cinnamyl amines, and *cis*-cinnamyl alcohol contained methoxy, halogens and nitro groups were obtained in high yields with moderate to high *E/Z* ratios.

**Keywords:** Deoxygenation; Nickel; Stereospecific; *cis*-Alkene; Epoxide



## Reference

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### ■ Professional Biography

Sunisa Akkarasamiyo received her bachelor's and master's degrees from Silpakorn University, under the supervision of Associate Professor Punlop Kuntiyong. She obtained her Ph.D. in 2014 from Kasetsart University under the Royal Golden Jubilee Ph.D. Program, under the supervision of Professor Ngampong and Professor Boonsong Kongkathip. After finishing Ph.D. studies, she was awarded the Erasmus Mundus postdoc scholarship to join the group of Professor Samec. Her research project focused on C–O bond activation of alcohols (2014–2018). She moved back to Thailand in 2018 and worked as research assistant at Chulabhorn Research Institute (CRI) in the group of Professor Poonsakdi Ployprodith (2018–2020). In 2020, she joined the Department of Chemistry, Faculty of Science, Kasetsart University as a lecturer and was promoted to Assistant Professor in 2022. Her research expertise includes catalysis, methodology development, and total synthesis using compounds from biomass as substrate.

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## Synthesis of curved nanographenes

Mihaela C. Stuparu

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Corannulene ( $C_{20}H_{10}$ ) is a polycyclic aromatic hydrocarbon that exhibits molecular curvature due to the arrangement of five six-membered rings around a central five-membered ring. It can, therefore, be considered as the cap region of fullerene  $C_{60}$ . This is the reason corannulene is sometime referred to as a ‘buckybowl’. The nonplanarity of the structure endows corannulene (and  $C_{60}$ ) with unique electronic properties that are not found in planar aromatic hydrocarbons such as anthracene and pyrene. In contrast to  $C_{60}$ , however, corannulene offers high solubility in common organic solvents and an avenue for multiple and well-defined substitutions on the aromatic nucleus. These two attributes are of high relevance to the synthetic and materials chemists as they allow for synthesis and unambiguous structural characterization of the synthesized materials. In this presentation, we will discuss our synthetic work revolving around this beautiful structural motif of carbon. We will focus on the synthesis of curved nanographenes based on the corannulene motif.

**Keywords:** Corannulene; Curved nanographenes; Fused-ring systems; Polycyclic aromatic hydrocarbons; Non-planar aromatics



### ■ Professional Biography

Mihaiela received her master's degree in Organic Chemistry from the Babes-Bolyai University (Romania). She then moved to Freie Universität Berlin (Germany) and finally to ETH-Zürich (Switzerland) to obtain her doctoral degree. After a one-year postdoctoral stay in the group of Prof. H. K. Hall Jr. at the University of Arizona at Tucson (USA), Mihaiela returned to Zürich as a member of the Prof. J. Siegel's group at the University of Zürich. In 2009, she received the Ambizione fellowship from the Swiss National Science Foundation. Her efforts at the University of Zürich were directed towards creating a research program focused on introducing the corannulene chemistry to the macromolecular science. After finishing her habilitation thesis work in 2014, she joined Nanyang Technological University (Singapore) as a Nanyang Assistant Professor. Since October 2023, she is an associate professor at the School of Chemistry, Chemical Engineering and Biotechnology.

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# Olefin metathesis-sustainable methodology for synthesis of valuable compounds

Anna Kajetanowicz

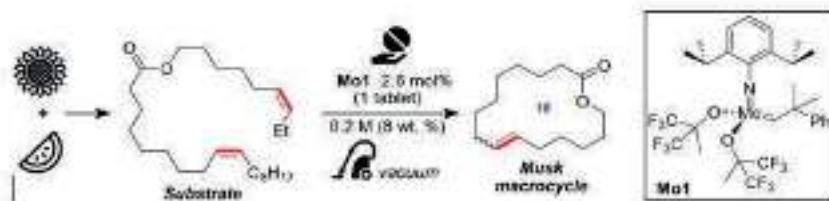
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Ruthenium-catalyzed olefin metathesis is an attractive and powerful transformation for the formation of carbon-carbon double bonds. This methodology is now familiar to most organic chemists as numerous catalysts are available that enable a multitude of olefin metathesis reactions.

Currently, one of the main research directions in this field involves the use of olefin metathesis to convert raw materials of natural origin. They can be transformed, for example, into macrocyclic musk compounds that are valuable raw materials for the flavor and fragrance industry. For many years, macroRCM was carried out at high dilutions to avoid the formation of undesired side products, but recently there has been increasing attention to developed conditions that allow the reaction concentration to be increased to 0.02-0.1 M. The use of reactive distillation, which allows the preparation of musk-scented compounds in the presence of both ruthenium and molybdenum catalysts at a concentration of 0.2 M or higher, makes us prominent participants in this general trend.<sup>1,2</sup> During the presentation, our key findings in this area will be highlighted.

**Keywords:** Olefin metathesis; Ethenolysis; Raw materials; Macrocyclization



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### ■ Professional Biography

Anna Kajetanowicz received a Master degree from Warsaw University of Technology, under the supervision of prof. Andrzej Jończyk, and a PhD degree from the Institute of Organic Chemistry PAS, under the supervision of prof. Mieczysław Mąkosza. She did two postdoctoral fellowships, first in Prof. Karol Grela's group in Warsaw and the second with prof. Thomas R. Ward in Basel. Next, she returned to IChO PAS and in 2015 she moved to the University of Warsaw. Since 2018 she has been deputy director of the Laboratory of Organometallic Synthesis at the Biological and Chemical Research Center. In 2021 she completed her Habilitation and in 2023 she became Professor of University of Warsaw. Her research interests are related to the development of new transition metal complexes, mainly based on ruthenium.

OM

## Macromolecular engineering: Well-defined model pentacrystalline pentablock quintopolymer

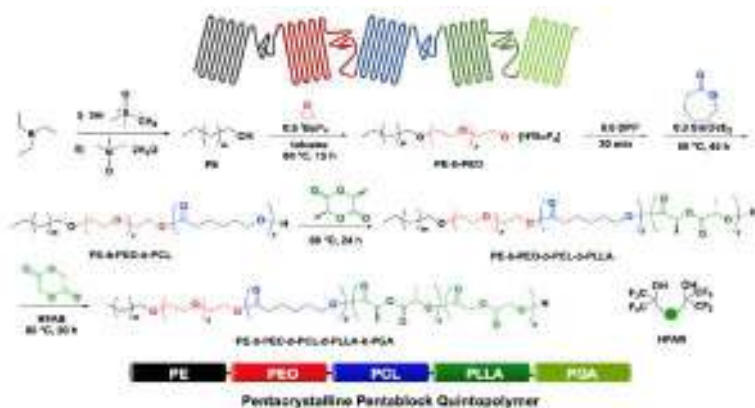
Nikos Hadjichristidis

*Polymer Synthesis Laboratory, Chemistry Program, KAUST Catalysis Center, Physical Sciences and Engineering Division, King Abdullah University of Science and Technology (KAUST)*

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After a short introduction on Macromolecular Engineering and its importance in Polymer Science and Industry, the talk will focus on a novel pentablock quinopolymer with five chemically different crystallites. Multicrystalline multiblock polymers are essential models for advancing polymer physics (crystallization, phase separation, self-assembly) and material science. However, due to the incompatibility of different synthetic methodologies, multicrystalline multiblock polymers with more than three crystallites have rarely been reported. By combining polyhomologation, ring-opening polymerization, and a new “catalyst switch” strategy, we synthesized the first pentacrystalline pentablock quintopolymer, poly(ethylene-b-poly(ethylene oxide)-b-poly( $\epsilon$ -caprolactone)-b-poly(L-lactide)-b-polyglycolide) (PE-b-PEO-b-PCL-b-PLLA-b-PGA). The pentacrystalline pentablock quintopolymer was characterized by 1D/2D liquid-state NMR, 1D/2D solid-state NMR, SEC, FTIR, and TGA. The coexistence of five crystallites was confirmed by DSC, WAXS, variable temperature  $^1\text{H}$ - $^{13}\text{C}$  CP-MAS NMR,  $^1\text{H}$ - $^{13}\text{C}$  INEPT NMR, and  $^1\text{H}$ - $^{13}\text{C}$  CP-MAS WISE NMR spectroscopy. This new synthetic strategy paves the way for the synthesis of well-defined complex multicrystalline macromolecular architectures.

**Keywords:** Crystalline polymers; Multiblock polymers; Ring-opening polymerization; Polyhomologation; Macromolecular engineering



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### ■ Professional Biography

Nikos Hadjichristidis is a Distinguished Professor of Chemistry at KAUST, Saudi Arabia. His research focuses mainly on the synthesis of novel, well-defined model homopolymers and copolymers with complex macromolecular architectures. These polymers are ideal for checking theories understanding/improving the performance of industrial polymers and are potential candidates for high-tech applications. Lately, he started research on vitrimers, and non covalent-based macromolecular architectures. He has published over 600 papers in peer-reviewed journals, has 35 patents, is the editor of four books, and is the author of one book on “Block Copolymers” (*h*-index: 89, citations: 36732). He is a Fellow of the Royal Society of Chemistry and has received several awards, including the Hermann F. Mark Medal, the UK Macro Group Medal, the ACS National Award for Polymer Chemistry, the ACS Chemistry of Thermoplastic Elastomers Award, the ACS Cooperative Research Award and the International Award of the Japanese Society of Polymer Science. (<https://polymer.kaust.edu.sa/>)

PC

## Bacterial cellulose as renewable polymeric platform for biosensing and biomedical applications

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Bacterial cellulose (BC) is a polysaccharide-based biopolymer synthesized extracellularly by bacteria (most effectively *Gluconacetobacter*). Its unique characteristics including high purity, high swelling, good mechanical strength and biocompatibility make it an attractive material for various applications. Reswellable hydrogel fabricated by direct deposition of water soluble carboxymethyl cellulose (CMC) into the BC network was developed into non-invasive colorimetric sensors for sweat pH and glucose. High analytical performance in terms of a wide linear detection range and a low limit of detection with low sample volume requirement was achieved. Gold nanoparticles (AuNPs) embedded in the BC/CMC hydrogel via *in situ* chemical reduction to form BC/CMC/AuNPs composite hydrogel can accommodate selective adsorption and preconcentration of an important thiol-containing biomarker of Alzheimer's disease, glutathione (GSH), prior to direct laser desorption/ionization mass spectrometric (LDI-MS) detection. Effective GSH ionization led to a low limit of detection which is a cut-off level for distinguishing between normal individuals and Alzheimer's patients. Guided tissue regeneration (GTR) membranes were developed by conjugating plant-derived recombinant human osteopontin (p-rhOPN) or calcium-binding domain of p-rhOPN, economically produced and RGD-containing biomolecules on the BC membrane chemically grafted with poly(acrylic acid) brushes or physically deposited with electrospun fibers of mixed CMC/poly(ethylene oxide). Results from immunocytochemistry, *in vitro* mineralization assay and two-stage quantitative real-time polymerase chain reaction strongly indicated that the developed membranes could enhance osteogenic differentiation of human periodontal ligament stem cells, suggesting their potential to be used as active GTR membranes to promote bone tissue regeneration.

**Keywords:** Sensor; Colorimetric; LDI-MS; GTR membrane; Osteopontin



### ■ Professional Biography

Professor Voravee Hoven earned her Ph.D. (1997) in Polymer Science and Engineering from University of Massachusetts, Amherst, USA and was a postdoctoral researcher at Rutgers University, USA (1997-1998). Currently, she is a faculty member and the head of Department of Chemistry, Faculty of Science, Chulalongkorn University, Thailand. She received a few national awards including L'Oreal Thailand "For Woman in Science" Fellowship for "Material Science" Research from L'Oreal Thailand and The Thai National Commission for UNESCO, Wiley-CST Outstanding Publication Award from John Wiley & Sons/the Chemical Society (Thailand), Outstanding Research Award in "Chemical and Pharmaceutical Science" from the National Research Council of Thailand. She has published more than 75 peer reviewed papers on polymer chemistry, polymer-hybrid materials and their biosensing, biomaterial and biomedical applications. Her recent research interest focuses on polymer-hybrid materials for biosensing and biomedical applications, polymeric hydrogel for therapeutic and diagnostic applications, polymeric nanoparticles as nanoreactors for green synthesis and catalysis.

PC

## Functional polymeric nanomaterials for controlled release systems in biomedical and cosmetic applications

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Mantana Opaprakasit<sup>2</sup>, Atitsa Petchsuk<sup>3</sup>, Chariya Kaewsaneha<sup>1</sup>  
Paiboon Sreearunothai<sup>1</sup>, and Abdelhamid Elaissari<sup>4</sup>

<sup>1</sup>School of Integrated Science and Innovation, Sirindhorn International Institute of Technology (SIIT),  
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Controlled release systems are of interest for preventing premature leakages and ensuring precise releases of active compounds at target sites. Various polymeric controlled-release systems have been developed in our laboratory for medical and cosmetic applications. Porous Eudragit micro-/nanoparticles embedded with thermoresponsive poly(N-isopropyl acrylamide) gatekeepers are fabricated. The materials possess high loading efficiency, with thermally triggered gatekeepers. The “on-off” switchable release mechanism enables precise drug release at the body temperature for effective treatments. Drug-encapsulated micro/nanoparticles with hollow structures have been prepared from polylactide (PLA) copolymers. As PLA is degradable and biocompatible, the materials are applied to encapsulate various active compounds, such as amoxicillin, eumelanin, and essential oils. The particle's hollow structure with a large surface area leads to high loading efficiency with tunable release mechanisms and UV scattering properties. The materials show high potential for antimicrobial systems and UV-shielding products in cosmetics. In addition, a process for sizing down commercial PLA resin to lactate oligomers is developed at a lower cost than a bottom-up synthesis from its monomer, employing an alcoholysis reaction by various polyols. The application of multifunctional 2,2-bis(hydroxymethyl) propionic acid (DMPA) generates lactate oligomers with hydroxyl and carboxylic acid terminals, which are subsequently used to synthesize PLA-based polyurethane (PUD) by reacting with appropriate diisocyanates. The resulting PUD is employed in encapsulating various active compounds, especially essential oils, without using any surfactant due to its self-stabilizability from carboxylate groups. The nanoparticles possess a small hydrodynamic size (300-500 nm), high encapsulation efficiency (80-88%), precise release mechanism, and non-toxicity to fibroblast cells. The products have high potential as drug encapsulation templates in biomedical applications.

**Keywords:** Encapsulation; PLA; Controlled release; Nanoparticle; Alcoholysis



**Figure 1** Structures and release mechanisms of PLA-based hollow nanoparticles and porous Eudragit nanoparticles with gatekeepers



### ■ Professional Biography

Pakorn Opaprakasit earned a B.Sc. (Hons.) in Chemistry from Chiang Mai University, Thailand, in 1997. He pursued postgraduate degrees, achieving an M.S. and Ph.D. in Materials Science and Engineering from Pennsylvania State University, USA, in 1999 and 2003, respectively. Presently, he serves as an Associate Professor and head of School of Integrated Science and Innovation at Sirindhorn International Institute of Technology (SIIT), Thammasat University, Thailand. His research interests span across functional materials, materials circularity, degradable polymers, nanomaterials, and materials characterization. He boasts a publication record of over 96 papers, holding an H-Index of 18 (Scopus), and has registered 13 patents. Additionally, he holds the position of Vice President at MRS-Thailand and is a board member of the Polymer Society of Thailand.

PC

## Green synthesis multi-stimuli responsive trimethyl chitosan-based nanogel and its promising application as nanocarrier for cancer photothermal chemotherapy

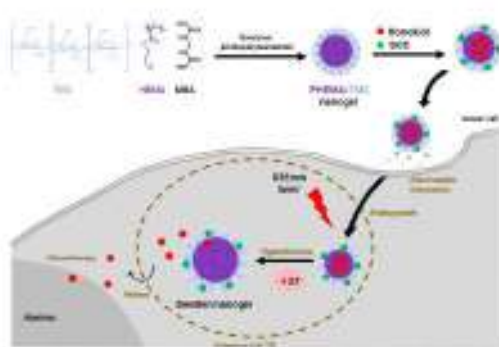
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Multi-stimuli responsive nanocarriers are highly attractive for being used as controlled-release drug delivery system in medical application. Herein, we introduce the green synthesis of multi-stimuli responsive biocompatible nanogel comprising crosslinked poly(2-hydroxyethyl methacrylate) core and trimethyl chitosan (TMC) periphery by a facile visible light-initiated surfactant-free emulsion polymerization. We found that some of polymerization parameters, such as TMC type and crosslinker concentration can affect the nanogel's thermal responsiveness. In addition, the synthesized nanogel exhibited a reversible upper critical solution temperature-type volume phase transition above 30 °C in acidic aqueous environment (pH 4.5-5). Furthermore, the incorporation of sodium copper chlorophyllin as a bio-based photosensitive agent and honokiol model drug to such nanogel not only introduced the hyperthermic effect when under exposure to light, but also activated the release of encapsulated honokiol. This co-loaded nanogel displayed the combined photothermal and chemotherapeutic effect, with the antitumor efficacy against Calu-3 cells. The nanogel synthesized through the green and facile method in this work exhibits pH- and light-dependent UCST-type thermoresponsiveness, which is promising for being used as nanocarrier for cancer photothermal chemotherapy.

**Keywords:** Nanogel; Visible light-induced surfactant-free emulsion polymerization; Trimethyl chitosan; PHEMA; Redox-responsive; Riboflavin





### ■ Professional Biography

Dr. Panya Sunintaboon is currently an Associate Professor in Polymer Science and Technology Program, Department of Chemistry, Faculty of Science, Mahidol University. Also, he has been appointed as the Polymer Society of Thailand Board member, and as Editorial Team for Asian Health, Science and Technology Reports journal. His research interests are in the scope of the following topics:

- Synthesis of amine-functionalized polymeric particles and their applications
- Heterogeneous polymerizations
- Fabrication of functional bio-based polymeric particles



# Synthesis of chiral cyclic oligomers and cyclic molecules based on planar chiral [2.2]paracyclophanes

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[2.2]Paracyclophane is a common cyclophane compound consisting of face-to-face benzene rings fixed by ethylene chains at the para-positions. Two eclipsed benzene rings are closely stacked, causing suppression of their rotatory motion. [2.2]Paracyclophane compounds with one or more substituents are planar chiral compounds depending on the substitution position(s). Enantiopure [2.2]paracyclophane compounds have been employed mainly as chiral ligands and chiral auxiliaries in organometallic and organic chemistry, respectively. However, there are only a few examples of their applications in the fields of polymer and materials chemistry.<sup>1</sup> Recently, we achieved optical resolutions of six kinds of di- and tetrasubstituted [2.2]paracyclophanes by the diastereomer method using appropriate chiral auxiliaries.<sup>2</sup> Subsequently, we synthesized various optically active molecules<sup>3</sup> containing planar chiral [2.2]paracyclophane units. The obtained chiral molecules exhibited excellent circularly polarized luminescence (CPL) properties.

We introduce syntheses of optically active cyclic oligomers<sup>4</sup> and molecules<sup>5</sup> based on the planar chiral [2.2]paracyclophanes as chiral building blocks. Their synthetic procedures and chiroptical properties, in particular good CPL profiles, are disclosed.

**Keywords:** Circularly polarized luminescence (CPL); Cyclic molecule; Cyclic oligomer; [2.2]Paracyclophane; Planar chirality

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3. For recent examples: (a) *Chem. Asian J.* **2022**, 17, e202200418. (b) *Bull. Chem. Soc. Jpn.* **2022**, 95, 1353-1359e. (c) *Science* **2022**, 377, 673-678.
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### ■ Professional Biography

Yasuhiro Morisaki is Professor at Kwansei Gakuin University. He graduated from Kyoto University in 1995, and then, he received Ph.D. from Kyoto University in 2000. After a six-month postdoctoral stay at Osaka National Research Institute, he joined the group of Professor Yoshiki Chujo as Assistant Professor at Kyoto University in 2000. From 2004 to 2005, he carried out postdoctoral work at the University of Alberta. He became lecturer at Kyoto University in 2008 and full Professor at Kwansei Gakuin University in 2015. His research interests focus on polymer and organic synthesis, in particular, cyclophane chemistry.

## Importance of noncovalent interactions in homogeneous and enzymatic catalysis

Seiji Mori

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Noncovalent interactions were very important in chemistry and biology. In my talk, I am going to emphasize the importance of noncovalent interactions in our recent research on the following topics.

(1) Oxovanadium-catalyzed asymmetric 1,2-oxytrifluoromethylation of olefins with chiral ligands, which enantioselectivities depend on C3-substituents of the ligands.<sup>1</sup>

(2) Direct hydride reduction of 5 $\alpha$ -dihydrotestosterone (5 $\alpha$ -DHT) Catalyzed by 3 $\alpha$ -Hydroxysteroid dehydrogenase (3 $\alpha$ -HSD) and by nicotinamide adenine dinucleotide phosphate (NADPH). We highlighted Tyr216 in human 3 $\alpha$ -HSD assisted the reaction by  $\pi/\pi$  interactions with the neighboring nicotinamide ring of NADP(H).<sup>2</sup>

(3) Systematic computational studies on a blue copper protein, pseudoazurin (PAz) and its Met16X (X = Phe, Leu, Val, Ile) variants.<sup>3</sup>

**Keywords:** Noncovalent interaction; DFT calculations; Reaction mechanisms; Catalysis; Enzyme

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### ■ Professional Biography

Prof. Seiji Mori was born in Tokyo, Japan, and obtained his PhD (chemistry) in 1998 under the guidance of Prof. Eiichi Nakamura from the University of Tokyo.

He was a postdoctoral fellow at Emory University, Atlanta, USA in 1998-2000 with Prof. Keiji Morokuma, and moved to Kyoto University as a JSPS postdoctoral fellow with Prof. Shigeki Kato. He became an assistant professor (2000-2001), an associate professor (2001-2012), and was promoted to a full professor in 2012 at Ibaraki University. He was an assistant vice president for international strategy at the same university from 2015-2017 and was charged with many MOUs, especially in ASEAN and the US universities. He has served as director of the Institute of Quantum Beam Science at Ibaraki University since 2022. His research interests include theoretical studies on homogeneous and enzymatic catalysis and functional organic molecules.

PT

## Theoretical study on the role of dynamics during enzyme catalysis

Toshifumi Mori

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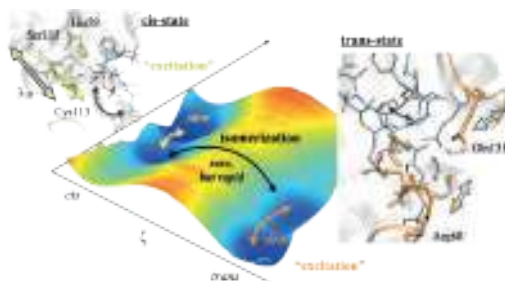
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Proteins constantly fluctuate in solution and often populate a variety of different states. The structural fluctuations and conformational transitions of proteins have been realized to be essential for function by recent experiments such as single-molecule FRET. However, since these dynamic personalities are not detectable in the ensemble-averaged measurements, and also occur a wide range of timescales, the understanding of how dynamics play a role in function, e.g., enzyme catalysis, remains highly controversial. Theoretical studies on enzyme catalysis, on the other hand, have mostly focused on free energy profiles and transition states along the minimum free energy paths where the enzyme dynamics are averaged-out and omitted.

In this talk, I will discuss how the gap between the ensemble-averaged and dynamic pictures of enzyme catalysis can be bridged using theoretical approaches. As an example, the mechanism of the catalytic cis-trans isomerization reaction of the peptidyl-prolyl bond catalyzed by Pin1 peptidyl-prolyl isomerase is examined. By comparing the reaction mechanisms from the static and dynamic perspectives, obtained by free energy calculations and transition path sampling, respectively, the conformational excited state of Pin1 is shown to play an essential role to promote the catalytic reaction events. I will also show how the optimal reaction coordinates for describing these reaction paths can be determined based on the dynamics information and machine learning approaches.

**Keywords:** Enzyme catalysis; Dynamics; Free energy; Simulation; Excited state





### ■ Professional Biography

Toshifumi Mori is an Associate Professor at the Institute for Materials Chemistry and Engineering in Kyushu University. He obtained his Ph.D. degree from Kyoto University in 2010 under the supervision of Prof. Shigeki Kato, and did his postdoc research in Stanford University with Prof. Todd Martínez and in University of Wisconsin Madison with Prof. Qiang Cui. In 2013, he joined the Institute for Molecular Science as an Assistant Professor, and in 2020 moved to the current affiliation. His research interest is in understanding the heterogeneous dynamics of biomolecules underlying conformational transitions and functional processes. He is currently focusing on chemical reactions and enzyme functions under complex environments, and develops molecular simulation and theoretical chemistry approaches to reveal the mechanisms in molecular detail.

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## Exploring human serum albumin modifications: Advancing screening and monitoring for non-communicable diseases

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Human Serum Albumin (HSA) is a pivotal protein prevalent in blood circulation, instrumental in transporting hormones, fatty acids, and drugs throughout the human body and maintaining oncotic pressure. Under conditions marked by elevated blood sugar levels, non-enzymatic linkage occurs between sugar molecules and HSA, forming Glycated Human Serum Albumin (GHSA). Consequently, GHSA levels serve as potential biomarkers for screening and monitoring Diabetes Mellitus and its associated complications. Since HSA is synthesized in the liver and undergoes filtration in the kidneys before entering the urinary system, its presence in urine samples can also signify kidney functionality. Therefore, measuring HSA in urine samples is a viable approach to monitor kidney functions.

Our research group has extensively studied the physical and biochemical properties of both HSA and GHSA. We have developed nanosensor devices capable of detecting HSA and GHSA in serum and urine samples, facilitating the screening and monitoring of Diabetes Mellitus and Chronic Kidney Disease. Our innovative devices, certified under ISO13485, have been implemented in various regions across Thailand, aiding in the early detection and management of these prevalent conditions.

**Keywords:** Human serum albumin; Diabetes mellitus; Non-communicable disease; Chronic kidney disease



### ■ Professional Biography

Dr. Deanpen Japrun currently serves as the Principal Researcher and Research Group Director of the Responsive Material and Nanosensor Research Group at the National Nanotechnology Center, National Science and Technology Development Agency in Thailand. Dr. Japrun holds a D.Phil. in Chemical Biology from the University of Oxford and has garnered an impressive array of academic qualifications, including an M.Sc. in Biochemistry from Mahidol University and a B.Sc. in Medical Technology with honors from Chulalongkorn University. An accomplished scientist, Dr. Japrun has an impressive portfolio of 47 published papers and holds 42 intellectual properties. Her research is primarily focused on the development of diagnostic tools, drug development processes, and pioneering advancements in nanopore technology and biosensor platforms. Dr. Japrun's significant contributions to the scientific community are recognized globally, which has led to her being a sought-after speaker at numerous esteemed conferences, including those organized by IEEE and the Gordon Research Conference.

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## Modeling the defective structure of MoS<sub>2</sub>: A first-principles kinetic Monte Carlo study

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Defect and vacancy sites play an essential role in the many catalytic processes. The literature has, for instance, discussed that the S-vacancies on MoS<sub>2</sub> can enhance its catalytic activity for hydrogen evolution and CO<sub>2</sub> conversion. Other studies have shown that the size and shape of the S-vacancies influence their electronic structures. Thus, it is reasonable to assume that the pattern and structures formed by the vacancies also affect the performance of a MoS<sub>2</sub> catalyst. In the present study, we have used density functional theory (DFT) calculations to explore the diffusion of the S-vacancy sites on a MoS<sub>2</sub> monolayer and investigate whether and how the direct environment affects the diffusion barrier of an S-vacancy site. These data are used as input for a kinetic Monte Carlo (kMC) model, which we use to study the behavior of these vacancy sites, e.g., what kind of surface pattern these vacancies form. The kMC results indicate that vacancies are highly dynamic and tend to form patterns consisting of alternating S-atoms and S-vacancy sites. The kMC model delivers a better understanding of the reshaping of the MoS<sub>2</sub> catalyst surface, which is a potential mechanism that may contribute to catalyst aging (and eventually deactivation).

**Keywords:** MoS<sub>2</sub>; Defect; Diffusion; Kinetic Monte Carlo



### ■ Professional Biography

Cheng-chau Chiu studied chemistry at the Technische Universität München in Germany, from which he obtained his BSc, MSc and PhD in 2008, 2010, and 2015, respectively. After graduation, he worked as a postdoc at the Institute of Atomic and Molecular Sciences, Academia Sinica, Taiwan. In 2020, he joined the Department of Chemistry of the National Sun Yat-sen University in Taiwan as an Assistant Professor. Prof Chiu started his scientific carrier with computational simulations on surface processes, with a focus on mechanistic details of chemical reactions in the context of heterogeneous catalysis. Recently he has been combing quantum chemical calculations with kinetic models to investigate various surface processes, e.g., how catalytic surfaces vary over time.

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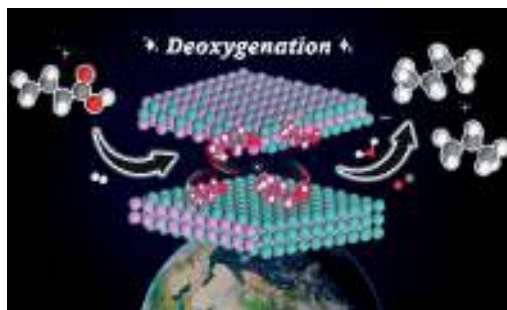
## A net zero climate-resilient future: A computational chemistry approach for energy solutions

Siriporn Jungsuttiwong

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Nowadays, theoretical study has helped to develop the nanotechnology industry, discovering effective and efficient catalysts is a crucial role in the industrial production of materials and environmental protection, chemical engineers, plant managers etc. This research focuses on a theoretical study on quantum chemistry of materials for energy applications and air treatment by using density functional theory. The results of this research project can be used for screening, type of catalyst/adsorbent and provide develop a real laboratory level to assist in the design, development of high-performance catalyst/absorbent materials for the removal of pollutants from the environment including smart and sustainable energy storage applications.



**Keywords:** Climate change; Energy materials; Catalyst; DFT



### ■ Professional Biography

Prof. Siriporn Jungsuttiwong received her B.S. degree in Chemistry from Khon Kaen University in 1994 and PhD degree in Chemistry in 2005 from Kasetsart University. She then became a lecturer in the Department of Chemistry, Ubon Ratchathani University in 2005. She was promoted to professor in 2018. Research interests focus on computational chemistry of development of new organic molecules for display and lighting technologies (OLEDs), transistors, power conversion, new catalysts/adsorbents for air treatment and hydrogen storage reactions including catalysts for energy materials as well as conversion of CO<sub>2</sub> to value-added product.

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# CST AWARDEE ABSTRACTS

## From liquid to gas to unconventional detections

Duangjai Nacapricha<sup>1,2\*</sup>, Prapin Wilairat<sup>1,2</sup>, Kanchana Uraisin<sup>1,2</sup>,  
Phoonthawee Saetear<sup>1,2</sup>, Nattapong Chantipmancee<sup>1,2</sup>, Nanthatchaphon Jantawong<sup>1,2</sup>,  
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Nuttamon Khoonrueng<sup>1,2</sup>, Takdanai Techarang<sup>1,2</sup>, Supakorn Kittikomoldej<sup>1,2</sup>,  
Vanlada Suksomphot<sup>1,2</sup>, Jirayu Sitanurak<sup>1,2</sup>, Nidup Wand<sup>1,2</sup>, Patiya Pasakon<sup>1,2</sup>,  
Nuanlaor Ratanawimarnwong<sup>1,3</sup>, Thitirat Mantim<sup>1,3</sup>, Nathawut Choengchan<sup>1,4</sup>,  
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This abstract invites you on a captivating journey through our research endeavors spanning over the past decades. Directly analyzing samples often poses a substantial hurdle in overcoming interferences. To address this, our focus lies on the *in-situ* transformation of analytes from liquid to gas, effectively separating them from interfering species. The gas is subsequently confined within a thin liquid layer, enabling successive in-situ detection using a suitable detector. Notably, our exploration extends to the unconventional utilization of various electrical detectors, including the capacitively coupled contactless conductivity detector and voltammetric sensors. Our journey is not a solitary endeavor but a collective symphony, shaped by the invaluable contributions of students, colleagues, and collaborators. Together, we have nurtured an environment where ideas flow freely, and knowledge is generously shared.

**Keywords:** Gas separation; In-situ; Contactless conductivity; Voltammetry



### ■ Professional Biography

Dr. Duangjai Nacapricha is an Associate Professor in the Department of Chemistry at the Faculty of Science, Mahidol University, Bangkok, Thailand. She earned her Bachelor's degree in Chemistry from Prince of Songkla University, followed by a Master's degree in Analytical Chemistry from Chiang Mai University. Dr. Nacapricha completed her Ph.D. at Liverpool John Moores University, UK, in 1993. After obtaining her Ph.D., she worked at the Thailand Institute of Scientific and Technological Research for one year before joining the Department of Chemistry at Mahidol University in 1995.

Her research focuses on analysis using flow-injection techniques, microfluidic paper-based analytical devices, and electrical sensors.

Dr. Nacapricha has authored and co-authored 132 international publications, and her current Scopus *h*-index is 28.

CST

## Multi-responsive chromism and luminescence in heteroatom-functionalized complexes

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CST

Complexes exhibiting multi-stimuli optical responses and luminescent sensing properties are the main topic of this presentation. The following complexes with various heteroatomic ligands were synthesized and structurally characterized: (1) a soft crystalline Ni(II) coordination polymer based on 5-(3-pyridyl)-1,3,4-oxadiazole-2-thiol (Hpzt), exhibiting mechanochromism, vapochromism, and thermochromism;<sup>1</sup> (2) a luminescent Cd(II) complex with 4-aminosalicylate (AS), which displays a luminescent sensing of NH<sub>3</sub> vapors through large blue-shifted emission spectra and undergoes structural transformation in different I<sub>2</sub> media;<sup>2,3</sup> (3) Cu(I) coordination polymers based on 2-amino-5-(4-pyridinyl)-1,3,4-thiadiazole (pyt-NH<sub>2</sub>) show a variety of luminescent colors and selective vapochromism and vapoluminescence when exposed to formaldehyde vapor.<sup>4</sup>

**Keywords:** Cu(I); Ni(II); Luminescent sensors; Multi-responsive chromism

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### ■ Professional Biography

Jaursup Boonmak is an associate professor in the Department of Chemistry, Faculty of Science, Khon Kaen University. His research interests include the synthesis and X-ray structure-function relationships of coordination polymers and supramolecular metal complexes for applications in magnetism, luminescence, and optical sensors. His honors include the Young Scientist Award from Thailand's Foundation for the Promotion of Science and Technology in 2018 and the Merck-CST Distinguished Dissertation Award 2011 from the Chemical Society of Thailand.

CST

## Pioneering sustainable futures: From enzyme-driven biocatalysis to revolutionary waste management in Thailand

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As global energy demands rise, our team concentrates on bioenergy and biorefinery. We leverage bioenergy's potential, dedicated to developing sustainable H<sub>2</sub> and CH<sub>4</sub> sources using advanced bio-methodologies. Our approaches include enzyme modification for cleaner chemical production, enhancing microorganisms for increased H<sub>2</sub> production, and advancing circular economy principles through efficient anaerobic digestion. A key achievement is converting Thai food and agricultural waste into valuable CH<sub>4</sub> sources, benefiting both the economy and environment. Our work in biocatalysis and green energy solutions is groundbreaking. We've enhanced the thermostability and efficacy of various enzymes and identified *Enterococcus faecalis* VT-H1 as crucial for H<sub>2</sub> production, highlighting the importance of microbial communities in CH<sub>4</sub> generation. Our SUZDEE digestion system, specifically designed for Thai food waste, operates in 29 stations across Thailand, turning waste into biogas and offering benefits like reduced heating costs and support for organic farming. This approach aligns with the UN's Sustainable Development Goals (SDGs). We aim to install 70 SUZDEE systems nationwide by 2026, reflecting our commitment to societal progress and environmental stewardship. Our vision is a future where bioenergy solutions and sustainability are intertwined, making a significant impact in Thai industries and society.

**Keywords:** Bioenergy; Biorefinery; Circular economy; Anaerobic digestion; Biocatalysis



### ■ Professional Biography

Dr. Thanyaporn Wongnate, serving as an Assistant Professor at the School of Biomolecular Science and Engineering, Vidyasirimedhi Institute of Science and Technology (Vistec), is a leading figure in green chemistry in Thailand. Her focus lies in bioenergy and biorefinery, with a particular emphasis on sustainable  $H_2$  and  $CH_4$  production. Dr. Wongnate's work transcends conventional energy paradigms, aiming to convert biomass into a variety of valuable bioproducts. Her initiatives include pioneering enzyme engineering for eco-friendly chemicals, boosting green  $H_2$  production through microorganism research, and promoting a circular economy via innovative anaerobic digestion techniques. Her efforts have led to significant advancements in transformative waste management strategies in Thailand, positively impacting both the economy and environment.

CST



## Origin classification of Thai agricultural products using chemical tools: Towards sustainable use of geographical indication

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### CST

Geographical indication (GI) has gained increasing interest as an effective tool in securing and sustaining the value of local products. In Thailand, over 200 GI products have been registered, with foods and agricultural products being the majority. Interestingly, in the registration process, only descriptive characteristics of the product are required, leading to possible conflicts and frauds for similarly described products. Hence, declaring more quantitative properties can help alleviate this issue, a task of which analytical instruments can play a vital role. In this presentation, the combination of chemical data acquisition by modern analytical instruments with chemometric analysis is demonstrated for the classifications of Thai agricultural products such as coffees, peppers, and durians. High performance liquid chromatography, gas chromatography, and various types of mass spectrometry were used to deliver chemical profiles such as volatile species, fatty acids, and carotenoids. These data are directly amenable to multivariate analysis, which in turn resulted in unambiguous differentiation of products from different origins. Importantly, the success of these studies can pave the way for similar studies in other economically important products. Also, they very well highlight the utility of advanced instruments in solving broad-impact problems.

**Keywords:** Geographical indication; Chemometrics; Mass spectrometry; Chromatography; Agricultural products



### ■ Professional Biography

Assoc. Prof. Dr. Thanit Praneenararat obtained his Ph. D. in chemistry from University of Wisconsin-Madison, USA under the Anandamahidol Foundation Scholarship. Since 2012, he served as a faculty member of the Department of Chemistry, Faculty of Science, Chulalongkorn University. Originally trained as a chemical biologist, Dr. Thanit embraces the interdisciplinary mindset, and has directed his research group towards the works involving the use of chemical tools and knowledge to solve problems across the fields of biology and food chemistry. More specifically, his recent research interests involve the applications of chromatography and mass spectrometry in the detection of food contaminants and geographical classifications. Also, his passion for adopting chemistry in an easy-to-understand manner also inspired him to follow a similar route in chemical education, leading to his winning of the 2022 Outstanding Science Teacher Award from the Science Society of Thailand Under the Patronage of His Majesty the King.

CST

## Highly enantioselective synthesis of chiral molecules at modified mesoporous metal electrodes

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Strategies for preferentially obtaining one enantiomer are critical for chiral technologies. This can be accomplished, among others, by employing alternatively enantioselective electrosynthesis. However, the long reaction time and the short lifetime of the electrodes used as electrocatalysts limit their practical use for the moment. Therefore, novel strategies to enhance the catalytic performances of these electrodes have been developed. For example, functionalizing the external surface of chiral mesoporous metal electrodes with organosulfur ligands can significantly decrease the degree of undesirable reactions, resulting in a high enantiomeric excess of 90% while reducing the reaction time from a week to a day.<sup>1</sup> Moreover, the design of chiral-encoded mesoporous metal Pt-Ir alloys was investigated, and these materials were subsequently applied as electrodes for asymmetric electrosynthesis. In this case, an enantioselectivity of almost 100% could be achieved, combined with outstanding electrochemical stability, even after several successive catalytic cycles.<sup>2</sup> This exceptional stability and activity of the developed surface layers also allowed their use for other applications, such as heterogeneous asymmetric hydrogenation and enantiomeric discrimination, by employing both traditional chemical processes and electrochemiluminescence (ECL).<sup>3,4</sup>

**Keywords:** Chiral imprinting; Mesoporous metals; Enantioselective synthesis; Electrosynthesis; Electroanalysis

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### ■ Professional Biography

Sopon Butcha is currently a lecturer at the Department of Chemistry, Faculty of Science and Technology, Thammasat University. He earned his Bachelor of Science in Chemistry with first-class honors at Suranaree University of Technology (SUT) in 2017, and his double degree program of Doctor of Philosophy in Materials Science and Engineering at Vidyasirimedhi Institute of Science and Technology (VISTEC) and Doctor of Philosophy in Physical Chemistry at University of Bordeaux, France in 2022, working with Assoc. Prof. Chularat Wattanakit and Prof. Alexander Kuhn. During his studies, he received full scholarships from the Development and Promotion of Science and Technology Talents Project (DPST), PTT Group, the Franco-Thai Scholarship Program, and the National Research Council of Thailand (NRCT). In his thesis work, he pioneered the novel designs of chiral-encoded mesoporous monometallic and alloyed metals for highly asymmetric electrosynthesis. His works have already resulted in several excellent publications, e.g., Nature Communications, Chemical Science, Chemical Communications, and Chemistry-An Asian Journal.

CST

## Tuning surface energy to enhance MoS<sub>2</sub> nanosheet production via liquid-phase exfoliation: Understanding the electrochemical adsorption of cesium chloride

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CST

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Environmental pollution caused by radionuclides like Cs-137 and Cs-134 has increased global attention toward public health. Electrochemical adsorption has emerged as a feasible, rapid, and scalable method to treat contaminated water sources. However, graphene and its derivatives have limitations in ion adsorption via physisorption, forming a double layer that restricts the electrode's adsorption capacity. To address this, we propose the use of molybdenum disulfide (MoS<sub>2</sub>) with its extensive intercalation galleries for cesium removal via an electrochemical route. Liquid-phase exfoliation with water and N-methyl-2-pyrrolidone (NMP) was then used to produce MoS<sub>2</sub> nanosheets in a scalable quantity (high-yield production). The formation of a mixed solvent possessing relatively equivalent surface energy for exfoliation enabled us to achieve a remarkable exfoliation yield of up to ca. 1.26 mg mL<sup>-1</sup>, which is one of the highest yields reported to date (without a surfactant being added) and to the best of our knowledge. The 35% v/v of water in NMP displayed a maximum yield while maintaining the structure of the as-exfoliated one. Water exceeding over 66.7% v/v led to the formation of MoO<sub>3</sub>. Moreover, an insight into the cesium ion removal mechanism through the electrochemical route was demonstrated. It is found that the Cs<sup>+</sup> removal follows electrochemical intercalation rather than adsorption. This work aids the understanding of cesium intercalation coupled with a mass-scale production method, which should lead to more efficient and cost-effective removal of radionuclides from contaminated water sources, opening new research avenues in materials and environmental science.

**Keywords:** MoS<sub>2</sub>; Liquid phase exfoliation; High-yield; Intercalation; Cesium removal





### ■ Professional Biography

I am currently pursuing a Master's degree in Engineering and Technology at the Sirindhorn International Institute of Technology (SIIT), Thammasat University. As a teaching assistant, I facilitated Chemistry Laboratory sessions at SIIT. Recently, I achieved First Place in the Best Presentation Award at the 1st Sustainable and Green Electrochemical Science and Technology (SGEST) Symposium held at VISTEC in 2023. My presentation, titled "Tuning Surface Energy for Enhanced MoS<sub>2</sub> Nanosheet Production via Liquid-Phase Exfoliation," focuses on optimizing MoS<sub>2</sub> production using water and NMP as solvents. This process fine-tunes surface tension, resulting in a high exfoliation yield. The research also explores electrochemical applications of MoS<sub>2</sub>, particularly in Cs<sup>+</sup> removal from wastewater. The study reveals that Cs<sup>+</sup> removal follows electrochemical intercalation rather than adsorption.

CST

## Sustainable supramolecular chemistry at the interface of environmental and materials science

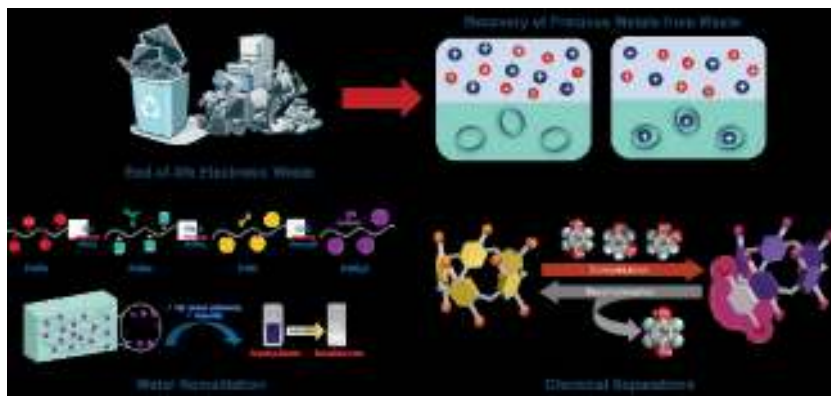
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In 2015, the United Nations General Assembly established the 2030 agenda for sustainable development. A key element of this plan was the encouragement of economic growth in concert with sustainable consumption of environmental resources and importantly chemical research can help accelerating achievement on the sustainable development goals. By learning from molecular recognition processes in nature, our lab has employed various forms of intermolecular non-covalent interactions through unusual supramolecular hosts that have been designed to self-assemble into complex nanostructures for tailored applications, especially in sustainable development. Herein, we will showcase our recent research focusing on applications of supramolecular chemistry and materials to address current global issues including the sustainable management of water and sanitation, the global energy consumption, and the preservation of resources to support transition from fossil fuels to clean and alternative energy.



**Keywords:** SDGs; Supramolecular chemistry; Sustainable resources; Water



### ■ Professional Biography

Assoc. Prof. Dr. Thanthapatra Bunchuay obtained a BSc (Hons) degree from Mahidol University where he did a senior project with Prof. Chutima Kuhakarn on iodine chemistry. After that, he carried on MSc degree in the field of MOFs materials under supervision of Assoc. Prof. Jonggol Tantirungrotechai. In 2014, he joined the group of Prof. Paul Beer at the University of Oxford, where he employed sigma-hole interactions incorporating into mechanically interlocked molecules for anion recognition in aqueous media. In 2019, he has established “The SupraValentine Research Lab” at Mahidol University. The prime research focus is the synthesis of novel macrocyclic molecules to study their unusual host-guest behaviour via advanced spectroscopic techniques. In addition, our synthetic macrocycles are used as the basis of functional materials for applications in sensing, extraction and recovery, delivery, and soft materials.

CST



# BILATERAL SYMPOSIUM BETWEEN THAILAND AND JAPAN ABSTRACTS

## Chiroptical properties of helical conjugated polymers synthesized in chiral liquid crystals

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BSTJ

We present a variety of  $\pi$ -conjugated polymers bearing helical structures and chiroptical properties. Helical polyacetylene, poly(ethylenedioxythiophene), helical aromatic copolymers, and helical network polymers are synthesized in chiral liquid crystals used as asymmetric reaction fields.<sup>1</sup> Helical carbon and graphite films with spiral morphologies are prepared through carbonizations of doped helical conjugated polymers.<sup>2</sup> Helically  $\pi$ -stacked assemblies between cationic conjugated polymers and anionic chiral compounds provide spherulites exhibiting circularly polarized luminescence.<sup>3</sup> Switching and amplification of circularly polarized luminescence of chiral conjugated polymers are achieved using selective reflection and transmission of chiral nematic liquid crystals.<sup>4</sup>

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**Keywords:** Conjugated polymers; Liquid crystal; Helicity; Chiroptical properties; Chiral luminescence



## ■ Professional Biography

Dr. Kazuo Akagi is an Eminent Research Professor, Research Organization of Science and Technology, Ritsumeikan University, and a Professor Emeritus of Kyoto University and University of Tsukuba, Japan.

He graduated from the Department of Hydrocarbon Chemistry at Kyoto University and obtained a Doctoral degree. He became a Research Associate at Fukui University, and an Assistant Professor, an Associate Professor, a Professor in the Institute of Materials Science at University of Tsukuba. He was a Director of Tsukuba Research Center of Interdisciplinary Materials Science. He moved to the Department of Polymer Chemistry at Kyoto University and became a Director of Fukui Institute for Fundamental Chemistry.

His research interests have involved electrically conducting polymers and liquid crystalline, luminescent, and photoresponsive conjugated polymers, with works focused on the synthesis of helical conjugated polymers in chiral liquid crystal field.

BSTJ

## Excited-state intramolecular proton transfer (ESIPT) molecules for optoelectronic materials, fluorescent sensors, and imaging agents

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Chromophores possessing excited-state intramolecular proton transfer (ESIPT) are of great importance in the past decades because of their desirable unique photophysical properties which can be used in various applications ranging from optoelectronic devices such as light emitting diodes and laser dyes, molecular switching to fluorescent probes both in chemical and biological systems. Therefore, the development of new chromophores based on the ESIPT process have been intensively developed using combined experimental approach and theoretical study. The identification of how structural modifications controlling their optical properties driven by ESIPT process and solvent media affecting their fluorescent emission are of great importance. Thus, our group is interested in studying several aspects in terms of electronic properties and ESIPT process through the computational chemistry as an effective tool. Moreover, the systemic study and molecular screening using certain criteria will be carried out to provide the best candidates for applications in fluorescent probes and light emitting diodes. The identification of the fundamental of conformational aspects of important ESIPT molecules in non-polar and polar solvents. These aspects include: (1) the molecular and electronic structures of the dyes, especially the multiple emission character from single proton transfer or double proton transfer; (2) the spectral tuning and (3) the sensitivity of ESIPT process to the environmental factors (solvent effect). The results obtained are useful for experimentalists in molecular designing high fluorescence efficiency and long lifetime of ESIPT molecules towards organic optoelectronic materials, fluorescent sensors, and imaging agents. Finally, the selected of designed compounds that pass the important criteria are recommended to synthesize and test for application uses in fluorescent probes and solid-state emitters based on ESIPT process.

**Keywords:** ESIPT; TD-DFT; Fluorescent; Optoelectronic



### ■ Professional Biography

Dr. Nawee Kungwan got his B.S. degree in Chemistry from Khon Kaen University in 2000 and PhD degree in Chemistry under the direction of Prof. Thanh N. Truong in 2007 from the University of Utah, USA. He then became a lecturer in the Department of Chemistry, Chiang Mai University in 2007 and did a postdoc research in 2009 at University of Vienna, Austria. He was promoted to assistant professor and associate professor in 2014 and 2019, respectively. His research interests focus on computational chemistry of light emitting materials, catalyst in ring-opening polymerization, catalytic materials for upgrading bio-oils, excited-state proton transfer and molecular design for fluorescent probes.

BSTJ

## Generation of circularly polarized electroluminescence from organic light-emitting diodes with optically inactive phosphorescent emitters under an external magnetic field

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Circularly polarized luminescence (CPL) is emission from a chemical substance oscillating in a left- or right-handed spiral manner. CPL is attracting much attention because it is expected to be applied to 3D displays, security technologies, and sensory systems. In this context, organic light-emitting diodes (OLED) affording circularly polarized electroluminescence (CPEL) should be reliable devices as the light sources, and chiral luminophores are required as CPL-active emitting materials. Development of such materials, however, require lots of costs and takes considerable time, through optical resolution and asymmetric synthesis. Here the author demonstrates generation of CPEL from OLEDs containing racemic or achiral phosphorescent organometallic complexes.

Racemic bis- and tris-cyclometalated iridium(III) complexes (*i.e.*, a mixture of  $\Delta$ - and  $\Lambda$ -optical isomers) and an achiral heteroleptic cyclometalated platinum(II) complex were employed as phosphorescent emitters. The OLED was placed between N- and S-poles of a permanent magnet, where the direction of the out-coupled electroluminescence is parallel and antiparallel to the longitudinal magnetic field, namely, N-up and S-up Faraday configurations, respectively. For OLEDs with the iridium(III) complexes, a pair of mirror-image CPEL spectra was obtained upon switching the Faraday configuration (N-up  $\leftrightarrow$  S-up), and the sign of CPEL depended on the coordination geometry around Ir(III) and the Faraday configuration. In the case of the Pt(II)-based OLED, a pair of mirror-image CPEL spectra was also obtained, and the spectral sign was completely regulated by the Faraday configuration. When the doping level of the platinum(II) complex was varied, the ratio of monomer and excimer emissions was varied, affording multi-color CPEL.

**Keywords:** Circularly polarized luminescence; Electroluminescence; Phosphorescence; Organic light-emitting diode; Organometallic complex



### ■ Professional Biography

Shigeyuki Yagi received his Master from Osaka Prefecture University (OPU) in 1993. After studying at Kyoto University (KU), he was appointed as an assistant professor at OPU in 1995. He received his Ph.D. from KU in 1999 under supervision of Prof. Susumu Kitagawa. He was promoted to an associate professor at OPU in 2003. In 2003–2004, he joined Prof. Timothy M. Swager's group at Massachusetts Institute of Technology, USA as a visiting scientist. He was promoted to a full professor at OPU in 2016. Since 2022, he has been a full professor at Osaka Metropolitan University, which has been established through reorganization of OPU and Osaka City University. His research interest lies in functional dyes for organic electronics, especially taken to emitting materials for organic light-emitting diodes.

BSIJ

## Sunlight-responsive photocatalysts for detoxification of organic dyes and antibiotics in natural water

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BSTJ

Low electron-hole separation efficiency is the main drawback influencing low photoactivity of the prepared photocatalyst. To solve this problem, either decoration of metals on the surface of semiconducting photocatalysts or creation of heterojunction can be regarded as the promising strategies to improve the photocatalytic activity of the final products. Firstly, the solvothermally grown BiOCl photocatalysts decorated with low silver content were prepared. The 2.5 wt% Ag/BiOCl showed complete photocatalytic degradation of Rhodamin B (RhB) dye and ofloxacin (OFL) antibiotic under sunlight. The improvement of the resultant photoactivity is mainly due to lowering of charge carrier recombination rate at the interface together with the generation of the Schottky barrier at the Ag/BiOCl interface so that an increase in quantum efficiency and enhancement of the photoactivity are expected. Besides, decoration of silver on BiOCl also leads to red shift in the absorption of light toward visible regime, attributed to the local surface plasmon resonance (LSPR) effect of Ag on BiOCl surface. The prepared Ag/BiOCl photocatalyst shows promising photoactivity with good structural stability after five cycles of use implying its excellent cycling ability. The present finding offers a new pathway to create a silver decorated BiOCl for complete removal of harmful dye and antibiotic in aqueous solution. Secondly, the degradation of the pollutants by ZnS/ZnO photocatalyst will also be presented. The photodegradation of the pollutants followed pseudo-first order kinetics. Charge transfer at the ZnO/ZnS heterojunction belongs to the Z-scheme type. The strategy based on interfacial engineering of heterojunctions for environmental protection will be discussed.

**Keywords:** Sunlight-active photocatalyst; Organic dyes; Antibiotics; Photodegradation; Environmental protection



### ■ Professional Biography

Dr. Suwat Nanan got his B.S. degree in Chemistry from Khon Kaen University in 2001 and MSc degree in Physical Chemistry from Mahidol University in 2003. He then became a lecturer in the Department of Chemistry, Khon Kaen University in 2004. He finished his PhD in Chemistry (Conducting Liquid crystals) from University of Leeds, UK in 2009. He was promoted to assistant professor and associate professor in 2015 and 2020, respectively. His research interests focus on the development and fabrication of semiconducting photocatalysts for environmental protection including the creation of visible-light-driven photocatalysts for removal of organic pollutants such as organic dyes, antibiotics, and insecticides in wastewater.

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## Visualization of electronic and magnetic transition moments aiming at the design of CPL chromophore having enhanced chiroptical properties

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The science of circularly polarized luminescence (CPL) and the technology using CPL and related phenomena have been attracting the attention of researchers worldwide. One of the most important physical constants attributable to the CPL chromophore is  $g_{\text{lum}}$  (equation 1) where  $I_L$  and  $I_R$  are the intensity of left and right circularly polarized CPL, respectively. It is clear from this equation that  $g_{\text{lum}}$  expresses *the purity of CPL*.  $g_{\text{lum}}$  is further defined using physical constants assigned to a chromophore, *i.e.*, the electronic transition moment  $\mu$ , the magnetic transition moment  $m$ , and the angle between  $\mu$  and  $m$ . Usually, the value of  $\mu$  is one thousand times larger than that of  $m$ . Therefore, the equation is approximated to the final item. This equation gives rise to an important molecular design strategy for the CPL chromophore having enhanced chiroptical properties, *i.e.*, the  $\mu$  and  $m$  values of a chromophore having a large  $g_{\text{lum}}$  value that emits “*pure CPL*” are small and large, respectively. This is a simple conclusion, but how do we translate this strategy to molecular design? These two values, particularly the latter  $m$ , are abstract and difficult to link to the molecular structure.

$$g_{\text{lum}} = 2 \frac{I_L - I_R}{I_L + I_R} = \frac{4|\mu| \cdot |m| \cos \theta}{|\mu|^2 + |m|^2} \simeq \frac{|m| \cos \theta}{|\mu|} \quad (m \ll \mu)$$

(equation 1)

This presentation will discuss the introduction of a simplified approach to gain a qualitative understanding of  $\mu$  and  $m$ . This approach takes into consideration the shapes of molecular orbitals (MOs) participating in the electronic transition. We can easily speculate the shapes of occupied and unoccupied MOs that show significantly large  $\mu$  and  $m$  values. In other words, we can design a molecule having such MOs.

**Keywords:** CPL;  $g_{\text{lum}}$ ; Electronic transition moment; Magnetic transition moment



### ■ Professional Biography

Ken-ichi Sugiura received a PhD (1992) in chemistry from the Institute for Molecular Science, the Graduate University for Advanced Studies. After the assistant professor at Osaka University, he became in 2005 professor of chemistry at Tokyo Metropolitan University.

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## New electrochemical detection strategies for clinical diagnosis

Kontad Ounnunkad\*, Patrawadee Yaiwong, Siriporn Anuthum, Supakeit Chanarsa, and Jaroon Jakmunee

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The power of ultratrace-level quantitative assays for disease biomarkers holds great potential. By detecting diseases at their earliest, most treatable stages, these assays help clinicians diagnose with unparalleled accuracy. They also provide researchers with insights into the body's responses to diseases and treatments, facilitating a better understanding of how to achieve in-body restorations. To detect such biomarkers, electrochemical immunosensors prove effective with good analytical performance. Their advancements rely on integrating functional materials using various fabrication and detection strategies to enhance sensitivity and specificity. The incorporation of novel state-of-the-art nanomaterials, such as nanoparticles, quantum dots, and two-dimensional nanomaterials, each with unique characteristics, has further propelled these developments. At Chiang Mai University, our research focuses on constructing innovative immunosensors with a sandwich-like configuration. These sensors, developed by our team, have the unique capability to detect both single and multiple target biomarkers. The responses, stemming from the amplification of redox probe/aptamer complexes situated on the immunocomplexes, demonstrate a proportional relationship to the targets. Our sensors exhibit outstanding sensitivity, selectivity, reproducibility, and stability, achieving low limits of detection suitable for identifying disease biomarkers at clinically relevant cut-off levels. The success of our work suggests the potential for practical applications in the field of clinical diagnoses.

**Keywords:** Nanomaterial; Immunosensor; Diagnosis; Amplification; Assay



### ■ Professional Biography

Kontad Ounnunkad received his Ph.D. in Chemistry from the University of Wollongong, Australia in 2010. He is currently an associate professor at Chiang Mai University, in Thailand. For his scientific achievements, Kontad received research fellowships from the French Embassy in Thailand, the Matsumae International Foundation, and the British Council in Thailand (Newton Fund). Moreover, he was awarded under Endeavour Research Fellowship from the Australian Embassy. His research focuses on the development of new electrochemical sensors for disease diagnosis and new energy storage devices. Recently, he was on the list of the World's Top 2% Scientists in 2022 and 2023 in the fields of Applied Physics and Analytical Chemistry, ranked by Stanford University.

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## Synthesis and chiroptical properties of strained paraphenylene anchoring chiral binaphthyl

Masashi Hasegawa\*, Xiao Wanli, and Yasuhiro Mazaki

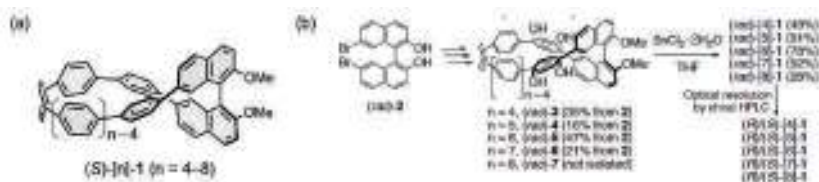
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Recently, our group reported the synthesis and chiroptical properties of a curved stereogenic [6]paraphenylene ([6]PP), anchoring a chiral binaphthyl scaffold at 7,7'- positions.<sup>1)</sup> In this study, a series of chiral PPs with the different number of paraphenylene rings ( $n = 4-8$ ) have been synthesized to investigate the relationship between chiroptical properties and the molecular distortion. The target molecules were synthesized via pre-aromatized precursors (3, 4, 6, 7, Scheme 1). X-ray analysis revealed a helically twisted structure of PP units induced by axial chirality of binaphthyl framework. Optical resolution by using a chiral HPLC method successfully provide (*R*)/(*S*)-[*n*]-PP. The chiroptical properties, including UV-vis absorption, fluorescence spectra, CD spectra, and CPL spectra, were thoroughly investigated, (Figure 2). As for the CPL spectra, with decreasing the ring size, the emission maxima are red-shifted and the value of  $|g_{lum}|$  are increased. In particular, [4]-1 exhibited a value of  $|g_{lum}| = 1.1 \times 10^{-2}$ , which is much larger than that of common organic compounds.

**Keywords:** Carbon nanoring; Macrocycle; Binaphthyl; Circularly polarized luminescence



Scheme 1 (a) Molecular structure of (*S*)-isomer. (b) Synthesis of [*n*]-1



## ■ Professional Biography

### Masashi Hasegawa

He earned his Ph.D. in 2004 from Tokyo Metropolitan University (TMU) under the supervision of Professor Masahiko Iyoda. He then served as a JSPS postdoctoral fellow with Professor Timothy M. Swager at MIT, and Professor Yohji Misaki at Ehime University, Japan. Then, he was appointed a faculty member at the School of Science, Kitasato University from September 2007 as associate professor, and his subsequent research has been recognized with the Daicel Chemical Industry Award in Synthetic Organic Chemistry (2010), Mazda Foundation Award (2009), and BCSJ Award (2011). His research focuses on the synthesis and development of novel chiral emitter for chiroptical materials.

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## Advancements in nanomaterials for augmenting electrochemical and photometric sensor performance

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Sensors and biosensors are compact devices widely employed for chemical analysis across diverse fields, owing to their attributes of high sensitivity, selectivity, cost-effectiveness, and user-friendly operation. Nevertheless, achieving heightened sensitivity and selectivity remains a challenge in numerous applications. The integration of nanomaterials into sensor design has emerged as a transformative strategy, resulting in significant enhancements in sensitivity, selectivity, and overall efficiency. Exploration into diverse nanomaterials, including carbon-based structures, metal/metal oxide nanoparticles, and quantum dots, has played a pivotal role in advancing sensor capabilities. Several illustrative examples highlight the impact of nanomaterials on sensor technology. For instance, copper oxide and carbon nanodots find application in a non-enzymatic amperometric glucose sensor. A nanocomposite comprising carbon nanotubes, nickel oxide, carbon black, and Nafion, when modified on a screen-printed carbon electrode, demonstrates the ability to discriminate electrochemical reactions of serotonin and dopamine in voltammetric analysis. Moreover, a composite of carbon black and graphene oxide exhibits enhanced sensitivity for uric acid determination. The sensitive detection of alpha-fetoprotein is achieved through a specific aptamer immobilized on platinum nanoparticles and carboxylated graphene oxide. Additionally, a label-free colorimetric aptasensor for the rapid detection of Aflatoxin B1, utilizing the surface plasmon resonance of gold or silver nanoparticles, has been investigated. This comprehensive analysis underscores the pivotal role of nanomaterials in propelling the evolution of electrochemical and photometric sensors, resulting in heightened performance and broader applicability across various domains.

**Keywords:** Nanomaterials; Sensor; Biosensor; Performance improvement; Electrochemical; Optical



### ■ Professional Biography

Jaroen Jakmunee is currently an Associate Professor at the Department of Chemistry, Faculty of Science, Chiang Mai University, Thailand. He finished Ph.D. in Chemistry from Chiang Mai University in 1997. He received many awards in research, such as an Outstanding Young Scientist of the Year 2003, by Foundation for the Promotion of Science and Technology under the Patronage of His Majesty the King Rama 9, FIA researcher awards from the Japanese Association for Flow Injection Analysis, and Outstanding Researcher of Chiang Mai University (Golden Elephant award).

His research interests are on the development of new materials, analytical methods and instrumentations for chemical analysis, including biosensors, microfluidics, and flow analysis for agricultural, environmental, and medical applications.

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## Newly developed systems for advanced CD and CPL measurements and their measurement methods and applications

Satoko Suzuki<sup>1,2</sup>, Yoshiro Kondo<sup>1</sup>, Akio Kaneta<sup>1</sup>, Yoshitane Imai<sup>3</sup>, Ken-ichi Akao<sup>1\*</sup> and Naoto Ishikawa<sup>2\*\*</sup>

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Circular dichroism (CD) spectroscopy has long been used for structural analysis of chiral compounds, and its applications have been expanding particularly in industrial fields for research, development and quality control for antibody and nucleic acid therapeutics. On the other hand, circularly polarized luminescence (CPL) spectroscopy has recently become a commonly used analytical method for characterizing the luminescence properties of chiral compounds. Here we describe newly developed systems and measurement methods for CD and CPL analysis. The topics covered include measurement methods of solid samples, a system for comprehensive high-throughput magnetic CD measurements that are difficult to perform manually, and a system for evaluating organic light-emitting diodes that emit CPL or magnetic CPL, which are being actively developed, together with measurement examples.

**Keywords:** Circular dichroism; Circularly polarized luminescence; Magnetic circular dichroism; Magnetic circularly polarized luminescence; High-throughput MCD system



Figure 1. High-throughput MCD system



### ■ Professional Biography

1. Manager, Applicative Solution Lab Division, JASCO Corporation
2. Graduated from the Department of Chemistry, Graduate School of Science, Osaka University in 2003.

Responsible for application development related to absorption, fluorescence, CD and CPL spectroscopy at JASCO since 2003.

3. Establishment of analytical methods for antibodies and nucleic acid therapeutics, and elucidation of magnetic and optical properties of phthalocyanine complexes using MCD and MCPL spectroscopy.

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## The synthesis and development of novel fluorescence compounds as heavy metal ion sensors

Anawat Ajavakom

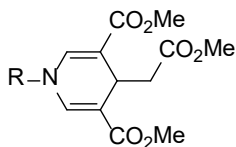
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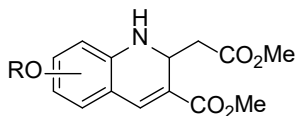
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Heavy metal ion in human body can potentially cause many serious health effects such as cancer, organ damage, and nervous system damage and in extreme cases, death. Hence, the method for detection of heavy metal ion has a vital role leading to the improvement of such contaminated environment, there is an extensive need for effective heavy metal ion sensing system. To overcome drawbacks of current analytical methods such as a complicated process, destructive to the sample, requiring expensive instrumentation, and necessity of a skillful operator, the fluorescence method has been a convenient alternative for detection of metal ion with on-top-advantages of high sensitivity and selectivity, and visualizing or imaging capability. Herein, a series of novel fluorescence compounds, basically designed and synthesized based on a 1,4-dihydropyridine (DHP), dihydroquinoline (DHQ) and other fluorophores, using newly developed methods, together with the development of such sensing probes into a heavy metal ion sensors will be explained. This presentation also focuses on how to determine the sensing mechanism by using several techniques such as  $^1\text{H}$  NMR experiment, UV-Vis spectrophotometry, and/or mass spectrometer and so on.

**Keywords:** Organic synthesis; Fluorescent chemosensor; 1,4-Dihydropyridine; Dihydroquinoline; Heavy metal ion detection



1,4-Dihydropyridine



Dihydroquinoline



### ■ Professional Biography

#### Anawat Ajavakom

An assistant professor in Chemistry Department, Faculty of Science, Chulalongkorn University. He is an expert in synthetic organic chemistry, synthetic methodological study for heterocyclic compounds and development of fluorescent sensors in sensing of heavy and transitional metal ions. His scientific interest also includes the methodological study, particularly for heterocyclic compounds, and the development of novel fluorescent sensing system incorporation with nanoparticles.

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## Development of aggregation-induced emissive materials exhibiting circularly polarized luminescence

Hiroyuki Nishikawa

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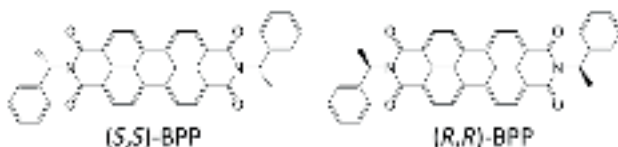
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There have been extensive studies in the development of organic light-emitting diodes (OLEDs) that emit circularly polarized light, so-called CP-OLEDs (circularly polarized light-emitting diodes), because of their potential applications across diverse area, including quantum computing, three-dimensional display technologies, chemical and biological sensing apparatus, and so on. The prevailing concern lies in the fact that most CP-OLEDs hitherto reported have suffered from insufficient device performance, such as low external quantum efficiency (EQE), as well as low circularly polarized electroluminescence (CPEL) characterized by the dissymmetry factors denoted as  $g_{EL}$ . In the investigation of materials exhibiting circularly polarized luminescence (CPL) with high photoluminescence  $g_{PL}$  values, the attainment of high  $g_{PL}$  values requires chiral arrangement of multiple luminophores. Within the device, however, the aggregation of luminophores induces aggregation caused quenching (ACQ). Therefore, the utilization of CPL-active aggregation-induced emission luminogens serves as a prospective material to overcome the conflict requisites. In this context, we have focused on chiral perylene diimide derivatives, specifically (*R,R*)- and (*S,S*)-BPP (Figure1), which demonstrate aggregation-induced enhanced (AIEnh) CPL. In this presentation, the origin of the AIEnh-CPL properties of chiral-BPP based on the spectroscopic examinations and theoretical calculations, along with the integration of chiral-BPPs into CP-OLEDs, will be expounded.

**Keywords:** Circularly polarized luminescence (CPL); Chirality; Aggregation-induced emission; Circularly polarized organic light-emitting diode (CP-OLED); Perylene diimide derivatives



**Figure 1** Molecular structures of (*S,S*)- and (*R,R*)-BPP



### ■ Professional Biography

Hiroyuki Nishikawa graduated from Kyoto University in 1988 and received his Ph.D. degree in 1993. Subsequently, he served as a postdoctoral fellow at Risø National Laboratory in Denmark from 1993 to 1994. In 1994, he joined Tokyo Metropolitan University as a Research Assistant in 1994, advancing to the position of Associate Professor at the University of Tsukuba in 2004. In 2009, he was appointed as Professor of Ibaraki University. His current interests cover organic electronics, including chiral luminescent materials for the application into light-emitting diodes and semiconducting devices associated with spin polarization phenomena.

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## Photophysical properties for excited-state intramolecular proton transfer (ESIPT) reaction of N-salicylidene-o-aminophenol: DFT based approaches

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Photophysical properties for excited-state intramolecular proton transfer (ESIPT) reaction of N-salicylidene-o-aminophenol (SA) Schiff base were comprehensively studied based on experimental methods combined with theoretical calculations. The results revealed that the SA was mainly presented in enol form in acidic solutions while it was predominantly existed in keto form in basic solutions. From UV-vis absorption and fluorescence emission studies, it showed that the ESIPT could effectively take place in non-polar and aprotic polar solvents. By using the CAM-B3LYP/6-311G(d,p) level of theory, it was found that the intramolecular proton transfer could preferably occur through six-membered ring transition rather than through five-membered ring transition. The dynamics of the ESIPT reactions of enol and keto tautomers were studied using TD-CAM-B3LYP with 6-311G (d,p) basis set. The potential energy curves for the intramolecular proton transfer in the ground (GSIPT) and excited state (ESIPT) exhibited that the GSIPT could occur through a low activation barrier, whereas in the case of ESIPT, the process could arise via low energy barrier.

**Keywords:** Photophysical properties; Schiff base; Excited-state intra-molecular proton transfer; Density functional theory



### ■ Professional Biography

Songwut Suramitr is currently an associate professor at Department of Chemistry, Faculty of Science, Kasetsart University. His research area is in Computational Chemistry, an area that focuses on study the photophysical properties of exciting molecules.

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# SMALL-SCALE CHEMISTRY TEACHERS NETWORKING ABSTRACT

## Microscale/Small scale chemistry experiments from Macedonia

Metodija Najdoski

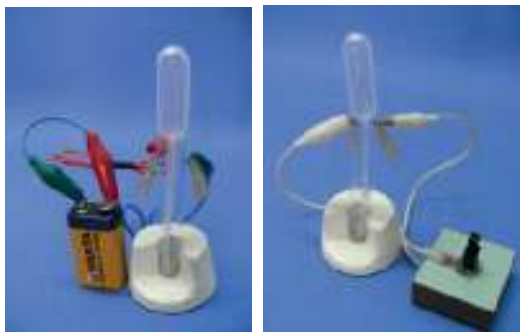
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SC

Microscale chemistry in Macedonia has been born in Turkey Istanbul on the the 18<sup>th</sup> International Conference on Chemical Education in 2004. Since then, many ideas born in this Balkan country has been presented worldwide. This abstract is about chemistry experiments parade with ideas tailored in Macedonia. An inspiration was driven by the enthusiastic, academic group known as microscale family. Many ideas have been presented on the educational events so the author got an impression that he has to give some contribution to the Microscale gas chemistry. Some of this ideas will be presented as an example of gas generation methods. One of these ideas goes further to designed experiment for determination of the oxygen content in the air. Some of the experiments are contributing into material science experiments. One of the main activity till today is related to educational, disposable chemistry experiments. These ideas were a kind of logic consequence from a survey made decades ago. A survey that answers the question: Why is so difficult, for the teachers to perform experiments in the classrooms? The answer, according to the author, for the solution of this problem are the proposed disposable chemistry kit. The author has designed around 50's such a kits and these cold be easily extended to more than 100 following this concept.

**Keywords:** Microscale gas chemistry; Disposable chemistry kits; Oxygen content; Plastic pipettes; Small scale experiments





### ■ Professional Biography

Metodija Najdoski received his Ph.D. in Materials Chemistry from the Ss. Cyril and Methodius University in 2000. He works at this University, Faculty of Natural Sciences, Institute of Chemistry since 1993. He teaches General and Inorganic Chemistry, Experimental Inorganic Chemistry, Methodology of Chemistry Experimentation, Microscale Chemistry Experimentation, Forensic Chemistry etc. He has published 115 papers, mainly in the area of Materials Science of Inorganic Thin Films and has significant number of educational papers related to the design of chemical experiments and Microscale Chemistry. In total, Prof. Najdoski gave 53 lectures, workshops from which 43 were conducted abroad by invitation. Ten books are also written by him in the area of Experimental chemistry, Experiments for Chemical Education and General Chemistry. Prof. Najdoski was visiting professor in Mexico at the Ibero-American University, Babes- Bolyai University, Romania and twice in Leipzig University in Germany. As an invited lecturer he has given lectures in Romania and many times in Israel.

SC



# SPECIAL SESSION ABSTRACTS

## Driving chemistry for sustainable change

Mandar Bodas<sup>1\*</sup>, Ryan Huang<sup>2</sup>, and Adeline Teoh<sup>3</sup>

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SS

Modern chemistry is the backbone of our society and has a profound impact on our lives. The chemical sector consumes 10% of the world's total energy and contributes to 8% of greenhouse gas emissions. 90% of global production depends on chemical products. Chemistry also is a major contributor to global environmental pollution, plastic waste and the ongoing climate crisis based on the products we use such as detergents, toothpaste, plastic, paints, drugs and beyond. The transition toward a sustainable future is the key for radical transformation towards sustainability to meet these global challenges on how chemistry is designed, developed, and executed. Sustainability-focused chemistry research is key to realizing lower pollution levels, less waste, safer chemicals, and greater energy efficiency. To adapt to a changing world, chemical syntheses and processes need to be adapted too.

Sustainable Chemistry makes a critical contribution to achieving the aims of all SDGs. Reaxys database along with the interoperability experience from ScienceDirect and Scopus database helps researchers in providing the right solutions which saves time and cost by improving efficiency and productivity.

Reaxys retrieves literature, compound properties and chemical reaction data faster than any other solution Reaxys offers a highly intuitive interface and robust database to help leading chemists retrieve relevant chemical literature, patent information, valid compound properties and experimental procedures in half the time. Designed to support the full range of chemistry research, including pharmaceutical development, environmental health & safety work and material science, Reaxys puts every scientist, from novice to expert, on the shortest path to answers.

**Keywords:** Green chemistry; Sustainable chemistry; Reaxys; Synthesis; Chemistry research

## NMR experiments for small molecule analysis and structure elucidation – quick update

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<sup>2</sup>*Bruker Switzerland AG, Sathorn City Tower 10th Floor, Thung Maha Mek, Sathorn, Bangkok, Thailand*

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Nuclear magnetic resonance (NMR) spectroscopy is an immensely powerful tool for the characterization of small molecule structures. Nowadays, with sophisticated pulse sequences, the core 2D NMR correlation experiments used in complete small molecules assignment can be recorded in a single measurement via NOAH (NMR by ordered acquisition using <sup>1</sup>H detection) supersequences. Meanwhile, Parallel Acquisition NMR Spectroscopy (PANSY), by taking advantage of multiple-receivers technologies which associated with the new spectrometer electronic, has expanded its analytical capability. The new group of PANSY experiments have enabling simultaneous acquisition of two or more signals arising from different nuclei in the standard analysis technique. For spectrometer which equipped with more sensitive cryogenically cooled probes, the aforementioned methods have opened up possibilities to incorporate insensitive but information rich 2D experiments. Furthermore, the ADEQUATE module (in NOAH-4) and HETCOR module (in PANSY) allow chemists to directly trace out carbon backbones with much greater certainty and higher resolution. With that, we greatly increasing the information content of NMR measurement within a single experiment. To date, single-scan acquisition, which avoids the need for tedious parameter optimization has significantly broaden the applicability on natural products which demonstrated extensive overlapped in <sup>1</sup>H NMR. The wide range of applications not only minimizing precious NMR instrument time but also enabling straightforward implementation for automation. Single-scan Gradient-Enhanced Multiplet-Selective Targeted-Observation NMR Experiment (GEMSTONE) and Single-scan Ultrasensitive Heteronuclear Polarization Transfer (UHPT) Method are among the key-highlights to this new approach.

**Keywords:** NMR; NOAH supersequences; PANSY; Pulse sequence

## Biocarbon value chain development from agricultural waste:

### A key driver in Thailand's Bio-Circular-Green economy

Pornthep Thanalertpipat\* and Tarnin Phanichewa

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Thai Carbon ([www.thaicarbon.bio](http://www.thaicarbon.bio)), a subsidiary of the Weng Group, demonstrates the synergy of the Bio-Circular-Green economy through its biochar production. By utilizing biological resources such as cassava rhizomes and bamboo, the company transforms renewable and biodegradable agricultural waste into biochar, embodying the 'Bio' aspect. This process seamlessly transitions into the 'Circular' model, as these agricultural by-products are repurposed into valuable biochar, showcasing waste reduction and resource efficiency. In alignment with 'Green' principles, Thai Carbon employs an emission-free pyrolysis process in biochar production, significantly contributing to carbon sequestration and climate change mitigation.

This presentation will delve into these aspects, highlighting how Thai Carbon's innovative practices contribute to sustainable development, efficient resource utilization, and environmental stewardship in Thailand.

**Keywords:** Biochar production; Circular economy; Sustainable agriculture; Zero-emission technology

# Analytical Chemistry (AC)

please access to the following QR code for abstracts



AC



## Oral Presentation

AC-O-01

### **Absolute quantification of phenylbutanoids in *Zingiber cassumunar* Roxb. rhizome by quantitative $^1\text{H}$ NMR**

Chatkamon Lekwongphaiboon, Boonwiset Seaho, Ngampuk Tayana, Wichayasith Inthakusol, Sumet Kongkiatpaiboon, Wiratchanee Mahavorasirikul, Saisuree Prateetpongkum, and Nongnaphat Duangdee\*

AC-O-02

### **Production and certification of certified reference material of Andrographolide in *Andrographis Paniculata* powder by a network of competent laboratories approach**

Ponhatai Kankaew\*, Kittiya Shearman, Kanjana Hongthong, Cheerapa Boonyakong, and Charun Yafa

AC-O-03

### **Gold nanoparticle-based dip strip immunoassay with silver enhancement method for cardiac troponin I detection**

Napakporn Poosinuntakul, Theeawut Chanmee, Sureerut Porntadavity, Orawon Chailapakul, and Amara Apilux\*

AC

AC-O-04

### **Synthesis of platinum on manganese (IV) oxide nanowires in chitosan scaffold as a catalyst in prostate immunosensor**

Suphaporn Chenkhuruthum, Anchana Preechaworapun, Pusit Pookmanee, and Tanin Tangkuaram\*

AC-O-05

### **Surfactant-free air bubble flotation for the rapid purification of basic dyes and drugs**

Koki Kodama, Ngo Thi Thu Thao, and Tohru Saitoh\*

AC-O-06

### **Electrical field-flow fractionation for separation and characterization of metal nanoparticles**

Takdanai Techarang\* and Atitaya Siripinyanond

AC-O-07

**An efficient method of tyramine detection in food and beverage products by capillary electrophoresis using silica-nanolayer coated capillary with UV detection**

Apinya Obma, Pattamaporn Hemwech, Sittisak Phoolpho, Rawiwan Bumrungpuech, Supa Wirasate, Sulawan Kaowphong, Prapin Wilairat, and Rattikan Chantiwas\*

AC-O-08

**Development of an electrochemical DNA super-sandwich assay for porcine adulteration detection via one-step immobilization using a poly-adenine oligonucleotide approach**

Vasita Lapee-e, Sudkate Chaiyo, and Abdulhadee Yakoh\*

AC-O-09

**Non-transferrin-bound iron (NTBI) quantification in human plasma using BODIPY-Pyridylhydrazone (BODIPY-PH) entrapped in a thin green film coupled with a portable fluorescence-based device**

Puttaraksa Naksen, Kantapat Chansaenpak, Siriporn Jungsuttiwong, Ratchadaree Intayot, Jaroon Jakmunee, Somkid Pencharee, Peter Lieberzeit,

AC-O-10

**Mickey mouse-shaped laminated paper-based analytical device in simultaneous total cholesterol and glucose determination in whole blood**

Akarapong Prakobkij, Suchada Sukapanon, Suticha Chunta, and Purim Jarujamrus\*

AC

AC-O-11

**Vanadium-doped porous cobalt oxide for its superior peroxidase mimic in simultaneous total cholesterol and glucose testing in whole blood on a 2D paper-based device**

Nattasa Kitchawengku, Budsakorn Wongsing, Akarapong Prakobkij, Wipark Anutrasakda, and Purim Jarujamrus\*

AC-O-12

**A distance-based paper device using polydiacetylene liposome as a chromogenic substance for rapid and in-field analysis of disinfectants against COVID-19**

Boonta Chutvirasakul, Nantana Nuchtavorn, Mirek Macka, and Leena Suntornsuk\*



AC-O-13

**Enhanced detection of favipiravir using a  $\text{Cu}_2\text{O}@\text{MnO}_2$  modified glassy carbon electrode**

Nuenghathai Chaiya, Anchana Preechaworapun, Phetlada Kunthadee, and Tanin Tangkuaram\*

AC-O-14

**Development of aptamer-based detection kit by electrochemistry for rapid assessment of vitamin D levels**

Sattawat Boonchaleaw, Supaporn Seetaha, and Kiattawee Choowongkomon\*

AC-O-15

**Ecological risk assessment of heavy metals in sediment from Klong Luang Reservoir, Chonburi, Thailand**

Sophit Buth, Lita chheang, and Sudtida Pliankarom Thanasupsin\*

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AC-O-16

**Effect of some short chain and long chain fatty acids on KOH number of concentrate natural rubber latex**

Najmee Hemmad\*, Wilairat Cheewasedtham, Thitima Rujiralai, and Nadeeya Samae

AC-O-17

**Sensitive and selective 3D-ePAD for dual simultaneous analysis of VMA and 5-HIAA tumor markers using graphene screen printed electrode modified with molecularly imprinted polymers for point-of-care application**

Kanpitcha Somnet, Supansa Chimjarn, Surasak Wanram, Purim Jarujamrus,

AC-O-18

**Electrochemical sensor based on amine-functionalized magnetite magnetic nanoparticles and reduced graphene oxide nanocomposites for determination of chloramphenicol**

Wasukamol Numphud, Wilai Siriwatcharapiboon, and Janjira Panchompoo\*

AC-O-19

### **Development of a paper-based analytical device for simultaneous detection of organophosphate pesticides and heavy metal in fruit and vegetable samples**

Supattra Arsawiset, and Siriwan Teepoo\*

AC-O-20

### **Microfluidic paper-based analytical devices for total amino acid detection in processed food**

Jaruwan Mettakoonpitak\* and Atcha Chanthabun

AC-O-21

### **A thread-based analytical device for nitrite detection in food samples**

David T. Ajayi and Siriwan Teepoo\*

AC-O-22

### **Development of a simple method for measuring nitrate ions in natural water samples**

Mika I. Umeda\*, Takatoshi Fujii, Eiichi Hino, Yusuke Date, Kaoru Aoki, Danchana Kaewta, and Takashi Kaneta

AC

AC-O-23

### **A novel immunosensor based on cobalt oxide nanocomposite modified single walled carbon nanohorns for the selective detection of aflatoxin B1**

Chulalak Damphathik, Chomphunuch Songsiriritthigul, Jamras Lerd Sri, Jaroon Jakmunee, Yutthana Wongnongwa, Siriporn Jungsuttiwong, Astrid Ortner, Kurt Kalcher, and Anchalee Samphao\*

AC-O-24

### **Effect of extraction solvent ratio in biosynthesis of silver nanoparticles, determination of phytochemicals, and investigation of antioxidant activity using *Artabotrys suaveolens* (Blume) Blume leaves**

Fode Bangaly Toure, Saowapa Chotisuwan, Somrak Phaphon, and Weeraya Treewanjutha\*



AC-O-25

**Effect of Mg compounds on fatty acids eduction in concentrated natural rubber (*Hevea brasiliensis*) latex**

Nadeeya Samae\*, Najmee Hemmad, Thitima Rujiralai,  
and Wilairat Cheewasedtham

AC

## Poster Presentation

AC-P-01

**Smartphone assisted digital image colorimetric determination of andrographolide and analogues in *Andrographis paniculata* extract**

Hathaichanok Karanasophonphun, Watcharaporn Seehun, Preeyanuch Sangtrirutnugul, and Atitaya Siripinyanond\*

AC-P-02

**A smartphone-assisted optosensor for ultrasensitive and highly selectivedetermination of diflunisal**

Angkana Pongprom and Opas Bunkoed\*

AC-P-03

**Point-of-care DNA testing device for simultaneous detection of HIV and HCV using alternating current electroluminescent display**

Chawin Srisomwat, Abdulhadee Yakoh, Tirayut Vilaivan and Orawon Chailapakul\*

AC-P-04

**Portable device for phosphate analysis in natural water**

Chayanuch Kijjamlerd, Siriwit Buajarern, and Kamonthip Sreenonchai\*

AC

AC-P-05

**Sequential determination of sucrose and phosphate in sugarcane juice by flow injection method**

Kamonthip Sreenonchai\*, Jiraporn Duangjan, and Siriwit Buajarern

AC-P-06

**Distance-based measurement of Ni(II) using a barrier-free paper device**

Siriporn Thongnantakun, Nanthatchaphon Jantawong, Takdanai Techarang, and Duangjai Nacapricha\*



AC-P-07

### **Development of distance-based paper device for measuring chloride ion in food**

Ruj Samarnworakit, Buddhima Phrirojchaikul, Wiput Tienwanpen,  
Chaiyarerk Homsirikamol, Kamonchanok Phoonsawat, and Wijitar Dungchai\*

AC-P-08

### **Paper-based test strip for analysis of organophosphate pesticides**

Wanchalearm Manchan, and Yupaporn Sameenoi\*

AC-P-09

### **Paper-based test strip for formaldehyde gas detection**

Wannisa Sroisarika, and Yupaporn Sameenoi\*

AC

AC-P-10

### **Paper-based devices for water hardness analysis**

Alicha Marut and Yupaporn Sameenoi\*

AC-P-11

### **Rapid test strip for malachite green detection**

Siriwan Teepoo\* and Khaunnapa Panapong

AC-P-12

### **Pencil lead electrode disks with rubbed prussian blue particle modification as cheap and ecological hydrogen peroxide sensors**

Thanakorn Hussana, Nattapol Ma, Sareeya Bureekaew, Satoshi Horike,  
and Albert Schulte\*

AC-P-13

### **Anodic stripping voltammetry of mercury (II) on a gold leaf sensor via flow analysis**

Paithoon Prasertying, Monrada Panuwatsuk, Phoonthawee Saetear, Kanchana Uraisin, and Duangjai Nacapricha\*

AC-P-14

### **An electrochemical sensor with gold leaf and nanoporous gold modification**

Supakorn Kittikomoldej, Nuttamon Khoonrueng, Paithoon Prasertying, Takdanai Techarang, and Duangjai Nacapricha\*

AC-P-15

### **Determination of rutin using a FeO nanoparticle-modified electrode**

Angwara Khiaomueang, Anurak Chitbuengphrao, Tanin Tangkuaram, and Anchana Preechaworapun\*

AC-P-16

### **Electrochemical detection chloramphenicol modified with tin on reduced graphene oxide by screen-printed carbon electrode**

Sirisupa Bunnasit, Chaiya Prasittichai\*, and Wilai Siriwatcharapiboon\*\*

AC

AC-P-17

### **Electrochemical determination of hydroquinone by activated glassy carbon electrode**

Wannasa Boonprom, Mathurada Artchakan, Anurak Chitbuengphrao, Tanin Tangkuaram, and Anchana Preechaworapun\*

AC-P-18

### **Squarewave voltammetry on a modified screen-printed electrode for selective detection of dopamine in the presence of uric acid**

Tharaton Nooin\*, Thaneeya Hawiset, and Prachak Inkaew



AC-P-19

### Simple electrochemical determination of favipiravir for anti-viral COVID-19

Tanin Tangkuarm\*, Kamonporn Prasertpornsut, Nuenghathai Chaiya, Jiraporn Kitikul, and Anchana Preechaworapun

AC-P-20

### Microflow injection analysis with electrochemical detection on cloth-based device

Tanaporn Boonnikom, and Yupaporn Sameenoi\*

AC-P-21

### Cost-effective gold leaf electrochemical sensor for voltammetric detection of chloride

Kumpirada Khamjoy, Paithoon Prasertying, and Duangjai Nacapricha\*

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AC-P-22

### Preparation and evaluation of ammonium ion reference material in salt matrix

Thararat Tangjit, Duangjai Nacapricha, Kanchana Uraisin, Nongluck Tangpaisarnkul, and Phoonthawee Seatear\*

AC-P-23

### Portable sensor for Dengue virus detection by modified screen-printed electrode

Wattanachai Boonprapha, Supaphorn Seetaha, Kiattawee Choowongkamon, and Chaiya Prasittichai\*

AC-P-24

### Development of an electrochemical immunosensor for the detection of oxytetracycline

Preeya Kusonpan, Astrid Ortner, Kurt Kalcher, and Anchalee Samphao\*

AC-P-25

**Monolithic  $\mu$ -SPE coupled with electrochemical sensor using screen-printed graphene electrode for the determination of urinary THC-COOH in forensic application**

Kesara Ar-sanork, Wichayaporn Kamsong, Chanpen Karuwan\*, and Patcharin Chaisuwan\*\*

AC-P-26

**A highly sensitive colorimetric sensor for detection and speciation of arsenic in soil samples**

Juthatip Ninlapan and Siriboon Mukdasai\*

AC-P-27

**Detection of histamine based on gold nanoparticles using UV-Vis spectrophotometer for analysis of histamine in seafood samples**

Monticha Photin, Orawan Kanluang, and Chacriya Malasuk\*

AC-P-28

**An optosensor based on quantum dots composited with molecularly imprinted polymers for the determination monuron**

Irin Prasertvetchatont and Opas Bunkoed\*

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AC-P-29

**An optosensor based on fluorescence quenching of nanocomposite sensing probe for the determination of non-steroidal anti-inflammatory drug**

Noppanut Longnapa and Opas Bunkoed\*

AC-P-30

**A highly sensitive and selective fluorescence sensor for the determination of piperacillin**

Nanthicha Chodchoy and Opas Bunkoed \*



AC-P-31

**A colorimetric sensing for arsenic (III) based on thiodiacetic acid functionalized gold nanoparticles**

Asmah Kuno, Nuryance Hama, Panwadee Wattanasin, and Thitima Rujiralai\*

AC-P-32

**Gingerol extract-stabilized silver nanoparticles and their applications: colorimetric and machine learning-based sensing of Hg (II) and antibacterial properties**

Kittiya Plaeyao, Ratchaneekorn Kampangta, Yuparat Korkokklang, Chanon Talodthaisong, Apichart Saenchoopa, Saengrawee Thammawithan, Krailikhit Latpala, Rina Patramanon, Navaphun Kayunkid, and Sirinan Kulchat\*

AC-P-33

**TAptamer-based lateral flow biosensor for the detection of cadmium**

Vorawan Yurayart, Sirowan Ruantip, Abdulhadee Yakoh, and Sudkate Chaiyo\*

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AC-P-34

**Investigation of carbon dots (CDs)-based fluorescence turn-on and turn-off sensing for detection of aspartame**

Rewat Nakwisai, Sayamol Choonnawan, Nattaporn Rosruen, Nakarin Noirahaeng, Thinnapong Wongpakdee, and Phoonthawee Seatear\*

AC-P-35

**The study of analysis method for sugar-based surfactant; alkyl polyglucoside in cleaning product**

Neungrutai Saesaengseerung\*, Darat Phathanakunkamchon, and Thanatcha Tongraya

AC-P-36

**A kinetic and spectroscopic study on the proteolytic activity of papain in organic solvents medium**

Jiraporn Thaithong, Phanuphong Sawatthitileat, and Nichanun Sirasunthorn\*

AC-P-37

### **Use of rice straw-cellulose nanofibril at a 2D-microcuvette for determination of fluorescein injection medicine**

Ratchanon Sangsriboonrueng, Panumart Thongyoo, Chutima Phechkrajang, Thanapat Intarawong, Chatdanai Sangson, and Nathawut Choengchan\*

AC-P-38

### **Tannin-modified membrane for preconcentration in the determination of lead using spectrophotometric techniques**

Vanlada Suksomphot, Chanpen Karuwan, Thitirat Mantim, Duangjai Nacapricha, and Nuanlaor Ratanawimarnwong\*

AC-P-39

### **Development of chitosan/graphene oxide nanocomposite for simultaneous extraction of antioxidants and bisphenol A**

Nurma Sulaiman, Nuryanee Hama, Saowanit Saithong, and Thitima Rujiralai\*

AC-P-40

### **A composite adsorbent for the extraction and determination of polycyclic aromatic hydrocarbons**

Onamon Chumsud, Opas Bunkoed, and Panwadee Wattanasin\*

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AC-P-41

### **A nanocomposite magnetic molecularly imprinted polymer adsorbent for the extraction and preconcentration of triazines**

Nurhasima Phirisi and Opas Bunkoed\*

AC-P-42

### **Determination of tetracycline residues in milk sample using biosorbents for a dispersive solid phase extraction by high performance liquid chromatography with UV detection**

Nongnapas Nakhonchai, Nattaya Prompila, Kraingkrai Ponghong\*, Watsaka Siriengkawut, Jitlada Vichapong, and Sam-ang Supharoek\*\*



AC-P-43

**Surfactant modified silica as effective sorbent for preconcentration of sulfonamides in water and honey samples prior to their determination by high-performance liquid chromatography**

Wannipha Khiaophong and Jitlada Vichapong\*

AC-P-44

**Monolithic-activated charcoal composite sorbent in micro pipette tips for micro-solid phase extraction**

Apiwat Muekhunthod, Kesara Ar-sanork, and Patcharin Chaisuwan\*

AC-P-45

**A composite magnetic solid phase extraction adsorbent for the extraction and determination of herbicides**

Suppawan Sillapawisut, Piyaluk Nurerk, and Opas Bunkoed\*

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AC-P-46

**Synthesis of non-polar and charged-monolithic materials in polypropylene pipette tips for micro-solid phase extraction**

Rawisara Woensanthia, Kesara Ar-sanork, and Patcharin Chaisuwan\*

AC-P-47

**Preparation and evaluation of zeolite composite monoliths for micro-solid phase extraction**

Manaphon Traswiman, Kesara Ar-sanork, Jatuporn Wittayakun, Sanchai Prayoonpokarach, and Patcharin Chaisuwan\*

AC-P-48

**Eco-friendly hydrophobic deep eutectic solvent-coated cellulose paper as a sorbent insorptive phase extraction for carbamate pesticides in fresh fruit and edible insect samples**

Phatchara Rattanaphonsaen, and Jitlada Vichapong\*

AC-P-49

### **Laser-induced biochar for the solid-phase extraction of organophosphorous pesticides**

Sherwin Hugo T. Lu1 and Puttaruksa Varanusupakul\*

AC-P-50

### **Melamine sponge impregnated with deep eutectic solvent for preconcentration of sulfonamides antibiotics prior to HPLC determination**

Jedsada Jaroensan and Jitlada Vichapong\*

AC-P-51

### **In situ ionic liquid-assisted in situ iron microparticles based on natural reagent for dispersive solid phase extraction of tetracyclines residues in honey prior to high performance liquid chromatography**

Tammanoon Nilnit, Janjira Jeenno, Jitlada Vichapong, Watsaka Siringkhawut, Sam-ang Supharoek\*, and Kraingkrai Ponghong\*\*

AC-P-52

### **Vortex-assisted dispersive liquid-liquid microextraction for determination of organophosphate pesticides using gas chromatography**

Andaman Thomthong, Anuwat Ratsamisomsi, and Warawut Tiyaongpattana\*

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AC-P-53

### **Determination of tetracycline oxytetracycline and chlortetracycline in *Macrobrachium rosenbergii* by liquid-liquid extraction and solid phase extraction using high-performance liquid chromatography with photodiode array detection**

Thinnakorn Sukkhunthod and Maliwan Subsadsana\*

AC-P-54

### **Optimization of ultrasonic extraction for the determination of PAHs in sediment by GC-MS**

Apinya Navakhun\* and Ausanee Saengin



AC-P-55

**Determination of the  $\Delta^9$ -tetrahydrocannabinol metabolite in urine by online-solid phase extraction coupled with liquid chromatography-mass spectrometry**

Waranyu Nachiangtai, Ajjima Thongbo, Chuleeporn Jantarasena, and Kraingkrai Ponghong\*

AC-P-56

**Assessing the quality of online-purchased alcohol-based hand sanitizers from Thailand online market using a GC-FID technique**

Orapan Apirakkan, Chompoonoot Paimoolpiam, Chaweewan Peangpitak, and Neungrutai Saesaengseerung\*

AC-P-57

**COVID-19 screening in sweat by volatile analysis using GC-MS and the relationship with military training dog results**

Suriwipa Chuachaina, Isaya Thaveesangsakulthai, Jantima Traipattanakul, Pornpawit Sinsukudomchai, Sorrawit Songsathitmetha, Kaywalee Chatdarong, Chadin Kulsing\*, and Thumnoon Nhujak\*\*

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AC-P-58

**Method development of peptide mapping characterization of monoclonal antibody (mAb) using liquid chromatography time-of-flight mass spectromete r(LC/Q-TOF)**

Ubonwan Chaiyo, Dalad Waropastrakul, and Ariya Chaisawadi\*

AC-P-59

**Development of analytical method for analysis of tetrahydrocannabinol and cannabidiol in tea infusion by high performance liquid chromatography**

Thoranin Yosbunruengsin\*, Thitiphan Chimsook, Anakhaorn Srisaipech, and Supaporn Sangsrichan\*\*

AC-P-60

**Chromatographic resolution of (+/-) -dimethyl *N,N*-dibenzyl-glutamate using modified silica with *N*-(pent-3-en-5-ol)ylglutarimide chiral selectors**

Varaporn Paradamit\*, Watcharapol Wong-iam, Tinnapat Thongngen, and Punlop Kuntiyong

AC-P-61

### **K9 Dogs sniff COVID-19 in Thailand trained by positive mixed biomarkers to improved screening test accuracy during pandemic**

Isaya Thaveesangsakulthai, Sorrawit Songsathitmetha, Pattama Torvorapanit, Kaywalee Chatdarong, and Chadin Kulsing\*

AC-P-62

### **Application of microbiology for COVID-19 volatile organic compounds biomarkers identification on surface swabbing and human secretion in Thailand community**

Isaya Thaveesangsakulthai, Sorrawit Songsathitmetha, Kanpat Vesessook, Pattama Torvorapanit, Naraporn Somboona, and Chadin Kulsing\*

AC-P-63

### **Derivatized alpha-cyclodextrin as gas chromatographic stationary phase for separation of chiral alcohols**

Atiptiya Sriprasit, Pinyada Jungkanjana, and Aroonsiri Shitangkoon\*

AC-P-64

### **Enhancing phenolic acid separation in capillary electrophoresis through surface modification using polyethyleneimine**

Nadia Mira Kusumaningtyas, Supa Wirasate, Apinya Obma, and Rattikan Chantiwas\*

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AC-P-65

### **Accuracy-based PT programs for determination of As, Cd and Pb in herbs**

Nunnapus Laitip\*, Usana Leekriangkrai, and Pranee Phukphatthanachai

AC-P-67

### **Method validation for determination of lead and cadmium in paper for food contact using microwave digestion followed by inductively coupled plasma mass spectrometry**

Netsirin Gissawong, Veerapat Ramanee, Warunrat Buranakul, Nootjarin Phonhong and Weera Suanthaisong\*



AC-P-68

**Using single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) for study silver nanoparticles (AgNPs) released from food packaging materials into different types of food simulants**

Kanokwan Dokprom, Kalyanee Sirisinha, and Atitaya Siripinyanond\*

AC-P-69

**Analysis of carbon-based microparticles released from plastic products with single particle inductively coupled plasma mass spectrometry**

Apinya Sakanupongkul, Kalyanee Sirisinha, Rattaporn Saenmuangchin, and Atitaya Siripinyanond\*

AC-P-70

**Using single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) for the study of zinc oxide nanoparticles suspension stability in various media**

Prawpan Pusuwan and Atitaya Siripinyanond\*

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AC-P-71

**Method validation for determination of heavy metals in alum (aluminium sulphate) by inductively coupled plasma mass spectrometer**

Inthuon Sukkseam, Jirasa Krongkrod\*, Sorada Khunhon, and Titiporn Wattanakul

AC-P-72

**Thailand reference material: TRM-F-2007 elements in turmeric powder**

Pranee Phukphatthanachai\*, Nunnapus Laitip, and Usana Leekriangkrai\*

AC-P-73

**Papain, as a specific removal treatment for conservative art**

Piyachat Sirikate, and Nichanan Sirasunthorn\*

AC-P-74

### Effect of catechin on the structures and activities of papain

Titinun Ubolsaard, Thidarat Jantho, and Nichanun Sirasunthorn\*

AC-P-76

### The removal of green and red reactive dyes by photolysis, oxidation and photooxidation processes using a simple UV reactor

Orawan Kritsunankul\*, Piyatida Kamlueng, Wanwisa Jaisarn, Tamisa Maporn, and Chanyud Kritsunankul

AC-P-77

### Development of a sensitivity enzyme-linked immunosorbent assay for detection of leucomalachite green

Rattawan Yoohanngoh and Siriwan Teepoo\*

AC-P-78

### One-step hydrothermal process for GO@FeO nanocomposite synthesis and characterization

Jirawan Khongyoo, Anurak Chitbuengphrao, Anchana Preechaworapun, Tanin Tangkuaram, and Kulwadee Pinwattana\*

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# Catalytic Chemistry (CC)

please access to the following QR code for abstracts

CC



## Oral Presentation

CC-O-01

### Uncovering insights in data-driven catalyst design: A case study in oxidative coupling of methane

Shun Nishimura\*, Xinyue Li, Junya Ohyama, and Keisuke Takahashi\*

CC-O-02

### Ethanol steam reforming using Ni catalyst supported on ZrO<sub>2</sub>-doped Al<sub>2</sub>O<sub>3</sub> with magnetic inducement

Marucheth Thongtheppairoj, Pattarika Tarawan, Sasimas Katanyutanon, and Pisanu Toochinda\*

CC-O-03

### Computational modeling of carbon monoxide oxidation on platinum supported on cerium dioxide

Iskra Z. Koleva, Hristiyan A. Aleksandrov, and Georgi N. Vayssilov\*

CC-O-04

### Chiral-induced spin selectivity effect at chiral-encoded Pt-Ir surfaces for enhanced oxygen reduction reaction

Zikkawas Pasom, Chularat Wattanakit\*, and Alexander Kuhn\*

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CC-O-05

### I-doped Bi<sub>2</sub>MoO<sub>6</sub> nanosheets for enhanced pollutant photodegradation and hydrogen evolution

Theeranun Siritanon\*, Anurak Wachayee, and Suwit Suthirakun

CC-O-06

### Role of incorporated metal/phosphorus acidity modification over low Si/Al ratio HZSM-5 catalysts in methanol-to-olefins process

Chotika Yoocham and Pattaraporn Kim-Lohsoontorn\*

CC-O-07

**Effect of manganese and magnesium promoter on catalytic hydrogenation of CO<sub>2</sub> over cobalt-based catalyst**

Sabaithip Tungkamani, Chutikan Tupmee, Jakkarin Hongsawong, and  
Saowaluk Intarasiri\*

CC-O-08

**Production of sustainable aviation fuel and green diesel from biodiesel via metathesis-deoxygenation over tungsten oxide based catalysts**

Mochamad Solehudin, Prataya Promchana, Kanokwan Wengwirat,  
Kittisak Choojun\*, and Tawan Sooknoi

CC-O-09

**Sol-gel preparation of copper cobaltite spinel for ciprofloxacin degradation via peroxymonosulfate activation**

Trung-Hieu Dinh and Minh-Vien Le\*

CC-O-10

**Cd<sub>0.5</sub>Zn<sub>0.5</sub>S/Bi<sub>2</sub>MoO<sub>6</sub> heterostructure for rhodamine B photodegradation under visible light**

Thitipong Choklap, Anurak Waehayee, Tharit Lerdwiriyanupap,  
Jeeranan Prachanat, and Theeranun Siritanon\*

## Poster Presentation

CC-P-01

### **Fabrication of metal-free g-C<sub>3</sub>N<sub>5</sub> photocatalyst for antibiotic removal in aqueous media**

Ngoc-Diem-Trinh Huynh, Huyen-Tran Tran, Chi-Hien Truong,  
Nhat-Mai Tran, Trung-Hieu Dinh, and Minh-Vien Le\*

CC-P-02

### **Synthesis of urea-derived Z-scheme photocatalyst LaFeO<sub>3</sub>/g-C<sub>3</sub>N<sub>4</sub> for tetracycline degradation under simulated natural irradiation**

Chi-Hien Truong, Ngoc-Diem-Trinh Huynh, Huu-Nhon Nguyen,  
and Minh-Vien Le\*

CC-P-03

### **Preparation of BiVO<sub>4</sub>/g-C<sub>3</sub>N<sub>4</sub> composite with enhanced visible-light-driven photocatalytic activity**

Tran-Huyen Tran, Pham-Ngoc-My Le, Triet-Han Ngo,  
and Minh-Vien Le\*

CC-P-04

### **Photocatalytic activity of N- and S-heteroatoms co-doped on graphene quantum dots under visible irradiation for degradation of organic dye**

Ilada Sanprasert, Okorn Mekasuwandumrong, and Joongjai Panpranot\*

CC

CC-P-05

### **The study of nanostructured graphitic carbon material prepared from sugarcane bagasse for chemical sensor**

Rawisara Tuncharoen and Patraporn Luksirikul\*

CC-P-06

### **A nanocellulose template for the controllable synthesis of hollow mesoporous aluminosilicate nanomaterials**

Panut Saelee and Karaked Tedsree\*



CC-P-07

**Solid acid catalyst development from rubber tire waste for biofuel and biochemical production**

Yanisa Doungkumchan and Sartrawut Tulapol\*

CC-P-08

**Bagasse heavy ash-derived Zn-loaded porous silica: Effects of bimodal mesopores on VOCs adsorption**

Kunpirom Chainarong, Waleeporn Donphai, and Metta Chareonpanich\*

CC-P-09

**Enhancing carbon capture efficiency: Optimization of ZIF-8 synthesis and integration into advanced adsorbent systems**

Kanoakwan Chanheeb and Pattaraporn Kim-Lohsoontorn\*

CC-P-11

**Tuning selectivity of Ni/Al<sub>2</sub>O<sub>3</sub> catalysts in CO<sub>2</sub> hydrogenation by incorporation of N, S-doped carbon**

Nipitpon Jarumalai, Suthasinee Watmanee, and Joongjai Panpranot\*

CC-P-12

**Tuning the morphology of PbBiO<sub>2</sub>Br nanosheets for photodegradation of methyl orange under visible light**

Jeeranan Prachanat, Anurak Wachayee, Thitipong Choklap, and Theeranun Siritanon\*

CC-P-13

**Catalytic LPG conversion over Ga/ZSM-5 zeolite catalyst: Effect of confined-space zeolite and external magnetic field**

Zehui Du, Waleeporn Donphai, and Metta Chareonpanich\*

## Poster Presentation

CC-P-14

**The use of copper phyllosilicate as a supported template to prepare  $\text{WO}_3/\text{SiO}_2$  catalyst for cross-metathesis of acetylene and ethylene**

Kanokwan Wengwirat, Pratya Promchana, Kittisak Choojun\*, and Tawan Sooknoi

CC-P-15

**Effect of pH precipitation on ceria–zirconia supported Ni-based catalyst via  $\text{CO}_2$  reforming of  $\text{CH}_4$  reaction**

Orrakanya Phichairatanaphong, Metta Chareonpanich, and Waleeporn Donphai\*

CC-P-17

**The study of magnetic inducement on Ni catalyst on  $\text{Gd}_2\text{O}_3\text{-CeO}_2$  doped  $\text{Al}_2\text{O}_3$  support for ethanol steam reforming**

Pattarachai Trongyuenyong, Patareesa Tulyapreecha, Sasimas Katanyutanon, and Pisanu Toochinda\*

CC-P-18

**Development of CaO promoted  $\text{Ni}/\text{Al}_2\text{O}_3$  catalyst for direct methanation of biogas into biomethane**

Jidapa Tatiyapantarak, Atthapon Srifa, Wanida Koo-Amornpattana, Choji Fukuhara, and Sakhon Ratchahat\*

CC

CC-P-19

**The production of fatty alcohol from methyl palmitate by selective hydrogenation over  $\text{CuMgAl}$  layered double hydroxide**

Chanisara Nooto, Warot Prasansang, Kittisak Choojan\*, and Tawan Sooknoi\*

CC-P-20

**Transesterification of refined palm oil with methanol catalyzed by anion-exchange resin in rotating packed bed reactor**

Rawipa Choknumchaisiri and Palang Bumroongsakulsawat\*



CC-P-21

**Effect of CH<sub>4</sub> impurity in flue gas feed on ethanol-assisted methanol synthesis from CO<sub>2</sub> hydrogenation over Cu-based catalyst**

Banthita Woraphan, Wen-Yueh Yu\*, and Pattaraporn Kim-Lohsoontorn\*

CC-P-22

**Conversion of amine-captured CO<sub>2</sub> to CaCO<sub>3</sub> by electrodialysis**

Wongchanok Chewathum and Palang Bumroongsakulsawat\*

CC-P-23

**Ternary photocatalyst based on ZnO for degradation of tetracycline antibiotic**

Khemika Wannakan and Suwat Nanan\*

CC

# Chemical Education (CE)

please access to the following QR code for abstracts





## Oral Presentation

CE-O-01

**Diagnosis of fundamental concepts of chemical basis of life among high school students**

Pongprapan Pongsophon

CE-O-02

**Promoting students' scientific explanation through the 6E STEM for BCG model on the topic of rate of reaction**

Parinya Mutcha and Chatree Faikhamta\*

CE-O-03

**Entrepreneurial STEAM-BCG in a cup: The development of high school student's sensemaking practices through dialogical argumentation with chemistry concepts**

Tharuesean Prasoplarb and Chatree Faikhamta\*

CE-O-04

**Using an esterification activity to enhance advanced placement (AP) chemistry students' competency in higher-order thinking (HOT)**

Sonthi Phonchaiya\* and Sanikan Saneewong

CE-O-05

**The effect of STEAM BCG through natural tie dye activities**

Tanchanok Poonsin and Ninna Jansoon\*

## Poster Presentation

CE-P-01

**The study on the conceptual changes in chemical equilibrium of science high school students using experimental-based learning**

Nuchutha Thamsumet

CE-P-02

**Intermolecular interactions that govern solute retention; thermodynamics learning in gas chromatography experiment**

Siriwit Buajarern\*, Kamonthip Sreenonchai, and Thetipat Phajan

CE-P-03

**An optimal representation of a small-scale chemistry experiment: A case of diffusion of substance lesson for 7th grade students**

Pongsaton Panyanukit\* and Chatree Faikhamta

CE-P-04

**Evaluating surface tension via smartphone-captured pendant drop method: Enhancing accuracy in simplified experimental designs**

Pannaporn Omee, Jutamas Changkian, Kanoksak Saelee, Akapong Suwattanamala, and Teeranan Nongnual\*

CE

CE-P-05

**Alcohol test kit: An integrated lesson in chemistry for high school students**

Sirihathai Srikwanjai, Sorachai Sae-Lim, and Duangkhae Srikun\*

CE-P-06

**Exploring betalain extraction from *Gomphrena globosa* L. as a green indicator in acid-base titration concepts**

Rattapol Meelapsom, Thitimaporn Kongkaew, Nattasa Kitchawengkul, Niyada Khunklong, Saksri Supasorn, and Purim Jarujamrus\*



CE-P-07

**Enhancing physical chemistry education: Active learning strategies, student engagement, and assessment alignment for successful learning outcomes**

Wissawat Sakulsaknimitr

CE-P-08

**Developing proficiency in applying exponential and logarithmic functions in the context of chemical kinetics for 11<sup>th</sup> grade students using the backward design teaching approach**

Sittichoke Som-am, Monsikarn Jansrang, and Usa Jeenjenkit\*

CE-P-09

**Environmental learning using problem-based learning and GLOBE protocol in the lotus field**

Usa Jeenjenkit and Weerawut Tiankao\*

CE-P-10

**Determination of ethanol content in disinfectant spray by color photo intensity measuring on mobile phone**

Metinee Mektan, Sasitorn Muncharoen, Sarayut Watchasit, and Jaray Jaratjaroonthong\*

CE-P-11

**A simple electrochemical experiment kit made from electrolyte gels**

Suchittra Channgan and Akapong Suwattanamala\*

# Environmental Chemistry and Renewable Energy (EE)

please access to the following QR code for abstracts



EE



## Oral Presentation

EE-O-01

### Microplastics and plastic additives in open dumping site soil from Thailand

Shinnosuke Yamahara, Voranop Viyakarn, Suchana Chavanich,  
Sujaree Bureekul, Atsuhiko Isobe, and Haruhiko Nakata\*

EE-O-02

### Preparation of porous biochar derived from avocado peel and its application on ciprofloxacin removal

Huynh Tran Hoang Thi, Tan Khanh Trinh Le, Suwadee Kongparakul,  
Chanatip Samart, and Thi Tuong Vi Tran\*

EE-O-03

### Minimize residual formaldehyde content in melamine-formaldehyde PCM microcapsules

Nichakorn Wangkajai, Apinan Soottitantawat, and Rungthiwa Methaapanon\*

EE-O-04

### Conversion of fat and oil contaminant waste produced by stationary wastewater treatment plant into calcium soap for ruminant feed

Aung Thae Oo and Suchat Leungprasert\*

EE

EE-O-05

### Exploring interphase instability in the LiTFSI-LiCl aqueous biphasic system through optical microscopy

Chalarat Chaemchamrat, Siraprapha Deebansok, and Olivier Fontaine\*

EE-O-06

### Nanostructured MoO<sub>2</sub>/MoS<sub>2</sub>/MoP heterojunction and N, S dual-doped reduced graphene oxide as high-performance electrode for supercapacitors

Kasira Kaewplod, Jeng-Yu Lin, Pimpa Limthongkul, and Panitat Hasin\*

EE-O-07

### **The fabrication of Ru<sub>2</sub>P nanoparticle decorated P-doped vegetable root-derived hierarchical porous carbon for supercapacitors with ultrahigh capacitance**

Sudarat Laihang, Pimpa Limthongkul, Jeng-Yu Lin, and Panitat Hasin\*

EE-O-08

### **Unveiling the potential of oxidative catalytic fractionation in spruce bark valorization**

Suthawan Muangmeesri, Daria Lebedeva, Lala Ramazanova, John Ralph, and Joseph S. M. Samec\*

EE-O-09

### **Conversion of food waste to a valuable soil resource in a day**

Apichat Junsod\*, Patomporn Pulsawad, Parichat Yamsri, and Sukhontha Silaart

EE-O-10

### **Comparative study of torrefaction and pyrolysis behavior on rice straw using thermogravimetry-mass spectrometry (TG-MS) technique**

Chakrya Theap, Penjit Srinophakun, Jatuporn Parnthong, Channarith Be, and Sanchai Kuboon\*

EE

EE-O-11

### **Copper calcium hydroxide nitrate derived from chicken eggshell and their catalytic activity in the removal of aqueous methylene orange**

Yiping Han, Taweechai Amornsakchai, Supakorn Boonyuen, and Siwaporn Meejoo Smith\*

EE-O-12

### **Photocatalytic degradation of organic dye and antibiotic by ZnO-based photocatalyst under natural solar light**

Suwat Nanan\* and Khemika Wannakan

EE-O-13

**Performance evaluation of phase change materials (PCMs) to improve energy saving potential of building**

Kanyamon Ausaman, Apinan soottitantawat, Rungthiwa Methaapanon\*

EE-O-14

**One-dimensional simulation of an alkaline-acid direct glycerol fuel cell**

Papitchaya Chaloeypanit, Supaporn Therdthianwong, and Apichai Therdthianwong\*

EE-O-15

**Simulation of hydrogen production from water-hyacinth with equilibrium reactors**

Sirikul Boonterm and Deacha Chatsiriwech\*

EE-O-16

**Unveiling novel mechanisms in energy storage materials with mimic battery concept**

Kulika Pithaksinsakul, Malinee Niamlaemand, Mathis Lorette, Siraprapha Deebansok, Dodzi Zigah, and Olivier Fontaine\*

EE

EE-O-17

**Efficient wastewater dye degradation using  $\text{Fe}_3\text{O}_4\text{-CuS@SiO}_2$  photocatalyst: Mechanism and performance**

Fatemeh Sadegh and Worawit Wongniramaikul\*

## Poster Presentation

EE-P-01

### Dual-analyte fluorescent chemosensor based on carbazole-based oxime for determinations of chlorpyrifos and $\text{Fe}^{3+}$

Punrada Thadatontichok and Krit Setthakarn\*

EE-P-02

### Fluorescence-based detection by using green-synthesized rutin and quercetin-modified gold nanoparticles

S. Boonyuen\*, S. Tantayanon, Y. Tangjaideborisut, P. Na Nakorn

EE-P-03

### Study of the content of particulate matter in office and working unit of Muban Chombueng Rajabhat University

Paitoon Mueanpetch\*, Juntima Donjuntai, and Khanatthapan Parnnarong

EE-P-04

### Synthesis of zeolite A from sugarcane bagasse ash and its application as a potential catalyst for amine solvent regeneration in $\text{CO}_2$ capture

Darunee Sukchit, Saisamorn Lumlong, Malee Prajuabsuk, Jitlada Deshativong, Prajakkit Rawee, Pharit Kamsri, Sasijuta Wattanarach, Pajaree Thavorniti, Bunjerd Jongsomjit, Natthawan Prasongthum and Pornpan Pungpo\*

EE

EE-P-05

### Synthesis of zeolite A from sugarcane bagasse ash and its application for adsorbent for removal of crystal violet dye

Jirawan Komuangmu, Wassana Soila, Patlada Boonsing, Darunee Sukchit, Saisamorn Lumlong, Malee Prajuabsuk, Jitlada Deshativong, Prajakkit Rawee, Pharit Kamsri, Sasijuta Wattanarach, Pajaree Thavorniti, Bunjerd Jongsomjit and Pornpan Pungpo\*

EE-P-06

### Synthesis of zeolite from industrial-waste coal fly ash for amine solution regeneration in $\text{CO}_2$ capture

Natthawan Prasongthum, Kritsakorn Janna, Banluesak Butphan, Darunee Sukchit, Amornrat Suemanotham, Lalita Attanatho, Pornpan Pungpo, and Yoothana Thanmongkhon\*



EE-P-07

**A prepared bio-sorbent from corn husk for the removal of crystal violet dye from aqueous solution**

Ornanong Aekkaphong, Chutima Yoothong, and Akapong Suwattanamala\*

EE-P-08

**Microplastic contamination in selected carbonated drinks in Thailand**

Napaphat Taechapattraporn, Panisara Suwannagate, Rattanaporn Suwansawang, Anh Tuan Ta and Sandhya Babel\*

EE-P-09

**Removal of chloride ions from wastewater through Friedel's salt chemical precipitation method**

Abhi Shrestha, Prakaidaw Panichvattana, Anh Tuan Ta, and Sandhya Babel

EE-P-10

**Decolorization and detoxification of solvent red 24 by *Bacillus* sp. FN1 producing laccase and lignin peroxidase**

Peraya Buapho and Sinthuwat Ritthitham\*

EE

EE-P-11

**Greenhouse gas-certified reference materials for tackling climate change in Thailand**

Kanokrat Charoenpornpukdee\*, Bunthoon Laongsri, Arnuttachai Wongjuk, Soponrat Rattanasombat, and Ratirat Sinweeruthai

EE-P-12

**A demonstration process of high quality biomass pellet produced from sugarcane wastes**

Pathompat Khowattana, Tosporn Phetyim, Apichat Junsod, Pathumrat Butniam, Natthawan Prasongthum, Amornrat Suemanotham, Yoothana Thanmongkhon, Chaiyan Chaiya and Lalita Attanatho\*

EE-P-13

### **A machine learning approach to gasification process model for environmental sustainability**

Kritsana Suwanamad and Phuet Prasertcharoensuk\*

EE-P-14

### **Efficient wastewater dye degradation using $\text{Fe}_3\text{O}_4\text{-CuS@SiO}_2$ photocatalyst: Mechanism and performance**

Fatemeh Sadegh and Worawit Wongniramaikul\*

EE-P-15

### **Effect of fuel type on the characteristics and photocatalytic activity of ZnO nanoparticles synthesized via solution combustion method**

Shabnam Purmahammad Abdollahi, Wuttichai Reainthippayasakul, and Karn Serivalsatit\*

EE-P-16

### **Purification of biomethanol synthesized from biogas by three stages distillation**

Rujira Jitrwung, Kuntima Krekkeitsakul\*, Nattawee Treerananont, Hiran Jinda, Parinya Thongyindee<sup>2</sup>, Sunisa Luadlai, and Boonsita Jantapoon

EE

EE-P-17

### **Flotation of surfactant-modified dispersive clay for the simultaneous removal of methyl orange and methylene blue from water**

Ngo Thi Thu Thao, Koki Kodama, and Tohru Saitoh

EE-P-18

### **High performance photodegradation of methyl orange with AgCl/Ag-impregnated glutaraldehyde-crosslinked alginate beads under sunlight irradiation**

Katananipa Wanchai\*, and Chaiwat Aiamsaard



EE-P-19

**Activated carbon derived from hemp core biowaste with a doped heteroatoms and large specific surface area for supercapacitor applications**

Pattaramon Meefang, Thanapat Jorn-am, Preeyanuch Supchocksoonthorn, and Peerasak Paoprasert\*

EE-P-20

**Development of pouch-cell Zn-ion battery using  $\text{MnO}_2$  synthesized from spent alkaline battery as cathode material**

Budsayamas kanthawong, Kamonpan Manowilaikun, Keeratipron Yoaharee, Kittima lolupiman, Rojana Pornprasertsuk\*

EE-P-21

**Preparation of composite polymer electrolytes based on poly (ethylene oxide) and cellulose nanofiber for solid-state zinc-ion batteries**

Weeraporn Treerittiwiattaya, Jitti Kasemchainan\*

EE-P-22

**Fabrication of  $\text{Sr}_2\text{Fe}_{0.9}\text{Ni}_{0.1}\text{MoO}_6$  anode supported solid oxide fuel cell by powder injection molding**

Kulanis Supprasert, Nutthita Chuankrerkkul, and Soamwadee Chianansutcharit\*

EE

EE-P-23

**Applying supercapacitors in emergency lights to extend their useful life**

Thanaporn Wongchanapiboon\*, Punika Yamsang\*, Natchapon Chuayin\*, and Peerasak Paoprasert

EE-P-24

**Preparation of bio-renewable corn starch-based electrolyte for a high performance, environmentally friendly supercapacitor**

Nichaphat Thongsai, Naruporn Jirawanichakun, and Peerasak Paoprasert\*

EE-P-25

### **Biodiesel production via the electrocatalytic process from pinari oil (*Sterculia foetida* L.)**

Anusorn Vorasingha

EE-P-26

### **Simulating cyclic voltammetry at porous electrodes considering faradaic and non-faradaic currents**

Vikrom Kiniman, Chanathip Kanokwhale, Phanuphong Boonto, Wasinee Pholauyphon, Kotchakarn Nantasaksiri, Patcharawat Charoen-amornkitt\*, Takahiro Suzuki, and Shohji Tsushima

EE-P-27

### **Topography optimized anode catalyst layer of polymer electrolyte membrane water electrolyzers under effects of gas coverage**

P Passakornjaras, P Orncompa, M Alizadeh, T Suzuki, S Tsushima, and P Charoen-amornkitt\*

EE-P-28

### **Effect of the hydroxyl groups in passivating molecules on the electronic quality of TiO<sub>2</sub> films**

Saranrat Asamo, Dharmendra Pratap Singh, Supa Hannongbua, and Pongthep Prajongtat\*

EE

EE-P-29

### **Improved hydrogen electrolysis in sodium hydroxide solution by stainless steel electrodes optimization**

Rujira Jitrwung\*, Kuntima Kreckeitsakul, Hiran Jinda and Parinya Thongyindee

EE-P-30

### ***In vivo* assessment and *in silico* prediction of estrogenic potency of endocrine disrupting chemicals using zebrafish (*Danio rerio*)**

Akira Kubota\*, Masashi Hirano, Yuka Yoshinouchi, Hisato Iwata, and Yusuke Kawai

# Food, Agriculture and Cosmetics (FA)

please access to the following QR code for abstracts



FA

## Oral Presentation

FA-O-01

### Development of coffee silver skin into food beverage and testing antioxidant activity

Kimsuy Vang, Assama Jewto, Wannika Jaipit,  
and Suddida Pliankarom Thanasupsin\*

FA-O-02

### Characteristics of pomelo cellulosepectin and its application in plant-based chicken nugget

Rattana Yooberg\*, Kamolwan Isrskarn, Janjira Buakaew,  
Pawadee Methacanon, and Chaiwut Gamonpilas

FA-O-03

### The application of coffee silver skin extract in pomegranate juice and study for its bioactivities

Thavy Kit and Suddida Pliankarom Thanasupsin\*

FA-O-04

### Construction and application of digital platform for predicting metabolism and toxicity of pesticides

Wenli Xu, Shuyang Jiang, Jia Li, and Jianhua Yao\*

FA-O-05

### The effect of ion exchange of clinoptilolite as a soil on the physiological response of radish

Yuri Kalvachev\*, Ermenegilda Vitale, Carmen Arena, Totka Todorova, Daniel Ilkov, and Violeta Velikova

FA-O-06

### Extracting bioactive protein from fish head using enzymatic hydrolysis

Poowanut Surachaisatikul, Polchanok Methakulnart, Photawan Chaoddee,  
and Supattra Supawong

FA



## Poster Presentation

FA-P-01

### Effect of solutions on retrogradation of cooked sticky rice

On-ong Chanprasartsuk, Kamolwan Jantranon, and Pornpen Atorngitjawat\*

FA-P-02

### Antioxidant activity of spent coffee ground and its extracts

Chitinsee Paidech and Chaleeda Borompichaichartkul\*

FA-P-03

### Fractionation of maltooligosaccharides from partial digested Hommali, Homnil and Sangyod rice starches

Wassaon Lerdkanjanapat, Sornsawan Sutthisamrueng,  
Suwapat Patarachayan, Tipaporn Subsomboon, Sukum Kositchaimongkol,  
and Pittaya Liewseeree\*

FA-P-04

### Pesticide residues in chilies collected from chili farms in Southern Thailand

Sujanya Jitlang\*, Panwadee Wattanasin, Kwanruthai Tadpetch,  
and Thitima Rujiralai\*

FA

FA-P-05

### Separation and partial purification of polysaccharides from mung bean meal using liquid extraction and non-chromatographic techniques

Monwadee Aiamsung, Lueacha Tabtimmai, Chanikan Sonklin, Phumin Chamsodsai, Kiattawee Choowongkamon, and Saranya Sedtananon\*

FA-P-06

### Sensomic approach characterization of odorants in fried chicken

Nattapon Deesom, Preecha Phuwapraisirisan, Suwimon Keeratipiboon,  
and Aphiniharn Phewpan\*

FA-P-07

### **Sensory attributes and antioxidant capacity of tomato meal extracts: A comparative analysis of enzymatic and ultrasonic extraction methods**

Pacharaporn Putthangkul, Phawinee Srinuan, Orrapun Selamassakul, Natta Laohakunjit, and Chanikan Sonklin\*

FA-P-08

### **Improvement of sensory attribute and antioxidant property of mungbean peptides by Maillard reaction**

Sarocho Sapcharoen, Nachomkamon Saengsuk, Natta Laohakunjit and Chanikan Sonklin\*

FA-P-09

### **Immobilization of transglucosidase enzyme via polymer-inorganic hybrid for isomaltooligosaccharide production**

Phassorn Khumfu, Areeya Phakpachai, and Yupin Phuphuak\*

FA-P-10

### **Encapsulation of turmeric extracts via complex emulsion-coacervation for active ingredients in dietary supplement foods**

Benjakarn Phungphian, Phassorn Khumfu, Phattaraphon Jampen, Waranya Rachayotha and Yupin Phuphuak\*

FA

FA-P-11

### **Optimized production of isomaltooligosaccharide prebiotics from homnin and sangyod rice flours by enzymatic hydrolysis processes**

Waranya rachayotha, Phassorn Khumfu, Ploypailin Buaban, Benjakarn Phungphian, and Yupin Phuphuak\*

FA-P-12

### **Evaluation of total phenolic contents and *in-vitro* antioxidant activity of hemp (*Cannabis sativa L.*) leaves extracts for its application in cosmetic product**

Nutlada Nusontra, Chakree Wattanasiri, Naphatsorn Ditthawutthikul, and Acharavadee Bunkoom\*



FA-P-13

**Evaluate the green tea quality through post-fermentation  
utilizing *Eurotium cristatum*, MFUTB001**

Daria Hayesalea, Antikan Klomchit, Phattharasaya Rattanawongkun,  
Nattakan Soykeabkaew, and Siraprapa Brooks\*

FA-P-14

**Evaluation of the chemical contents of avocado oil extracted with  
coconut oils for cosmetic application**

Wassana Sangkhara, Nutlada Nusontra, Chakree Wattanasiri,  
and Acharavadee Bunkoom\*

FA-P-15

**Development and optimization of spray-dried kaffir lime peel  
essential oil microparticles using emulsion stabilized by modified  
Cassava Starch**

Nipaporn Rungjitvaranont, Rattiya Tangratniyom, Sirapat Jitanawasan,  
and Suthida Boonsith\*

FA-P-16

**Method validation of QuEChERS-GC- $\mu$ ECD method for  
pyrethroid pesticides analysis in mango**

Padungrat Toopmuang, Pattama Prangchan and Juthathip Thepsit

FA

FA-P-17

**Exploration approach to differentiate Khao Dawk Mali 105 rice  
located in the northern and northeastern region of Thailand based  
on Rb, Sr, Mo, Mg, P, K analyzed by ICP-MS.**

Wiranee Sriwiang\*, Piriya Kacopookum, and Nantanat Chailanggar

FA-P-18

**Unveiling MUS-7: A promising domain antibody for combating  
*Klebsiella pneumoniae* infections**

Pattamawan Rerkprakhon, Kanyanat Kongrin, Kiattawee Choowongkamon,  
and Lueacha Tabtimmai\*

FA-P-19

**Analysis of manganese, cobalt, copper and arsenic in unpolished rice (*Oryza sativa* L.) using inductively coupled plasma mass spectrometry (ICP-MS)**

Sirirat Sookkham, Ratchadawan Tamklang, Chunyapuk Kukusamude, and Supalak Kongsri\*

FA-P-20

**Determination of heavy metals in honey using inductively coupled plasma mass spectrometry (ICP-MS)**

Ratchadawan Tamklang, Sirirat Sookkham, Supalak Kongsri, Chunyapuk Kukusamude\*, and Kanokporn Boonsirichai\*

FA-P-21

**Optimization of lignin-loaded nanostructured lipid carrier using box-behnken design**

Krittin Intaraopart, Suthida Boonsith, and Warangkana Pornputtapitak\*

FA-P-22

**Fungal endophyte isolated from nibung palm (*Oncosperma* sp.) enhances the growth rate of red coral lettuce (*Lactuca sativa* L.)**

Sutarat Nitdanklang, Machima Saengket, Antikan Klomchit, and Siraprapa Brooks\*

FA-P-24

**Preparation and properties of wet wipes from water hyacinth**

Worakrit Chanai, Jamecharun Srikeaw, Ketsak Trerawaranun, and Sa-ad Riyaja\*

FA-P-25

**Preservation of plums (*Prunus salicina*) via the application of edible packaging films developed from tapioca starch/gelatin incorporating Hass avocado extract**

Van-Huy Tran, Trong-Phuc Pham, Thi-Quynh-Nhu Tran, Thi Tuong Vi Tran\*, and Thi-Van-Linh Nguyen\*

FA



FA-P-26

**Preparation of complex carrier from aloe vera mucilage/gelatin for kaempfer essential oil**

Supathida Patthanaprasitchai, Athitaya Boonmas and Jirada Singkhonrat\*

FA-P-27

**Effect of cooking process on physicochemical and biological properties of resistant starch content in Jasmine rice cultivated in saline soil area**

Kwanyuen Leamsamrong, Piyanete Chantiratikul,  
Walaiporin Tongjaroenbuangam, and Noppakun Pakdeenarong\*

FA-P-28

**$\alpha$ -Glucosidase inhibitory activity of *Cyperus rotundus* rhizome extracts**

Lalita Pimsawang, Vasakorn Bullangpoti, and Wanchai Pluempunupat\*

FA-P-29

**Evaluation of enzyme inhibitory activity of *Ganoderma lucidum* (antler shaped lingzhi fruiting body) extracts**

Apisara Bungarat, Prapassorn Rugthaworn, Udomlak Sukatta\*,  
and Wanchai Pluempunupat\*

FA

FA-P-30

**Algal-based protein: Tempeh produced from *Cladophora glomerata* (Sarai-Kai)**

Kangsadan Boonprab\*, Kitima Wongreanrod, and Yanutsara Wongpukdee

FA-P-31

**The effect of ethanol and water ratios of star fruit (*Averrhoa carambola*) extract on total phenolic, total flavonoid, tartaric acid contents and an inhibitory of tyrosinase activity**

Arunrat Sunthitikawinsakul\*, Rapeepan Kongtoom,  
and Wanpen Saengthongpinit

FA-P-32

### **Analysis of carnosine and anserine from the black chicken Nin-Kaset by high performance liquid chromatography**

Chalita Kaewkhow, Chokwan Chumang, Tharinee Saleepoch,  
Piboon Pantu, Patraporn Luksirikul, Prapasiri Pongprayoon, Thanathip  
Suwanasopee , Skorn Koonawootrittriron\* and Sutasinee Kityakarn\*

FA-P-33

### **Efficiency of commercial tea against *Escherichia coli* and *Staphylococcus aureus***

Mantana Boonnucht, Paweena Kumpai, Kotchapon Martpaijit, Rawinan  
Chanthabut, Siriporn Pranee, Jiravich Methewiroon, Sirapan Sukontasing,  
Patamaporn Umnahanant<sup>1</sup>, and Sirinit Tharntada\*

FA-P-34

### **Preparation and physical properties of cassava starch/poly (vinyl alcohol)/clay nanocomposite films**

Saad Riyajan\* and Nopporn Poolyarat

FA

# Inorganic Chemistry (IC)

please access to the following QR code for abstracts



IC

## Oral Presentation

IC-O-01

### Highly dispersed and stable palladium(II) species anchoring on ethylenediamine-grafted-MIL-101(Cr) for styrene oxidation

Nuttapong Makmeesub, Kittisak Choojun\*, Chonlada Ritvirulh,  
and Tawan Sooknoi

IC-O-02

### Biodegradable polyester composites, containing various metal oxide particles: A model study as shelf-life extendable packaging for bananas

Nattawut Yuntawattana

IC-O-03

### A low-cost SFX-based hole transporting material for perovskite solar cells

Jeeranun Manit, Pongsakorn Kanjanaboos, and Supavadee Kiatisevi\*

IC-O-04

### Switchable metal-ion selectivity in sulfur-functionalised pillar[5]arenes and their host-guest complexes

Bunyaporn Todee, Patharaporn Sanae, Araya Ruengsuk, Pattarapapa Janthakit, Vinich Promarak, Jonggol Tantirungrotechai, Mongkol Sukwattanasinitt, Taweetham Limpanuparb, David J. Harding, and Thanthapatra Bunchuay\*

IC-O-05

### Pillararene supramolecular assembly in supramolecular organic frameworks (SOFs) and mechanically interlocked molecules (MIMs)

Pipatpong Laoviwat, Korawit Khamphaijun, David J. Harding, and Thanthapatra Bunchuay\*

IC

IC-O-06

### Synthetic studies and the applications of BINOL coordinated metalloporphyrins

Shafikul Islam, Masatoshi Ishida, and Ken-ichi Sugiura\*

IC-O-07

**Neutral isocyanide-templated assembly of pillar[5]arene [2] and [3]pseudorotaxanes**

Korawit Khamphaijun, Phitawat Namnouad, Andrew Docker, Araya Ruengsuk, Jonggol Tantirungrotechai, Raúl Díaz-Torres, David J. Harding, and Thanthapatra Bunchuay\*

IC-O-08

**Development of chiral metal complexes coordinated by axial chiral ligands exhibiting circularly polarized luminescence**

Daiki Tauchi, Masashi Hasegawa, Yasuhiro Mazaki, Kazunori Tsubaki, Ken-ichi-Sugiura, and Hiroyuki Nishikawa\*

## Poster Presentation

IC-P-01

### Spectroscopic evidence of heme and antimalarial drugs interaction

Chaipat Lapinee\*, and Nitipol Srimongkolpithak

IC-P-02

### The adsorption efficiency of composited magnetic biochar for tetracycline adsorption in an aqueous solution

Sukrit Pemmakitti, and Thitipone Suwunwong

IC-P-03

### Hydrothermal preparation of heteroatoms doped mangosteen peel carbon dots and their sensing abilities

Pongsiri Rueangprat and Chomchai Suksai\*

IC-P-04

### Titanium complexes of phenoxy-azo and phenoxy-imine ligands: A comparative study for the ring-opening polymerization of rac-lactide and $\epsilon$ -caprolactone

Wasan Joopor, and Pimpa Hormnirun\*

IC-P-05

### Controlled and effective ring-opening (co)polymerization of rac-lactide, $\epsilon$ -caprolactone and $\epsilon$ -decalactone by $\beta$ -pyrimidyl enolate aluminum complexes

Sirawan Kamavichanurat, Kunamon Jampakeaw, and Pimpa Hormnirun\*

IC-P-06

### Enhanced aerobic alcohol oxidation activity of multinuclear copper catalysts featuring amine-bis(triazoyl) ligands

Attawit Jehdaramarn, Teera Chantarojsiri, Kitipong Chainok and Preeyanuch Sangtrirutnugul\*

IC



IC-P-07

**Preparation of lead tree wood composite with zeolite NaA, NaX, NaP**

Rachata Jaikla, Chalida Upan, Panot Krukkratoke, Chalermpan Keawkumay, and Jatuporn Wittayakun\*

IC-P-08

**Aluminum complexes of tridentate [ONN]-phenolate ligands the ring-opening polymerization of rac-lactide and  $\epsilon$ -caprolactone**

Kunanon Jampakaew, and Pimpa Hormnirun\*

IC-P-09

**Synthesis of silver nanoparticles using carboxymethyl cellulose from water hyacinth biomass for the colorimetric detection sensor of Hg (II) ions**

Panida Thepwat, Apichart Saenchoopa, Wipada Onnet, Sirinan Kulchat, and Suppanat Kosolwattana\*

IC-P-10

**Titanium complexes bearing tridentate [ONN]-phenolate ligands for the ring-opening polymerization of cyclic ester monomers**

Suppakan Vongfak, and Pimpa Hormnirun\*

IC

IC-P-11

**A study of N-heterocyclic imidazolium-functionalized cage-like silsesquioxane on transition metals as a catalyst**

Wannipa Phansuwan, and Vuthichai Ervithayasuporn\*

IC-P-12

**Facile synthesis of silsesquioxane appended with 1,8-naphthalimide benzo-15-crown-5 chemosensor**

Boonsita Chanyong, Pattara Siripanich, and Vuthichai Ervithayasuporn\*

IC-P-13

### Synthesis of zeolite sodium A, X, Y from silica gel bead

Chalida Upan, Ratchata Jaikla, Panot Krukkratoke, Chalermpan Keawkumay,  
and Jatuporn Wittayakun\*

IC-P-14

### Electrochemical self-coupling of benzyl halides catalyzed by cobalt complex with pincer based ligand

Pornwimon Kongkiatkrai and Teera Chantarojsiri\*

IC-P-15

### The effect of polyethylene glycol chain length of nickel bis(aminomethyl)pyridine on hydrogen evolution reaction

Kanrawee Dechdang and Teera Chantarojsiri\*

IC

# Industrial and Engineering Chemistry (IE)

please access to the following QR code for abstracts



## Oral Presentation

IE-O-01

### Synthesis of silicon carbide by using rice husk ash from power plant wastes

Benchanaree Singrattananaphan and Anurak Petiraksakul

IE-O-02

### Development of neural network architectures for prediction of energy consumption and carbon dioxide emission in natural gas separation process

Bhiranat Pongsri and Pornchai Bumrungsri\*

IE-O-03

### Heat transfer analysis of a microwave reactor using computational fluid dynamics for polymer recycling

Aung Khant Zaw, Issadaporn Wongwanichkangwarn, Hidetoshi Sekiguchi, Somboon Otarawanna, and Tanyakarn Treeratanaphitak\*

IE-O-04

### Beyond the extraction limit – molecular cages as membranes for chemical separations

Jiratheep Pruchyathamkorn\*, Laura M. Torrente, and Jonathan R. Nitschke

IE



## Poster Presentation

IE-P-01

### Investigation of dyeing polyester with disperse dyes in an oil/water dual-phase system

Praifon Puangsing, Jantip Setthayanond, and Potjanart Suwanruji\*

IE-P-03

### Effect of fly ash to alkali activator ratios on pore properties of porous fly ash-based geopolymer under curing by microwave irradiation

Komchan Meecharoen, Khanthima Hemra, and Sirithan Jiemsirilers\*

IE-P-05

### Amino acid fertilizer derived from poultry bio-waste

Natdanai Supawongchuwinit and Supakit Achiwawanich\*

IE-P-06

### Ion exchange capacity and ionic conductivity of polyvinyl alcohol and nanocellulose based anion exchange membranes

Piyamad Kaewkoon, Supatta Midpanon, and Pinsuda Viravathana\*

IE

IE-P-07

### The opinion of citizens on governance management of the very small solid waste power plant in Thailand

Suwannee Missita and Wisakha Phoochinda

IE-P-08

### Synthesis of biphasic calcium phosphate porous ceramic from fish scales

Laksana Wangmooklang\*, Parawee Pumwongpitak, Saengdoen Doungdaw, Siriporn Tong-On, and Siriporn Larpmkiattaworn

IE-P-09

### **Preparation and characterization of oil palm fibers from oil palm trunks for industrial applications**

Parawee Pumwongpitak\*, Sureeporn Kumneadklang, Busarin Noikaew, Laksana Wangmooklang, Saengdoen Daungdaw, and Siriporn Larпкиattaworn

IE-P-10

### **Effect of grog and cement on physical and mechanical properties for unfired brick production**

Soravich Mulinta

IE

# Material Chemistry and Nanotechnology (MN)

please access to the following QR code for abstracts



MN

## Oral Presentation

MN-O-01

**Asymmetric D-A-D' type hybridized local and charge transfer fluorophores as deep-red/near-infrared emitters for efficient non-doped OLEDs**

Teerapat Itsoponpan, Wijitra Waengdongbung, Taweesak Sudyodsuk, and Vinich Promarak\*

MN-O-02

**Boosting OLEDs performance via hot exciton mechanism: The study of heteroatom and different the number of donor unit effects on D- $\pi$ -A type emitters**

Takdanai Unjarern, Chokchai Kaiyasuan, Suangsiri Arunlimsawat, Panida Surawatanawong, Teera Chantarojsiri, Vinich Promarak, Taweesak Sudyodsuk, and Nopporn Ruangsapapichat\*

MN-O-03

**Development of near-infrared phosphorescent organoiridium(III) complexes bearing 2-arylquinoxaline-based cyclometalated ligands**

Ryuta Shikura, Keima Yoneda, Naoya Suzuki, Shintaro Kodama, Takeshi Maeda, Shigeyuki Yagi\*, and Seiji Akiyama

MN-O-04

**Facile synthesis of highly active and durable carbon composite as a non-precious metal oxygen reduction reaction electrocatalyst in alkaline media**

Kittimaporn Nernprom, Jakkid Sanetuntikul, Nattawan Pitipuech, Apichat Saejio, Noppavan Chanunpanich, Chedhawut Poompipatpong and Kriangsak Ketpang\*

MN-O-05

**Preparation and characterization of MoS<sub>2</sub>/lignin-based carbon nanocomposite fibers for supercapacitor electrodes**

Kamonluk Sirikarint, Autchara Pangon, and Thitirat Inprasit\*

MN

MN-O-06

**Solution plasma-assisted integration of Mxene nanosheets with iron and nitrogen-doped carbons as electrocatalysts for oxygen reduction reaction**

Kasidit Janbooranapinij, Wisit Hirunpinyopas, and Gasidit Panomsuwan\*



MN-O-07

**Parameter optimization for the synthesis of hybrid gold nanoparticle-carbon dot colloids and their luminescent properties alteration**

Thammika Srisaman, Dakrong Pissuwan, and Anyarat Watthanaphanit\*

MN-O-08

**Development of colloidal cellulose nanocrystal suspensions as a sprayable PM<sub>2.5</sub> remover**

Benyapha Kheawmanee, Parinton Jangtawee, and Tewarak Panklang\*

MN-O-09

**Colorimetric sensing of polymers by using polydiacetylene/zinc (II) ion/zinc oxide nanocomposites: Effects of solvents and cationic surfactant**

Sasiwan Boonmak, Rakchart Traiphol\*, and Nisanart Traiphol\*

MN-O-10

**Polydiacetylene-based materials for colorimetric sensing of fatty acids**

Nannapat Kaewnukulkit, Nisanart Traiphol, and Rakchart Traiphol\*

MN-O-11

**Quercetin mediated Ag@Au core-shell nanoparticles: Synthesis, characterization and applications**

Amtul Qayoom, Neha Kanwal, Shaz Asrar, Saeeda Nadir Ali, and Dilshad Hussain

MN-O-12

**Synthesis of gold nanoparticles supported on carbon nanomaterials via solution plasma sputtering as electrochemical sensors for mercury(II) ion detection**

Jidapa Chantaramethakul, Wisit Hirunpinyopas, and Gasidit Panomsuwan\*

MN-O-13

### Synthesis and characterization of nitrogen-doped carbon dots from bird's nest for heavy metal detection

Supakorn Boonyuen\*, Paramasivam Shanmugam, A. Lim Teik Zheng, Siwaporn Meejoo Smith, Teeraphat Prachayanipon, and Weeraphat Praphasmontien

MN-O-14

### Voltammetry of paraquat-based bismuth nanoparticles screen-printed electrodes for environmental surveillance

Porntip Khownarumit\*, Patima Phumsathan, Sirimarn Ngamchana, Wachira Chaiworn, Warinthorn Detpisuttitham, and Patsamon Rijiravanich

MN-O-15

### pH-Responsive polymer as a new stable solid electrolyte interphase for water-in-salt battery

Rossukon Jommongkol, Nantawat Kaekratoke, Yachao Zhu, Tobias Burton, Siraprapha Deebansok, Daniel Crespy\*, and Olivier Fontaine\*

MN-O-16

### Preparation and characterization of silver nanowires/cellulose nanofibrils-based conductive paper

Noppamas Thongsiri, Saowaluk Inpaeng, Chaisak Issro, and Karaked Tedsree\*

MN-O-17

### Plasmon enhancement of photodetectors based on CsPbBr<sub>3</sub> quantum dots

Zar Ni Thein Htay, Chaturika Madhuwanthi, Sakoolkan Boonruang, and Shu-Han Hsu\*

MN

MN-O-18

### Influence of chemical surface-treatment agent on mechanical and neutron-shielding properties of recycled high-density polyethylene (r-HDPE)/gadolinium oxide (Gd<sub>2</sub>O<sub>3</sub>) composites

Donruedee Toyen, Ekachai Wimolmala, Kasinee Hemvichian, Pattra Lertsarawut, and Kiadtisak Saenboonruang



MN-O-19

**Metal-organic chalcogenolates – An emerging family of low-dimensional hybrid semiconductors**

Watcharaphol Paritmongkol

MN-O-20

**Bio-CaCO<sub>3</sub> from *Perna viridis* shells for plant coating**

Orakanya Kumphon, Chutiparn Lertvachirapaiboon, Sanong Ekgasit, and Tewarak Parnklang\*

MN-O-21

**Microstructural modification of nickel aluminium bronze against erosion corrosion**

Methawat Keereerakwattana and Napachat Tareelap\*

MN-O-22

**Synthesis of RGB fluorescent helical network polymers in chiral liquid crystals and evaluation of their circularly polarized luminescence**

Hiromasa Yamamoto, Satoru Yoshida, Keita Horie, Kosuke Kaneko, Tomonori Hanasaki, and Kazuo Akagi\*

MN-O-23

**Synthesis of achiral fluorene derivatives exhibiting circularly polarized luminescence induced in chiral nematic liquid crystal medium**

Yuki Fujita, Keita Horie, Kosuke Kaneko, Tomonori Hanasaki, and Kazuo Akagi

MN

## Poster Presentation

**MN-P-01**

**Activated biocarbons prepared by chemical activation of cashew nut shells as potential electrode materials for supercapacitors**

Myo Myo Thu, Veeramuthu Vignesh, Nattapat Chaiammart, Thandavarayan Maiyalagan, and Gasidit Panomsuwan\*

**MN-P-02**

**Cobalt/nitrogen-doped carbons derived from teak sawdust as low-cost and stable electrocatalysts for oxygen reduction reaction in fuel cells**

Jirayu Kongtip, Thandavarayan Maiyalagan, and Gasidit Panomsuwan\*

**MN-P-03**

**Synthesis of  $\text{MnO}_2/\text{C}$  composite from spent alkaline battery by one-step hydrothermal process for rechargeable Zn-ion battery application**

Auscha Thongsri, Kamonpan Manowilaikun, Keeratipron Yoaharee, and Rojana Pornprasertsuk\*

**MN-P-04**

**Mesoporous carbons synthesized via solution plasma process: A potential electrode material for mesoscopic perovskite solar cells**

Chanatip Sungprasit, Myo Myo Thu, Masakazu Nakamura, Pongthep Prajongtat, and Gasidit Panomsuwan\*

**MN-P-05**

**Improving photocatalytic efficiency of zinc oxide immobilized on glass slides by using plasma surface modification**

Pamika Na-Ranong, Yuttida Sangsri, Watis Kongchanpat, Darapond Triampo, and Duangkhae Srikun\*

**MN**

**MN-P-06**

**Synthesis of chemically activated carbons from waste macadamia shells through potassium hydroxide activation for symmetric supercapacitors**

Nattapat Chaiammart, Ariya Taechamahaphan, Parinya Chakartnarodom, Wichit Prakaypan, and Gasidit Panomsuwan\*



MN-P-07

**Formulation a catechol-based copolymer for the creation of MXene dispersible in organic solution**

Jeongmin Kim, Jemin Yeon, Seongmin Park, Young Ho Park, and Insik In\*

MN-P-08

**Organic ligand enhanced MXene based water dispersible polymer composite as a source for hybrid aerogel fabrication**

Jemin Yeon, Jeongmin Kim, Seongmin Park, Young Ho Park, and Insik In\*

MN-P-09

**Organic processing and applications of MXenes: Surface-modified ligand library**

Seongmin Park, Jeongmin Kim, Jemin Yeon, Young Ho Park, and Insik In\*

MN-P-10

**Wireless preparation of Ni-Ag alloyed janus objects using bipolar electrochemistry**

Oranit Phuakkong\* and Suttisuk Plongnui

MN-P-11

**Synthesis of mesoporous silica film from sodium silicate by electrochemically assisted self-assembly method**

Thida Ounjaidee, Krittanun Deekamwong, Nichakorn Pornnongsan, Sudarat Sombatsri, and Sanchai Prayoonpokarach\*

MN-P-12

**High surface area electrode for direct CO<sub>2</sub> capturing in air**

Theeratrorn Treeintong and Chaiya Prasittichai\*

**MN-P-13**

**Surface modification of titanium with poly(amidoamine) dendrimer and its impact on bacterial adhesion and biofilm formation**

Wanida Wattanakaroon\*, Kidtiya Boonkasam, Rossanee Fordsoongnern, Yanisa Jongrakwit, and Nareenart Sripho-on

**MN-P-14**

**Green synthesis of ultrasound-assisted Fe<sub>3</sub>O<sub>4</sub>/berry extract nanocomposites for enhanced antibacterial activity and 4-NP reduction reaction**

Supakorn Boonyuen\*, Paramasivam Shanmugam, Chayanut Samanram, and Chuthathip Phutthikit

**MN-P-15**

**Green synthesis of gold nanoparticles from macadamia nut shell extracts and their antioxidant, antibacterial and catalytic activities**

Supakorn Boonyuen\*, Paramasivam Shanmugam, A. Lim Teik Zheng, S. Tantayanon, Siwaporn Meejoo Smith, and P. Yugala

**MN-P-16**

**Green preparation method of silver nanoparticles for cosmetic applications**

Nakadech Youngwilai\* and Suttinun Phongtamrug

**MN-P-17**

**Preparation of silver nanoparticles by orange peel extract for antibacterial paper packaging**

Warisara Petphisit, Piyada Sailen, Pitt Supaphol, Narumol Kreua-ngarjnuakool, and Saowapa Thumsing Niyomthai\*

**MN**

**MN-P-18**

**Enhanced adsorption of ceftriaxone antibiotic from hospital wastewater by modified granular activated carbon**

Attajaree Smata, Chayanin Hanwarinroj, Areerat Kanarat, Eknarin Thanayupong, Sineenat Thaiboonrod, Peerakarn Banjerdkiij, Saowaluk Chaleawlwert-umpon, and Nuttaporn Pimpha\*



MN-P-20

**Development of the cellulose microcrystalline as a potential carrier of biologics delivery**

Phatheera Kachai and Chaiya Prasittichai\*

MN-P-21

**Cationic chitosan-fluorescein tagged BSA nano-delivery system**

Jirayu Sudchada\*, Theerachart Leepasert, and Thitinun Karpkird

MN-P-22

**Microwave-assisted green synthesis of gold nanoparticles using amino acids and their antibacterial and catalytic activities**

Supakorn Boonyuen\*, T. Therdkiet, T. Sanyawut, S. Tantayanon, and Siwaporn Meejoo Smith

MN-P-23

**Carbon dots from latex using microwave-assisted pyrolysis for tyrosine detection**

Thanathip Sitthichot and Sirilux Poompradub\*

MN-P-24

**Development of antibacterial and wound dressing hydrogels based natural biopolymer composite with curcumin stabilized gold nanoparticles-loaded nanoliposome**

Apichart Saenchoopa, Sarawut Lapmanee, La-or Somsakeesit, and Sirinan Kulchat\*

MN-P-25

**Morphology-controlled microwave synthesis of tetragonal copper bismuth oxide with needle-like flower architecture**

Rapeepat Muankaew, Chompunut Banphot, Punyanuch Thammaacheep, and Duangdao Channei\*

**MN-P-26**

### **Microwave synthesis of nitrogen and boron co-doped carbon dots from ascorbic acid**

Antika Boonruanganan, Karn Serivalsatit, and Wuttichai Reainthippayasakul\*

**MN-P-27**

### **Effect of graphene quantum dots in enhancing plant growth and anti-oxidant activity of mung bean**

Warawut Kongseangchai\*, and Joongjai Panpranot\*

**MN-P-28**

### **One-pot synthesis of magnetic activated carbon by consecutive hydrothermal pretreatment and pyrolysis of cassava rhizome for methylene blue adsorption**

Jenjira Phuriragpitikhon\*, Warinda Fuangchoonuch, Kittiya Pluamjai, and Laemthong Chuenchom

**MN-P-29**

### **Synthesis and characterization of cellulose aerogel composite from pineapple leaves and polyvinyl alcohol**

Arisa Jaiyu\*, Julaluk Phunnoi, Passakorn Sueprasit, and Niphaporn Yawongsa

**MN-P-30**

### **The study of rheological properties of silk fibroin in ionic liquids**

Tanissara Pinijmontree\*, Sathish K. Sukumaran, Masataka Sugimoto, Adisak Takhulee, and Yoshiaki Takahashi

**MN**

**MN-P-31**

### **The metal nanoparticles coupling with carbon quantum dots via solution plasma discharge and embedding in metal-organic frameworks for dye degradation**

Sasimaporn Treepet, Chayanaphat Chokradjaroen, Kyusung Kim, Nagahiro Saito, and Anyarat Watthanaphanit\*



MN-P-32

### **Fabrication and characterization of MOF-808/PVDF films**

Nathakrit Trianreal and Jonggol Tantirungrotechai\*

MN-P-33

### **ZIF-8 synthesis for oil removal from water surface**

Wachirapun Punkrawee\*, Nimit Palee, and Amornpon Changsuphan

MN-P-34

### **Trimethylamine adsorption and host-guest interaction within UiO-66-NH<sub>2</sub> framework**

Aimwipa Sasiprapa, Ketsiree Sooncharoen, Thomas M. Roseveare, Chadchalerm Ruksakoon, and Ramida Rattanakam\*

MN-P-35

### **Pomelo peel nanocellulose for pickering stabilization of oil-in-water emulsion**

Kanthida Bunyapong, Naphatson Chanthathamrongsiri, and Karaked Tedsree\*

MN-P-36

### **Performance of lignin as eco-friendly reinforced filler in dental adhesives**

Siripatsorn Maimansomsuk, Thanamas Koolthi, Pannaree Srinoi, Chomdao Sinthuvanich, and Khrongkhan Akkarachaneeyakorn\*

MN

MN-P-37

### **Preparation of activated carbon from spent coffee grounds by radiation processing for methylene blue adsorption**

Phunkamon Khantiakarapat, Jariyaporn Sangkaworn, Threeraphat Chutimasakul, and Jonggol Tantirungrotechai\*

MN-P-38

### **Surface modification of porous titanium complex with bioactive RGD for bone tissue regeneration**

Jirut Meesane, Si Thu Myint Maung, Kantida Juncheed, and Pemikar Srifa\*

MN-P-39

### **The effect of calcination temperatures on NIR reflection of lateritic soil pigments**

Chumphol Busabok\*, Wasana Khongwong, Sittichai Kanchanasutha, and Yotin Kallayalert

MN-P-40

### **Optimizing color conversion and luminance enhancement in ultra-thin films through aerosol-deposited perovskite quantum dot/metal oxide composites**

Changmin lee, Seokwoo kang, Hyukmin Kwon, and Jongwook Park\*

MN-P-41

### **White electroluminescence emission using perovskite nanocrystals and organic emitters**

Hyukmin Kwon, Sunwoo Park, Hayoon Lee, Changmin lee, and Jongwook Park\*

MN-P-42

### **Hydrogels containing liquid crystal droplets for stretchable display applications**

Teerapat Lapsirivatkul, Daniel Crespy, and Pichaya Pattanasattayavong\*

MN

MN-P-43

### **Encapsulation of *Mitragyna speciosa* (Roxb.) korth. using coaxial electrospray technique**

Chutatip Tongped, Prapatsorn Pansawat, Natchaya Sawatdirak, and Nisalak Trongsirawat,\*



MN-P-44

**X-ray absorption studies on emerald and jade-like glass prepared from glass waste**

Sivapa Sukluntanasorn, Pawanrat Nakniam, Warunphorn Kungkapradit, Kamolwan Samkongngam, and Radchada Buntam\*

MN-P-45

**Effect of flux treatment process on photocatalytic dye degradation of aluminium-doped strontium titanate**

Natruja Towiratkit, Thanakorn Wasanapiarnpong, Wuttichai Reainthippayasakul, Noppakhate Jirabornvornpongsa, and Pornapa Sujaridworakun\*

MN-P-46

**Effect of shape stabilizers on properties of calcium chloride hydrate composite phase change materials for solar cell cooling**

Peerakarn Mongkolsin, Karn Serivalsatit, and Thanakorn Wassanapiarnpong\*

MN-P-47

**Corrosion inhibition studies of tamarind shell tannins on mild steel in acidic medium**

Abdalmajid Abdullahi and M. Hazwan Hussin\*

MN

# Natural Products, Biological Chemistry and Chemical Biology (NP)





## Oral Presentation

NP-O-01

### NMR-based stability evaluation of (*E*)-1-(3,4-dimethoxyphenyl)butadiene (DMPBD) from *Zingiber cassumunar* Roxb. rhizome

Boonwiset Seaho, Chatkamon Lekwongphaiboon, Wichayasith Inthakusol, Saisuree Prateepthongkum, Wacharee Harnying, Albrecht Berkessel, and Nongnaphat Duangdee\*

NP-O-02

### Molecular docking simulation tool CB-Dock2 confirmed high binding affinity between curcuminoids and IkBa/p50/p65 protein complex

Sompot Jantarawong and Yutthana Pengjam\*

NP-O-03

### *In silico* and *in vitro* studies on nucleoside-based inhibitors for pan-antiviral drug repurposing

Pitchayathida Mee-udorn, Pornthip Aunbamrung, Jaraspim Narkpuk, Peera Jaruampornpan, Suppachoke Onnome, Amporn Suphatrakul, Bunpote Siridechadilok, Chanya Srisaowakarn, Suwimon Manopwisedjaroen, Arunee Thitithanyanon, Tanaporn Uengwetwanit, and Nitipol Srimongkolpithak\*

NP-O-04

### Chemical constituents and their biological activities from the rhizomes and leaves of *Curculigo orchoides*

Phornnapa Saentao, Ratsami Lekphrom, Sarawut Tontapha, and Florian T. Schevenels\*

NP-O-05

### Immobilized chitinase as an effective biocatalytic platform for producing bioactive chitobiose from biomass-derived chitin

Ailada Charoenpol, Daniel Crespy, Albert Schulte, and Wipa Suginta\*

NP

## Poster Presentation

NP-P-01

### Effects of mangosteen peel extract against *Staphylococcus aureus* and *Candida parapsilosis*

Nahathai Weerapatiwat, Apichaya Kwansud, Yossakorn Kerdpon, Srisuda Pannanusorn\*, and Worawat Surarit

NP-P-02

### Antibacterial effect of *Syzygium aromaticum* essential oil against normal flora on the skin

Nitchakarn Phimthong, Jomkwan Meerak, Churdsak Jaikang, Nitwara Wikan, Wutigri Nimlamoon, and Saranyapin Potikanond\*

NP-P-03

### Selection of the membrane for centrifugal ultrafiltration and protein profile analysis of human primary keratinocyte secretome

Natthakit Bunkam and Kwanchnok Viravaidya-Pasuwat\*

NP-P-04

### Live-cell imaging of intracellular esterases using a rhodol-based fluorescent ester surrogate substrate

Tanatorn Boonklang\* and Palangpon Kongsaree\*

NP-P-05

### Alpha-glucosidase inhibition of major cannabinoids from the leaves of *Cannabis sativa*: preliminary results, isolation, bio-assay, and kinetic study

Khoa Nguyen-Anh, Sutida Othapornchai, Areeba Nayab, and Preecha Phuwapraisirisan\*

NP

NP-P-06

### Bacterial cellulose for wound dressing with preventing infection with Mangosteen peel (*Garcinia mangostana*) and Pa Thalai Chon (*Andrographis paniculata*) extracts

Jiratchaya Threerodjanataworn\*, Pattarawadee Hongthong\*, Passawuth Nopphakunwong\*, Thirawatthana Pharamat, and Chanan Phonprapai

NP-P-08

**First report of indole-3-carbinol in vegetables from local market, Southern Thailand**

Supinya Tanyaros\*, Pinyapat Petchpan, Pimchana Rojanahasadin, Kosin Teeparuksapun, and Nicha Prasongchan

NP-P-09

**Total phenolic content and antioxidant activity of *Brassica napus* var. *pabularia* (Red Russian Kale)**

Sukanya Keawsa-ard and Patcharaporn Saengratwatchara\*

NP-P-10

**A novel organic fluorescent molecule for protease enzyme detection**

Kittiporn Nakprasit and Anawat Ajavakom\*

NP-P-11

**Chemical constituents from the roots of *Zygotelma benthamii***

Tanakiat Chompupong, Florian T. Schevenels, Thanaset Senawong, and Ratsami Lekphrom\*

NP-P-12

**New chromone from the stems of *Harrisonia perforata***

Thawatchai Sriwongsa, Waraluck Chaichompoo, Wachirachai Pabuprapap, and Apichart Suksamrarn\*

NP

NP-P-13

**Antibiotic resistance progress and challenges among gram-negative and gram-positive pathogens in Southern Thailand: A retrospective 10-year study**

Phanvasri Saengsuwan\*, Narongdet Kositpantawong, Soontara Kawila, and Wichien Patugkaro

NP-P-14

### **Fabrication and releasing of anonaine encapsulated in sodium alginate beads**

Pantharee Kaewvichien, Chayapol Kaewsakul, Boonyisa Pechkao, and Nopparat Plucktaveesak\*

NP-P-15

### **A comparison of TLC and HPLC methods for the quantitative analysis of mitragynine in Kratom products**

Sirithorn Srithorn, Namphet Seekham, Thanapich Santiwat, Nakorn Niamnont, Atitaya Samontha, and Nilubon Sornkaew\*

NP-P-16

### **Isolation and screening of antimicrobial properties of the actinobacteria isolated from Thailand**

Koech Samson and Amit Jaisi\*

NP-P-17

### **Inhibition of *Staphylococcus aureus* biofilm formation by natural coumarins**

Nattaruja Raksasat, Suphat Chantawarin, Natthapat Sawektreeratana, Sakchai Hongthong, Chutima Kuhakarn, and Chutima Jiarpinitnun\*

NP-P-18

### **Syntheses of curcumin derivatives and their biological activity against *Staphylococcus aureus***

Krit Ruechai and Chutima Jiarpinitnun\*

NP

NP-P-19

### **Siamfuranones B and C, two new furanone derivatives from the flowers of *Uvaria siamensis***

Awat Wisetsai\*, Florian T. Schevenels, Supachai Jadsadajerm, Ratsami Lekphrom, and Nuttapon Yodsin



NP-P-21

**Heterologous expression of *aristolochene synthase* and its site-directed mutagenized form from *Menisporopsis theobromae* BCC 4162 in *Aspergillus oryzae* NSAR1**

Thirat Anumon, and Pakorn Wattana-Amorn\*

NP-P-22

**Biosynthetic study of alternapyrone: A highly methylated polyene  $\alpha$ -pyrone**

Inthira Tapeng, Jaiyfunghong Phakeovilay, and Pakorn Wattana-Amorn\*

NP-P-23

**Dicarboxylic acids as substrates for a new type III polyketide synthase from *Cavenderia subdiscoidea***

Nattapong Dedkad, Sukhita Sathinaitham, Supachai Vuttipongchaikij, Passorn Wonnapijij, and Pakorn Wattana-Amorn\*

NP-P-24

**Heterologous expression of the fungal reducing polyketide synthase genes in *Aspergillus oryzae***

Thanakorn Deelee and Pakorn Wattana-Amorn\*

NP-P-26

**LC-ESI-MS based structural elucidation of major chemical compounds in *Boesenbergia rotunda* (L.) Mansf. ethanol extract and its antioxidant activity**

Laksana Charoenchai\* and Thaniya Wunnakup

NP

NP-P-27

**Inhibition effect of cytochrome P4502A6 enzyme mutant alleles 7 (CYP2A6\*7) activity by Luteolin**

Weeraphat Hassa, Supattra Boonruang, and Songklod Sarapusit\*

NP-P-28

**Computational studies of inhibitory effect of brazilin and hematein from *Caesalpinia sappan* Linn. against *Cutibacterium acnes***

Manceenuch Pengsawang, Apaporn Boonmee, Phoom Chairatana, and Prapasiri Pongprayoon\*

NP-P-29

**The binding mechanism of Atazanavir to drug-resistant HIV protease: A simulation study**

Phonphiphat Bamrung, Borvornwat Toviwek, and Prapasiri Pongprayoon\*

NP-P-30

**The computational studies of Rilpivirine – resistant HIV Reverse Transcriptase for drug design and development**

Narumon Wanluer, Borvornwat Toviwek, and Prapasiri Pongprayoon\*

NP-P-31

**Metabolite profiling of *Spirodela* by LC-QTOF**

Wacharakorn Patumanon, Kyoya Onishi, and Witcha Imaram\*

NP-P-32

**Chemical profile of hexane fraction of hydrosol from fresh *Wolffia globosa***

Ratchaphon Lertchaiyongphanit and Witcha Imaram\*

NP-P-33

**Bioactive substances in the Peel of immature *Dictyophora indusiata* mushrooms expressed antioxidant and anti-tyrosinase properties**

Sebian Yusbani, Wuttisak Kunu, and Supawadee Patathananone\*

NP-P-34

**Extraction, preliminary phytochemical screening and antioxidant properties of ethanolic crude extract of Madan (*Garcinia schomburgkiana* Pierre)**

Supraanee Pimpila, Worawat Chanmin, Irawan Cheunangul, and Winai Oungpipat \*

NP

# Organic Synthesis and Medicinal Chemistry (OM)

please access to the following QR code for abstracts



OM

## Oral Presentation

OM-O-01

### Stannylation as the key strategy for the synthesis of C2-substituted cordycepin derivatives for antiviral drug development

A. Thiraporn, P. Mee-udorn, R. Thiabma, N. Sooksai, S. Onnome, A. Suphatrakul, T. Uengwetwanit, B. Siridechadilok, and N. Srimongkolpithak\*

OM-O-02

### Synthetic study of natural antimalarial, (+)-febrifugine, from D-glucose and D-serine: Development of new pathways via azide and azide free approaches

Suwanan Uipanit and Nutthawat Chuanopparat\*

OM-O-03

### Amination of 1,2,4-oxadiazol-5(4H)-ones with tertiary amines

Mookda Pattarawarapan, Muh Alfiadhi, Nittaya Wiriya, Surat Hongsibsong, and Wong Phakhodee\*

OM-O-04

### Comparison synthesis of picric acid from phenol and salicylic acid for crystallization of mitragynine as picrate salt at difference percent purity

Suntisuk Sinthunakorn and Muhammad Niyomdechachai\*

OM-O-05

### Synthesis and evaluation of chrysin derivatives as histone deacetylase inhibitors

Thitiporn Kamloon\*, Narissara Namwan, Thanaset Senawong, Pakit Kumboonma, Somying Leelasubcharoen, and Chanokbhorn Phaosiri

OM-O-06

### Structural simplification of maytansine and synthesis efficiency for antitumor activity

Tomomi Uchida, Mayuka Fujimoto, Maina Minamino, and Masaki Kuse\*

OM



OM-O-07

**Syntheses and mechanistic investigations of formamides, formamidines, and formimidates**

Chhorvy Kong\*, Piyabutr Wanichpongpan, and Kittichai Chaiseeda

OM-O-08

**Synthetic and chiroptical studies on novel fluorophores based on chiral bipyrenyl platform**

Reichi Kobayashi\*, Syunso Robert Kozuma, Masatoshi Ishida, Masashi Hasegawa, Yasuhiro Mazaki, Yasuyuki Araki, Takehiko Wada, and Ken-ichi Sugiura\*

OM-O-09

**Gallic acid encapsulated Pamam dendrimers: A promising antioxidant delivery system for controlled release and reduced toxicity**

Aorada Sripunya, Chuda Chittasupho, Alexander Angerhofer, and Witcha Imaram\*

OM-O-10

**Synthesis of azanorbornadienes as building blocks to complex aryl products**

Thomas Whatton, Dr Ben Emery, Dr James Taylor, and Prof. Steven Bull\*

OM-O-11

**Synthesis and properties of helical oligothiophenes anchored to binaphthyl**

Hikari Kawashima, Masashi Hasegawa\*, and Yasuhiro Mazaki\*

OM

## Poster Presentation

OM-P-01

### Development of visible-light-induced hydrogen atom transfer (HAT) process as a tool for C–H functionalization of indole derivatives

Prakansi Naksing, Rungroj Saruengkhanphasit, and Worawat Niwetmarin\*

OM-P-02

### Synthetic and theoretical study on the homodimerization mechanism of coumarin derivatives

Kristina B. Simeonova, Ana I. Koleva, Anna-Mariya R. Zlatanova, Nevena I. Petkova-Yankova, Hristiyan A. Aleksandrov, Petko St. Petkov, and Rositca D. Nikolova\*

OM-P-03

### Synthesis of ceramide IIIB, a natural skin protective lipid barrier, from commercially available protected L-serine

Punyisa Laovilas and Nutthawat Chuanopparat\*

OM-P-04

### Investigation of the aqueous-mediated green synthesis of squarate esters and squarate thioesters

Siraporn Soonthonhut and Peera Acharasatian\*

OM-P-05

### Synthesis, structural modification and biological activity evaluation of triazole derivatives derived from S-benzylhomocysteines

Teesuda sirichai and Nutthawat Chuanopparat \*

OM-P-06

### An *In Silico* study of phloretin as a potential of class I glucose transporters inhibitor for targeted hepatocellular carcinoma treatment

Worarat Boonpech, Pemikar Srifa, and Kantida Juncheed\*

OM



OM-P-07

**Applications of methyl itaconate-anthracene adducts as chiral resolving agents for binaphthol derivatives**

Wichai Saema, Puracheth Rithchumpon, Nopawit Khamto,  
and Puttinan Meepowpan\*

OM-P-08

**Cyclodextrin conjugated fluorescein dye for drug delivery**

Kanniga Poatchongrak\* and Thitinun Karpkird

OM-P-09

**Synthesis and characterization of gallic acid derivatives for investigating antioxidant properties**

Sorachai Sae-Lim, Chanjira Jaramornburapong,  
and Muhammad Niyomdecha\*

OM-P-10

**The synthesis of benzazepine analogs via intramolecular ritter reaction**

Suthimon Boonmee\*, Gunniga Tanomsiri, Jumreang Tummatorn,  
Charnsak Thongsornkleeb, and Somsak RuchirawatSomsak Ruchirawat,  
and Nopporn Thasana\*

OM-P-11

**Phospha-1,4-addition promoted highly regioselective cyclization of *N*-propargyl azlactone: Unprecedented synthesis of benzopyrroloazepine**

Papitchaya Patangwasa, Takumi minami, Naiyana Saesian,  
Rattana Worayuthakarn, Somsak Ruchirawat, and Nopporn Thasana\*

OM

OM-P-12

**Synthesis and anticancer evaluation of indolo[1,2-*a*]quinoline derivatives**

Kredmanee Yimnoi and Paiboon Ngermmeesri\*

OM-P-13

**Potential of flavonoids from Thai natural products as SARS-CoV-2 3CLPro inhibitor: *In silico* and experimental perspectives**

Nopawit Khamto, Panida Boontawee, Kraikrit Utama, Atchara Janthong, Suriya Tatieng, Supakorn Arthan, Chavi Yenjai, Padchanee Sangthong, Nutee Suree, and Puttinan Meepowpan\*

OM-P-14

**A novel synthetic approach to 2,3-diaryl-1,3-thiazolidin-4-ones and their anticancer activity**

Chaiyawat Aonsri\*, Arnatchai Maiuthed, and Kittisak Sripha

OM-P-15

**Synthesis and molecular docking studies on SAR-CoV-2, AChE and MPO inhibitors of chalcone-caffeine hybrids**

Napasawan Chumnavej\*, Kulyada Charnrit, Rachanon Manakom, Pornthip Wanpen, Kamolchanok Kitpaiboonwattana, and Sunan Kitjaruwankul

OM-P-16

**The synthesis of phenanthrene-9-ols *via* palladium-catalyzed annulation**

Kamonlak Chatrangsan\*, Phornphan Yongpanich, Charnsak Thongsornkleeb, Jumreang Tummatorn and Somsak Ruchirawat

OM-P-17

**Development of the cobra antivenom production efficiency by using radioactive tracer techniques**

Wiranee Sriwiang\*, Piriya Kaeopookum, Sarinya Wongsanit, Nantat Chailangar, and Wanpen Rangsawai

OM-P-18

**Studies toward the synthesis of dibenzo[*b,f*]azepine derivatives**

NorAsian Boosaman and Paiboon Ngermmeesri\*

OM



## Poster Presentation

OM-P-19

### Design, synthesis, and biological activity evaluation of novel colchicine derivative as anticancer agent

Gbenga Olorunmodimu, Takorn Chow, and Tanatorn Khotavivattana\*

OM-P-20

### Acid-catalyzed formylation reaction of indole derivatives with trialkyl orthoformate

Kiratipong Charoensawas, Jirapat Yimyaem, and Jaray Jaratjaroonphong\*

OM-P-21

### Development of a PSMA-11 lyophilized kit for convenient radiolabeling with $^{68}\text{Ga}$

Boon-Uma Jowanaridhi\*, Thidarat Kohud, Kanyapat Lumyong, Suppamat Makjan, Chonticha Phaophang, and Sudkanung Phumkem

OM-P-22

### Toward the synthesis of dauphinol B, a novel antimalarial natural product

Pichaipol Tungtaweekool and Nutthawat Chuanopparat\*

OM-P-23

### Chemical synthesis research of sea urchin feeding inhibitory substances

Saki Tanaka and Masaki Kuse\*

OM

OM-P-24

### The modified formula of aggregated human albumin in lyophilization form (MAA-Cold kit) by adding human albumin solution.

Thidarat Kohud\*, Wanpen Rangsawa, Sanguansak hykunya, Boon-Uma Jowanaridhi, Krittika Somruedee, Kanyapat Lumyong, Suppamat Makjan, Chotiwid Wiriyaachailerd, Sudkanung Phumkem, Siriwat Thida, and Chonticha Phaophang

OM-P-25

**Design, synthesis, and evaluation of  
*N*<sup>2</sup>-phenylurea-*N*<sup>4</sup>-aminoquinazolines targeting  
*Plasmodium falciparum* histone lysine methyltransferase**

Nattakarn Pobsuk, Tanapa Srito, Jennifer Riley, Mark C. Anderson,  
Nicole Mutter, Lauren Webster, Supa Hannongbua\*, Duangkamol Gleeson,  
Kanokthip Boonyarattanakalin, Kevin D. Read and M. Paul Gleeson\*

OM-P-26

**Synthesis and structural modification of thymidine derivatives via  
multicomponent Pd-catalyzed coupling reaction**

Kamonwan Jaithum and Nutthawat Chuanopparat\*

OM-P-27

**Production and quality control of <sup>177</sup>Lu-PSMA for prostate  
cancer treatment**

Suppamat Makjan\*, Kanyapat Lumyong, Chotiwid Wiriyaichalerd,  
Sudkanung Phumkem, Boon-Uma Jowanaridhi, and Thanete Duangta

OM-P-28

**Radiolabeling of DFO-NCS and DFO\*-NCS siderophore chelator  
with zirconium-89 radiometal**

Kanyapat Lumyong\*, Thidarat Kohud, Suppamat Makjan, Thanete Duangta,  
Boon-Uma Jowanaridhi, Chotiwid Wiriyaichalerd, Sudkanung Phumkem,  
Siriwat Thida, Wiranee Sriwiang, and Piriya Kaepookum

OM-P-29

**The development of new azobenzene derivatives within  
three-colors range absorption for biological applications**

Waraporn Pimboonma, Chanikan Wongkaew,  
Tonman Lim-o-pas Phannoudej, Nuttakorn Jewyeen,  
and Nopporn Ruangsapapichat\*

OM-P-30

**Diastereoselective synthesis of  
spiro[indolizidine-oxindole]-isoxazolidine via  
tandem Cope oxidation/[3+2]-nitron cycloaddition**

Sasipa Booranamonthol, Phongsathon Khlengkhlao, Sucharat Sanongkiet,  
Jitnapa Sirirak, and Punlop Kuntiyong\*

OM



## Poster Presentation

OM-P-31

### Synthesis of dibenzylamino derivative of (+)-and (-)-chabamide

Phongsathon Khlongkhlaeo, Thorfan Saelim, Nanthanapas Madphol,  
Ratikorn Sangwirat, and Punlop Kuntiyong\*

OM-P-32

### Asymmetric heptamethine cyanine photosensitizer for near-infrared photodynamic cancer therapy

Onnichia Khaikate, Kantapat Chansaenpak, and Anyanee Kamkaew\*

OM-P-33

### Synthesis and $\alpha$ -glucosidase inhibitory activity of bis-coumarin derivatives

Tipanan Wisarutwanit and Wanchai Pluempanupat\*

OM

# Polymer Chemistry and Bio-Based Materials (PC)

please access to the following QR code for abstracts



PC



## Oral Presentation

PC-O-01

**A study of pre-vulcanization time affected on the nano-porous structure preservation in silica aerogel/natural rubber composite**

Chayanan Boonrawd\*, Thutiyaporn Thiawong, Ittipol Jangchud,  
and Darapond Triampo

PC-O-02

**Production and characterization of cellulose powders from brewery' spent grain**

Kawalee Kumpangnil and Sasithorn Kongruang\*

PC-O-03

**Development and characterization of amidated pectin-PVA hydrogels for enhanced drug delivery and antimicrobial properties**

Supatcha Suankhe, Woranart Jonglertjunya, Warangkana pornputtapitak,  
and Suthida Boonsith\*

PC-O-04

**Comparison properties of hybrid carbon-based nanocomposites between engineering-thermoplastic acrylonitrile-butadiene-styrene and commodity-thermoplastic polypropylene for electrical and thermal application**

Sorawit Duangsripat\*, Pajaera Patanathabutr, and Nattakarn Hongsriphan

PC-O-05

**Apatite growth of bioactive glass containing elephant dung cellulose**

Phimmada Nithipongwarodom, Kasamol Phomsombut,  
and Radchada Buntum\*

## Poster Presentation

PC-P-01

### **Tumor microenvironment modulation using nano-formulated drug for cancer immunotherapy**

Jung Min Shin\*, Sung Ryong Kim, and Hongkyeong Kim

PC-P-02

### **Exploring electrohydrodynamically printed organic semiconductors for high-performance solution-processed organic field-effect transistors and integrated logic devices**

Tae Kyu An, and Jihoon Lee\*

PC-P-05

### **Release characteristic of Curcumin (Zingiberaceae) from sodium alginate and polyvinyl alcohol-based hydrogel composite: Antioxidant properties**

Thanyaluck Thanyacharoen \*, Piyachat Chuysinuan, Supanna Techasakul, Pongpat Sukhavattanakul, and Sarute Ummartyotin\*

PC-P-05

### **Preparation of hyaluronic acid-PVA-cyclodextrin biocompatible film**

Kunyalux Stapornpiriyadaj\* and Thitinun Karpkird

PC-P-06

### **Hyaluronic acid conjugated amino-beta-cyclodextrin schiff base hydrogels for drug control releasing**

Parichat Sutthisawatkul\*, Theerachart Leepasert, and Thitinun Karpkird

PC-P-07

### **Preparation and properties of poly(vinyl chloride) composites recycled from used peritoneal dialysis solution containers and reinforced with silane-treated pineapple leaf fibers**

Bongkodporn Khonpet and Nonsee Nimitsiriwat \*

PC



PC-P-08

**Dyeing silk fabric with natural dyes from *Garcinia dulcis* (Roxb.) Kurz bark**

Napawan Martjarern<sup>1</sup>, Pacharapol Sirisoontorn, Pornpen Atorngitjawat, and Kanitta Watcharaporn\*

PC-P-09

**Natural and synthetic fibers on mechanical properties and degradation of fiber cements**

Piyalak Ngernchuklin\*, Wuttinai kokkamhang, and Suwatchai Thongnoi

PC-P-10

**Bacterial cellulose from kombucha for oil adsorption**

Sira Amatsaena, Supak Suksawat, Chanunthon Chanawit, Phoom Sangsuwan\*, and Kamonchanok Phoonsawat\*

PC-P-11

**Simulated gastrointestinal digestion of microencapsulated *Lactobacillus salivarius* culture in biopolymer**

Kiattisak Kaewkaenkhun, Thitinun Pradubsang, and Sasithorn Kongruang\*

PC-P-12

**Chitosan coated on magnetic nanoparticles for a simple *Escherichia coli* detection**

Kamonluck Witthayasutthaphon, Piyaporn Na Nongkhai, and Thanida Trakulsujarithchok\*

PC-P-13

**Preparation of carboxymethylcellulose (CMC)-polyethylene glycol (PEG) hydrogel for the growth of plants**

Pattrawadee Toprangkobsin

PC-P-14

### **Preparation of HPMC/chitosan blend films incorporated with chrysin and wintergreen essential oil for strawberry preservation**

Thussanee Mananunsap and Nopparat Plucktaveesak\*

PC-P-16

### **Mechanical properties of hybrid fibers paper sheet from pineapple leaf fiber and banana fiber for packaging**

Borwon Narupai\*, Arisa Jaiyu, Malinee Leekrajang, Nattaporn Chutichairattanaphum, Teerakorn Kongkaew, Julaluk Phunnoi, Niphaporn Yawongsa, and Passakorn Sueprasit

PC-P-17

### **Preparation of microcrystalline cellulose from corn cob and synthesis of microcrystalline cellulose-derived polyol for polyurethane foam**

Sudarat Kulabphet, Chanchai Thongpin, and Sudsiri Hemsri\*

PC-P-18

### **Study and development process for reed dyeing with *Garcinia Mangostana* Linn. leaves dyes extraction**

Katsinee Nammakorn, Pornpen Atorngitjawat, and Kanitta Watcharaporn\*

PC-P-19

### **Hybrid interpenetrating polymer networks of $\kappa$ -carrageenan/poly(vinyl alcohol) films**

Kamonwan Kanphai, Anan Athipornchai, and Thanida Trakulsujaritchok\*

PC-P-20

### **Investigation of mechanical properties on TPS/PLA bio-plastic composite with oil palm fiber**

Busarin Noikaew\*, Punthinee Somwongsa, Saengdoen Doungdaw, Sureeporn Kumneadklang and Siriporn Larpiattaworn

PC



PC-P-21

**Enhancing the mechanical properties of pineapple leaf fiber paper sheets with a dispersing agent**

Malinee Leekrajang\*, Nattaporn Chutichairattanaphum, Borwon Narupai, and Teerakorn Kongkaew

PC-P-22

**Developing hydrophobic cellulose fibers from pineapple leaves for oil absorption**

Nattaporn Chutichairattanaphum\*, Malinee Leekrajang, and Borwon Narupai

PC-P-23

**Synthesis of conjugated network polymers from thieno[3,4-b]pyrazine derivatives**

Prapassorn Ongjaroon, Worawan Bhanthumnavin, and Yongsak Sritana-Anant\*

PC-P-24

**Volatile organic compound absorption and photocatalytic degradation of natural rubber foam with modified TiO<sub>2</sub> composites**

Sassawat Mailaecciad, Siriluk Chiarakorn, and Yeampon Nakaramontri\*

PC-P-25

**Effects of plasticizers on light transmission of silk fibroin films**

Sitthichai Audtoom and Supranee Kaewpirom\*

PC

PC-P-26

**Preparation of levan from *B. subtilis* under different cultivation conditions**

Pornpun Aramsangtienchai\* and Warisara Raksachue

PC-P-27

### **Production of nanocellulose from green algae**

Anurak Khiewchaon, Kanitta Watcharaporn, and Pornpen Atorngitjawat\*

PC-P-28

### **Silk yarn dyeing with extracted dye from spent coffee grounds using a moka pot**

Wanrudee Kaewmesri\*, Nattida Pinjai, Manat Jaimasith, and Sorachai Khamsan

PC-P-29

### **Utilization of silk sericin as an ingredient in acne hydrogels: effects of tea tree oil on the inhibitory effect against *Staphylococcus aureus***

Patchareeya Khaopenyai, Waraporn Phokka and Supranee Kaewpirom\*

PC-P-30

### **Influence of functionalized graphene on properties of short glass fiber reinforced polyamide12 composites**

Nattakarn Hongsriphan\* and Pajaera Patanathabutr

PC-P-31

### **Investigation of physicochemical properties of pomegranate extract loaded nanoliposome for cosmetic application**

Punyaporn Thongprasert, Thanyaluck Thanyacharoen, Piyachat Chuysinuan\*, and Supanna Techasakul\*

PC

# Physical and Theoretical Chemistry (PT)

please access to the following QR code for abstracts



## Oral Presentation

PT-O-01

**The development of a new hypothetical MOF database for high-efficiency MOFs targeted for CO<sub>2</sub> utilization**

Poobodin Mano and Supawadee Namuangruk\*

PT-O-02

**Computational investigation of double-atoms catalysts decorated on defective boron nitride for catalyzing CO oxidation: A DFT study**

Ratchadaree Intayot and Siriporn Jungsuttiwong\*

PT-O-03

**Enhanced formic acid production through catalytic CO<sub>2</sub> hydrogenation on frustrated Lewis pair functionalized UiO-67**

Pimjai Pimbaotham, Yuwanda Injongkol, Siriporn Jungsuttiwong\*, and Nuttapon Yodsin\*

PT-O-04

**A DFT study on a single transition metal doped C<sub>3</sub>N for oxidation reaction**

S. Kamchompoo, M. Kunaseth\*, and S. Jungsuttiwong\*

PT-O-05

**The effect of non-metal doped graphitic carbon nitride for carbon dioxide reduction reaction: A DFT study**

Wassana Mongkonkan, Kaito Takahashi, Supawadee Namuangruk\*, and Siriporn Jungsuttiwong\*

PT-O-06

**Enhancing carbon dioxide reduction through single and dual heteroatoms doped diamond: A DFT study**

Yuwanda Injongkol, Rui-Qin Zhang, Pemikar Srifa, Alejandro Montoya\*, Thanyada Rungrotmongkol\*, and Siriporn Jungsuttiwong\*

PT

PT-O-07

**How many water molecules react with simplest Criegee intermediates at atmospheric conditions?**

Kaito Takahashi

PT-O-08

**Enhancing  $V_2O_5$  cathodes in magnesium-ion batteries through aqueous electrolyte-induced hydrogen insertion:  
A first-principles approach**

Panupol Untarabut, Sirisak Singesen, Lappawat Ngamwongwan, Ittipon Fongkaew, Anchalee Junkaew\*, and Suwit Suthirakun\*

PT-O-09

**Roles of reactants for Suzuki C-C cross-coupling reaction using molecular volcano plots**

Kwanchanok Kaewkwan, Vudhichai Parasuk, and Boodsarin Sawatlon\*

PT-O-10

**Molecular docking and dynamic simulations of anti-apoptotic Bcl-2 proteins as targets for bioactive compounds in *Durio Zibethinus* for anti-cancer activity**

Ayomi Vidana Pathiranage, Kulpavee Jitapunkul, Pisanu Tooichinda, and Luckhana Lawtrakul\*

## Poster Presentation

PT-P-01

### **Transient luminescence studies for excited-state kinetics of organic sensitizer dyes in solar cells**

Kanon Ie and Koichiro Mitsuke\*

PT-P-02

### **Modeling metal-atom-based hydrogen storage materials in the presence of non-inert gaseous species**

Ming-Jia Chiu, Po-Ching Huang, and Cheng-chau Chiu\*

PT-P-03

### **Structural investigation on chiral recognition of dapoxetine enantiomers with methylated cyclodextrins**

Arthiwath Anyamaneearmornrath, Chetsada Thanin, Potcharadanai Pitakannop, Nat Triamchaisri, and Luckhana Lawtrakul\*

PT-P-04

### **Chiral recognition of terbutaline enantiomers with $\beta$ -cyclodextrin and its three methylated derivatives: Molecular modeling approaches**

Yodfa Jantam, Sasicha Namkeaw, Nat Triamchaisri, and Luckhana Lawtrakul\*

PT-P-05

### **Cross-docking, ONIOM and molecular dynamic studies of potent antiviral HIV-1 nonnucleoside reverse transcriptase inhibitors**

Suwicha Patnin, Arthit Makarasen\*, Pongsit Vijitphan, Apisara Baicharoen, and Supanna Techasakul

PT-P-06

### **A DFT study on cracking and dehydrogenation of propane on H-ZSM-5**

Natthatida Khanom and Tanin Nanok\*

PT



PT-P-07

**Investigating electronic and phosphorescent characteristics in cycloplatinated complexes through DFT/TD-DFT analysis: Insights for OLED applications**

Wilaiwan Rosungnoen, Supa Hannongbua, and Songwut Suramitr\*

PT-P-08

**Density functional theory study on the antioxidant mechanism and electronic properties of hydroxybenzoic acid derivatives**

Nilawan Tantiwatanaworakul, Mutita Homchan, Aurisaya Boonpaen, Supanan Tanapakpolkul, Pornthip Boonsri, Supa Hannongbua, and Malinee Promkatkaew\*

PT-P-09

**Binding investigation of 7,8-dimethoxy-4-isochromanone derivatives as acetylcholinesterase inhibitors by computational study**

Apinya Patigo, Supa Hannongbua, and Patchreenart Saparpakorn\*

PT-P-10

**In silico screening for repurposing anticancer drugs against *Plasmodium falciparum* dihydrofolate reductase-thymidylate synthase (PfDHFR-TS)**

Sasipha Seetin, Patchreenart Saparpakorn, Jarunee Vanichtanankul, Sumalee Kamchonwongpaisan, and Supa Hannongbua\*

PT-P-11

**Evaluating the binding modes of hepatitis B e-antigen inhibitor by in silico method**

Wigrom Yogboworn\* and Pornthep Sompornpisut

PT-P-12

**Charaterization of volatile compound adsorbed on metal oxide**

Apisara Kuapan, Kanyanee Thapklay, and Nattawadee Wisitruangsakul\*

PT

PT-P-13

**Binding study of acetylcholinesterase inhibitors from *Centella asiatica* using molecular dynamics simulations**

Warunyu Chockchowwat, Apinya Patigo, Supa Hannongbua,  
and Patchreenart Saparpakorn\*

PT-P-14

**A theoretical investigation on depsidones as potential candidates for small cell lung cancer targeting PARP-1 enzyme**

Chartniwat Suksamrarn, Patchreenart Saparpakorn, and Supa Hannongbua\*

PT-P-15

**Transient luminescence studies for excited-state kinetics of organic indoline dyes adsorbed on nanocrystalline TiO<sub>2</sub> films**

Kanon Ie, Rina Watanabe, and Koichiro Mitsuke\*

PT-P-16

**Theoretical study on butylone inclusion complexes with  $\beta$ -cyclodextrin and its three methylated derivatives**

Waraitip Laosangprateep, Watanyuta Jantarose, Nat Triamchaisri,  
and Luckhana Lawtrakul\*

PT-P-17

**Virtual screening of “Prab-Chompoo-Taweep” remedy targeting acetylcholinesterase for Alzheimer disease**

Nonthaphon Platoon, Jaruporn Srisarakham, Supa Hannongbua,  
and Patchreenart Saparpakorn\*

PT-P-18

**Improving hydrophobicity in 3D printing of resin inks with porogen additives and micro-pillar structures**

Bantita Chomdee, Natthawut Butphom, Kanoksak Saelee,  
Supranee Kaewpirom, and Teeranan Nongnual\*

PT



PT-P-23

**Elucidation of the specific interactions between benzimidazole derivatives and InhA based on *ab initio* fragment molecular orbital calculation**

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# Analytical Chemistry (AC)

## Oral Presentation



## Absolute quantification of phenylbutanoids in *Zingiber cassumunar* Roxb. rhizome by quantitative $^1\text{H}$ NMR

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Quantitative NMR spectroscopy (qNMR) has gained substantial popularity as a powerful and effective technique for both qualitative and quantitative analyses of natural products. In this work, the direct quantification of four characteristic phenylbutanoids, i.e. (*E*)-1-(3',4'-dimethoxyphenyl)butadiene (DMPBD, **1**), (*E*)-1-(2',4',5'-trimethoxyphenyl)butadiene (TMPBD, **2**), (*E*)-4-(3',4'-dimethoxyphenyl)but-3-en-1-ol (**3**), and (*E*)-4-(3',4'-dimethoxyphenyl)but-3-en-1-yl acetate (**4**), in *Z. cassumunar* rhizome crude extract by qHNMR using an internal standard (ethyl *p*-methoxycinnamate, EPMC) was achieved, with high specificity and sensitivity. The selected  $^1\text{H}$  NMR signals could unambiguously be assigned and did not overlap with other resonances, including the highly similar compounds DMPBD and TMPBD. The method provides the linear response with a concentration range of 0.71-14.29 mg/mL, with a limit of quantification of 0.46-0.68 mg/mL. The relative standard deviation values of intraday and interday precisions are in the range of 0.20-0.49% and 0.01-0.71%, respectively. Recovery tests at three concentrations (50, 100, and 150%) yield average recoveries of 99.54-100.18%. Our qNMR method was applied to determine the contents of **1**, **2**, **3**, and **4** in the *Z. cassumunar* rhizome *n*-hexane crude extract derived from Plai samples. For this purpose, two amount levels (5.00 and 10.00 mg) of the crude extract, per 2.00 mg of the internal standard (EPMC) were analysed. The contents of **1**, **2**, **3**, and **4** were found to be in the ranges of 31.87-38.39%, 6.45-12.26%, 7.17-15.85%, and 2.86-8.43%, respectively. This method provides excellent accuracy, precision, and reliability for quantifying phenylbutanoids in the crude extract of *Z. cassumunar* rhizome. The advantages of qNMR are simplicity, rapidity, and non-destructiveness.

**Keywords:** *Zingiber cassumunar*; Phenylbutanoids; qNMR

## Production and certification of certified reference material of Andrographolide in *Andrographis Paniculata* powder by a network of competent laboratories approach

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*Andrographis paniculata* is in Thailand's official list of essential medicines (Herbal medicine list) of the Ministry of Public Health for the management of respiratory and gastrointestinal disorders including COVID-19 treatment. It was recommended that the proper amount of active pharmaceutical ingredient (Andrographolide) for COVID-19 treatment was 180 mg/day. Accurate measurement of the amount of active ingredient in herbal medicine is therefore important, not only for the effectiveness of treatment but also for minimizing the side effect of drug overdose. There were no certified reference materials available to allow laboratories to access their analytical method performances. A matrix-matched Certified Reference Material (CRM), TRM-F-5011, was prepared at the National Institute of Metrology, Thailand (NIMT), from freeze dried, ground, Green Chiretta (*Andrographis Paniculata*) leaves. Homogeneity and stability of the material were rigorously assessed. Characterization of the reference material was carried out by a network of competence laboratories. The interlaboratory results were statistically analyzed, and robust mean was calculated as assigned value of CRM. Measurement uncertainty of the certified value was evaluated from the between-unit inhomogeneity, long-term storage stability of the material at -20 °C and laboratory biases from characterization by a network of competence laboratories. The results showed that TRM-F-5011 contained Andrographolide at  $(18.7 \pm 1.3)$  mg/g.

**Keywords:** Andrographolide; Certified reference material; *Andrographis paniculata*; Production of Certified reference material

## Gold nanoparticle-based dip strip immunoassay with silver enhancement method for cardiac troponin I detection

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The dip strip immunoassay for simple and sensitive cardiac troponin I (cTnI) detection was developed. Silver-enhanced gold nanoparticles (AuNPs) method was employed on the developed dip strip to enhance sensitivity of the detection. In the presence of silver enhancer, the color of AuNPs changed from red to dark brown. This was due to the precipitation of silver ions on AuNPs which caused their enlargement. The concentration of cTnI was quantified by measuring the color intensity on the dip strip using smartphone analysis with RGB application. Under optimal conditions, the limit of detection (LOD) was found to be 0.5 ng/mL by the naked eye which exhibited 50-fold more sensitive than without the silver enhancement. For quantitative analysis using smartphone, the cTnI concentration could be measured in the range of 0.5 to 50 ng/mL with good linearity ( $R^2=0.9955$ ) and LOD was 0.12 ng/mL. The developed dip strip immunoassay was successfully applied to the detection of cTnI in serum samples (the relative standard deviation and recovery were in the range of 2.91 – 5.13% and 96.10 – 119.17%, respectively) with no cross-reactivity with the potential interferences toward cTnI.

**Keywords:** Silver enhancement; Gold nanoparticles; Cardiac troponin I; Dip strip immunoassay; Smartphone analysis



## Synthesis of platinum on manganese (IV) oxide nanowires in chitosan scaffold as a catalyst in prostate immunosensor

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Label-free electrochemical immunosensor was designed for the detection of prostate-specific antigen (PSA) using platinum on manganese (IV) oxide nanowires (Pt-MnO<sub>2</sub> NWs) for signal amplification. A one-pot oxygen-evolution reaction was employed to synthesize MnO<sub>2</sub> NWs, while the Pt-MnO<sub>2</sub> NWs was synthesized through the electrostatic adsorption technique of PtCl<sub>6</sub><sup>3-</sup> on MnO<sub>2</sub> NWs. This material enhanced the loading of prostate-specific antibodies (Ab) and efficiently catalyzed hydrogen peroxide (H<sub>2</sub>O<sub>2</sub>) reactions, ultimately leading to signal amplification. Pt-MnO<sub>2</sub> NWs was dispersed in chitosan cross-linked glutaraldehyde solution and it was drop-cast onto the electrode surface and followed by an aliquot of Ab. Amperometry was employed to evaluate the amount of specific recognition of PSA through the partial blocking of H<sub>2</sub>O<sub>2</sub> on the electrode surface of the NWs-based immunosensor. This prostate immunosensor operated at an applied potential of +0.90 V, employing 4 mg of Pt-MnO<sub>2</sub>, along with 0.15 µg of antibody (Ab), and exhibited a limit of detection of 5 pg/mL.

**Keywords:** PSA biosensor; Pt-MnO<sub>2</sub> nanowire; Cancer immunosensor; Prostate-specific antigen

## Surfactant-free air bubble flotation for the rapid purification of basic dyes and drugs

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Surfactant-free air bubble flotation method was developed for the rapid purification of basic drugs. The method was conducted by adding small amount of alcohol (typically 0.2% (v/v) of ethanol) to the aqueous solution containing crude product of a basic drug in a cylindrical glass vessel having a sintered glass filter at the bottom and feeding air passed through the filter to generate air bubbles. The basic drug in water was concentrated to temporally generated foam on the water surface. Moreover, the concentrated basic drug formed precipitate when it exceeded its solubility. The precipitate was readily collected from the water surface by a suction method. The results of dynamic surface tension measurement and molecular dynamic simulation indicated that the basic drug orientated at air-water interface and, therefore, adsorbed on the surface of air bubble. On the other hand, source materials and intermediate compounds remained in the bulk aqueous solution. The strength of adsorption at the air-water interface had a significant impact on purification efficiency. After the repeated air bubble flotation, the crude product of a basic drug containing source materials and intermediate compounds was highly purified corresponding to its analytical grade agent. The proposed method did not require large amount of toxic and volatile organic solvents that are usually used for drug purification by crystallization method or chromatographic techniques. The applicability to the purification of a basic dye, Rhodamine B, and a basic drug, chloroquine, was examined. Conditions for the efficient separation were studied in detail.

**Keywords:** Air bubbles; Flotation; Purification; Basic dyes; Basic drugs

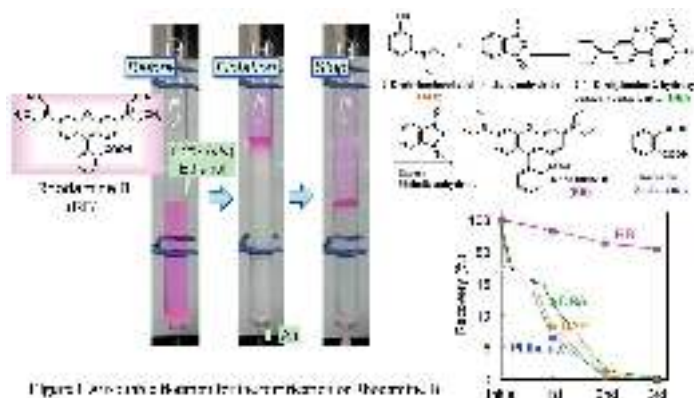


Figure 1. Schematic diagram of the air bubble flotation method for the purification of Rhodamine B.

## Electrical field-flow fractionation for separation and characterization of metal nanoparticles

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Electrical field-flow fractionation (EIFFF) is a separation-based technique utilized for separation of charged nanoparticles. The separation is achieved in separation channel (44 cm long x 2.6 cm wide x 125  $\mu\text{m}$  thick) using electrical field (direct current, DC, voltage) and carrier liquid flow. However, electrical double layer (EDL) interferes the electrical field which is major parameter for separation in EIFFF result in poor separation efficiency. This work demonstrated the use of additive substances including sodium carbonate, FL-70, acetonitrile and Triton X-100 for preparation of carrier liquid in deionized (DI) water in order to improve the separation in EIFFF by minimizing EDL and increasing electrical field. The condition of 0.01% (V/V) Triton X-100 carrier liquid provides the maximum improvement in the effective field and in separation resolution of 1.11 for mixture of 5 nm and 15 nm gold nanoparticles (AuNPs) stabilized by polyvinylpyrrolidone (PVP) as comparing to other carrier liquids. In addition, EIFFF was applied for characterization of nanoparticle size and charge associated with single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) which is size determination technique. The nanoparticles were separation by using EIFFF under separation condition of 1.50 V applied voltage in DI water carrier prior to size determination by using SP-ICP-MS. With retention time from EIFFF and determined size from SP-ICP-MS under the EIFFF theory, this method was able to characterize AuNPs and silver nanoparticles (AgNPs) as individual and mixture.

**Keywords:** EIFFF; SP-ICP-MS; Nanoparticles; Separation; Characterization

## An efficient method of tyramine detection in food and beverage products by capillary electrophoresis using silica-nanolayer coated capillary with UV detection

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Tyramine is a prevalent biogenic amine in many food products. High levels of tyramine can cause health risks, including high blood pressure and migraines. Especially for patients on monoamine oxidase inhibitor (MAOI) antidepressants, even a low concentration (6 mg per meal) of tyramine can trigger these symptoms. Thus, the development of an efficient method for the separation of tyramine is a necessity. In this work, we applied a hydrothermal sol-gel process to create a uniform silica nanolayer coating on the inner wall of a silica capillary to adjust the surface properties to improve the electrophoretic separation. Optimized sol-gel compositions and coating conditions were established for the reproducible formation of the coating layer by observation of uniform gel formation on an optical microscope. The selection conditions for the sol-gel mixture will be discussed. Surface characterization of the coated layer was studied by *in-situ* scanning electron microscopy (SEM), contact angle measurements, Fourier-transform infrared spectroscopy (FT-IR), and X-ray powder diffraction (XRD). This procedure resulted in the coating of a *ca.* 100 nm thick silica layer on the capillary walls. EOF mobility measurements were used to evaluate the reproducibility and the uniformity of the coating layer. The nanolayer-coated capillary provides higher efficiency for separation of eight standard amines (histamine, benzylamine, phenylethylamine, tyramine, benzhydrylamine (IS, internal standard), dopamine, propranolol and atenolol) and consequently higher peak heights with plate number  $N \geq 3.0 \times 10^4$  m<sup>-1</sup> and higher peak resolution  $R_s \geq 2$  for all adjacent peaks than non-coated capillary. The coated capillary was applied to analyze tyramine in food and beverage products, successfully separating tyramine from matrix peaks, which was not achieved with the non-coated capillary. Our work achieved lower limits of detection (LOD) of 4.9  $\mu\text{g L}^{-1}$  than previous works, wide dynamic range (5 – 200  $\mu\text{g L}^{-1}$ ), high precision (%RSD of RMT < 2%), high separation efficiency for tyramine and reasonable percent recovery (95 – 106%).

**Keywords:** Silica coated capillary; Nanolayer coating; Hydrothermal sol-gel process; Amines; Tyramine; Food and beverage products

## Development of an electrochemical DNA super-sandwich assay for porcine adulteration detection via one-step immobilization using a poly-adenine oligonucleotide approach

Vasita Lapee-e<sup>1,2</sup>, Sudkate Chaiyo<sup>2</sup>, and Abdulhadee Yakoh<sup>2\*</sup>

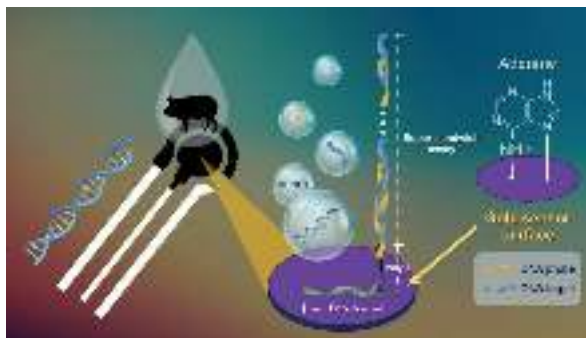
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Amid escalating meat consumption, concerns over meat adulteration and mislabeling have intensified. This undermines consumers trust, especially among those driven by cultural, religious, or allergic consideration, amplifying the need for devices to identify meat adulteration. Traditional molecular tests, such as polymerase chain reaction (PCR), have been employed for meat identification, but they are time-consuming, user-unfriendly and inconvenient. In this work, we developed an electrochemical DNA biosensor to detect porcine mitochondrial DNA. This combined a gold nanoparticle-modified screen-printed graphene electrode (AuNPs/SPGE) with a one-step DNA probe immobilization via the poly-adenine (poly-A) oligonucleotide approach. Importantly, the detection mechanism utilizes a DNA super-sandwich assay, enhancing sensitivity without requiring extensive sample amplification. The DNA super-sandwiched structure allows for monitoring the hybridization of target porcine DNA to the poly-A probe through the labeled-ferrocene, using differential pulse voltammetry (DPV). The results highlighted a clear difference between positive and negative control. Additionally, measurement conditions such as DNA probe concentration, incubation time and signal concentration were studied. The linear range was established between 10 to 10<sup>6</sup> pmol/L, with the limit of detection (LOD) and limit of quantification (LOQ) of 1.136 pmol/L and 1.531 pmol/L, respectively. To our knowledge, most meat adulteration biosensors primarily use optical techniques, with only a few being electrochemical. Given this, the developed DNA super-sandwich assay, coupled with the simple poly-A probe immobilization method, offers an efficient, affordable, and user-friendly alternative for detecting porcine adulteration, applicable across the meat industry chain and even by end consumers.

**Keywords:** Electrochemical detection; DNA biosensor; Super-sandwich assay; Meat Adulteration; Porcine



## Non-transferrin-bound iron (NTBI) quantification in human plasma using BODIPY-Pyridylhydrazone (BODIPY-PH) entrapped in a thin green film coupled with a portable fluorescence-based device

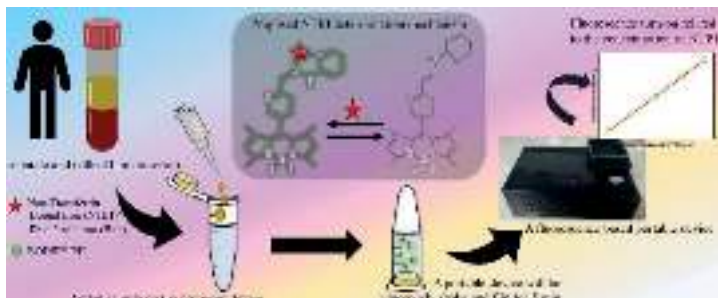
Puttaraksa Naksen<sup>1,2</sup>, Kantapat Chansaenpak<sup>3</sup>, Siriporn Jungstutwong<sup>4</sup>, Ratchadaree Intayot<sup>4</sup>, Jaroon Jakmunee<sup>5</sup>, Somkid Pencharee<sup>6</sup>, Peter Lieberzeit<sup>7</sup> and Purim Jarujamrus<sup>1,2\*</sup>

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Free iron in human serum, known as non-transferrin-bound iron (NTBI), poses a risk by generating free radicals and causing oxidative damage. It's also a crucial biomarker for assessing iron loading in thalassemia patients, with healthy individuals typically having NTBI levels below one  $\mu\text{M}$ . In this study, we present a novel method that involves entrapping the BODIPY-PH molecule within a tapioca starch-sealed microcentrifuge tube lid for NTBI detection in human serum samples using a portable fluorometer. The fluorescence intensity of BODIPY-PH exhibited a notable increase as NTBI concentration rose, providing a responsive "turn-on" signal. Within 5 minutes, fluorescent products were generated, their intensities directly correlating with NTBI concentration. Under optimal conditions, utilizing the developed portable fluorescence device and a fluorescence spectrometer, we achieved satisfactory detection limits (LOD) of 0.003 and 0.0015  $\mu\text{M}$ , respectively. Importantly, our NTBI detection method showed no significant variance from established values when tested in human serum samples from thalassemia patients. Our innovative approach, employing the developed portable device with a fluorometer, demonstrates remarkable speed, accuracy, cost-effectiveness, and reproducibility in NTBI quantification from human serum samples. This system holds promise for efficient clinical applications.

**Keywords:** Thalassemia; BODIPY-PH; Portable fluorometer; Human serum



## Mickey mouse-shaped laminated paper-based analytical device in simultaneous total cholesterol and glucose determination in whole blood

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We developed a mickey-mouse-shaped laminated paper-based analytical device (LPAD) for efficient point-of-care testing. This LPAD was created by integrating cutting and reagent deposition techniques. Based on a colorimetric enzymatic reaction, it enables simultaneous glucose and total cholesterol (TC) determination in only two simple steps. Lamination with adhesive tape finalizes the device, consistently delivering results in agreement with clinical standards. The LF1 membrane selectively isolates plasma from whole blood through size exclusion, offering plasma for subsequent enzymatic reaction steps. Using a reagent-filled technical pen instead of the knife allows continuous reagent deposition without manual switching, enhancing efficiency and automation. Our approach provides hydrophobic reagent-free, and suitable for rapid, cost-effective, and high-reproducibility mass production (can make 146  $\mu$ PADs in under 10 minutes). This method is innovative because it streamlines the process, enabling all-in-one fabrication. This versatile device is ready for use and can be adapted as a prototype for various diagnostic applications involving whole blood samples, promising significant benefits in point-of-care testing.

**Keywords:** Paper-based; Total cholesterol; Glucose; Colorimetric; Whole blood



## Vanadium-doped porous cobalt oxide for its superior peroxidase mimic in simultaneous total cholesterol and glucose testing in whole blood on a 2D paper-based device

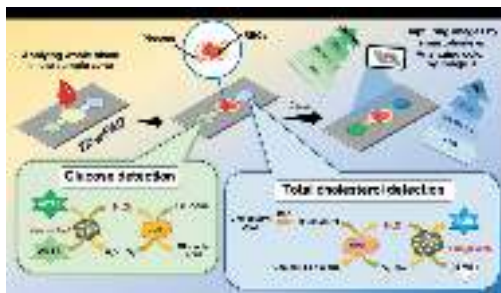
Nattasa Kitchawengku<sup>1,2</sup>, Budsakorn Wongsing<sup>1,2</sup>, Akarapong Prakobkij<sup>1,2</sup>,  
Wipark Anutrasakda<sup>3,4</sup>, and Purim Jarujamrus<sup>1,2\*</sup>

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We synthesized vanadium-doped porous cobalt oxide (V-porous  $\text{Co}_3\text{O}_4$ ) as a superior peroxidase mimic for rapid colorimetric assessment of glucose and total cholesterol (TC) in whole blood on a 2D microfluidic paper device (2D- $\mu\text{PAD}$ ). The V-porous  $\text{Co}_3\text{O}_4$  demonstrated excellent catalytic activity due to its dual-metal composition and large surface area, with low Michaelis–Menten constants ( $K_M$ ) of 0.1301 and 0.0141 mM for 2,2'-azino-bis(3-ethylbenzthiazoline-6-sulfonic acid) (ABTS) and 3,3',5,5'-tetramethylbenzidine (TMB), respectively. Our 2D- $\mu\text{PAD}$  was created using simple wax screen printing and cutting techniques. This device enables the simultaneous colorimetric analysis of glucose and TC in whole blood, with results in 5 minutes and requiring only a 15  $\mu\text{L}$  blood drop with zero sample preparation on the LF1 membrane. The enzymatic reaction on the sample zone led to the oxidation of generated hydrogen peroxide ( $\text{H}_2\text{O}_2$ ) by V-porous  $\text{Co}_3\text{O}_4$ , producing hydroxyl radicals ( $\cdot\text{OH}$ ). This initiated the generation of green and blue color products, indicating glucose and TC levels. The V-porous  $\text{Co}_3\text{O}_4$  combined with 2D- $\mu\text{PAD}$  offers a rapid, cost-effective, and straightforward solution for point-of-care blood biomarker detection without the need for specialized technical support.

**Keywords:** Vanadium-doped porous cobalt oxide (V-porous  $\text{Co}_3\text{O}_4$ ); Peroxidase mimic; Microfluidic paper-based analytical device ( $\mu\text{PAD}$ ); Glucose; Total cholesterol



## A distance-based paper device using polydiacetylene liposome as a chromogenic substance for rapid and in-field analysis of disinfectants against COVID-19

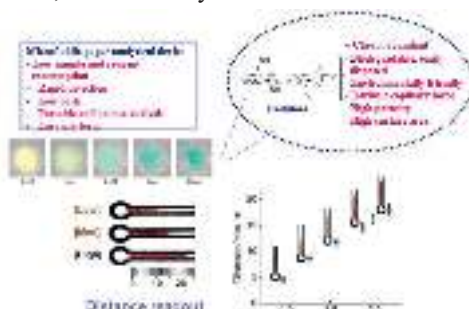
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A simple distance-based paper device ( $\mu$ PAD) with a smartphone-based photo editor was invented for rapid and in-field analysis of disinfectants to ensure their antimicrobial activity and user safety. The disinfectants were widely utilized in households and hospitals against COVID-19, which included dodecyl dimethyl ammonium chloride (DDAC), benzyl dimethyl tetradecyl ammonium chloride (BAC) and cetylpyridinium chloride (CPC). The  $\mu$ PAD device was wax-printed as a thermometer-like shape consisting of a sample reservoir and a microchannel as the detection zone. This zone was pre-deposited with polydiacetylene (PDA) liposome as a chromogenic substance. The PDA changed from blue to red upon reacting with the disinfectants at pH 4.0 to 10.0 for 7 min. Validation data of the device showed good specificity, accuracy (96.1–109.4%), and precision (%RSDs  $\leq$  9.3%). Sensitivity in terms of limits of detection and quantitation were in the ranges of 20 to 80 and 70 to 250  $\mu$ M, respectively. The device was applied for in-field analysis of the disinfectant in fumigation solution compared to the colorimetric assay ( $P > 0.05$ ). The  $\mu$ PAD complies with the World Health Organization-ASSURED concept (i.e., affordable, sensitive/specificity, user-friendly, rapid, equipment-free, and delivery to end-user), which can be helpful in resource and skill-limited areas.

**Keywords:** Distance-based paper device; Polydiacetylene; Quaternary ammonium compounds; COVID-19; In-field analysis





## Enhanced detection of favipiravir using a $\text{Cu}_2\text{O}@\text{MnO}_2$ modified glassy carbon electrode

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The accurate and rapid quantification of favipiravir (FAV) is of paramount importance for pharmaceutical development, clinical monitoring, and epidemiological research. This research presented the development of an electrochemical sensor for the determination of FAV based on copper (I) oxide at manganese (IV) oxide ( $\text{Cu}_2\text{O}@\text{MnO}_2$ ) in chitosan scaffold modified on the glassy carbon electrode (GCE). The analytical specification of this sensor was studied by the square wave voltammetry technique that it was observed at a peak potential of 1.37 V. Under optimized conditions, linearity was obtained from 1-200  $\mu\text{M}$  with a detection limit of 0.79  $\mu\text{M}$ . This sensor showed good selectivity without interfering from glucose, sucrose, ascorbic acid, cholesterol, molnupiravir,  $\text{Cl}^-$ ,  $\text{CO}_3^{2-}$ , and  $\text{NO}_3^-$ . The repeatability and reproducibility were obtained at 4.49 and 4.75 %RSD (N=5), respectively. This sensor was successfully applied to the FAV tablet, and percent recoveries were found in the range of 96.06-99.23%. The validation between the standard method and this sensor found that the result was not significantly different for the analysis of favipiravir.

**Keywords:** Copper (I) oxide at manganese (IV) oxide; Favipiravir sensor

## Development of aptamer-based detection kit by electrochemistry for rapid assessment of vitamin D levels

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Vitamin D deficiency is a widespread health concern affecting both general populations and patients, exerting diverse effects beyond bone health, encompassing several vital organ systems. Prompt and accurate monitoring of vitamin D levels is imperative to ensure timely intervention and management of deficiencies. However, the existing methodologies for vitamin D detection often demand specialized expertise and present financial constraints. To address these challenges, we propose a novel detection kit employing a DNA aptamer immobilized on a screen-printed carbon electrode and an electrochemistry assay for precise measurement. Our investigation into DNA aptamers specific to vitamin D revealed the efficacy of VD2-VD3 aptamer in detecting both vitamin D2 and D3, and VD3 aptamer specifically targeting vitamin D3, with an optimal concentration of 20  $\mu\text{M}$ . The resultant detection kit demonstrates the capability to identify both forms of vitamin D, exhibiting a detection limit of 10 ng/ml and a detection range spanning 10-100 ng/ml. This innovation holds promising implications for the efficient and cost-effective diagnosis and management of vitamin D deficiencies, thereby positively impacting public health outcomes.

**Keywords:** Ergocalciferol; Cholecalciferol; Detection kit; Aptamer; Electrochemistry

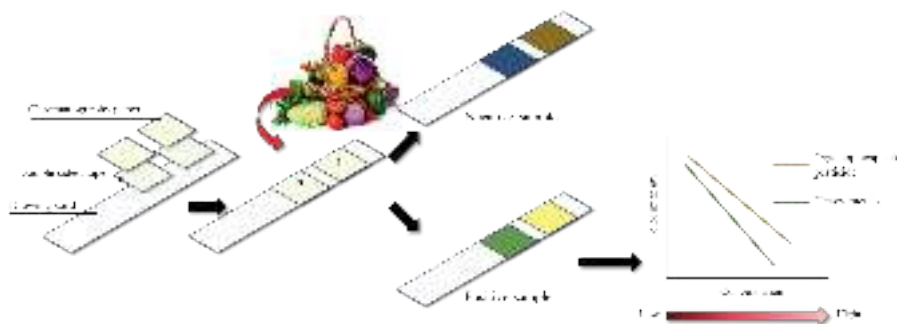


Figure 1. Illustration of the paper-based analytical device for simultaneous organophosphate pesticide

## Ecological risk assessment of heavy metals in sediment from Klong Luang Reservoir, Chonburi, Thailand

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Heavy metals (HMs) in the aquatic system are a global problem and environmental hazard, and sediment is widely recognized as the repository and sink pollutants of HMs. The increasing concentration of heavy metals (HMs) in the Klong Luang reservoir can be attributed to natural origin (i.e., weathering processes of soil and rocks) and anthropogenic origin, including discharge from various urbanization, industrialization, and agricultural activities. Direct and indirect discharges from open dumping, industry effluent, vehicle emissions, agriculture, and road runoff can release HMs to the reservoir. The potential harm posed by HMs has emerged as a significant concern for human health and ecological risk. Therefore, this study aims to quantify the concentration of HMs including cadmium (Cd), nickel (Ni), zinc (Zn), manganese (Mn), lead (Pb), and copper (Cu) in the sediment by using Inductively Coupled Plasma-Optical Emission Spectrometry (ICP-OES) technique. The Monitoring data, modified degree of contamination (mCd), pollution index (PI), and potential ecological risk index (PER) were conducted to provide a detailed of the HMs contamination. The result demonstrated Mn concentration (270.96 mg/kg) was the highest among those HMs (Mn>Pb>Zn>Cu>Ni>Cd). The mCd was found in a moderate degree of contamination ( $2 \leq \text{mCd} < 4$ ) and the PI showed moderate pollution conditions ( $2 \leq \text{PI} < 3$ ). The value of PER indicated moderate potential risk ( $50 \leq \text{PER} < 100$ ) and the dominant is Cd. Considering environmental quality, our study findings reservoir status in a moderate potential ecological risk. hence, it is imperative to monitor pollution in the future.

**Keywords:** Ecological risk; Heavy metal; Klong Luang reservoir; Sediment

## Effect of some short chain and long chain fatty acids on KOH number of concentrate natural rubber latex

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The potassium hydroxide number, or KOH number, is an important indicator of latex quality. The total number of fatty acids in the latex that can react with KOH is indicated by the KOH number. Currently, no verification of the KOH number method for concentrated latex has been available. Thus, the purpose of this work is to investigate the types of fatty acids, both long- and short-chain, that influence the KOH number of concentrated natural rubber latex. The long-chain fatty acids in this study were represented by oleic acid and lauric acid, and the short-chain fatty acids by acetic acid and formic acid. It was found that oleic acid, a long chain carboxylic acid, was the best spiking agent. The recovery percentages were found at 103.28, 93.34, 81.64 and 60.12% for oleic acid, acetic acid, lauric acid and formic acid, respectively.

**Keywords:** KOH number; Short chain fatty acids; Long chain fatty acids; Concentrate natural rubber latex

## Sensitive and selective 3D-ePAD for dual simultaneous analysis of VMA and 5-HIAA tumor markers using graphene screen printed electrode modified with molecularly imprinted polymers for point-of-care application

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Levels of vanillylmandelic acid (VMA) and 5-Hydroxyindole-3-acetic acid (5-HIAA) biomarkers in the human body fluids are valuable tools for clinical diagnosis not only of neuroblastoma or carcinoid syndrome, but also of essential hypertension, depression, migraine, and Tourette's syndrome. In this work, we developed a novel dual-imprinted sensor for selective and simultaneous determination of VMA and 5-HIAA using graphene quantum dots (GQDs) coated with molecularly imprinted polymer (MIP) and explore the well-suited for use as a facile and a ready-to-use disposable device for point-of-care testing in urine and plasma samples. The dual-MIP was successfully coated on the GQDs core via co-polymerization of (3-aminopropyl) triethoxysilane (APTES) and tetraethyl orthosilicate (TEOS), acting as functional and cross-linking monomers, respectively. In addition, we fabricated a facile and ready-to-use Origami three-dimensional electrochemical paper-based analytical device (Origami 3D-ePAD) for simultaneous determination of VMA and 5-HIAA using a GQDs@ dual-MIP modified graphene electrode (GQDs@ dual-MIP/SPGE). Quantitative analysis relying on square wave voltammetry reveals excellent linear dynamic ranges of around 0.001 to 25  $\mu\text{M}$ , with detection limits of 0.023 nM for 5-HIAA and 0.047 nM for VMA ( $3S_b$ ,  $n = 3$ ). The synthetic recognition sites are highly selective for 5-HIAA and VMA molecules with an imprinting factor of 8.46 and 7.10, respectively. The proposed Origami 3D-ePAD showed good accuracy and precision when applied to actual samples, including urine and plasma samples validated by a conventional HPLC method.

**Keywords:** Dual sensor; ePAD, Biomarkers; Carcinoid tumors; Molecularly imprinted polymers

# Electrochemical sensor based on amine-functionalized magnetite magnetic nanoparticles and reduced graphene oxide nanocomposites for determination of chloramphenicol

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Antibiotics, such as chloramphenicol (CAP), have been widely used to treat bacterial infections and prevent the growth of bacteria in both humans and animals. The misuse and overuse of antibiotics have led to trace amounts of antibiotic residue being found in animal products for consumption. Excessive antibiotic residue may contribute to the development of antibiotic resistance in animals and humans, which has continuously impacted human safety and health. The accurate and rapid assessment of antibiotic residue has been a challenge for controlling the quality and quantity of antibiotics used in animal products. In this work, an electrochemical sensor has been fabricated and developed for electrochemical determination of CAP in animal products. The synthesized magnetite magnetic nanoparticles functionalized with amine groups ( $\text{Fe}_2\text{O}_3@\text{NH}_2$ ) and electrochemically reduced graphene oxide (rGO) nanocomposite were modified on the surface of an in-house fabricated magnetic screen-printed graphene electrode (mSPGE). The morphology, elemental composition, and size of the  $\text{Fe}_2\text{O}_3@\text{NH}_2/\text{rGO}$  nanocomposites were characterized by FE-SEM, EDS, and DLS, respectively. The sensitive electrochemical detection of CAP could be achieved through the electro-reductive pretreatment of CAP, followed by the oxidation of its reduced CAP formed, thereby enhancing the sensor's performance. The results obtained from the  $\text{Fe}_2\text{O}_3@\text{NH}_2/\text{rGO}/\text{mSPGE}$  sensor exhibited electrocatalytic oxidation towards CAP with high sensitivity, excellent selectivity, and good stability. Additionally, a wide linear range (5 nM–50  $\mu\text{M}$ ) and a low detection limit ( $\text{LOD} = 14.7$  nM) could be achieved. This proposed electrochemical sensor was successfully applied to determine CAP in animal products (e.g. milk and honey) with acceptable recoveries.

**Keywords:** Chloramphenicol; Electrochemical sensor; Magnetic screen-printed graphene electrode; Amine-functionalized magnetite magnetic nanoparticles; Electro-reductive pretreatment

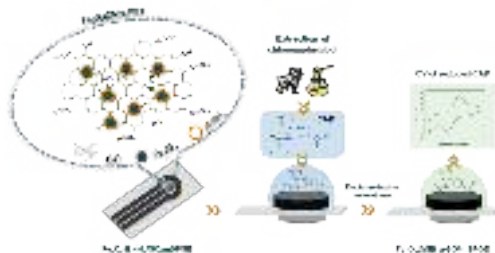


Figure 1. Scheme illustrating the sensitive determination of CAP through electro-reductive pretreatment followed by CV measurement using the  $\text{Fe}_2\text{O}_3@\text{NH}_2/\text{rGO}/\text{mSPGE}$  sensor.

# Development of a paper-based analytical device for simultaneous detection of organophosphate pesticides and heavy metal in fruit and vegetable samples

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In this work, we report the simultaneous detection of organophosphate pesticides and heavy metals using a paper-based analytical device with a smartphone as a detector. Chromatography paper was selected to create two distinct detection zones. The preparation of samples differs for organophosphate pesticides and heavy metal detection. For organophosphate pesticide detection, the sample was extracted by adding methanol and acetone. In heavy metal detection, the sample was extracted by adding nitric acid and perchloric acid. The color of the extracted sample solution does not affect the measurement. Zone 1 for organophosphate pesticide detection and zone 2 for heavy metal analysis. In the organophosphate pesticide detection process, when organophosphate pesticides are present in the sample, based on the inhibition effect of cholinesterase activity from malathion and using CuONPs to react with hydrogen peroxide obtained from the first process, the color in zone 1 changes from brown to colorless. When there is an increased presence of malathion, it leads to a higher degree of inhibition, resulting in a decrease in the color intensity of the product. In the case of heavy metal presence, cadmium was studied as a heavy metal in this research by using urease activity for detection, resulting in a color change from blue to green in zone 2. The linear range of organophosphate pesticide is from 0.1–5.0 mg/L ( $R^2 = 0.9986$ ) with a detection limit of 0.08 mg/L, and the linear range of heavy metals is from 0.1–1.0 mg/L ( $R^2 = 0.9983$ ) with a detection limit of 0.06 mg/L. The limit of the quantitative value was determined to be 0.27 and 0.19 mg/L for organophosphate pesticide and heavy metals detections, respectively. The recoveries of organophosphate pesticide and heavy metals were within 82–105% and 94–107%, respectively. This simultaneous detection of organophosphate pesticides and heavy metals was achieved within 10 minutes. The developed method for simultaneous detection of organophosphate pesticides and heavy metals in fruits and vegetables in the field demonstrated high precision (%RSD = 0.93 for organophosphate pesticides and %RSD = 0.69 for heavy metal) and accuracy, a low detection limit, time efficiency, high stability, and a portable format enabling rapid on-site testing.

**Keywords:** Organophosphate pesticides; Heavy metals; Paper-based analytical device; Smartphone

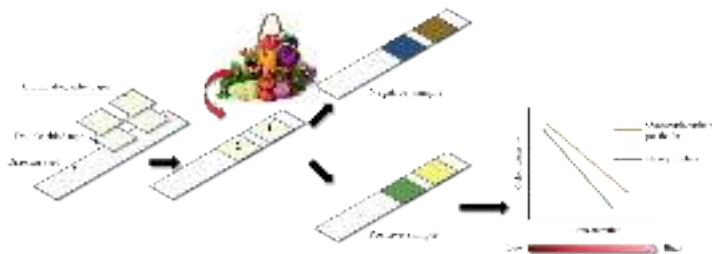


Figure 1. Illustration of the paper-based analytical device for simultaneous organophosphate pesticide and heavy metal analysis.

## Microfluidic paper-based analytical aevices for total amino acid detection in processed food

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Some amino acids reacting with sugar at high temperature are reported to produce acrylamide, a group 2A carcinogen classified by the International Agency for Research on Cancer. Expensive, huge, and complicated instrument is typically required for amino acid analysis hindering people to reach a simple test. Herein, microfluidic paper-based analytical devices ( $\mu$ PADs) for total amino acid detection based on the ninhydrin reaction were introduced. The ninhydrin test is normally performed at high temperature; however, it is not ideal in fieldworks. Consequently,  $\text{SnCl}_2$  was added to the reaction to make the test possible on  $\mu$ PADs due to its ability for preventing oxidative side reactions. Moreover, the device platform allowed automatic sample introduction to offer user-friendly tools. The optimum parameters including  $1 \text{ mg mL}^{-1}$  ninhydrin,  $1 \text{ mg mL}^{-1}$   $\text{SnCl}_2$ ,  $0.1 \text{ M}$  phosphate buffer pH 6, and reaction time of 2 min were obtained. A detection limit and a linear working range were  $0.16 \text{ mg mL}^{-1}$  and  $0.5\text{-}10 \text{ mg mL}^{-1}$ , respectively. Finally, the method was applied for total amino acid detection in raw food ingredients such as cooking powder and processed food such as potato chips. The developed device will be further applied for other application such as agricultural assessments.

**Keywords:** Microfluidic paper-based analytical devices; Amino acid detection; Processed food



## A thread-based analytical device for nitrite detection in food samples

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The use of nitrate and nitrite in food processing has been associated with hazardous effects, including cancer, methemoglobinemia, and thyroid disorders. Hence, determining nitrate/nitrite levels in food is critical for public health protection. Conventional methods for nitrate/nitrite assays require expensive instrumentation, have poor portability, and cannot meet the requirements of rapid on-site detection. Therefore, a simple, fast, and low-cost microfluidic thread-based analytical device ( $\mu$ TAD) was developed for detecting nitrite in processed meats. The study was based on the modified Griess reaction. The proposed  $\mu$ TAD utilized a distance-based detection technique wherein the length of the color change was measured using a digital caliper. Optimization studies established HCl concentration of 1 M, sample volume of 6  $\mu$ L, sulfanilamide volume of 5  $\mu$ L, N-(1-naphthyl) ethylenediamine (NED) volume of 5  $\mu$ L, sulfanilamide concentration of 22 mM, NED concentration of 12 mM, and detection time of 5 min. A linear response was observed in a range of 5 – 25 mg/L ( $R^2 = 0.9991$ ). The LOD and LOQ were 1.47 mg/L and 4.47 mg/L, respectively. The method demonstrated good selectivity, precision, and accuracy. The proposed  $\mu$ TAD offers an equipment-free platform for nitrite detection in food samples.

**Keywords:** Thread-based analytical device; Distance-based detection; Modified Griess reaction; Nitrite

## Development of a simple method for measuring nitrate ions in natural water samples

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When measuring pollutants in environmental water, samples are generally taken back to a laboratory for instrumental analysis. However, on-site analysis is desirable if the samples can deteriorate during transportation. In this study, we focused on the quantification of  $\text{NO}_3^-$  in natural water using paper-based analytical devices (PADs) without instruments and complicated operations. The PADs were fabricated by wax printing on filter paper sheets, as shown in Figure 1, followed by heating the sheets to penetrate wax ink into the backside. The PADs consisted of sample introduction, reduction, and detection zones. Zinc powder applied to the reduction zone reduced  $\text{NO}_3^-$  to  $\text{NO}_2^-$ . When the resultant  $\text{NO}_2^-$  reached the detection zone, the pre-deposited colorimetric reagent (Griess reagent) turned reddish-purple. The detection zone was processed using ImageJ to calculate absorbance. Griess reagent is known to be selective for  $\text{NO}_2^-$ , so interference studies are not attempted in this study. However, when a sample contains both  $\text{NO}_2^-$  and  $\text{NO}_3^-$ , the  $\text{NO}_3^-$  concentration should be determined by subtracting the  $\text{NO}_2^-$  concentration that is measured using PADs without zinc. A calibration curve was constructed under optimum conditions where the reaction times with zinc and colorimetric reagent were 20 and 30 min, respectively. The calibration curve shows good linearity in the range of 0-15  $\text{mg L}^{-1}$ , and the LOD is 0.06  $\text{mg L}^{-1}$ . A natural water sample was taken from a pond and measured to demonstrate a practical application. The result showed a reliable concentration of  $\text{NO}_3^-$  that was validated using a conventional spectrophotometric method.

**Keywords:** PADs; Paper-based analytical devices; On-site measurement; Griess reaction; Nitrate ion

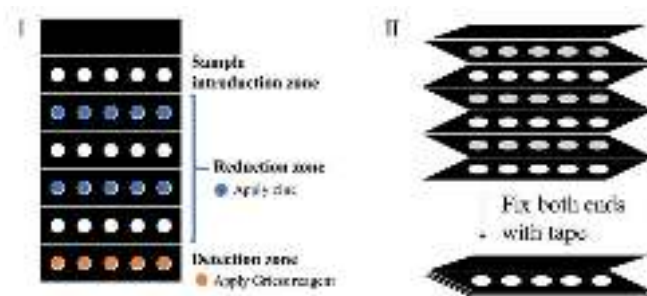


Figure 1 The optimized device (I: The design, II: The image after isocentrality)



## A novel immunosensor based on cobalt oxide nanocomposite modified single walled carbon nanohorns for the selective detection of aflatoxin B1

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We developed a novel, sensitive, and selective platform for the specific determination of aflatoxin B1 (AFB1). Single-walled carbon nanohorns decorated by a cobalt oxide composite and gold nanoparticles were created to provide facile electron transfer and improve the sensor's sensitivity. In addition, we attributed the selectivity of the proposed sensor to the specific binding property of the anti-aflatoxin B1 antibody and clarified the specific interaction of the proposed immunosensor to AFB1 using homology modeling combined with molecular docking. In the presence of AFB1, the current signal of the modified electrode reduced; this involved specific antibody-antigen binding, including hydrophobic hydrogen bonding and pi-pi stack interactions. The new AFB1 sensor platform showed two linearity ranges of 0.01 – 1 ng mL<sup>-1</sup> and 1 – 100 ng mL<sup>-1</sup>, with the limit of detection at 0.0019 ng mL<sup>-1</sup>. The proposed immunosensor was applied in certified reference material of a peanut sample (labeled 206 µg kg<sup>-1</sup> AFB1) and actual samples (peanuts, corn, and chicken feed). The sensor's accuracy yielded 86.1 – 104.4% recovery, which agrees with the reference HPLC technique using paired t-test analysis. The present work shows excellent performance for AFB1 detection and could be applied for food quality control or modified to detect other mycotoxins.

**Keywords:** Immunosensor; Mycotoxin; Aflatoxin B1 (AFB1); Single-walled carbon nanohorns; Cobalt oxide

## Effect of extraction solvent ratio in biosynthesis of silver nanoparticles, determination of phytochemicals, and investigation of antioxidant activity using *Artabotrys suaveolens* (Blume) Blume leaves

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The green synthesis of silver nanoparticles (AgNPs) is a potential and exponentially attractive area of research. The green synthesis of silver nanoparticles is regarded as a cost-effective, eco-friendly, and sustainable approach to nanoparticle manufacture. In this study, the effect of extraction solvent ratios was investigated. Different ratios (3:7, 4:6, 5:5, 6:4, 7:3) of the mixture of ethanol-distilled water (EtOH/DW) were used to extract the phytochemicals from *Artabotrys suaveolens* (Blume) Blume leaves. The crude extracts of different ratios were used to perform phytochemical determination by Total Phenolic Content (TPC) and Total Flavonoids Content (TFC) methods and antioxidant activities by DPPH, ABTS, and FRAP methods. The ratio (7:3) showed the highest content in both phytochemical contents determination and antioxidant activities. Additionally, the best ratio of EtOH/DW mixture was utilized for the green synthesis of AgNPs in optimized conditions such as precursor concentration, crude extract concentration, ratio of silver nitrate ( $\text{AgNO}_3$ ) to crude extract, temperature, reaction time, and pH. The characterization techniques revealed that UV-Vis spectra showed a specific surface plasmon resonance (SPR) absorbance peak around 420-450 nm, which confirmed the formation of AgNPs. The functional groups (O-H and C-O) are responsible for the synthesis of AgNPs revealed by FTIR. The crystal structure was confirmed by XRD which showed cubic face centered AgNPs. The TEM techniques revealed morphological structure of AgNPs in average size around 20-50 nm and mostly in spherical shape. In summary, this study clearly showed the effect of extraction solvent ratios and the successful synthesis of AgNPs using *Artabotrys suaveolens* (Blume) Blume leaves.

**Keywords:** Extraction solvent; Solvent ratio effect; Phytochemical; Antioxidant; Silver nanoparticles





## Effect of Mg Compounds on Fatty Acids Reduction in Concentrated Natural Rubber (*Hevea brasiliensis*) Latex

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Concentrated latex (CL) is a field natural rubber (*Hevea brasiliensis*) latex product with a total solids content of 60%. The concentrated latex preserved by using ammonia solution makes the condition in the latex alkaline, affected by hydrolysis of phospholipids surrounding the rubber particles. After centrifuging, the concentrated latex must be allowed for at least two weeks to allow the fatty acid hydrolysis to gradually rise until maturation is reached, which can be investigated by the mechanical stability time (MST) of latex. Nonetheless, to expedite the rise of the MST value to the intended norm, latex manufacturers typically add ammonium laurate, an ammonium salt of fatty acid, into their latex. Unfortunately, the process of hydrolysis fatty acids is ongoing and continues to be influenced by the enzymatic activity of bacteria and alkaline environments. As a result, by the time ammonium laurate-added latex reaches the latex user, the fatty acid content of the latex may be excessive, which could have a negative impact on the latex user industry. Research is still ongoing to get the fatty acid content of latex down to the appropriate amount. In this work, we propose using compounds of magnesium, by adding of magnesium sulfate and magnesium carbonate in latex to 180 mM, which is an indigenous metal in latex, to create fatty acid salts that may be centrifuged to remove them from the latex concentrate. The potassium hydroxide number (KOH number) has been used to study the effectiveness of fatty acid. The latex batch with 180 mM magnesium sulfate added was found to reduce fatty acid in latex the best-quality, the KOH number of concentrated latex reduced 0.021. Magnesium compounds significantly ( $p < 0.05$ ) affected fatty acid reduction.

**Keywords:** Concentrated latex; Magnesium compound; Potassium hydroxide number

# Analytical Chemistry (AC)

## Poster Presentation



## Smartphone assisted digital image colorimetric determination of andrographolide and analogues in *Andrographis paniculata* extract

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*Andrographis paniculata*, known as Fa-Ta-Lai-Chon, is a well-known medical plant useful for treating COVID-19 disease. Many people take Fa-Ta-Lai-Chon capsules for treating COVID-19 disease. Fa-Ta-Lai-Chon capsules contain many diterpene lactones, such as andrographolide, neoandrographolide, etc. Thus, a simple method to quantify the andrographolides in Fa-Ta-Lai-Chon capsules is needed. In this work, we developed a simple colorimetric determination of andrographolide analogues by using smartphone detection based on the reaction between andrographolides and 3,5-dinitrobenzoic acid under the basic conditions to form the purplish-red complex. However, the green color from Fa-Ta-Lai-Chon extract can interfere with the determination of andrographolide. To solve this problem, we proposed the use of color subtraction method of the digital images to remove the green color from the mixed color after the reaction, by using a free function available on the colorhexa.com website. The RGB values from digital images were put on this website to perform subtraction. The RGB values of green colors were subtracted from the RGB values of mixed colors. The RGB value results from the subtraction were then converted to the  $R/(R+G+B)$  ratio. The plot between the  $R/(R+G+B)$  ratio and the standard andrographolide concentration was linear up to  $150 \text{ mg L}^{-1}$ . The concentrations of andrographolide in the real samples obtained from the smartphone color subtraction method were in good agreement with the UV-Vis spectrophotometer, with a relative value of 80-120%. Based on our findings, the proposed smartphone color subtraction is a simple and reliable method for the determination of andrographolide analogues in Fa-Ta-Lai-Chon capsules.

**Keywords:** Andrographolide; 3,5-Dinitrobenzoic acid; Smartphone; Color subtraction; Colorimetric analysis

## A smartphone-assisted optosensor for ultrasensitive and highly selective determination of diflunisal

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Diflunisal is a nonsteroidal anti-inflammatory drug (NSAID) commonly used in human and veterinary medicine. However, high-dose or long-term use can lead to potential health risks. Therefore, it is important to determine the presence of diflunisal in foods to minimize possible harmful effects on consumers. An optosensor was designed and fabricated for the ultrasensitive and highly selective determination of diflunisal. The determination is based on the fluorescence quenching of sensing probe and smartphone image processing. The fluorescent sensing probe integrated nitrogen-doped graphene quantum dots and selective molecular imprinted (N-GQDs@MIP). The combination of these materials can improve the sensitivity and selectivity of an optosensor. A smartphone was used to capture fluorescence color and read out the RGB value. Under the optimum conditions, the smartphone-assisted optosensor demonstrated a good linearity ranging from 1.0 to 50.0  $\mu\text{g L}^{-1}$  ( $r^2=0.995$ ). The limit of detection (LOD) for diflunisal is 0.80  $\mu\text{g L}^{-1}$ , determined through the application of the  $3\sigma$  criteria ( $3\sigma/S$ ), where  $S$  signifies the slope of the linear calibration, and  $\sigma$  denotes the standard deviation of the blank response. The developed optosensor using N-GQDs@MIP probe was successfully applied to determine diflunisal in milk, yogurt, and egg samples. Recoveries were obtained in the range of 94.9 to 106.9% with RSDs less than 6%. The analysis results correlated well with HPLC analysis. The developed smartphone-assisted optosensor provided high sensitivity, good selectivity, low cost, portability, easy implementation, and presented great potential for onsite monitoring.

**Keywords:** Diflunisal; Nitrogen-doped graphene quantum dots; Optosensor; Molecularly imprinted polymer; Smartphone

## Point-of-care DNA testing device for simultaneous detection of HIV and HCV using alternating current electroluminescent display

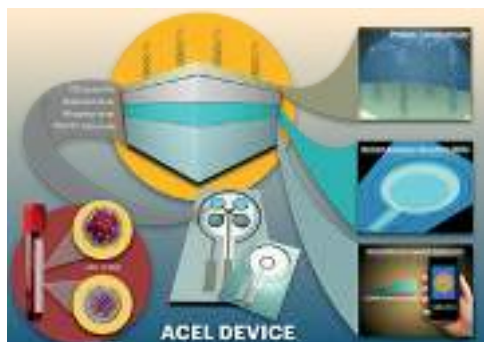
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In this study, we introduced an innovative approach by utilizing an alternating current electroluminescent (ACEL) display as a DNA sensor for the first time. The ACEL display offers many advantages, such as low energy consumption, high luminosity, and the ability for naked-eye detection. The sensing mechanism relies on conductance-based luminescence, specifically proton conduction. Thus, light emission is observed in the presence of target DNA since the proton hops along the negatively charged phosphate backbone groups on a target DNA, facilitating a label-free DNA detection approach. Our sensor presents noteworthy advantages, including the use of small sample volume, high sensitivity, and selectivity, and using only smartphone's camera to detect the light intensity. To expand the application, we developed a 2X2-ACEL device for simultaneous detection of HIV and HCV cDNA, addressing the significant global public health issue of coinfection between HIV and HCV, which increases the risk of liver cancer in co-infected individuals. Under optimal conditions, linear range from 1 nM to 1000 nM of both target cDNAs with the LODs of 1.86 pM (HIV cDNA) and 1.96 pM (HCV cDNA) were achieved. Importantly, no cross-reactivity was observed between the two target DNAs, thanks to the high specificity of an acpcPNA probe. Besides, our developed device can be successfully applied to detect HIV and HCV cDNA extracted from patient serum, with results that showed 100% agreement with the real-time PCR method.

**Keywords:** Alternating current electroluminescent device; DNA sensor; Smartphone-based detection; Infectious disease; Label-free detection



## Portable device for phosphate analysis in natural water

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This work aims to develop method for detecting phosphate at typical concentration of 0.3 mg PO<sub>4</sub><sup>3-</sup>/L (or 0.1 mg P/L) in water samples using a developed portable device. The developed device was fabricated from available materials including a cardboard with LED light for being a lightbox studio, and small test tubes with home-made sample holder for being reaction vessels. The sample and reagent solutions will be mixed into the tube to produce phosphoantimonymolybdenum blue complex (PAMB) via molybdenum blue reaction. A smartphone camera was used for taking a photo inside the lightbox studio and then evaluating the blue color intensity of PAMB by ImageJ program in RGB mode. Variable parameters affecting the analysis method were optimized *i.e.* reaction time, solution volumes and chemical concentrations. The applicability of the method was evaluated by analyzing natural water samples.

**Keywords:** Phosphate; Colorimetric detection; Smartphone



**Figure 1.** A schematic drawing of the proposed portable device



## Sequential determination of sucrose and phosphate in sugarcane juice by flow injection method

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This work presents a flow injection (FI) system with visible spectrophotometric detection at 880 nm for sequential analysis of sucrose and phosphate in sugarcane juice. The FI system was designed for firstly instantaneous measurement of sucrose based on the schlieren effect which is the physical phenomenon of light refraction at liquid interfaces between a sample plug and water carrier. Subsequently, the same sample plug was continuously flowed out of the detector and reacted with the molybdenum blue reagent to produce phosphomolybdenum blue complex (PMB). The PMB was then flowed back to the detector after the sucrose signal returned to baseline. The presented FI system provides fast analysis of both important analytes within 3.5 min per analysis cycle. The linear working ranges were obtained from 1-50 degree Brix for sucrose and 5-300 mg  $P_2O_5$  L<sup>-1</sup> for orthophosphate, with the determination of coefficient more than 0.990. The limit of detection (3S/N) of 1 degree Brix and 1.25 mg  $P_2O_5$  L<sup>-1</sup> was obtained. The analysis was highly precise (RSD < 2.94%) and accurate (recovery 104 - 106%). Furthermore, a semi-automatic method of sample preparation was proposed for supporting a large number of sugarcane juice samples.

**Keywords:** Flow injection; Phosphate; Sucrose; Green method; Colorimetry

**Reference:** Flow injection spectrophotometric system for sequential determination of sugar and orthophosphate in soft drinks and sugarcane juice. **Sreenonchai, K.**, Atsawawiphart, P., Duangjan, J., Nacapricha, D., & Buajarern, S. *Science and Technology Asia*, 27 (2022) 95-108.

## Distance-based measurement of Ni(II) using a barrier-free paper device

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This study introduces a barrier-free paper device as an analytical platform for distance-based determination of Ni(II). The paper device was created by scissors-cutting Whatman No. 1 filter paper, measuring 3 mm wide × 65 mm long, with the backside adhered with transparent tape. The determination process involves the reaction between Ni(II) and dimethylglyoxime (DMG), resulting in the vivid pink Ni(DMG)<sub>2</sub> complex formation on the paper strip, which functions as the detection zone. Prior to analysis, the paper strip is segmented into 13 sections (each measuring 3 mm × 5 mm). Each of the 12 sections is spotted with 2 µl of a 0.5 mM DMG solution to coat the reagent onto the detection zone. Subsequently, a 20 µL of Ni(II) standard solution is loaded onto the last uncoated section (sample loading zone). The length of the pink reaction band is measured along the detection zone using a ruler scale. The linear relationship between the pink band length and Ni(II) concentration (20 -100 mg L<sup>-1</sup> Ni(II)) is expressed as  $y = (0.102 \pm 0.008)x + (6.12 \pm 0.52)$ , with an R<sup>2</sup> value of 0.9826. The limit of detection or LOD ( $3.182 \times (\text{SD of intercept}) / (\text{slope of calibration line})$ ) was found to be 16.2 mg L<sup>-1</sup> Ni(II). Featuring a hydrophobic barrier-free design, this paper device holds promise as a simple and cost-effective paper-based analytical tool for on-the-spot Ni(II) detection.

**Keywords:** Barrier-free; Paper device; Ni(II) determination; Ni(DMG)<sub>2</sub>; Distance-based measurement

## Development of distance-based paper device for measuring chloride ion in food

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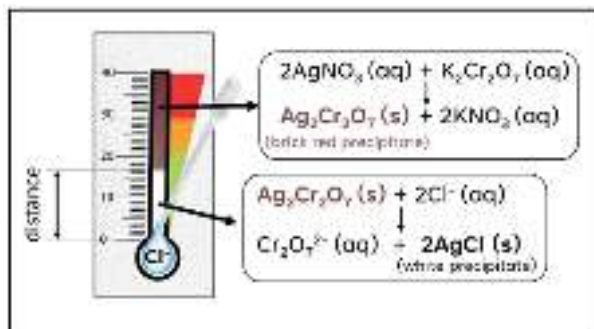
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Chloride ( $\text{Cl}^-$ ) is a necessary mineral for humans, but the effect of an inappropriate amount of  $\text{Cl}^-$  can cause health problems.  $\text{Cl}^-$  in food is typically in form of table salt, which can indicate the amount of sodium. A distance-based paper device (dPAD) for measuring  $\text{Cl}^-$  in food allowing people to control  $\text{Cl}^-$  intake is considered one of the easy-to-use, affordable, and portable; nevertheless, dPAD required sample dilution before analysis due to the limited measurement of  $\text{Cl}^-$ . For these reasons, the purpose of this research is to develop the dPAD to measure  $\text{Cl}^-$  in food with the most-reduced dilution ratio by increasing the reagent concentration. The effects of pH, viscosity, precipitate, and anion interferences were also studied. The results showed that the concentration of  $\text{AgNO}_3$  and  $\text{K}_2\text{Cr}_2\text{O}_7$  reagents on the detection zone at 0.50 M and 0.25 M respectively, provided a range of 0.5–20  $\text{g L}^{-1}$  for 30  $\mu\text{L}$  of  $\text{Cl}^-$  sample volume and the detection time of 20 minutes. The effects of pH, sediment, and anion interferences in food were insignificant. To develop the prototype test-kit, a plastic dropper with single drop of sample was used instead of a micropipette. The effect of viscosity in detection can be modified by using clear packing tape to assist the flow. In conclusion, this dPAD is reliable and should be tested with more samples and for the shelf life to see its possibility in commercialization.

**Keywords:** Chloride; Distance-based paper device; Measuring chloride in food



## Paper-based test strip for analysis of organophosphate pesticides

Wanchalearm Manchan<sup>1,2</sup> and Yupaporn Sameenoi<sup>1,2\*</sup>

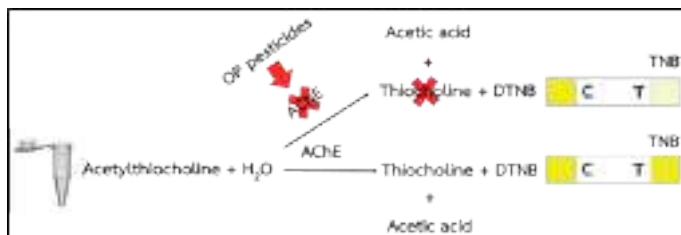
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A paper-based test strip for analysis of organophosphate pesticide using enzyme inhibition assay has been developed. The strip composed of two ends for control and sample test zones. Both zones were immobilized with the acetylcholinesterase (AChE) enzyme and Ellman's Reagent (DTNB). In the absence of pesticides, the enzyme AChE catalyzed the formation of thiocholine (TC) that reacts with DTNB to produce a yellow product (TNB). After incubation with organophosphate pesticide, the activity of AChE was inhibited and produced less TC, and hence, reduced yellow product. Color intensity was analyzed by scanning the paper-based test strip and measuring the intensity using ImageJ software. This developed assay is able to analyze organophosphate pesticides with the detection limits of two model organophosphate pesticides as low as 25.0 ng/mL of methyl-paraoxon and 6.1 ng/mL of chlorpyrifos-oxon. The developed method has been successfully applied to detect methyl-paraoxon in spiked cabbage and kale obtaining recovery values about 94% and 95%, respectively. Therefore, the developed method is promising for analysis of organophosphate pesticides in real samples.

**Keywords:** Paper-based device; Organophosphate pesticide; Enzyme inhibition assay



## Paper-based test strip for formaldehyde gas detection

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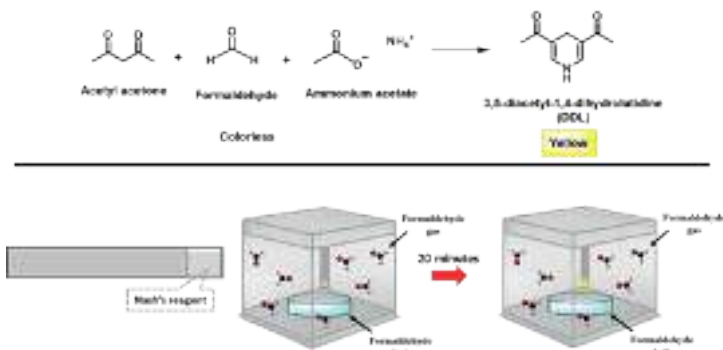
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This work aims to develop a novel, and one-step analysis method for formaldehyde gas using a paper-based test strip. The proposed method relies on the reaction between formaldehyde and acetyl acetone in the presence of ammonium acetate (Nash's reagent), which yields a yellow-colored product of 3,5-diacetyl-1,4-dihydropyridine (DDL). The paper-based test strip has a rectangular shape, measuring 6 cm long and 1 cm wide. The test zone, which is 1 cm long and 1 cm wide, is located at one end of the strip. To prepare the test zone, the paper is dipped into Nash's reagent and then dried at 40°C. The formaldehyde test is performed by exposing the test strip to formaldehyde gas, and if formaldehyde is present in the sample, the test area will appear yellow. The intensity of the yellow color is directly proportional to the amount of formaldehyde in the sample being tested. The yellow that appeared on the test zone was measured for color intensity using a scanner and ImageJ software. It was found that the developed device was able to measure formaldehyde in the linear range of 0.25–1 ppmV, with the limit of detection of 0.16 ppmV, which is lower than the air quality threshold set by the Occupational Safety and Health Administration (OSHA). These preliminary results demonstrated that the developed paper-based test strip is promising to be used for measuring formaldehyde in air samples.

**Keywords:** Paper-based test strip; Formaldehyde; Nash's reagent



## Paper-based devices for water hardness analysis

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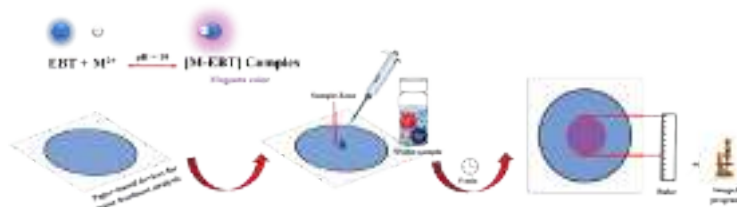
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A diameter-based measurement paper device for analysis of water hardness has been developed. The device was designed to have a circular test zone with diameter of 3 cm and fabricated using wax-printing method. Eriochrome Black T (EBT) in glycine buffer solution (pH 10) was stored in the test zone and allowed to dry. The device was then laminated with plastic sheets where the top layer was hole-punched with 0.5 mm diameter at the center and used for sample inlet. The analysis of water hardness is based on the complex reaction of  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  with EBT at pH 10. As the sample solution containing  $\text{Ca}^{2+}$  and  $\text{Mg}^{2+}$  diffuses from sample inlet outward radially towards the edge of the test zone, the ions react with EBT and the magenta color is formed whose diameter measured by a ruler within 5 min is proportional to the ion concentration. The method provided limit of detection for  $\text{Ca}^{2+}$ ,  $\text{Mg}^{2+}$  and total hardness as equivalent to  $\text{CaCO}_3$  of 0.03, 0.025 and 0.013 mM, respectively. The linear range of 0.13-1.5 mM for  $\text{Ca}^{2+}$ , 0.025-0.5 mM for  $\text{Mg}^{2+}$  and 0.025-0.5 mM for total hardness was obtained using the developed devices. The device has been used to analyze hardness in drinking water, tap water, and pond water giving the recovery in the range of 80-105% indicating the high accuracy of the developed device for water hardness analysis.

**Keywords:** Paper-based devices; Water hardness; Diameter-based readout





## Rapid test strip for malachite green detection

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Malachite green (MG) is a toxic chemical that is mostly utilized as a dye; however, it has been determined to be highly effective in treating parasites, fungal infections, and bacterial infections in aquatic animals. MG can cause significant health hazards for consumer such as carcinogenicity and mutagenicity. Therefore, a rapid test strip was fabricated for detection of MG based on competitive immunochromatographic assay (ICA). Gold nanoparticles were used as labels for detecting MG. The proposed strip achieved both qualitative and quantitative detections of MG. The strip was able to be completed in 10 min and detected by a naked eye for qualitative detection and read by a smartphone for quantitative detections of MG. The established test strip was evaluated for the quantitative determination of MG with limit of detection as 0.17  $\mu\text{g/L}$  and the visual cut-off level was 2.0  $\mu\text{g/L}$ . The limit of quantification was 0.56  $\mu\text{g/L}$ . The developed test strip was found to be linear in the range of 0.7 to 2.0  $\mu\text{g/L}$  with an excellent correlation coefficient of 0.9990. The advantages of the rapid test strip are rapidity, low cost, portability, without the need of any instruments and suitable for the on-site rapid detection of MG.

**Keywords:** Malachite green; Test strip; Immunochromatographic assay; Gold nanoparticles

## Pencil lead electrode disks with rubbed prussian blue particle modification as cheap and ecological hydrogen peroxide sensors

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Hydrogen peroxide ( $H_2O_2$ ) is valued reagent in numerous industrial processes, and an active ingredient of many commercial end products, too. In living organisms,  $H_2O_2$  is a redox release of cellular metabolism and for many of the oxidase-based biosensors on the market it is the detected signaling molecule. Modern electroanalysis of the multifaceted small molecule is taken advantage of cathodic detection at sensor surfaces with a Prussian Blue (PB) modification that catalyzes the reduction of the target at the electrode tips. Standard for the placement of electrocatalytic PB on electrode discs or cylinders is the electrochemical or chemical deposition from customized aqueous ferric and ferricyanide solutions. The two procedures work but their successful execution requires experience, complex chemical blends, careful parameter optimization and significant time and a freshly obtained reasonable  $H_2O_2$  sensitivity is often of short-lived or instable nature. For two not yet as  $H_2O_2$  sensor modification explored homemade PB powders and a commercial PB powder equivalent a new, very simple strategy for practical PB sensor adaption was explored. A few milligrams of the PB powder of choice were placed on a soft pad and the tip of disk-shaped pencil lead electrodes (PLEs) was then with gentle pressure and in an eight-shaped loop moved through the material. The details of the fabrication of PLEs with PB impregnation will be presented, their response in amperometric cathodic  $H_2O_2$  calibration trials at - 0.15 V vs. Ag/AgCl/3M KCl reference electrode be outlined and the performance in  $H_2O_2$  determinations in the standard addition mode be discussed.

**Keywords:** Hydrogen peroxide; Prussian blue; Amperometry; Electrocatalysis

## Anodic stripping voltammetry of mercury (II) on a gold leaf sensor via flow analysis

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Mercury is widely recognized as a highly toxic heavy metal to human health. This work presents a cost-effective gold leaf sensor (7.2 THB per device) for the quantification of mercury (II) ions. The sensor, measuring 10 mm x 35 mm, comprises a hand-hammered gold leaf serving as the working electrode, a printed carbon ink strip, and a printed silver/silver chloride ink strip, which function as the counter and reference electrodes, respectively. Prior to detecting mercury (II), the performance of the sensor was tested using a standard solution of potassium hexacyanoferrate at 6 mmol L<sup>-1</sup> in a 0.1 mol L<sup>-1</sup> potassium chloride. The resulting CV scans resemble those obtained from a commercial gold-printed electrochemical sensor, with the  $I_{pa}/I_{pc}$  ratio being close to 1. For the determination of mercury (II) through anodic stripping voltammetry (ASV) in a flow injection setup, the constructed sensor was integrated into the flow-through detection cell. ASV was conducted for 2.5 minutes in a stop-flow mode. Under optimal conditions, the sensor delivered satisfactory results for a range of Hg(II) standard solutions (10-100 µg L<sup>-1</sup> Hg(II)) in a 0.6 mol L<sup>-1</sup> NaCl solution. The limit of detection (3xSDblank/slope) was determined to be 4.5 µg L<sup>-1</sup> Hg(II), with an acceptable level of precision (%RSDs:1.2-1.8). This study marks the pioneering use of the in-house gold leaf sensor within an electrochemical flow cell for heavy metal quantification. Further applications of this sensor in quantitative analysis of mercury (II) will be discussed.

**Keywords:** Gold leaf sensor; Electrochemical flow cell; Mercury (II); Heavy metal; Anodic stripping

## An Electrochemical Sensor with Gold Leaf and Nanoporous Gold Modification

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Nanoporous gold leaf (NPG) is a 3D structure composed of interconnected gold atoms, featuring numerous tiny pores distributed within its composition, due to its remarkable characteristics, like high electrical conductivity, specific surface area, ease of modification, and resistance to bio-fouling. NPG has attracted considerable attention in the development of electrochemical sensors. This study presents a fusion of NPG with an internally developed gold leaf electrochemical sensor. The synthesis of NPG entails the chemical dealloying of a white gold leaf 12K, achieved through the use of concentrated nitric acid. This process dissolves the silver component, leaving the porous structure intact within the leaf's framework. In our investigation, we explored dealloying times ranging from 10 to 45 minutes using an electron microscope. Cyclic voltammograms of 0.5 M H<sub>2</sub>SO<sub>4</sub> with a scan rate of 0.05 V s<sup>-1</sup> indicated that the reduction peak of gold oxide increased as dealloying time extended. Upon comparing the modified gold leaf electrode with its unaltered counterpart, we observed a marked enhancement in sensitivity, along with a clear linear relationship. This improvement in sensitivity is primarily attributed to an increase in electrochemically active surface area, leading to a twofold increase, shifting from 13.8±0.6 to 26.7±0.6 during the anodic scan, and from 14.8±0.2 to 25.3±3.6 during the cathodic scan.

**Keywords:** Nanoporous gold; Electrochemical sensor; Dealloying; Cyclic voltammetry; Sensitivity

## Determination of rutin using a FeO nanoparticle-modified electrode

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Rutin is natural flavonoids, which have anti-oxidative, anti-bacterial, and anti-tumor medical effects. FeO nanoparticle was synthesized with hydrothermal and subsequently characterized by Fourier transform infrared spectroscopy, and scanning electron microscopy. Then, a pencil carbon electrode (PCE) modified with FeO nanoparticles (FeO/PCE) was constructed for the electrochemical determination of rutin. Cyclic voltammetry was used to investigate the electrochemical behaviors of rutin on the FeO/PCE and bare PCE. The oxidation signal of rutin was found at the same peak potential of 0.57 V for both of bare PCE and FeO/PCE. The modified FeO/PCE provides a sharper peak and higher anodic peak current of 35  $\mu\text{M}$  rutin than that obtained from bare ( $\sim 1.5$  times). The quantitative determination of rutin was performed by square wave voltammetry. The linearity of FeO/PCE was obtained in two ranges of 0.5  $\mu\text{M}$  – 82  $\mu\text{M}$  and 100 – 520  $\mu\text{M}$  rutin. The low detection limit ( $S/N=3$ ) was calculated to be 0.2  $\mu\text{M}$  with an excellent sensitivity of 0.45  $\mu\text{A}/\mu\text{M}$ .

**Keywords:** Rutin; FeO nanoparticle; Pencil carbon electrode; Electrochemistry; Square wave voltammetry

## Electrochemical detection chloramphenicol modified with tin on reduced graphene oxide by screen-printed carbon electrode

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Tin (Sn) and reduced graphene oxide (rGO) were synthesized by the electrochemical method. They were used to modify the working electrode surface of a disposable screen-printed carbon electrode (SPCE) for the direct detection of an antibiotic drug chloramphenicol (CAP) in real samples. CAP has been used to treat many bacterial infections in veterinary practice. However, it has side effects and serious adverse reactions. The modification of the electrode was used to enhance sensitivity and selectivity of the disposable and applicable SPCE. The CAP determination was performed by using differential pulse voltammetry (DPV) method under optimum conditions. The Sn/rGO/SPCE showed a linear working range of 0.5  $\mu\text{M}$  to 30  $\mu\text{M}$  and 30  $\mu\text{M}$  to 100  $\mu\text{M}$ . The linear regression of the lower range was  $I_{pc} (\mu\text{A}) = 0.3895C (\mu\text{M}) + 0.1599$  with  $R^2 = 0.9957$ , and that of the higher range was  $I_{pc} (\mu\text{A}) = 0.1161C (\mu\text{M}) + 8.1342$  with  $R^2 = 0.9941$ . The limit of detection and limit of quantification were 0.2  $\mu\text{M}$  (S/N=3) and 0.7  $\mu\text{M}$  (S/N=10), respectively. The sensitivities were  $0.934 \mu\text{A}\mu\text{M}^{-1}\text{cm}^{-2}$  for the lower concentration range and  $0.278 \mu\text{A}\mu\text{M}^{-1}\text{cm}^{-2}$  for the higher concentration range. As a result, the use of Sn and rGO was considered a promising approach to enhance the detection toward CAP with high sensitivity. The purposed disposable sensor was successfully applied to determine CAP in milk, honey and eye drop samples with satisfactory recovery.

**Keywords:** Chloramphenicol; Antibiotic; Food contaminants; Screen-printed carbon electrode



## Electrochemical determination of hydroquinone by activated glassy carbon electrode

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In this research, we investigated simple electrochemical sensor for hydroquinone (HQ) analysis by electrochemically pretreated glassy carbon electrode (PGCE) comparison with bare glassy carbon electrode (GCE). The electrochemical pretreatment of GCE was done in phosphate buffer solution and characterized by cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). The PGCE shows a significant enhancement in redox peak of HQ. The quantitative determination of HQ was performed by square wave voltammetry using the oxidation signal. The anodic peak current increased linearly with the concentration of HQ. The linear concentration range is 81 to 1,100  $\mu\text{M}$  and 3.3 to 155  $\mu\text{M}$  for GCE and PGCE, respectively. The PGCE showed excellent sensitivity and low detection limit at 0.43  $\mu\text{A}/\mu\text{M}$  and 1  $\mu\text{M}$ , respectively. The other electrode, GCE was received 0.02  $\mu\text{A}/\mu\text{M}$  and 30  $\mu\text{M}$  for sensitivity and low detection limit, respectively.

**Keywords:** Hydroquinone; Activated glassy carbon electrode; Electrochemistry

## Squarewave voltammetry on a modified screen-printed electrode for selective detection of dopamine in the presence of uric acid

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Dopamine, a neurotransmitter compound, is associated with several important diseases of the nervous system such as Parkinson's disease, depression, and schizophrenia. Dopamine in the blood can be detected by several methods. Voltammetric analysis is one of the preferred methods for dopamine detection. However, squarewave voltammetric analysis of dopamine in blood is hindered by interference from ascorbic acid and uric acid; the oxidation peak of dopamine on most solid electrodes appears at about the same potential as the aforementioned acids. In this study, a modified electrode based on activated carbon powder coated on a screen-printed gold electrode was prepared and used for dopamine detection. The prepared electrode enhanced the responses for dopamine and suppressed the interfering effect from uric. The modified electrode showed a good linear range of 5.3- 2500.0  $\mu\text{M}$  ( $R^2=0.997$ ) with a detection limit ( $3.3 \sigma/\text{slope}$ ) of 3.6  $\mu\text{M}$  (scan rate of 100 mV/s, amplitude of 0.04V, frequency of 50 Hz and  $e$  step 0.01V). Analysis of dopamine in blood samples confirmed the ability of this modified electrode for dopamine detection. The concentrations of dopamine in blood samples obtained from squarewave voltammetric analysis were in good agreement with the values obtained from UV-visible spectroscopy.

**Keywords:** Dopamine; Modified electrode; Activated carbon; Screen-printed electrode



## Simple electrochemical determination of favipiravir for anti-viral COVID-19

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We present a simple determination of favipiravir (FAV) used against anti-viral COVID-19 on a bare glassy carbon electrode via the electrooxidation of FAV. The reaction process was recorded by the cyclic voltammetry while an amperometry was used for FAV quantitation. Analytical parameters such as applied potential, supporting electrolytes, and pH were varied. The optimum condition was found to be +1.30 V, Na<sub>2</sub>B<sub>4</sub>O<sub>7</sub> – NaOH buffer, and pH 10.20, respectively. The electrochemical sensor was characteristic studied and it showed a linear range of 0.25  $\mu$ M to 500.0  $\mu$ M ( $y$  ( $\mu$ A)) = 0.0326x( $\mu$ M) + 0.1547) with a limit of detection of 0.13  $\mu$ M FAV (S/N=3). This technique exhibited high repeatability at 4.64 %RSD and interferences such as NaCl, molnupiravir, ascorbic acid, sucrose, and glucose were unaffected. It was successful in analyzing FAV in real tablet samples with high accuracy as the relative error was lower than 1.96 percent.

**Keywords:** Favipiravir sensor; Cyclic voltammetry; Glassy carbon electrode; COVID-19

## Microflow injection analysis with electrochemical detection on cloth-based device

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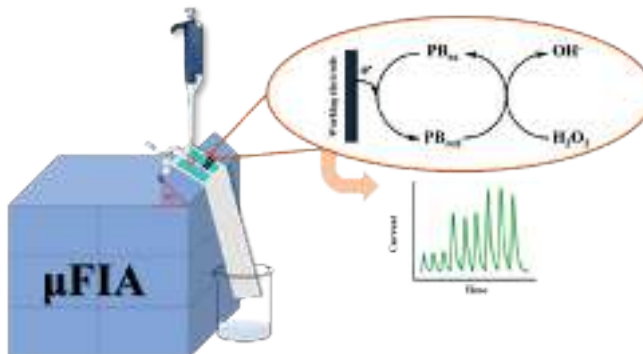
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A microflow injection analysis ( $\mu$ FIA) system with integrated electrochemical detection has been developed on a cloth-based device (CAD). The CAD was designed to have a long channel to allow the capillary flow and fabricated by polymer screen-printing method using polystyrene as a hydrophobic material. The electrodes was screen-printed on the CAD at the end of the channel using silver-silver chloride, carbon paste with Prussian blue and carbon paste as reference, working and auxiliary electrodes, respectively. A  $\mu$ FIA system is created by immersing the top end in a microtube containing the carrier solution. The area next to the electrode is inclined at an angle of 50 degrees to the plane and the end of the channel is dipped in the lower reservoir. The flow analysis was performed by injecting the  $\text{H}_2\text{O}_2$  used as model analyte for proof-of-concept at the sample injection zone which is located at 0.4-cm away from the reference electrode. Using this system, the solution flowed on the CAD by the capillary wicking and the gravitational force from the carrier upper reservoir and push the analyte to pass through the electrodes to the lower reservoir. Under optimal conditions, the method provided a linear range of 0.5-30 mM ( $R^2 = 0.9933$ ) for  $\text{H}_2\text{O}_2$  analysis with the limit of detection as low as 0.33 mM, demonstrating that it could be used as a platform for chemical analysis in several areas.

**Keywords:** Cloth-based device; Microflow injection analysis; Electrochemical detection



## Cost-effective gold leaf electrochemical sensor for voltammetric detection of chloride

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The assessment of chloride levels in water is crucial for evaluating water quality, with elevated concentrations serving as indicators of pollution. This work introduces a cost-effective, in-house electrochemical sensor designed specifically for monitoring chloride (Cl<sup>-</sup>) levels. The sensor features a gilded gold leaf (12mm × 27mm) as the working electrode (WE), while printed carbon and silver-silver chloride function as the counter electrode (CE) and reference electrode (RE), respectively. In cyclic voltammetry tests using 2-10 mM K<sub>3</sub>Fe(CN)<sub>6</sub> in 0.1 M KCl, the sensor exhibited good performance compared to the commercial gold screen-printed electrode. The ratio of oxidation peak current to reduction peak current ( $I_{pa}/I_{pc}$ ) approaching 1 indicates a reversible redox process. Furthermore, the sensor demonstrated well-defined responses in the voltammetric detection of various chloride standard solutions (50-300 μmol L<sup>-1</sup> Cl<sup>-</sup>) in a 60 mmol L<sup>-1</sup> phosphate buffer solution at pH 5, yielding an  $r^2$  value exceeding 0.998. The limit of detection (3SD of intercept/slope) was determined to be 12.5 μmol L<sup>-1</sup> Cl<sup>-</sup>, accompanied by a satisfactory level of precision (%RSD 0.6-1.2). Remarkably, this marks the debut of a gold leaf electrochemical sensor for halide determination. Further potential applications of this sensor in the quantitative analysis will be explored.

**Keywords:** Gold-leaf electrochemical sensor; Screen-printing technique; Voltammetry; Chloride; Halide

## Preparation and evaluation of ammonium ion reference material in salt matrix

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An ammonium ion ( $\text{NH}_4^+$ ) plays a pivotal role in the nitrogen cycle within aquatic environments. Elevated  $\text{NH}_4^+$  levels, reaching up to  $1.0 \text{ mgN L}^{-1}$ , poses health risks to shrimp and other aquatic organisms. Consequently, regulating ammonium concentration in shrimp farming water is crucial to mitigate potential health issues. As a result, the reliability and accuracy of  $\text{NH}_4^+$  measurements are essential for addressing this matter effectively. Ensuring measurement accuracy requires the calibration and verification of instruments using ammonium ion reference material ( $\text{NH}_4^+$ -RM). While numerous commercial reference materials cater to freshwater, this work introduces the development of the  $\text{NH}_4^+$ -RM within a salt matrix (aquacultural water). This approach ensures the suitability of RMs for instrument validation before their application in measuring water in shrimp ponds. Potentiometric technique with ion selective electrode (ISE) is selected for selective determination of  $\text{NH}_4^+$  in the developed RMs, prepared with ammonium chloride in synthetic sea salt water. Salinity (0-15 ppt) is observed as the effect of ionic strength. Magnesium sulfate solution as ionic strength adjuster (ISA) is also investigated. According to the preliminary results, the linearity range is  $0.8 - 10 \text{ mgN L}^{-1}$  with a limit of detection (LOD) of  $0.25 \text{ mgN L}^{-1}$  and limit of quantitation (LOQ) of  $0.80 \text{ mgN L}^{-1}$ . The  $\text{NH}_4^+$  value slightly increases with increasing salinity. With increasing the amount of ISA, the  $\text{NH}_4^+$  concentrations are then more reliable due to the reduction of ionic strength effect. Verification and its application of the developed  $\text{NH}_4^+$ -RM to aquacultural water for shrimp pond will be investigated and discussed.

**Keywords:** Ammonium ions standard solution; Reference materials (RM); Ion selective electrode (ISE); Aquaculture sample

## Portable sensor for Dengue virus detection by modified screen-printed electrode

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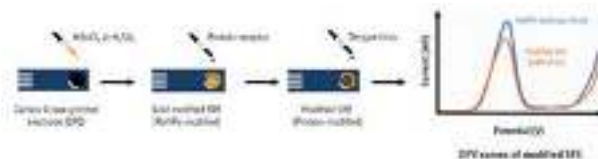
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Dengue hemorrhagic fever, a severe disease transmitted by infected mosquitoes, can lead to circulatory system failure, shock, and even death. Traditional detection methods, such as immunoassays, polymerase chain reaction (PCR) test, enzyme-linked immunosorbent assay (ELISA) and mass spectroscopy, are commonly used for identifying the dengue virus. However, these methods may not be suitable for on-site testing. In this study, we developed portable electrochemical electrodes using gold nanoparticles (AuNPs) on screen-printed carbon electrodes (SPEs) for dengue virus detection. The AuNPs were carefully deposited on the electrodes through electrochemical reduction of chloroauric acid in a concentrated sulfuric solution. Following this modification, the SPEs were immersed in a specific protein receptor solution to accurately identify and quantify the dengue virus in a suitable solution. A correlation between the reduction in electrochemical signal and the concentration of the dengue virus was seen, enabling the detection of the virus at concentrations as low as 0.01 PFU/mL. Additional tests are currently performed in the real samples to verify the effects of interferences. These findings provide valuable insights for the development of electrodes for measuring pathogenic microorganisms, offering potential applications in the field of rapid and on-site virus detection.

**Keywords:** Screen-printed electrode; Gold nanoparticles; Dengue virus; Differential pulse voltammetry; Impedance spectroscopy



## Development of an electrochemical immunosensor for the detection of oxytetracycline

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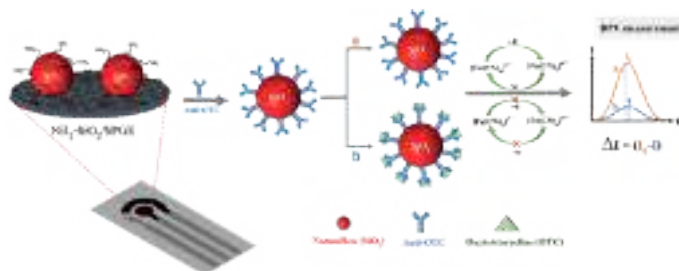
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Among the commercially available antibiotics, oxytetracycline (OTC) is one of the most applied antibiotics to human medicine, veterinary medicine, and the welfare of livestock. The unreasonable utilization of antibiotics results in environmental pollution residues in foodstuffs and endanger the health of human. Especially, OTC may cause serious threats to human health, such as hypersensitivity, drug resistance, and toxicity. Hence, it is an important to explore high-efficient, sensitive, selective, and inexpensive detection systems for the determination of OTC. This developed immunosensor was fabricated by modifying screen-printed graphene electrode with amine-functionalized nanosilica for improvement sensitivity. The amine-functionalized nanosilica was further used as a scaffold for monoclonal antibody oxytetracycline immobilization to detect oxytetracycline sensitively. OTC detection was determined by differential pulse voltammetry (DPV). The proposed electrochemical immunosensor exhibited two linear responses for oxytetracycline detection as 1-10 and 10-500 ng/mL with reliability coefficient ( $r^2$ ) of 0.9947 and 0.9958, respectively. The detection limit and quantification limit of OTC were 0.50 ng/mL and 1.74 ng/mL, respectively. Additionally, the developed immunosensor showed good reproducibility (RSD = 4.61%,  $n = 5$  electrodes).

**Keywords:** Immunosensor; Antibiotics; Amine-functionalized nanosilica; Oxytetracycline



## Monolithic $\mu$ -SPE coupled with electrochemical sensor using screen-printed graphene electrode for the determination of urinary THC-COOH in forensic application

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Cannabis is the most widely consumed illicit drug worldwide. 11-Nor- $\Delta^9$ -tetrahydrocannabinol-9-carboxylic acid (THC-COOH) is commonly used as a marker for identifying cannabis consuming. In this work, a simple, sensitive, and high-throughput analysis method for THC-COOH was introduced. The method involved the combination of a parallel in-tip monolithic micro-solid phase extraction (IT monolithic  $\mu$ -SPE) system with an electrochemical sensor utilizing screen-printed graphene electrode (SPGE). IT monolithic  $\mu$ -SPE was constructed through *in situ* synthesis of poly(stearyl methacrylate-ethylene dimethacrylate) in modified polypropylene pipette tip. The  $\mu$ -SPE condition for THC-COOH was thoroughly investigated. The parallel IT monolithic  $\mu$ -SPE enabled simultaneous processing of 12 samples within 30 min (2.5 min/sample). The IT monolithic  $\mu$ -SPE method was coupled with the electrochemical sensor using SPGE. Under optimum condition, the developed method demonstrated good linearity in concentration range of 10 - 250 ng mL<sup>-1</sup> ( $r^2 = 0.9992$ ). Limit of detection of 2.68 ng mL<sup>-1</sup> and limit of quantification of 8.93 ng mL<sup>-1</sup> were achieved. An 18-fold pre-concentration factor with 91 % extraction efficiency was provided by the developed method. The method was applied in forensic application, authentic human urine samples were analyzed, revealing THC-COOH concentrations ranging from 119 to 178 ng mL<sup>-1</sup> with good recovery of 85 - 108 %.

**Keywords:** Cannabis; THC-COOH; In-tip monolithic  $\mu$ -SPE; Screen-printed graphene electrode; Forensic application

## A highly sensitive colorimetric sensor for detection and speciation of arsenic in soil samples

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A colorimetric sensor based on amino silane modified on surface of silica sol was developed for determination and speciation of inorganic arsenic (As) species. The colorimetric probe was fabricated by loading ammonium molybdate (Mo) in amino silane/silica sol before As detection. The As(V) was performed the arsenomolybdenum blue complex on the colorimetric probe and was directly determined. The As(III) concentration was determined by subtracting As(V) from total As following oxidation of As(III) to As(V) by  $K_2S_2O_8$  in acidic medium. The quantitative data is obtained by UV-Vis spectrophotometry and naked-eye detection based on the changing of color which is captured by smartphone in combination with Image J program. Under optimal conditions, the linear range was in the range of 0.04 - 0.10 mM with the correlation coefficient of 0.9923 and limit of detection (LOD) was 4.57  $\mu$ M. Good precision was obtained with relative standard deviation (%RSD) less than 1.0% for intra-day and inter-day. The proposed colorimetric sensor was successfully applied for detection and speciation of arsenic in soil samples and the obtained results were comparable to those from inductively coupled plasma atomic emission spectroscopy (ICP-OES) method.

**Keywords:** Colorimetric sensor; Inorganic arsenic species; Silica sol; Molybdenum blue; Soil samples



## Detection of histamine based on gold nanoparticles using UV-Vis spectrophotometer for analysis of histamine in seafood samples

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This study aimed to determine histamine content in seafood samples using gold nanoparticles (AuNPs) and NaCl solution with a UV-Vis spectrophotometer. Electrostatic interactions between histamine and AuNPs cause increase in electron density and surface amino group content resulting aggregation of AuNPs. The AuNPs were simply synthesized for analysis of histamine in NaCl solution using citrate reduction. The optimization of the concentration of AuNPs and the concentration of NaCl were performed for highly sensitive detection. It was found that under the optimum condition using 0.25 mM AuNPs with 0.9% of NaCl solution, quantitative analysis of histamine was achieved in a concentration range of 1-1,000 nM by monitoring decrease in absorbance at 520 nM due to red shift of AuNPs absorption peak. The limit of detection and the limit of quantitation of the method were 0.9 and 1.3 nM, respectively. Selectivity of the method was investigated showing no effect of interferences. The developed method was applied for determination of histamine in real samples including tuna and salmon. It was found that the mean concentrations of histamine in tuna and salmon were 0.013 and 0.003 mg/kg, respectively, which do not exceed the FDA limit that may cause allergy to human. The accuracy and precision of the method was confirmed by %recovery values of 92.5-95.2% and %RSD values of 2.9-5.3% in tuna and salmon samples, respectively. The results showed that this developed method is effective for the analysis of histamine in real samples and is suitable for monitoring seafood spoilage to ensure food safety.

**Keywords:** Histamine; Gold nanoparticles; UV-Vis spectroscopy; Seafoods; Food safety

## An optosensor based on quantum dots composited with molecularly imprinted polymers for the determination monuron

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An optosensor based on the fluorescence quenching of nanocomposite sensing probe was fabricated for the determination of monuron. The nanoprobe consists of nitrogen doped graphene quantum dots (N-GQDs) and molecularly imprinted polymer (MIP). The composite probe was synthesized through a sol-gel polymerization process using (3-aminopropyl) triethoxysilane (APTES) as a monomer, tetraethyl orthosilicate (TEOS) as a cross-linking agent and monuron as template molecule. Various parameters that affect the sensitivity were investigated and optimized. The fabricated N-GQDs@MIP nanoprobe exhibited the maximum fluorescence emission intensity at 406 nm. The intensity of sensing probe decreased linearly with increasing concentration of monuron in the range of 0.3 to 25.0  $\mu\text{g/L}$ , the coefficient of determination ( $R^2$ ) of 0.9917. Limit of detection (LOD) and limit of quantitation (LOQ) were 0.10 and 0.30  $\mu\text{g/L}$ , respectively. The optosensor was applied to determine monuron in tea, fruit juice and vegetable. The analysis results were also compared with high-performance liquid chromatography technique (HPLC). The advantages of the developed optosensor is rapid, low-cost, simple produce, high sensitivity and good selectivity which can be used for the determination of trace monuron in food samples.

**Keywords:** Monuron; Optosensor; Quantum dots; Molecularly imprinted polymers; Fluorescence



## An optosensor based on fluorescence quenching of nanocomposite sensing probe for the determination of non-steroidal anti-inflammatory drug

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Non-steroidal anti-inflammatory drugs (NSAIDs) are widely used in veterinary medicine for the treatment of inflammation, pain and bovine respiratory diseases. However, the overuse of these drugs can cause a potential risk to human health due to their residue can enter the food chain. Therefore, the determination of NSAIDs is necessary. An optosensor based on nanocomposite sensing probe was developed and utilized for the determination of NSAIDs. The nanocomposite sensing probe was fabricated by incorporating of graphene quantum dots (GQDs) with excellent optical property into molecularly imprinted polymer (MIP). The nanocomposite sensing probe was prepared via a sol-gel polymerization process using meclofenamic acid as a template molecule, 3-aminopropyltriethoxysilane (APTES) as a functional monomer and tetraethyl orthosilicate (TEOS) as a cross-linker. Under the optimal conditions, the fluorescence emission intensity of the nanocomposite sensing probe at 408 nm was linearly quenched with increasing concentration of meclofenamic acid from 0.30 to 50.0  $\mu\text{g L}^{-1}$  ( $R^2 = 0.993$ ). The limit of detection and the limit of quantitation were 0.10  $\mu\text{g L}^{-1}$  and 0.30  $\mu\text{g L}^{-1}$ , respectively. The nanocomposite sensing probe was utilized to detect meclofenamic acid in dairy products with satisfactory recoveries were obtained ranging from 94.1 to 104.5% and RSD lower than 3.1%. This developed optosensor is highly sensitive and selective for the determination of target analyte. The results of the developed optosensor were also in good agreement with high-performance liquid chromatography (HPLC).

**Keywords:** Non-steroidal anti-inflammatory drugs; Fluorescence; Graphene quantum dots; Molecularly imprinted polymer; Quenching

## A highly sensitive and selective fluorescence sensor for the determination of piperacillin

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Piperacillin is widely used for anti-infective treatment in poultry and livestock aquaculture. The misuse of piperacillin leads to its residue in foods. Therefore, it is important to develop a sensitive and selective analytical method for the determination of piperacillin. In this work, a nanocomposite sensing probe was designed and fabricated for the determination of piperacillin. The nanocomposite probe was synthesized by integrating of quantum dots into molecularly imprinted polymer (MIP). The MIP nanoprobe was prepared via a sol-gel process using 3-aminopropylethoxysilane (APTES) as a functional monomer, tetraethoxysilane (TEOS) as a cross-linker and piperacillin as a template molecule. The fabricated nanocomposite probe was characterized using scanning electron microscope (SEM), transmission electron microscope (TEM) and fourier transform infrared spectrometer (FTIR) techniques. The fabrication of nanocomposite sensing probe and the determination conditions were optimized. Good linearity was obtained in the range of 0.10 to 20.0  $\mu\text{g L}^{-1}$  with a coefficient of determination ( $R^2$ ) of 0.9914. The limit of detection (LOD) was 0.03  $\mu\text{g L}^{-1}$ . The developed method was applied to determine piperacillin in dairy products and recoveries were obtained between 90.4% and 99.9% with RSD lower than 5%. The developed optosensor provided the analysis results agree well with high-performance liquid chromatography. However, the developed method is easy to fabricate, cost-effective, high sensitivity and good selectively.

**Keywords:** Piperacillin; Optosensor; Fluorescence; Quantum dots; Molecularly imprinted polymer

## A colorimetric sensing for arsenic(III) based on thiodiacetic acid functionalized gold nanoparticles

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Arsenic ( $\text{As}^{3+}$ ) is one of the most common heavy metals in the environment and is considered as a global health risk factor. Exposure to inorganic arsenic through consumption of contaminated food and water can lead to serious effects on human health. According to the International Agency for Research on Cancer (IARC), arsenic was categorized in group 1 relating to carcinogenic to humans. Herein, we have developed a novel and simple colorimetric method for the detection of  $\text{As}^{3+}$  in water samples. The colorimetric detection is based on the aggregation of gold nanoparticles (AuNPs) functionalized with 2,2'-thiodiacetic acid (TDA) in the presence of  $\text{As}^{3+}$ . The interaction between oxygen groups in TDA and  $\text{As}^{3+}$  induced the aggregation of AuNPs and the resulting solution color changed from red to blue, depending on the concentration of  $\text{As}^{3+}$ . The presence of  $\text{As}^{3+}$  can be monitored by the colorimetric response and UV-Vis analysis in the range of 400–800 nm. Two parameters, the TDA concentration and pH of solution, were optimized and the value of absorbance ratio between 610 and 520 nm ( $A_{610}/A_{520}$ ) was used for optimized response. The results presented that 1.0 mM of TDA concentration and a solution pH of 5 were the best conditions. Our colorimetric method also exhibited good selectivity of  $\text{As}^{3+}$  among other metal ions ( $\text{As}^{5+}$ ,  $\text{Co}^{2+}$ ,  $\text{Fe}^{2+}$ ,  $\text{Fe}^{3+}$ ,  $\text{Pb}^{2+}$ ,  $\text{Al}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Cd}^{2+}$ ,  $\text{Ni}^{2+}$ ,  $\text{Zn}^{2+}$ ).

**Keywords:** Chemical sensor; Gold nanoparticles; TDA; Arsenic; Aggregation

## Gingerol extract-stabilized silver nanoparticles and their applications: Colorimetric and machine learning-based sensing of Hg (II) and antibacterial properties

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This study focused on synthesizing ginger-stabilized silver nanoparticles (Gin-AgNPs) using more eco-friendly method that utilized AgNO<sub>3</sub> and natural ginger solution. These nanoparticles underwent a color change from yellow to colorless when exposed to Hg<sup>2+</sup>, enabling the detection of Hg<sup>2+</sup> in tap water. The colorimetric sensor had good sensitivity, with a limit of detection (LOD) of 1.46 μM and a limit of quantitation (LOQ) of 3.04 μM. Importantly, the sensor operated accurately without being affected by various other metal ions. To enhance its performance, a machine learning approach was employed and achieved accuracy ranging from 0% to 14.66% when trained with images of Gin-AgNP solutions containing different Hg<sup>2+</sup> concentrations. Furthermore, the Gin-AgNPs and Gin-AgNPs hydrogels exhibited antibacterial effects against both gram-negative and gram-positive bacteria, indicating potential future applications in the detection of Hg<sup>2+</sup> and in wound healing.

**Keywords:** Silver nanoparticles; Zingiber officinale; Mercury sensing; Antibacterial; Silver nanoparticles in hydrogel



## Aptamer-based lateral flow biosensor for the detection of cadmium

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Currently, chemical test kits are popular for detecting cadmium ( $\text{Cd}^{2+}$ ) contamination in food and the environment. However, this device still has many steps of operation. Here, an aptamer-based lateral flow biosensor was developed for the rapid detection of  $\text{Cd}^{2+}$ . This sensor combines a flow test strip with an aptasensor not only to increase the specificity for  $\text{Cd}^{2+}$  detection but also to reduce the detection steps of the device. In the operating principle of this strip test, the Cd-aptamer probe was mixed with the sample before being applied to the sample pad. In the absence of  $\text{Cd}^{2+}$ , the Cd-aptamer probe was free, and then this solution continuously flowed into a conjugate pad coated with an AuNPs-aptamer-conjugated probe. This free Cd-aptamer probe was hybridized with the AuNPs-aptamer conjugated probe so that the test line did not appear as a color band. The cadmium detection was interpreted as negative. In the case of positive,  $\text{Cd}^{2+}$  ions are specifically bound to the Cd-aptamer probe. Next, this solution continued to flow to the conjugate pad, which could not bind to the AuNPs-aptamer conjugated probe. For this reason, the test line appears as a colored band from the binding of the AuNPs-aptamer conjugated probe, and the aptamer sequences match on the test line. This test strip has been shown to detect as low as 3 ppb of  $\text{Cd}^{2+}$ . In addition, this test strip has been applied to detect  $\text{Cd}^{2+}$  in tap water samples, where it represents a simple, rapid, and field-ready application.

**Keywords:** Cadmium ions; Aptasensor; Lateral flow assay; Strip test;

## Investigation of carbon dots (CDs)-based fluorescence turn-on and turn-off sensing for detection of aspartame

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Aspartame is widely used as an artificial sweetener in various foods and beverages. There have been some reports concerning its potentially carcinogenic effects on humans. This work aims to develop and describes an investigation of a simple fluorescence-based method using carbon dots (CDs) for detection of aspartame. CDs are synthesized from citric acid and urea (1:1 mass ratio) via a rapid one-step microwave-assisted pyrolysis method (750 Watt for 5 min). When exposed to UV light, the CDs emit intense blue fluorescence ( $\lambda_{\text{ex}} = 357 \text{ nm}$ ,  $\lambda_{\text{em}} = 444 \text{ nm}$ ), whereas the CDs solution appear as a yellow color under visible light ( $\lambda_{\text{max}} = 338 \text{ nm}$ ). We employ a concept of fluorescence turn-on/turn-off of CDs for detection of aspartame. When silver ions are added to the native CDs solution, there is increased quenching (turn-off) of fluorescence as the concentration of silver ions increases. A possible quenching mechanism is silver ions interact with the functional groups present on the surface of CDs in a carbonate solution. Consequently, aspartame solution is then added to the quenched CDs solution, causing return enhancement of the CDs' fluorescence (turn-on), due to the complex formation of silver and aspartame. According to the preliminary result, increasing concentrations of 0 - 45  $\mu\text{mol L}^{-1}$  of aspartame gives gradually enhanced fluorescence of the CDs solutions with the linear calibration of  $y = 0.0059x + 1.0077$ ,  $r^2 = 0.975$ . Physical and chemical parameters to obtain sufficient sensitivity will be discussed. Applications of our proposed method in beverages analysis will also be investigated.

**Keywords:** Carbon dots; Fluorescence; Turn-on/Turn-off; Aspartame; Microwave-assisted pyrolysis method

## The study of analysis method for sugar-based surfactant; alkyl polyglucoside in cleaning product

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Alkyl polyglucoside (APG) is a sugar-based surfactant working as nonionic surfactant. Due to its biodegradable property, alkyl polyglucoside is therefore more popular formulated in liquid detergent products. However, quantification of alkyl polyglucoside in cleaning products is difficult and expensive because of the surfactant consists of a complex mixture of a variety of homologues and isomers which requires the pure standard chemicals and advance instrumental techniques. To simplify the test method, a more classical method based on TIS 474 - 1999 and anthrone method for carbohydrate were studied to testing amount of alkyl polyglucoside in the products. Although FT-IR spectrum of the extracts obtained from the TIS: 474 - 1999 method was identified as their alkyl polyglucoside used as ingredients, amount of extracted alkyl polyglucoside was lower than the expected to 75%. For the anthrone method, seven cleaning products containing 0.13 - 5.08% of alkyl polyglucoside were analyzed using anthrone reagent in acid condition and measured UV absorbance at wavelength of 620 nm. Then results of each product were compared to standard calibration curve obtained from their alkyl polyglucoside used in raw material and alkyl polyglucoside bought this study. The *t-test* of amount of the surfactant obtained from both sources of standard calibration curve was not different significantly from the amount contained in the cleaning products at the 95% confidence.

**Keywords:** Alkyl polyglucoside; Anthrone; Sugar-based surfactant

## A kinetic and spectroscopic study on the proteolytic activity of papain in organic solvents medium

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Traditional chromatographic methods, capillary electrophoresis, mass spectrometry, and immunoassay are effective for various small molecule determinations but have certain limitations such as complexity, time-consuming sample preparation, and the requirement of expensive instruments. In recent years, the enzyme-based biosensor has emerged as the alternative method with simplicity, high sensitivity, and multi-residue detection. Despite its wide use, few studies have been published showing the inhibitory effect of organic solvents in enzyme kinetic assays. Here, the effect of organic solvents on enzymatic reactions and structure was investigated using the selected papain model, a protease enzyme that can be found in *Carica papaya*. The activity of papain was monitored by the hydrolysis of *N* $\alpha$ -benzoyl-arginine-*p*-nitroanilide (BAPNA). The presence of a yellow color produced by a product, *p*-nitroaniline, can be measured at 430 nm. In the first step, the calculation of UV-visible molar absorption coefficients of *p*-nitroaniline was carried out in various organic solvents including acetonitrile (ACN), dimethyl sulfoxide (DMSO), methanol (MeOH), ethanol (EtOH), and chloroform (TCM). A change is observed in the range of 51.0-107.3% depending on the solvent polarity. Moreover, the fluorescence emission of papain exposed to organic solvents-aqueous mixtures shows a shift of the emission maximum towards shorter wavelengths. These modifications also affect the active catalytic site in the particular in case of DMSO and EtOH according to kinetic measurements. These results can be used as guidance for employing organic solvents for biosensor purposes.

**Keywords:** Biosensors; Kinetic and spectroscopic study; Papain; Organic solvents

## Use of rice straw-cellulose nanofibril at a 2D-microcuvette for determination of fluorescein injection medicine

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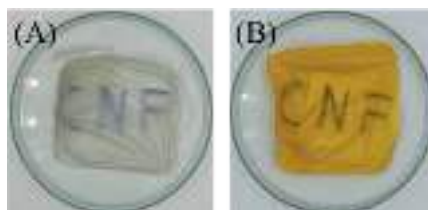
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Cellulose nanofibrils (CNF) has been attracting great attention due to their properties such as flexible, transparent, and biodegradable. Many applications of CNF as smart materials have been reported. Herein, we are interested in fabrication of a two-dimensional (2D)-microcuvette from CNF for determination of fluorescein injection. Fluorescein injection is a kind of medicine, used for diagnostic angiography of the retina. Excess amount of injected fluorescein can result in optics and eyes damage. Quality control of commercially available fluorescein injection is therefore necessary. By using a 2D-microcuvette for fluorescein injection analysis instead of fluorescent cells the advantage is that low cost and more flexible than fluorescent cells and reduces the volume of samples required for analysis. In this work, the CNF was prepared from rice straw waste. The waste was mechanically pulverized. The rice straw powder was then chemically modified using TEMPO (2,2,6,6-Tetramethylpiperidine 1-oxyl)-mediated oxidation reaction in the presence of NaBr (99.0%) and NaClO (4.00%). The solution was disintegrated by household blender. The obtained bare-CNF suspended solution was divided into five aliquots. Each aliquot (10 mL) was spiked with the standard fluorescein solution (15 mL) in the concentration range from 1 to 20 % w/v. These solutions were dried at ambient temperature around 30 hr. The fluorescein-CNFs were achieved and were then used as the standard fluorescein strips (Figure 1). These strips were directly inserted into the compartment of the fluorometer. The emission wavelength of the immobilized fluorescein-CNF was located at 518 nm. The determination of the fluorescein injection is like the standard solution; however, the medicine solution was immobilized instead. Discussion will be made on optimization and validation of the method with using a standard fluorescence quartz cell

**Keywords:** Cellulose nanofibrils; Fluorescein injection; Fluorescein sensing; Fluorometry; 2D-microcuvette



**Figure 1.** The optical images of: (A) the bare-CNF and (B) the fluorescein immobilized-CNF.

## Tannin-modified membrane for preconcentration in the determination of lead using spectrophotometric techniques

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This study examines the use of tannin, an abundant and cost-efficient natural biomass, that contains multiple adjacent hydroxyl groups capable of chelating heavy metal ions such as lead, copper, and nickel in water-based solutions. Tannin's unique property makes it an attractive alternative for metal ion adsorption. The research focuses on creating a tannin-modified membrane (TM) designed to concentrate and detect lead using a complex formation between lead and (4-2-pyridylazo)-resorcinol (PAR). To prepare the TM, tannin was immobilized on a cellulose filter paper using a gelatin cross-linking agent, and then cut into small circular shapes (13-mm diameter) to fit a syringe filter holder. A 50 mL sample containing lead at pH 5 was loaded onto the TM using a syringe connected to the filter holder, followed by washing and elution with 5 mL of 0.1 M HCl. The eluent (3 mL) was mixed with the PAR reagent at pH 9, and the solution's absorbance at 522 nm was measured. Under optimized conditions, a linear calibration range of 0.1-1.25 mg/L for lead solutions, is achieved with a low detection limit (LOD) of 0.07 mg·L<sup>-1</sup> and a satisfactory relative standard deviation (%RSD, n=5) of 2.0%. The developed TM was successfully utilized for lead detection in drinking water samples, showing high recoveries of 90.4% and 92.0%. Additionally, an enrichment factor of 7.4 times was achieved using 0.5 mg/L lead with the TM, indicating its significant potential for lead absorption and preconcentration.

**Keywords:** Lead; Tannin; Gelatin; Tannin-modified membrane; Preconcentration

## Development of chitosan/graphene oxide nanocomposite for simultaneous extraction of antioxidants and bisphenol A

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Butylated hydroxytoluene (BHT), butylated hydroxyanisole (BHA), and bisphenol A (BPA) are widely used in industrial products, food, and water. Excessive amounts or over a long period of time are considered to be a health risk. Therefore, this work was developed based on the dispersive solid phase extraction (DSPE) for simultaneous extraction of antioxidants and bisphenol A coupled with gas chromatography-flame ionization detection (GC-FID). A chitosan/graphene oxide (CH/GO) based polymer nanocomposite was synthesized by using chitosan (CH), methacrylic acid as a monomer, ethylene glycol dimethacrylate as a cross-linker, and graphene oxide (GO). Further, the synthesized CH/GO polymer nanocomposite was applied as adsorbent for DSPE of BHT, BHA and BPA in the water sample. The adsorption of BHT, BHA, and BPA was attributed to  $\pi$ - $\pi$  stacking and hydrogen bonding. The best extraction conditions, 50 mg of CH/GO adsorbent, 900  $\mu$ L of GO, extraction time of 20 min, and ethyl acetate as a desorption solvent were achieved. We found the linear calibration curve in the concentration ranges of 0.01-5.00 mg/L for three analytes with a coefficient of determination ( $R^2$ ) greater than 0.9931. The limit of detections for BHT, BHA, and BPA were found to be 0.01 mg/L.

**Keywords:** Antioxidants; Bisphenol A; Nanocomposites; DSPE; GC-FID

## A composite adsorbent for the extraction and determination of polycyclic aromatic hydrocarbons

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A porous composite magnetic solid-phase extraction (MSPE) adsorbent was developed by incorporating of metal-organic framework (MOF) and calcium carbonate into alginate beads. The porous MSPE adsorbent was applied to extract five polycyclic aromatic hydrocarbons (PAHs) in food samples prior to HPLC-FLD analysis. The porous alginate beads were formed by the reaction of incorporated calcium carbonate with hydrochloric acid which produced carbon dioxide bubbles resulting in micropore. The extraction efficiency was enhanced through hydrophobic and  $\pi$ - $\pi$  interactions between target analytes and the porous composite adsorbent. The extraction conditions including the amount of adsorbent, sample volume, sample pH, the effect of ionic strength, stirring rate, extraction time, type and volume of eluting solvent and desorption time were investigated and optimized. Under the optimum condition, good linearity was achieved from 0.05 to 100  $\mu\text{g L}^{-1}$  and the limit of detection (LOD) was 0.01  $\mu\text{g L}^{-1}$ . The developed method was successfully applied to determine PAHs in coffee, cocoa and tea samples. Relative recoveries were obtained in the range of 70 to 96%, with RSDs below 10%. The developed adsorbent exhibited good stability which can be reused and the extraction procedure was simple and rapid isolation.

**Keywords:** Alginate; Polycyclic aromatic hydrocarbons; Magnetic solid-phase extraction; Metal-organic framework; Porous adsorbent



## A nanocomposite magnetic molecularly imprinted polymer adsorbent for the extraction and preconcentration of triazines

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A nanocomposite magnetic molecularly imprinted polymer (MMIP) adsorbent was fabricated by incorporating of magnetite nanoparticles and mesoporous carbon into the molecularly imprinted polymer (MPC@Fe<sub>3</sub>O<sub>4</sub>-SiO<sub>2</sub>-NH<sub>2</sub>@MIP). The nanocomposite adsorbent was applied in a dispersive magnetic solid-phase extraction (d-MSPE) procedure to extract triazines (simazine, atrazine, and propazine) in fruit juice sample. The developed MMIP adsorbent was prepared via the sol-gel polymerization process using 3-aminopropyltriethoxysilane as a functional monomer, tetraethyl oxysilicate as a cross-linker and target triazines as template molecules. MPC was used as an additional adsorption material to enhance the affinity binding between triazines and the adsorbent via hydrogen bonding and hydrophobic interaction. The amino-functionalized magnetite nanoparticles (Fe<sub>3</sub>O<sub>4</sub>-SiO<sub>2</sub>-NH<sub>2</sub>) embedded in the nanocomposite adsorbent for rapid isolation of the adsorbent from sample solution. The extracted triazines were determined by high-performance liquid chromatography (HPLC). Under the optimum conditions, the developed method provided good linearity from 1.5 to 100 µg L<sup>-1</sup> with a low detection limit of 0.5 µg L<sup>-1</sup>. Satisfactory recoveries of the spiked sample were achieved in the range of 70 to 110%, with a relative standard deviation of less than 6%. The developed nanocomposite adsorbent provided good selectivity, high extraction efficiency, easy to fabricate and good stability.

**Keywords:** Magnetic solid phase extraction; Triazines; Magnetic molecularly imprinted polymer; Mesoporous carbons; Adsorbent

# Determination of tetracycline residues in milk sample using biosorbents for a dispersive solid phase extraction by high performance liquid chromatography with UV detection

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The simple, rapid, cost-effective and eco-friendly extraction method, namely dispersive solid phase extraction (DSPE), was developed for extracting tetracycline antibiotic prior to high-performance liquid chromatography (HPLC) with UV detection. Hair basil seed (*Ocimum basilicum* L.) represented highlight of adsorption feature was used as biosorbent to enrich tetracyclines (TCs). TCs are widely used for treating bacterial infections in veterinary, leading to the accumulation in animal-derived food products, which can be transmitted to humans. All experimental parameters for extraction of oxytetracycline (OTC), tetracycline (TC) and doxycycline (DC) were optimized. The good linear ranges were obtained at 15.0-500  $\mu\text{g L}^{-1}$  with  $r^2$  more than 0.9994. The limits of detection (LODs) ranged were 5.0-7.0  $\mu\text{g L}^{-1}$  and limits of quantitation (LOQs) were 15.0  $\mu\text{g L}^{-1}$  (all TCs), while the relative standard deviations (RSDs) were lower than 13%. The proposed method based on DSPE-HPLC-UV was successfully applied to enrich and determine TCs residues in milk samples. Recovery values for TCs were found in the range of 83.1-109.9%.

**Keywords:** Antibiotic; Food sample; Dispersive solid phase extraction; Biosorbent; Sample preconcentration

## Surfactant modified silica as effective sorbent for preconcentration of sulfonamides in water and honey samples prior to their determination by high-performance liquid chromatography

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Silica gel is extremely porous, hydrophilic, and highly absorbent. This work proposes an application of silica modified with cetyltrimethylammonium bromide (CTAB) as sorbent for solid phase extraction (SPE) method. The sorbent was simply in-situ synthesis under facile condition. Transmission electron microscopy, fourier transform infrared spectroscopy, and  $N_2$  adsorption measurements were used to characterize the sorbent. Various parameters affect the extraction efficiency were studied, such as the amount of sorbent, the kind and concentration of surfactant, and kind and volume of desorption solvent. Under the optimum condition, a good analytical performance for the proposed SPE method was obtained with a wide linear range within the range of 0.09-3  $\mu\text{g mL}^{-1}$ , and low limits of detection (0.003  $\mu\text{g mL}^{-1}$  for Sulfamethazine and 0.001  $\mu\text{g mL}^{-1}$  for Sulfathiazole Sulfamethoxazole and Sulfadimethoxine) were obtained. The intra and interday precision values were evaluated in terms of percentage relative standard deviations (%RSD) and were less than 2.85 and 5.99% for the retention time and peak area, respectively. The recoveries in a satisfactory range of 50.0–144.3% were obtained and Analytical Eco-Scale (AEC) of this method were all found to have a value of 82, which can be considered a green method. Moreover, the proposed method provided enrichment factors (EF) ranging from 4 to 13 folds.

**Keywords:** Sulfonamide antibiotic; Extraction; Surfactant; Silica gel; HPLC

## Monolithic-activated charcoal composite sorbent in micro pipette tips for micro-solid phase extraction

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Solid sorbent extraction (SPE) is widely used for sample clean up and pre-concentration due to its high extraction efficiency and simplicity. Organic polymer-based material of monoliths in pipette tips has been continuously developing for various SPE applications. Monolithic materials can be *in situ* synthesized in pipette tips without need of retaining frits and requiring of complex equipment. In order to enhance extraction efficiency by monolith, we composited the material with activated charcoal which is aromatic-based material containing various functional groups such as carbonyl, carboxyl, phenol, lactone and quinones. Activated charcoal content and polymerization condition for the sorbent preparation were investigated at a selected monomer to porogenic solvent of 23:77. The composite materials containing 5% activated charcoal (compared to total monomer weight) were fabricated inside surface-pretreated micro pipette tip, with UV light irradiation for 20 min and then heated at 70 °C for 1 h 10 min. Extraction characteristic of the materials were tested for three model compounds of Bisphenol-A, Serotonin, and 5-Hydroxyindoleacetic Acid using High-Performance Liquid Chromatography technique. In summary, the developed material shows high loading capacity for the extraction of the model compounds.

**Keywords:** Micro-solid phase extraction; Solid sorbent extraction; Monolithic materials

## A composite magnetic solid phase extraction adsorbent for the extraction and determination of herbicides

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A composite adsorbent was developed by incorporating of hypercrosslink polymer decorated graphene oxide and magnetic nanoparticle into alginate hydrogel bead ( $\text{Fe}_3\text{O}_4\text{@HCP-GO/alginate}$  bead). The composite bead was fabricated and applied to extract and enrich phenylurea herbicides (PUHs) prior to instrumental analysis. The composite bead was assembled and utilized as a dispersive magnetic solid phase extraction adsorbent. The developed  $\text{Fe}_3\text{O}_4\text{@HCP-GO/alginate}$  bead could adsorb target herbicides via hydrogen bonding and  $\pi$ - $\pi$  interactions. The fabricated adsorbent was characterized using FTIR, FL microscope, SEM and BET techniques. The different composite absorbent beads were investigated and the extraction conditions were optimized. Under the optimum conditions, the developed method provided a good linearly from 20 to 100  $\mu\text{g L}^{-1}$  for metoxuron and monolinuron and 10 to 100  $\mu\text{g L}^{-1}$  for monuron, chlortoluron, isoproturon and buturon. The limits of detection ranged from 5 to 10  $\mu\text{g L}^{-1}$ . Satisfactory recoveries were in the range of 70-110%. The fabricated composite hydro bead has many advantages including easy to prepare, simple extraction and rapid operation. It could be used as an alternative adsorbent for the extraction of herbicides in food sample.

**Keywords:** Composite beads; Dispersive magnetic solid phase extraction; Herbicides;

## Synthesis of non-polar and charged-monolithic materials in polypropylene pipette tips for micro-solid phase extraction

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Monoliths are increasingly employed in micro-solid phase extraction ( $\mu$ -SPE) due to their tunable chemical and physical properties. In this work, we introduced hydrophobic and charged-functional monolithic materials *in situ* synthesized in polypropylene pipette tips for  $\mu$ -SPE. Stearyl methacrylate (SMA) and methacrylic acid (MAA) monomers were co-polymerized with the crosslinker, ethylene dimethacrylate (EDMA), resulting in SMA-co-EDMA and MAA-co-EDMA monolithic sorbents, respectively. Rapid synthesis method was carried out using photo-induced polymerization under UV irradiation at 365 nm, allowing for the preparation of twenty in-tip monolithic  $\mu$ -SPEs within 10 min (2 min/tip) with a 100 % success rate. These monoliths were evaluated for their  $\mu$ -SPE capabilities by extracting two model compounds, serotonin, and bisphenol A (BPA). The negatively charged MAA-co-EDMA monolith indicated high adsorption for the polar, positively charged-molecule, serotonin, while relatively non-polar compound was strongly retained to the SMA-co-EDMA monolith. Pre-concentrations were achieved by desorbing serotonin and BPA using 150  $\mu$ L of 10:90 (v/v) acetonitrile (ACN):20 mM phosphate buffer pH 2.0 and 60:40 (v/v) ACN:H<sub>2</sub>O, respectively. Pre-concentration factor of 13 (loading volume of 2.00 mL and eluting volume of 150  $\mu$ L) was observed with 100 % extraction efficiency for both analytes (%RSDs were 0.25 % and 0.11 % for serotonin and BPA, respectively). This confirms the successful preparation of alternative non-polar and charged-monolithic materials for in-tip  $\mu$ -SPE.

**Keywords:** Monoliths; In-pipette tip  $\mu$ -SPE; Serotonin; Bisphenol A



## Preparation and evaluation of zeolite composite monoliths for micro-solid phase extraction

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Currently, monoliths are garnering interest as excellent adsorbents for micro-solid phase extraction ( $\mu$ -SPE) due to the high surface area and high permeability. In this work, we proposed a preparation method of zeolite composite monoliths for  $\mu$ -SPE. The composite monoliths were synthesized through photo-assisted co-polymerization of methacrylic acid and ethylene dimethacrylate (MAA-EDMA), which were not only used as a support but also functional monomers. Two different types of zeolites, NaX and NaY, were composited with the MAA-EDMA monolith to obtain NaX-MAA-EDMA and NaY-MAA-EDMA monoliths, respectively. The synthesized materials were characterized by scanning electron microscope and energy dispersive X-ray spectroscopy. To assess the capability of the sorbents, 8-hydroxyl-2'-deoxyguanosine (8-OHdG) was employed as the adsorbed model. The adsorption abilities were investigated by comparing % trapping of 8-OHdG on NaX-MAA-EDMA, NaY-MAA-EDMA and MAA-EDMA monoliths. The crucial extraction parameter, including zeolite contents, amount of sorbents, and pH of sample loading were examined. The results provided a maximum trapping of 69 % for adsorbing 8-OHdG on NaY-MAA-EDMA. Meanwhile, NaX-MAA-EDMA and MAA-EDMA exhibited % trapping of 31 % and 4 %, respectively.

**Keywords:** Composite monoliths; Zeolite; Micro-solid phase extraction; 8-OHdG

# Eco-friendly hydrophobic deep eutectic solvent-coated cellulose paper as a sorbent in sorptive phase extraction for carbamate pesticides in fresh fruit and edible insect samples

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In this work, an alternative sample preparation method was investigated for extraction of carbamate insecticides in fruit and edible insect samples followed by high performance liquid chromatography. This method is based on sorptive phase extraction (SPE) using cellulose paper coated with hydrophobic deep eutectic solvent (HDES) as a sorbent (CP-HDES-SPE). In this CP-HDES-SPE method, HDES prepared from decanoic acid and tetrabutylammonium bromide (TBABr) in the ratio 4:1 is synthesized and deposited on precut cellulose paper strips. Fourier transform infrared spectrometer and scanning electron microscope were used to characterized the synthesized sorbent. Various parameters affected the extraction efficiency were studied, such as kind and volume of the deep eutectic solvent components, soaking time, centrifugation time, kind and volume of the eluent. The developed method was found to be advantageous as compared with other methods. Under the optimum conditions, the proposed method provides a good linear range in the range of 0.09-1.00  $\mu\text{g/kg}$  ( $R^2 \geq 0.99$ ) for all analysis, low limit of detection in the range of 0.03-0.3  $\mu\text{g/kg}$  and the accuracy expressed as relative standard deviation in the range of 0.75-5.83%, percentage recoveries in the range of 62-158% and the proposed method provided enrichment factor of all analytes up to 10 folds. In addition, the preparation of CP-HDES is simple and involves short time and less consumption of toxic organic solvents. The greenness of the investigated method was assessed using Analytical Eco-Scale.

**Keywords:** Cellulose paper; Deep eutectic solvent; Carbamate insecticides; Sorptive phase extraction; High performance liquid chromatography

## Laser-induced biochar for the solid-phase extraction of organophosphorous pesticides

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Biochar is a carbon-rich material made from the combustion of biomass. It is considered to be a potential sustainable material for sorbents, however conventional research uses an energy-intensive slow pyrolysis method to produce biochar sorbents. In this study, a more energy-efficient approach, using a laser irradiation process, was explored to produce a biochar sorbent for the solid-phase extraction of organophosphorous pesticides (OPPs). Various biomass materials rich in lignin were tested to produce laser-induced biochar. From characterization data by Raman spectroscopy and SEM-EDS, cork sheet was found to be the most consistent and, hence, selected as the main biomass material. A central composite design was employed in optimizing the following laser parameters: lasing speed, power of laser, and number of times lased. Lasing speed was found to be best at high settings (200-250 mm/s), and number of times lased was optimal at 1 lase time. Power varied according to the physical properties and functionalities of the analyte. As a result, OPPs that are non-polar and aromatic favored high power (10.5-12 W), while OPPs that are non-aromatic favored low power (6-7.5 W). The optimized parameters that covered most OPPs were 9 W, 250 mm/s, and 1 lase time. This new application of laser-induced biochar shows the potential for low-energy production of a biochar sorbent for solid-phase extraction.

**Keywords:** Laser-induced biochar; Biochar; Solid-phase extraction; Organophosphorous pesticides



## Melamine sponge impregnated with deep eutectic solvent for preconcentration of sulfonamides antibiotics prior to HPLC determination

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This work presents the preparation of a simple impregnation of a melamine sponge (MS) with deep eutectic solvents (DES) as effective sorbent for preconcentration of sulfonamides. The selected DES were prepared and impregnated on MS to get DES-MS. Scanning electron microscope (SEM), Fourier Transform Infrared Spectrometer (FT-IR) and N<sub>2</sub> adsorption were used to characterize the synthesis sorbent. The process parameters that affect the sorption capacity of DES-MS were types of fatty acid, mole ratio and volume of DES, size of MS, types, concentration and volume of surfactant, types and volume of desorption solvent. The presented method was then analyzed by high-performance liquid chromatography. Under the selected condition, method validation of developed method was investigated in term of linearity, repeatability, reproducibility, limit of detection and limit of quantitation. This technique has been prosperously applied for the extraction of sulfonamides antibiotics in various samples. The developed method was found to be advantageous as compared with other methods. In addition, the preparation of DES-MS is simple, short time and less consumption of toxic organic solvent. The greenness of the developed method was assessed using Analytical Eco-scale.

**Keywords:** Melamine sponge; Deep eutectic solvent; Sulfonamides antibiotics; Solid phase extraction; High performance liquid chromatography



## In situ Ionic Liquid-assisted In situ Iron Microparticles Based on Natural Reagent for Dispersive Solid Phase Extraction of Tetracyclines Residues in Honey Prior to High Performance Liquid Chromatography

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Honey is a healthy food, but it is often found that antibiotics like tetracyclines (TCs) was residue, which come from their used in to treat or prevent diseases in beekeeping such as American foulbrood (AFB) and European foulbrood (EFB). As a result, the trace determination of TCs poses a serious challenge for researchers. In this research, we developed an iron microparticles adsorbent through in situ complexation between betel nut natural reagent and iron (III) for dispersive solid phase extraction (d-SPE) to extract oxytetracycline (OTC), tetracycline (TC), chlortetracycline (CTC) and doxycycline (DC) in honey. To increase extraction efficiency, hydrophobic ionic liquid of [Hmim][PF<sub>6</sub>] was synergistically utilized as an extraction solvent to extract and accumulate adsorbent bound with TC before quantitation by HPLC-UV. The chemical and physical parameters affecting the extraction efficiency were evaluated, and it was found that the developed method was able to provide low limit of detection (1–3 µg L<sup>-1</sup>) and limit of quantification (5–10 µg L<sup>-1</sup>). The enrichment factors for OTC, TC, DC and CTC were 61, 114, 121 and 197 respectively. Therefore, the developed method was successfully applied to determine TC residues in honey samples with recoveries ranging 80.0 to 121%.

**Keywords:** Tetracyclines; Natural reagent; Dispersive solid phase extraction; HPLC-UV; Ionic liquid

## Vortex-assisted dispersive liquid-liquid microextraction for determination of organophosphate pesticides using gas chromatography

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A method for determining trace levels of organophosphate pesticides (chlorpyrifos and ethion) in mango, orange, and tomato juices was developed using a dispersive liquid-liquid microextraction coupled with a vortex agitation approach. In this method, hexane served as a low-density extraction solvent, and acetone was employed as the dispersive solvent. These solutions were added sequentially to the diluted sample solution, which was spiked with carbophenothion as the internal standard. After vortexing and centrifugation at room temperature, the solution was frozen at -25 °C for 60 minutes, and hexane was subsequently decanted into a vial before injection into gas chromatography with flame ionization detection. Under optimal conditions, the proposed method exhibited a satisfactory linearity over the range of 0.5 to 500  $\mu\text{g L}^{-1}$ , achieving the coefficient of determination ( $R^2$ ) higher than 0.999. The detection and quantification limits were 0.1 – 2.0  $\mu\text{g L}^{-1}$  and 0.5 – 5.0  $\mu\text{g L}^{-1}$ , respectively. The recoveries were ranged from 84 to 110 % at the spiked concentration of 100  $\mu\text{g L}^{-1}$ , with relative standard deviations (RSDs) below 2.86 %. The validated method successfully met the criteria outlined in SANTE 11312/2021. This proposed approach is characterized by its simplicity, cost-effectiveness, and demonstrated effectiveness in determining chlorpyrifos and ethion in fruit juice samples.

**Keywords:** Organophosphate; Chlorpyrifos; Ethion; Low-density solvent; Vortex-assisted dispersive liquid-liquid microextraction; Gas chromatography with flame ionization detection



## Determination of tetracycline oxytetracycline and chlortetracycline in *Macrobrachium rosenbergii* by liquid-liquid extraction and solid phase extraction using high-performance liquid chromatography with photodiode array detection

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Tetracycline (TC), Oxytetracycline (OTC), and chlortetracycline (CTC) in *Macrobrachium rosenbergii* (shrimp) were detected by using a rapid sensitive and reliable method via high-performance liquid chromatography (HPLC). Shrimp samples were extracted to liquid-liquid extraction (LLE) and cleaned-up using solid-phase extraction (SPE). The analytes were eluted 0.10 M McIlvaine- $\text{Na}_2\text{EDTA}$  (pH 4.0)/methanol (80:20, %v/v), followed by an octadecyl  $\text{C}_{18}$  SPE cartridge clean-up procedure. The HPLC separation was carried out on a column C-18 (250 mm x 4.5 mm i.d., 5  $\mu\text{m}$ ) at 30 °C with mobile phase elution of acetonitrile (A) and 0.01% trifluoroacetic acid (B), a gradient elution 15(A):85(B), %v/v at 0-4 min, switching to 30(A):70(B), %v/v at 7 min and hold time 5 min after that adjusting to 15(A): 85(B), %v/v for 13-14 min, the flow rate was 1.0 ml/min using photodiode array detection at 365 nm. Calibration curves in the studied concentration ranges of 1.0-10.0  $\mu\text{g/ml}$  was obtained linear with a correlation coefficient ( $R^2$ ) of greater than 0.995. The limits of detection of TC, OTC, and CTC were 0.012, 0.018 and 0.010  $\mu\text{g/ml}$  in shrimp, respectively. The limits of quantitation of TC, OTC, and CTC were 0.039, 0.062 and 0.033  $\mu\text{g/ml}$  in shrimp, respectively. The recoveries of TC, OTC, and CTC from spiked sample at the three concentrations (1.0, 6.0 and 10.0  $\mu\text{g/ml}$ ) were in the range 91.1-97.5%, 96.8-97.5% and 93.2-96.6%, respectively. This method was applied for determination of TC, OTC, and CTC residues in shrimp samples from local markets of Nakhon Ratchasima Province.

**Keywords:** Tetracycline; Oxytetracycline; Chlortetracycline; *Macrobrachium rosenbergii*; Solid-phase extraction

## Optimization of ultrasonic extraction for the determination of PAHs in sediment by GC-MS

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The extraction of 6 polycyclic aromatic hydrocarbons (PAHs) including naphthalene, acenaphthylene, acenaphthene, fluorene, phenanthrene, and fluoranthene in sediment samples by ultrasonic extraction method was studied. The amount of PAHs was analyzed by gas chromatography-mass spectrometry. The extracted solvent of 25 mL dichloromethane: hexane (1:1 v/v), ultrasonic extraction time of 30 minute, drying temperature of 40°C, and addition of 2.50 g sodium chloride was achieved for good extraction efficiency. Under the optimum conditions, the limit of detection and the limit of quantification were in the range of 0.0008-0.2970 and 0.0024-0.9000 µg/kg, respectively. The correlation coefficient of the calibration curves were in the range of 0.9802-0.9960. For the precision study, repeatability of 0.83-5.83% and reproducibility of 16.42-25.46% were obtained.

**Keywords:** Ultrasonic extraction; Polycyclic aromatic hydrocarbons; GC-MS



## Determination of the $\Delta^9$ -tetrahydrocannabinol metabolite in urine by online-solid phase extraction coupled with liquid chromatography-mass spectrometry

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Delta-9-tetrahydrocannabinol (THC) is the bioactive compound in marijuana (*Cannabis sativa* L.) that can be used for medical purposes at low concentrations. THC is metabolized in the liver and transformed to 11-nor- $\Delta^9$ -tetrahydrocannabinol-9-carboxylic acid (11-nor- $\Delta^9$ -THC-COOH), which is excreted in urine. Therefore, this study aims to develop a sensitive analytical method for the determination of the THC metabolite in urine at trace level. Online-solid phase extraction (HyperSep Retain PEP Online-SPE column) was employed to extract of 11-nor- $\Delta^9$ -THC-COOH in urine before analysis by liquid chromatography-mass spectrometry (LC-MS). The online-SPE is a simple and rapid that reduces the preparation steps by passing the sample through the SPE cartridge and then eluting with appropriated solvent before separating by LC-MS. This method demonstrated the detection limit and quantitative limit at 0.20 ng mL<sup>-1</sup> and 1.00 ng mL<sup>-1</sup>, respectively. The linearity range was 1.00-100.00 ng mL<sup>-1</sup>. According to the SWGTOX guidelines, the accuracy value (%bias) and precision value of the developed method were considered within the acceptable criteria ( $\pm 20\%$ ). The percentage of recovery was observed in the range 99.16–101.60%. Therefore, this method is accurate, precise and appropriate for analyzing 11-nor- $\Delta^9$ -THC-COOH metabolite in urine sample at low-level concentrations.

**Keywords:** Delta-9-tetrahydrocannabinol; Marijuana; Urine; Online-solid phase extraction

## Assessing the quality of online-purchased alcohol-based hand sanitizers from Thailand online market using a GC-FID technique

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Since the COVID-19 pandemic, the proliferation of online marketplaces has provided consumers with convenient access to a wide range of alcohol-based hand sanitizers. However, without a rigorous post-marketing surveillance, the quality of these products remains a significant concern, given the potential risks associated with substandard or counterfeit formulations. This research conducted the post marketing surveillance for quality investigation of alcohol-based hand sanitizers purchased from Thailand online markets. The alcohol content and ingredient authenticity were examined compliance with Thai industrial standards (TIS:3302-2021) using gas chromatography-flame ionization detector (GC-FID) technique. Each of the hand sanitizer samples was diluted tenfold with deionized water; isobutanol was added as an internal standard prior to the analysis. The results show that the random purchase during March 2023 to August 2023 of the 41 alcohol-based products bought from Thai online markets come in various formulations, 29 liquid forms, 8 gel forms and 4 wet wipe forms. Products that have ethanol content compliance with TIS:3302-2021 ( $\geq 70\%v/v$ ), were found to be 65.9% of all products. However, 25 products out of 65.9% found alcohol content label mismatch in either higher or lesser than the maximum acceptable deviation in the active substance content specified on label. 3 products found methanol content exceed the TIS: 3302-2021 limit, among of these, 1 product spotted as a counterfeit formulation of using methanol instead of ethanol/isopropanol. Methanol is harmful and hardly distinguishable by odor from ethanol. These results reveal that the post-marketing surveillance of alcohol-based hand sanitizers by laboratory testing is therefore very necessary to ensure safety for consumers.

**Keywords:** Alcohol-based hand sanitizer; Thailand online market; Post-marketing surveillance; TIS-3302-2021; GC-FID

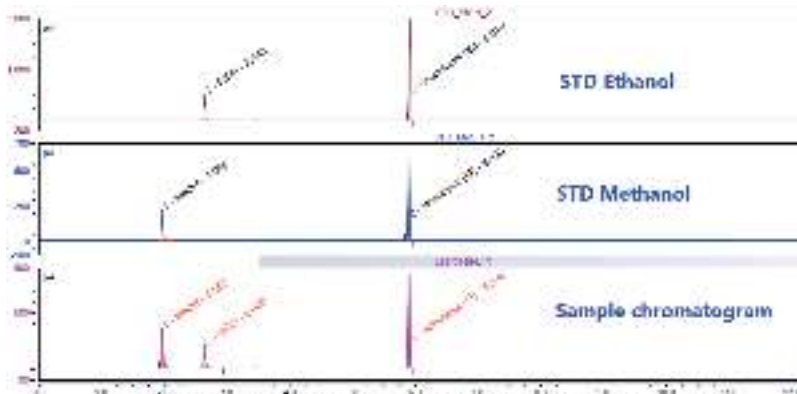


Figure 1: Chromatograms of the detection of methanol and ethanol in sample

## COVID-19 screening in sweat by volatile analysis using GC-MS and the relationship with military training dog results

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Several approaches have been recently developed as an alternative method for COVID-19 screening due to the pandemic of SAR-CoV-2 since 2019 based on rapid, non-invasive and cost- effectiveness. Sniffer dog is one of those alternative methods successfully developed with the performance results showing as > 90% of accuracy. Six military training dogs were trained to recognize unique smells of positive COVID-19 patient's sweat as well as smells of negative cases. Then, this training dogs could differentiate among patients who were infected and uninfected with COVID-19. We worked with gas chromatography – mass spectrometry (GC-MS) for volatile analysis in sweat samples of volunteer patients together with statistical analyses to clarify the potential markers of VOCs/odors with the relationship of COVID-19 screening results obtained from military training dog. This work was under the collaboration of Phramongkutklao hospital and Chulalongkorn university in Bangkok, Thailand. Two sets of sweat samples were collected from each volunteers using sterile cotton rods as an absorbent material. A set of sweat samples included two cotton rods after sweat absorption from both right and left sides of armpits. the first sample set was brought to military training dog and the second sample set was brought to GC-MS method for volatiles analysis. In addition, all results were validated by comparison with RT-PCR results. Finally, several volatile compounds were identified and reported as possible markers in human sweat that the canines recognized. This study is expected to provide a new insight into the area of dogs' odor recognition for improved screening of COVID-19 and the other related diseases in the future.

**Keywords:** COVID-19 screening; Training dog; GC-MS; Sweat analysis; VOCs

## Method development of peptide mapping characterization of monoclonal antibody (mAb) using liquid chromatography time-of-flight mass spectrometry (LC/Q-TOF)

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A method for characterization on peptide mapping parameter using liquid chromatography time-of-flight mass spectrometry (LC/QTOF) have been developed and validated. Sample preparation steps and gradient ratio of mobile phase were modified to improve the protein coverage percentage. Qualitative validation such as repeatability and reproducibility were performed with monoclonal antibody, Trastuzumab. The Protein Metrics software was also used for analyzing the coverage percentage of peptide mapping. The samples were prepared by reduced disulfide bond of the monoclonal antibody with dithiothreitol (DTT) and alkylated free thiol group with Iodoacetamide (IAA) then digested the peptides with restriction enzyme, trypsin, which specifically cleaves C-terminal to Arginine (R) and Lysine (K). The digestion reaction was performed at 37 °C and incubated overnight then stop the reaction using formic acid. The liquid chromatography was performed by using C18 column and 0.1% formic acid and 0.01% TFA in water and 0.1% formic acid and 0.01%TFA in acetonitrile (ACN) as mobile phases. The QTOF was operated using positive mode electrospray ionization using data dependent acquisition. The m/z were selected to second fragmentation according to priority list which generate by calculated m/z of the interested molecule. The other data acquisition processing was performed as in-house method which able to adjust to new molecules of interest. This method gives the coverage percentage over 90% in both heavy chain and light chain of the monoclonal antibody molecule. The use of LC-MSMS technique gives the highly efficient and robust approach to confirm the characteristic of the Trastuzumab molecule in peptide mapping parameter which can be updates to use with other protein molecules for further characterization.

**Keywords:** Trastuzamab; Method development; Liquid chromatography; QTOF; monoclonal antibody

## Development of analytical method for analysis of tetrahydrocannabinol and cannabidiol in tea infusion by high performance liquid chromatography

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In accordance with the Notification of Ministry of Public Health No. 427 (2021), the amount of tetrahydrocannabinol (THC) and cannabidiol (CBD) in food products containing certain parts of cannabis or hemp, shall not exceed 1.6 and 1.41 mg per package, respectively. This study aims to develop a simple analytical method to determine THC and CBD in tea infusion by High Performance Liquid Chromatography (HPLC). THC and CBD from tea samples were extracted by using solvent extraction then cleaned-up by SPE before HPLC quantitation. HPLC mobile phase consisted of 5 mM ammonium acetate and acetonitrile with gradient elution program operated at a flow rate of 1.0 mL/min. A Photodiode array detector (DAD) was set at a wavelength of 220 nm. The standard calibration curves of CBD and THC were linear in the concentration range of 0.5-10.0 µg/mL and the correlation coefficient ( $r^2$ ) were 0.9998 and 0.9992, respectively. The limits of detection and quantitation of this method for CBD and THC were 0.20 µg/mL and 0.50 µg/mL, respectively. The accuracy of the method was between 83% and 92%, with a precision of 10.75% to 11.72%RSD. The optimal method was successfully tested on the commercial infusion tea samples purchased in Thailand.

**Keywords:** Tetrahydrocannabinol (THC); Cannabidiol (CBD); High Performance Liquid Chromatography

## Chromatographic resolution of (+/-) -dimethyl *N,N*-dibenzyl-glutamate using modified silica with *N*-(pent-3-en-5-ol)ylglutarimide chiral selectors

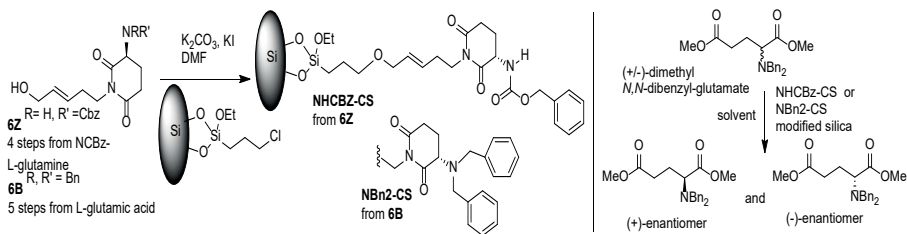
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Chiral resolution or the separation of enantiomers though can be performed by various techniques, the chromatographic resolution by chiral stationary phases (CSP) has proven to be the most attractive and applicable method for separating and acquiring pure enantiomer. Over the past few decades, huge numbers of CSPs have been widely studied and developed to be used in the HPLC system to give enantiomerically pure substrates which are of great importance in the early steps of medicinal synthesis. This can reduce overall cost of the synthesis process. Herein, we describe new chiral selectors for modification of the silica gel used for column chromatography. The chiral selectors are derivatives of *N*-(pent-3-en-5-ol)ylglutarimide with different substituted amino group at C2 position. The chiral selectors **6Z** and **6B** were synthesized in 4 steps from L-*N*-CBz-glutamine and 5 steps from L-glutamic acid, respectively. They were coupled to the triethoxychloropropylsilane-modified silica gel to give NHCBZ-CS chiral selector and NBN2-CS chiral selector. In order to prove chromatographic resolution of racemic mixture, the modified silica was used for separation of racemic (+/-) -dimethyl *N,N*-dibenzyl-glutamate and resulted in partial resolution to give enantioenriched (+)- and (-)- enantiomers. The results, conditions and hypothesis of the resolution based on three-point interaction between the analyte and a chiral selector approach that resulted in different polarity value from each eluted fraction will be discussed in the presentation.



**Keywords:** Chiral resolution; Chiral stationary phase; Chiral selector; Modified silica gel; Enantio-separation



## K9 Dogs sniff COVID-19 in Thailand trained by positive mixed biomarkers to improved screening test accuracy during pandemic

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This study developed a reliable, rapid, and non-invasive diagnostic approach for screening of populations with SARS-CoV-2 infection. Sniffer dogs were trained to perform the screening test according to differentiation of sweat samples by sniffing on the volatile organic compounds (VOCs) collected under armpits and socks of the asymptomatic or uninfected people, symptomatic with RT-PCR confirmed cases. The six sniffer dogs performed sniffing based on a double-blind trial for diagnosis of 100 SARS-CoV-2 infected and 100 uninfected samples in Thailand. They were able to improve the screening test with positive mixed biomarkers derived from statistical analysis of headspace-solid phase microextraction-gas chromatography-mass spectrometry (HS-SPME-GC-MS) was applied to analyze volatile compounds in the samples for the potential markers in armpit samples and socks such as aldehyde and aromatics compound. The screening test of the samples improved specificity and sensitivity up to 94% and 99% with respectively, with the accuracy of 98% regardless of the sweat sampling materials (cottons and socks) and sweat origins. The deploy dogs as an alternative point-of-care test would help stopping silent spread in the public areas, point of entry screening and quarantine areas, airports and seaports when the new normal situation is resumed.

**Keywords:** K9 dogs; COVID-19; Non-invasive; Biomarkers; HS-SPME-GC-MS

## Application of microbiology for COVID-19 volatile organic compounds biomarkers identification on surface swabbing and human secretion in Thailand community

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Since the start of the coronavirus disease 2019 (COVID-19) pandemic and its subsequent years, there has been a demand for a quick, cost-effective, and, most importantly, non-invasive approach to screen for the SARS-CoV-2 virus in suspected patients. Various solutions have shown up throughout the years, in this research mainly focus on the volatile organic compound (VOCs) detection of aldehyde and aromatic compounds of COVID-19 biomarkers in secretion objects in the environments contaminated with COVID-19. The samples were obtained from surface swabs taken from market and community, Nonthaburi, Thailand. A headspace solid-phase microextraction coupled with gas chromatography-mass spectrometry (HS-SPME/GC-MS) was used to investigate the concentration of volatile organic compounds biomarkers from the samples during specific time intervals over the total intensity of peak area. The data of the intensity and the time interval coupled with the use of computational and statistical analysis of the data yields a cut-off for determining total positive or negative cases with an overall specificity and sensitivity of 95% and 96%, respectively. This method of utilizing secretion objects in the environment, GC-MS, and computational analysis provides a non-invasive detection method for COVID-19 and the test results were confirmed to be as effective, accurate, fast and timely.

**Keywords:** COVID-19; Volatile organic compounds; HS-SPME; GC-MS; Non-invasive



## Derivatized alpha-cyclodextrin as gas chromatographic stationary phase for separation of chiral alcohols

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Many chiral compounds are important in pharmaceutical industries. The use of pure single enantiomer is desired to avoid unwanted properties. Gas chromatography (GC) is a common technique used to analyze volatile organic compounds. Derivatized beta-cyclodextrins (CDs) were largely used as chiral GC stationary phases to separate enantiomers. In this work, the small-size methylated alpha-CD mixed with polysiloxane was explored as a chiral stationary phase. A capillary column of 15 m long, 0.25 mm i.d., and 0.25  $\mu$ m film of stationary phase was used. Underivatized chiral alcohols were examined including aliphatic alcohols (e.g. 2-octanol, 2-nonanol) and alcohols with aromatic or cyclic structure (e.g. 1-phenylethanols, 1-phenylpropan-2-ol, 1-cyclohexylethanol, 1,2,3,4-tetrahydro-2-naphthol). Separations of all analytes were investigated by GC equipped with a split injector (250 °C) and a flame ionization detector (250 °C). Hydrogen was used as a carrier gas at a velocity of 50 cm/sec. Conditions for complete enantiomeric separation of each analyte were determined. It was found that all aliphatic alcohols could be separated into their enantiomers. Enantiomeric separations of alcohols with aromatic or cyclic structure depended on position of stereogenic center and type and position of substitution. While enantiomers of 1-phenylethanol could be completely separated (at 127 °C,  $k'_2 = 2.74$ ,  $\alpha = 1.03$ ); enantiomers of 1-phenylpropan-2-ol could not be separated with this column. The influence of column temperature on enantioselectivity and retention were compared. This methylated alpha-CD showed good enantioselectivity towards chiral alcohols of different structures, especially aliphatic alcohols. It can be an alternative supplement to other chiral columns.

**Keywords:** Gas chromatography; Cyclodextrin; Chiral alcohol

## Enhancing phenolic acid separation in capillary electrophoresis through surface modification using polyethyleneimine

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Phenolic acids are anionic compounds with structurally similar characteristics, which makes it challenging to obtain high separation efficiency. Capillary electrophoresis (CE) offers an advanced analytical solution with rapid analysis, high resolution, and minimal reagent requirements. Current advancements in CE aim to enhance separation efficiency, primarily by modifying electric osmotic flow (EOF). EOF adjustments can be made by incorporating additives into the buffer or altering the inner wall of the capillary. We attempt to chemically modify the capillary surface for providing surface stability, and reusability. In this work, we employed 0.1 % (w/v) polyethyleneimine (PEI) as a coating to suppress EOF mobility, thereby extending the migration time of target analytes with higher separation efficiency. This surface modification is intended to adjust electrokinetic chromatographic separation efficiency with detection by capacitively coupled contactless conductivity detection (C<sup>4</sup>D). The PEI layer imparts positive charges, influencing the direction and magnitude of EOF. The comparison between two separation systems; System 1: PEI modified capillary, run buffer of 40.0 mM MES/His buffer (pH 6.0) and System 2: non-modified capillary, the same buffer with CTAB addition is investigated using a mixture of nine compounds (benzoic acid, gentisic acid, 4-hydroxyphenyl acetic acid, vanillic acid, coumaric acid, syringic acid, caffeic acid, ferulic acid, and sinapic acid). The developed system (System 1) provided higher separation efficiency with the increment of 3-fold peak resolution ( $R_s$ ) compared to System 2. The  $R_s$  and plate number  $N$  of system 1 were 0.98 – 3.14, and  $\geq 1.35 \times 10^4 \text{ m}^{-1}$ , respectively.

**Keywords:** Polyethyleneimine surface modification; Phenolic acids; Capacitively coupled contactless conductivity detection; C<sup>4</sup>D

## Accuracy-based PT programs for determination of As, Cd and Pb in herbs

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Accuracy-based proficiency test program (PT) is a powerful quality control tool to evaluate laboratory performance. National Institute of Metrology (Thailand), NIMT, had organized two PT programs for the determination of As, Cd and Pb in herb powders to serve the herbal medicine product industry. Green Chiretta (*Andrographis Paniculata*) and Turmeric (*Curcuma longa L.*) are prioritized as commercial herbs, the former is known for Covid-19 treatment. PTs were carried out in accordance with ISO/IEC 17043 to evaluate laboratories performance. Their results were statistically evaluated using the z score,  $E_n$  score and Zeta score with the metrologically traceable assigned values from NIMT which their Calibration and Measurement Capabilities (CMCs) were internationally recognized. More than two-thirds of participating laboratories were found their performance satisfactory ( $|z \text{ score}| \leq 2$ ) in both PT programs. It was found that 60% of all laboratories reported measurement uncertainties which their performances were evaluated using the Zeta score and  $E_n$  scores as supplementary. PT results revealed that 60 % of those laboratories were evaluated satisfactory on the As analysis, whereas only 25 % of the participants achieved satisfactory results on Cd and Pb analysis. Unsatisfactory Zeta score/  $E_n$  score results can be explained by a large deviation of the reported result from the assigned value as well as an inappropriate estimation of its uncertainty. Accuracy-based PT program allows the participating laboratories to monitor their measurement capability performance and check the appropriateness of each laboratory measurement uncertainty by comparing against metrologically traceable reference values and uncertainties provided.

**Keywords:** Accuracy-based proficiency testing program (PT); Metrologically traceable assigned values; Calibration and Measurement Capabilities (CMCs); Measurement uncertainties

## Method validation for determination of lead and cadmium in paper for food contact using microwave digestion followed by inductively coupled plasma mass spectrometry

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Nowadays, paper-based materials are one of food contact materials (FCMs), extensively used worldwide to fulfill eco-friendly trend due to its degradation. However, paper is often treated with coating, additive, and adhesive materials to enhance its functional properties. Therefore, contaminants such as optical brightening agents, antimicrobial constituents and heavy metals can migrate from paper based FCMs to food. This work proposed the method validation for lead (Pb) and cadmium (Cd) analysis in the paper. It is necessary that the laboratory has to validate this testing method to evaluate whether the validated method is fit for intended use. The paper based FCMs was digested using microwave digestion in acidic condition. All metals were then analyzed by inductively coupled plasma mass spectrometry (ICP-MS) which is instead of European Standard (EN) 12498 method referred in Thai Industrial Standard (TIS) 2948-2019 standard due to unacceptable accuracy in adsorbent-paper. The results indicated that this method can detect the metals in the acceptable range of TIS criteria as Pb lower than  $3.0 \text{ mg kg}^{-1}$  and Cd lower than  $0.50 \text{ mg kg}^{-1}$ . The bias and precision studies showed that percentage of recovery and relative standard deviations of two elements were between 85-105% and less than 10%, respectively. Moreover, the expanded uncertainties of all elements were less than  $\pm 15\%$  at the confidence level of 95%. Thus, this test method for determination of two heavy metals in food contact paper by ICP-MS using microwave digestion was valid and fit for the intended use.

**Keywords:** heavy metals; paper for food contact; method validation; microwave digestion; ICP-MS



The schematic diagram of determination of lead and cadmium in food contact paper using microwave digestion followed by ICP-MS.

## Using single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) for study silver nanoparticles (AgNPs) released from food packaging materials into different types of food simulants

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Due to their antimicrobial properties, silver nanoparticles (AgNPs) are used extensively in food packaging technology to help maintaining food freshness for longer storage time. However, the potential risks to humans from AgNPs exposure are of concern as AgNPs can be released from the packaging into foods. Therefore, evaluating the potential migration of AgNPs from food packaging is required. In this study, we used a single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) technique that can offer information on size and particle concentration of nanoparticles in liquid medium at low concentration to track the change of AgNPs at several steps of their route from synthesis to food packaging containing AgNPs in various food simulants. The AgNPs migration study was carried out by incubating AgNPs in various food simulants, including, ultrapure water, acetic acid, ethanol at the storage conditions as 20 °C, 40 °C for 1, 7 and 10 Days, and 70 °C for 2 hours and 6 hours. The migration solution was characterized with SP-ICP-MS to observe particle size, size distribution, and particle concentration. It was found that AgNPs were potentially migrated into food simulants, especially when in contact with acetic acid or acidic substances.

**Keywords:** Silver nanoparticles; Single particle inductively coupled plasma mass spectrometry; Food packaging; Migration; Food simulants

## Analysis of carbon-based microparticles released from plastic products with single particle inductively coupled plasma mass spectrometry

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A method based on single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) was developed for investigation of microplastics released from consumer products. In SP-ICP-MS, a standard type nebulizer was used for sample introduction with the flow rate at 0.18 mL min<sup>-1</sup> in order to minimize background signal of dissolved carbon species which can blind carbon particle signal leading to incorrect measurement. Under this condition, the calibration graph of dissolved forms of carbon was prepared in the range of 1 – 5 µg L<sup>-1</sup> by using sucrose solution as a source of carbon. The calibration of polystyrene particles was linear in the range of 1 – 6 µm with the size detection limit of 400 nm. This proposed method was applied to the determination of particle size of laboratory synthesized polystyrene latex in ethanol solution. The particle sizes measured by SP-ICP-MS were larger than the sizes reported by scanning electron microscopy (SEM) which was due to matrix interferences of ethanol solution. Ethanol was then removed from polystyrene particles suspension before the analysis by centrifugation at 6000 rpm for 10 minutes, then the supernatant was discarded, followed by adding deionized water to suspend the particles. After the washing process, the sizes observed from SP-ICP-MS were similar with sizes observed from SEM. Then, the developed SP-ICP-MS method was applied to observe the release of microplastics from consumer products with the results compared with the results from dynamic light scattering (DLS) and SEM.

**Keywords:** Microplastics; Release; Plastic products; Single particle inductively coupled plasma mass spectrometry

## Using single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) for the study of zinc oxide nanoparticles suspension stability in various media

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Since zinc oxide (ZnO) nanoparticles have antimicrobial and UV light-absorbing properties, they are widely employed in industry, particularly in food packaging, paint, and consumer products such as sunscreen. It is essential to control the size and stability of ZnO nanoparticles. In this study, ZnO nanoparticles dispersed in deionized water, triton X-100 as a non-ionic surfactant media, cetyltrimethylammonium bromide (CTAB) as a cationic surfactant media, and sodium dodecyl sulfate (SDS) as an anionic surfactant media were analyzed using single particle inductively coupled plasma mass spectrometry (SP-ICP-MS) along with settling experiment which gathered at various temporal and vertical distances. The combination of SP-ICP-MS and the settling process allows for the investigation of particle concentration and size distribution at very low concentrations, offering a new approach for investigation of the stability of ZnO suspension. The ZnO nanoparticles were found to be more stable in an anionic surfactant, SDS, than in other media, based on the mean size and total concentration observed which suggested to have slow sedimentation. Transmission electron microscopy, zetasizer and conventional mode ICP-MS confirmed the same trend as observed by SP-ICP-MS technique, implying that this newly developed method can be used as a characterization tool to evaluate the stability of nanoparticles.

**Keywords:** Zinc oxide nanoparticles; Single particle inductively coupled plasma mass spectrometry; Surfactant; Suspension stability; Settling

## Method validation for determination of heavy metals in alum (aluminium sulphate) by inductively coupled plasma mass spectrometer

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Aluminium sulphate (Alum) is widely used in water purification and wastewater treatment. It can remove the suspended impurities by coagulating them into larger particles which will settle to the bottom of the container or will be filter out easily. However, the present of heavy metals like Manganese (Mn), Chromium (Cr), and Cadmium (Cd) in large amounts can negatively impact the water quality. At present, the analysis of heavy metal content in alum according to Thai Industrial Standard (TIS) 165 - 2011 uses the graphite furnace atomic absorption spectrophotometer. However, a limitation of this technique is a time-consuming and not suitable for routine work. The linearity range of these heavy metals were narrow between 0 – 20 µg/L; therefore, the high-concentrated sample need to be diluted about 200 times from the initial concentration. Additionally, the determination of Cd required to use standard addition techniques, due to a matrix interference effect, which was more tedious to prepare the calibration plot for each sample separately. In this work, the heavy metals in alum were tested by digesting the sample with 1:1 nitric acid and then quantifying the amount of Mn, Cr, and Cd simultaneously by using an Inductively Coupled Plasma Mass Spectrometer (ICP-MS). The linear range of three elements was 0 - 1000 µg/L. The bias and precision studies showed that percentage of recovery and relative standard deviations of three elements were between 80 - 110% and less than 10%, respectively. Thus, this test method offered several advantages, including simultaneous detection and quantification of a broader range of elements and a linearity range over a higher range of concentration level reducing the necessity of sample dilution process. As a result, this developed method was suitable for routine work in the analysis of heavy metals in alum using ICP-MS.

**Keywords:** Aluminium sulphate; Alum; Heavy metals; ICP-MS

## Thailand reference material: TRM-F-2007 elements in turmeric powder

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The application of certified reference material (CRM) in analytical chemistry for quality control purposes is recognized and recommended by international, national and professional organizations worldwide. Due to the unavailability of matrix matched CRMs in our country, TRM-F-2007:elements in turmeric powder (*Curcuma longa*) was initiated by National Institute of Metrology (Thailand) (NIMT) for the analysis of key elements. It was developed under the trade name of Thailand Reference Material (TRM).

Quantification of 15 elements was performed by ICP-MS and ICP-OES using three analytical techniques: isotope dilution mass spectrometry (IDMS), gravimetric standard addition (GSA) and external calibration. Homogeneity and short-term stability were studied using external calibration technique, while long-term stability was studied using IDMS or GSA. Statistical data shows that TRM-F-2007 is homogeneous and stable at temperature 45 °C for 3 weeks and it is stable at room temperature at least 3 years. Characterization of the elements requires at least two analytical methods. Eleven elements (As, Ca, Cd, Cu, Fe, K, Mg, Ni, P, Pb and Zn) are certified by weighting method from 2 – 6 analytical methods to provide accuracy and measurement uncertainty whereas 4 elements (Cr, Hg, Mn and Na) are mentioned as information value.

The entire process of production, measurement and the statistical models used are all controlled according to the quality system ISO 17034:2016, ISO/IEC 17025:2017 and ISO Guide 35:2017, respectively. Therefore, TRM-F-2007 is reliable and traceable to SI units through unbroken chain. This TRM is suitable for quality control purposes such as method validation, and quality control sample.

**Keywords:** Thailand Reference Material; Turmeric Powder; Element, National Institute of Metrology (Thailand)

## Papain, as a specific removal treatment for conservative art

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Protein-based glues are natural polymers used as adhesives, binders, and consolidants in the conservation of artifacts. With the fluctuating environment, the aging mechanisms and behavior on light exposure may alter the physical and chemical properties of the artwork such as shrunk, cracked, rigid, and brittle. Although there are many techniques to remove these adhesive materials, the specific removal method of working under mild conditions is still a shortcoming. Herein papain, belonging to a proteolytic enzyme group capable of digesting large-sized proteins into smaller molecules, has been proposed as an alternative specific treatment. The activity of papain was monitored by the hydrolysis of *N* $\alpha$ -benzoyl-arginine-*p*-nitroanilide (BAPNA). The presence of a yellow color produced by a product, *p*-nitroaniline, can be measured at 430 nm. . To identify the optimum condition for the use of papain, various factors including enzyme concentration, reaction temperature, incubation time, the presence of metal ions and enzyme deactivation time were optimized. Finally, the effectiveness of papain on adhesive paste removal was studied on the canvas samples. Scanning electron microscopy (SEM) photo revealed different degrees of parallel ridges, characteristic of fiber, reflecting the different amounts of remaining adhesive pastes.

**Keywords:** Conservative arts; Low-cost enzyme treatment; Papain; Protein-based glues;



## Effect of catechin on the structures and activities of papain

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The development of polyphenol-protein complexes has gained increasing attention due to their potential to enhance the antioxidant activities of proteins. In this study, changes in enzymatic activity after the addition of catechin (flavanols or flavan-3-ols), the major ingredient in green tea, were investigated. Papain was incubated in the presence of catechin, the precipitate discarded, and the remaining enzyme activity in the supernatant was determined with N- $\alpha$ -benzoyl-arginine-p-nitroanilide (BAPNA) as a substrate. Complex formation between catechin and papain markedly affects the activity of the enzyme resulting in the diminishes of the yellow-colored product observed at 410 nm. The presence of catechin enhanced the papain activity at low concentrations, while the high concentrations substantially decreased the formation of the yellow product. The activity of complexes was detectable throughout the entire studied pH range, but it was especially high close to the pH optima of the enzymes. Moreover, the effect of catechin on the papain structures was investigated by UV-visible absorbance and fluorescence methods. Preliminary results show that upon catechin binding, the alteration of the main papain's absorption band (290 nm) reflects the transformation of the microenvironment of their aromatic amino acids. These results could provide valuable guidance for the future food industries.

**Keywords:** Catechin; Papain; Protein-polyphenol interactions; Structural properties

## The removal of green and red reactive dyes by photolysis, oxidation and photooxidation processes using a simple UV reactor

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This research investigates the efficiency of advanced oxidation processes for the removal of green and red reactive dyes. These processes are photolysis (with only UV lamp), oxidation (with only potassium persulfate) and photooxidation (with UV lamp plus potassium persulfate) processes. All processes were done in a simple UV reactor. Firstly, the absorption spectra and linear calibration graphs of both reactive dyes were carried out using UV-Visible spectrophotometer. After that the conditions of treatment processes were examined such as flow rates, types of tubing for roll round the UV lamp, sample volumes, UV lamp powers, potassium persulfate concentrations and dye concentrations. Under optimum conditions, a  $1.13 \pm 0.06$  mL/min of flow rate, a PTFE tubing (200 cm length, 0.86 mm i.d.), a 10 mL of sample volume, a 36 W of UV power, a 3.0 %w/v of potassium persulfate and a 350 mg/L of green and red dye were selected. From the results, the photolysis process of green and red dyes achieved 100% dye removal in 80 mins, respectively. For the oxidation process, a green dye was removed 35.95% of the dye in 90 min, while a red dye was removed 18.33% of the dye in 60 min. And for the photooxidation process, green and red dyes achieved 100% dye removal in 25 mins, respectively. Results also revealed that the photooxidation process was higher efficiency for green and red removals than the photolysis and oxidation processes, respectively.

**Keywords:** Green dye; Red dye; Photolysis; Oxidation; Photooxidation

## Development of a sensitivity enzyme-linked immunosorbent assay for detection of leucomalachite green

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Leucomalachite green (LMG) is produced through the transformation of malachite green (MG). LMG is commonly used in the aquatic industry to control and treat diseases caused by fungi, parasites, and protozoa in aquatic animals. Its popularity stems from being readily available, cost-effective, and efficacious in treatment. LMG residues can accumulate in the tissues of aquatic animals, potentially leading to adverse effects on humans. Therefore, enzyme-linked immunosorbent assay (ELISA) was developed for detection of LMG based on the immunocomplex binding between antibodies labeled with biotin and HRP-streptavidin. After adding the 3,3',5,5'-tetramethylbenzidine and  $H_2O_2$ , the blue immunocomplex was obtained. By measuring using the method UV-vis spectrophotometry. The linear range of LMG is from 0.1– 4 ug/L with a detection limit of 0.039 ug/L. The limit of the quantitative value was 0.13 ug/L. The ELISA developed for the detection of LMG in aquatic animals had high precision and low detection limit. This LMG biosensor showed considerable potential as a testing tool for the sensitive detection of trace LMG. The selectivity and the ability of quantitative analysis of the method were validated in real food samples. This LMG biosensor showed considerable potential as a testing tool for the sensitive detection of trace LMG.

**Keywords:** Leucomalachite green, Enzyme-linked immunosorbent assay, Aquatic animal

# One-step hydrothermal process for GO@FeO nanocomposite synthesis and characterization

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The nanocomposite of graphene oxide and FeO (GO@FeO) was synthesized by a simple one-step hydrothermal process at 160 °C. The synthesized particle was characterized by UV-Vis spectroscopy, Fourier transform infrared (FT-IR), and CHNS analyzer. The UV-visible absorption spectra of GO@FeO demonstrated peaks around 290 and 370 nm. The FT-IR spectra showed bands corresponding to the functional groups such as –OH, –C=C, and –C=O groups. The element analysis from CHNS analyzer demonstrated GO@FeO particles mainly consisted of C and H. Furthermore, electrochemical cyclic voltammetry was studied by modified GO@FeO particles at glassy carbon electrode (GCE) comparison with bare GCE in 5 mM Fe(CN)<sub>6</sub><sup>3-/4-</sup> solution. The difference in anodic and cathodic peak was 0.10 V and 0.25 V for GO@FeO/GCE and bare GCE, respectively. Also, the anodic and cathodic currents obtained from GO@FeO/GCE were higher than those from the bare GCE, which were due to effective electron transfer between the GO@FeO/GCE electrode surface and electrolyte, suggesting that its suitability to be applied as electrochemical sensor.

**Keywords:** GO@FeO; Nanocomposite; Hydrothermal

# Catalytic Chemistry (CC)

## Oral Presentation

# Uncovering insights in data-driven catalyst design: A case study in oxidative coupling of methane

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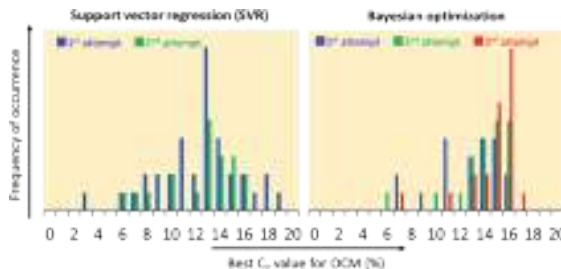
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Catalyst Informatics has received a lot of attention [Takahashi et al., *Chem. Commun.* 2023, 59, 2222.], where the multiple relationship analyses in the datasets of high-throughput experimentations (HTE), published data, and/or computational development are performed by data management techniques to guide access to the demand for desired catalyst performance. Herein, Support vector regression (SVR) and the Bayesian optimization processes based on systematic HTE data [Taniike et al., *ACS Catal.* 2020, 10, 921; *ibid.* 2021, 11, 1797] and literature data [Shimizu et al., *ChemCatChem* 2021, 13, 3636] are applied to the design of catalysts for the oxidative coupling of methane (OCM), which produces C<sub>2</sub> compounds (C<sub>2</sub>H<sub>4</sub> and C<sub>2</sub>H<sub>6</sub>) from CH<sub>4</sub>. SVR can find eight catalysts showing C<sub>2</sub> yield higher than 15.0% in the 1<sup>st</sup> validation under the present reaction conditions, however the 2<sup>nd</sup> attempt of SVR using the updated dataset including the 1<sup>st</sup> validation results was not able to suggest any other potential OCM catalyst. While, Bayesian optimization was examined repeatedly for three cycles of prediction, validation, and dataset updating processes. It could guide the new catalyst design toward the upper range for C<sub>2</sub> yields: the number of occurrences with the best C<sub>2</sub> yield value higher than 15.00% was 3, 8, and 14 catalysts, respectively, in the 1<sup>st</sup>, 2<sup>nd</sup>, and 3<sup>rd</sup> validation. However, the best C<sub>2</sub> yield value did not change at around 16.5%. Accordingly, data-driven catalyst design involves a different set of defect issues from the conventional style of catalyst investigations [Nishimura et al., *Catal. Sci. Technol.* 2023, 13, 4646].

**Keywords:** Heterogeneous catalyst informatics; Oxidative coupling of methane (OCM); Uncovering insights, Machine learning (ML); Support vector regression (SVR); Bayesian optimization processes



**Figure 1.** Results of SVR and Bayesian optimization-driven catalyst investigation

# Ethanol steam reforming using Ni catalyst supported on ZrO<sub>2</sub>-doped Al<sub>2</sub>O<sub>3</sub> with magnetic inducement

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Nickel catalysts are used to enhance catalytic activity in ethanol steam reforming; however, they suffer from deactivation due to coke formation. Alumina support possesses acidic sites which increase coke formation. It has been shown that partially doping alumina support with ZrO<sub>2</sub> can improve the stability, adjust the acidity, and influence coke formation. The dispersion of the dopant in the support is essential to ensure homogeneity of the dopant effect. The application of magnetic inducement has been shown to affect the dispersion of cerium in alumina support. Therefore, in this study, magnetic fields will be used during the preparation of ZrO<sub>2</sub>-doped-Al<sub>2</sub>O<sub>3</sub> and their effect on catalytic activity for ethanol steam reforming and coke reduction will be discussed.

**Keywords:** Ethanol steam reforming; ZrO<sub>2</sub> -doped-Al<sub>2</sub>O<sub>3</sub>; Ni catalyst; Magnetic inducement

## Computational modeling of carbon monoxide oxidation on platinum supported on cerium dioxide

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In order to contribute to clarification of the mechanism of CO oxidation on platinum supported on  $\text{CeO}_2$  we modeled the process on mononuclear platinum species and Pt clusters employing periodic density functional calculations with PW91 functional and cut-off of the planewave basis of 415 eV. For localization of the f-electrons of Ce we used U parameter of 4 eV. The models represent regular  $\text{CeO}_2(111)$  surface and  $\text{Ce}_{21}\text{O}_{42}$  nanoparticle. This approach and models were confirmed to provide reliable results in previous computational studies.

The mechanism involves two reaction steps, oxidation of CO and restoration of the catalyst via reoxidation. The lowest activation barriers are calculated for the reaction paths via  $\text{Pt}^{2+}(\text{CO})_2$  or  $\text{Pt}^{4+}(\text{CO})$  complexes: 22 – 35 kJ/mol. Via the dicarbonyl complexes,  $\text{Pt}^{2+}(\text{CO})_2$ , the barriers are 24 - 40 kJ/mol, while the barriers for the reoxidation of the catalyst with  $\text{O}_2$  are somewhat higher, 49 - 69 kJ/mol. Under oxidative conditions, in presence of  $\text{Pt}^{4+}$ , the calculated barriers are 35 - 53 kJ/mol on  $\text{CeO}_2(111)$  surface, and 22 - 27 kJ/mol on the nanoparticle.

The CO oxidation on platinum clusters occurs with relatively low activation barriers when the clusters are completely covered by CO, namely 40 and 50 kJ/mol on ceria surface and 47 or 19 kJ/mol on ceria nanoparticle. Thus, both platinum clusters and cationic species feature relatively low activation barriers, in agreement with experimental results.

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**Keywords:** Heterogeneous catalysis; Cerium dioxide; Platinum; Density functional theory

## Chiral-induced spin selectivity effect at chiral-encoded Pt-Ir surfaces for enhanced oxygen reduction reaction

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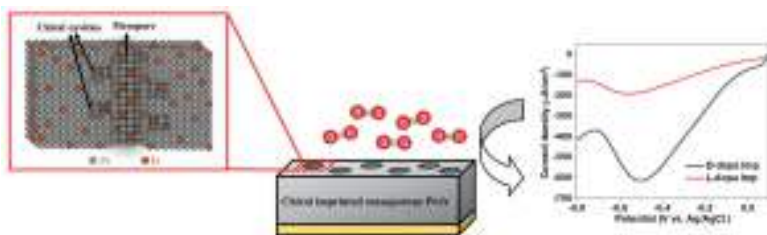
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The Chiral-Induced Spin Selectivity (CISS) effect has been recently proposed as an interesting concept for many different applications. In particular, it has a significant impact on the oxygen reduction reaction (ORR), which plays an important role in clean energy production such as with fuel cells, due to the high electron transfer efficiency from chiral electrode surfaces to oxygen molecules. To date, this perspective is still in an early stage of development, and it has been mostly investigated for electrodes modified with chiral organic monolayers or chiral assemblies. However, it has not been reported so far that a similar effect can also be achieved with intrinsically chiral metal surfaces without chiral monolayer adsorption. Recently, we have successfully developed chiral imprinted Pt-Ir alloys with mesoporous features by electrodeposition of metal salts in the simultaneous presence of non-ionic surfactants and various chiral compounds such as the enantiomers of phenylethanol. These designer materials can perfectly retain molecular chiral information, even after template removal. This allows using them for various applications such as asymmetric synthesis of chiral compounds and enantioselective analysis. In this contribution, we study chiral imprinted mesoporous Pt-Ir obtained by electrodeposition at -0.05 V vs Ag/AgCl with charge density 8 C cm<sup>-2</sup> as an electrocatalyst for ORR. We show that such electrodes can significantly improve ORR due to the CISS effect, eventually leading to higher current intensities. However, this effect cannot be observed when using an achiral electrode of analog composition or which has been imprinted with the opposite enantiomer with the spin selectivity percent up to 49 %. This work opens up novel perspectives for developing catalysts for ORR based on the CISS effect, promoted at intrinsically chiral metal surfaces.

**Keywords:** Electrocatalyst; Oxygen reduction reaction; CISS effect



**Figure 1.** Illustration of the concept using a chiral imprinted mesoporous Pt-Ir electrode to promote ORR.

# I-doped $\text{Bi}_2\text{MoO}_6$ nanosheets for enhanced pollutant photodegradation and hydrogen evolution

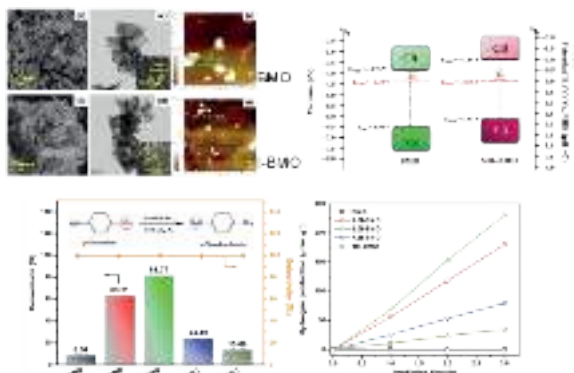
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In recent years, photocatalysis has emerged as a promising technology to address various environmental and energy-related challenges. To improve the efficiency of the photocatalysts, several strategies are commonly employed. Among them, ion substitution stands out due to its ability to influence the intrinsic properties of materials, modifying both crystal and electronic structures. This work investigates the preparation and properties of I-doped  $\text{Bi}_2\text{MoO}_6$  nanosheets. While the overall crystal structure remains unchanged, the substitution of iodate groups in the  $\text{Bi}_2\text{MoO}_6$  lattice influences the growth of lattice planes, resulting in thinner nanosheets (5 nm vs 15 nm) with different exposed facets. Moreover, this substitution alters the band edge potentials of the catalysts, influencing the generation of active species. Consequently, I-doped  $\text{Bi}_2\text{MoO}_6$  nanosheets effectively degrade 100% of Rhodamine B in 60 minutes. Additionally,  $\text{H}_2$  evolution efficiency of the doped catalysts reaches  $75 \mu\text{molg}^{-1}\text{h}^{-1}$ , surpassing the performance of pristine  $\text{Bi}_2\text{MoO}_6$  ( $1 \mu\text{molg}^{-1}\text{h}^{-1}$ ) by several orders. Our comprehensive characterizations indicate that the improved activities stem from the increased surface area, exposure of appropriate facets, and enhanced carrier separation. This research sheds light on the crucial role of ion substitution in tailoring photocatalytic materials for advanced environmental and energy applications.

**Keywords:** Photocatalyst; Photodegradation; Hydrogen evolution



## Role of incorporated metal/phosphorus acidity modification over low Si/Al ratio HZSM-5 Catalysts in Methanol-to-Olefins process

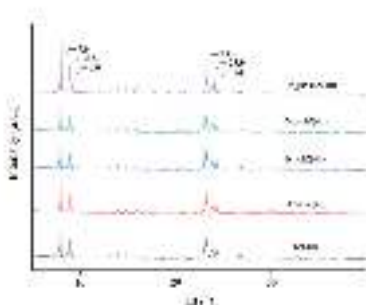
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Methanol has garnered considerable attention as a renewable and environmentally friendly energy source, derived from non-petroleum feedstocks such as CO<sub>2</sub>-based products. This has led to a significant market volume, making it an attractive and cost-effective feedstock. Consequently, value-added hydrocarbon products can be produced through remarkable processes, such as methanol to olefins (MTO). In this current work, the MTO process was investigated under atmospheric pressure, maintaining a reaction temperature of 500°C. This investigation was conducted using a nitrogen carrier within a continuous-flow stainless steel fixed-bed reactor, packed with 0.2 grams of modified HZSM-5 catalyst. The high acidity of low SiO<sub>2</sub>/Al<sub>2</sub>O<sub>3</sub> ratio (SAR=40) HZSM-5 catalysts were impregnated by 1 wt.% metal/non-metal of Fe, Ni, Mg, and Mg-P respectively, to enhance the selectivity of light olefins, mainly propylene and ethylene. As a result, the catalytic performance was notably influenced by the reaction conditions, with the addition of metals affecting acid strength and the quantity of strong/weak acid sites. Mg-P/HZSM-5, magnesium modification results in a reduction of strong acid sites, specifically a decrease in Bronsted acid, hindering the aromatization of olefins to aromatics. Additionally, the micropore volume decreases to mitigate the retained species that lead to coke precursors within the zeolite structure. While phosphorus promoter could neutralize the catalyst by enhancing catalyst stability, effectively suppressing coke deposition, and promoting olefins selectivity particularly propylene via the oligomerization of ethylene and cracking of higher olefins.

**Keywords:** HZSM-5; MTO; C<sub>2</sub>-C<sub>4</sub> Olefins; Methanol; Fixed-bed reactor



**Figure 1** XRD patterns of the parent and modified zeolites.

## Effect of manganese and magnesium promoter on catalytic hydrogenation of CO<sub>2</sub> over cobalt-based catalyst

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Concerning the problem of greenhouse gas, this attention has been focused on the conversion of CO<sub>2</sub> to value-added hydrocarbons via catalytic hydrogenation. This research aimed to improve the property of cobalt-based catalysts in CO<sub>2</sub> hydrogenation by adding the Mn and Mg as promoters. A parent 20CS and promoted catalysts (20CS1Mn and 20CS1Mg) were synthesized and characterized by N<sub>2</sub>-adsorption, XRD, H<sub>2</sub>-TPR, H<sub>2</sub>-TPD and CO<sub>2</sub> TPD techniques. The catalytic performance in CO<sub>2</sub> hydrogenation was investigated in a fixed-bed reactor at 220 °C under atmospheric pressure. The promoters influence the physical and chemical properties of the catalyst. A significant increase in pore sizes and average crystallite sizes of 20CS1Mn and 20CS1Mg catalysts leads to the ease of catalyst reduction. This is due to the structural effect of promoter. CO<sub>2</sub>-TPD profiles of promoted catalyst hint that CO<sub>2</sub> strongly adsorbs on the promoted catalysts because of electronic promoter. The CO<sub>2</sub> hydrogenation over the promoted catalyst demonstrates the possibility of chain polymerization during the reaction time (2, 4 and 6 hrs.) even low CO<sub>2</sub> conversion (approximately 2-4%). The reactions over 20CS1Mg and 20CS1Mn catalysts present the selectivity of C<sub>2</sub><sup>+</sup> approximately 1.5%, whereas the parent catalyst could not be observed. This could be the result of promoter effect.

**Keywords:** CO<sub>2</sub> hydrogenation; Cobalt-based catalyst; Mn promoter; Mg promoter

## Production of Sustainable Aviation Fuel and Green Diesel from Biodiesel Via Metathesis-Deoxygenation Over Tungsten Oxide Based Catalysts

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Biofuels, such as sustainable aviation fuel (SAF) and hydrogenated vegetable oil (HVO) provide eco-friendly alternatives to fossil fuels, reducing greenhouse gas emissions. Fatty acid methyl ester (FAMES), especially from palm oil, is a favored feedstock for jet fuel and green diesel. The main objective of this study is to produce components of SAF and HVO through metathesis-deoxygenation processes, utilizing  $\text{WO}_3/\text{SiO}_2$  as a catalyst, all without relying on molecular hydrogen in hydro-processing. Furthermore, the research aims to establish a connection between the active species of the catalyst and catalytic performance while also delving into the reaction pathways. The active species of the catalyst have been investigated by XRD and Raman spectroscopy. The reaction was performed in a continuous fixed bed reactor at atmospheric ethylene pressure, operating at 460°C, and utilizing 8%  $\text{WO}_3/\text{SiO}_2$  as a catalyst and biodiesel B100 as a feedstock. The results demonstrated that this process effectively produces SAF and HVO, with the yield of 15.54% and 13.47%, respectively. The SAF mainly composes of 1-decene which is produced together with methyl-9-decenoate from cross-metathesis of methyl oleate in B100 and ethylene. A small amount of unsaturated C9 could be generated from decarboxylation/decarbonylation of methyl-9-decenoate. Furthermore, the methyl oleate undergoes self-metathesis forming octadecene and dimethyl octadecenedioate that are a precursor of SAF. Moreover, hexadecene plays a major part in HVO yield resulting from the deoxygenation of methyl palmitate in B100. Some of C15 hydrocarbon in HVO is also produced through the decarbonylation of methyl palmitate.

**Keywords:** Deoxygenation; FAMES; Green Diesel; Metathesis; SAF.

## Sol-gel preparation of copper cobaltite spinel for ciprofloxacin degradation via peroxymonosulfate activation

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By a simple sol-gel route,  $\text{CuCo}_2\text{O}_4$  spinel nanoparticles were successfully synthesized and utilized as an efficient catalyst for peroxymonosulfate (PMS) activation to eliminate ciprofloxacin (CIP) for the first time. The material was characterized by X-ray diffraction (XRD), field-emission scanning electron microscopes (FESEM) combined with energy dispersive X-ray spectroscopy (EDX), and  $\text{N}_2$  adsorption-desorption isotherms. The material exhibited a stable spinel structure with a crystallite size of about 26 nm and a uniform morphology. Within the interval of 30 minutes, the  $\text{CuCo}_2\text{O}_4$ /PMS catalytic system could reach approximately 85% of CIP degradation efficiency ( $k \approx 0.08 \text{ min}^{-1}$ ) in the optimal experiment conditions. Besides, only relatively low concentrations of copper and cobalt ions were leached into the experiment solution after the reaction, indicating the high stability of the catalyst. Based on its safety and high catalytic activity,  $\text{CuCo}_2\text{O}_4$  can be a feasible approach for the treatment of highly stable pharmaceuticals.

**Keywords:** PMS activation; Heterogeneous catalyst;  $\text{CuCo}_2\text{O}_4$  nanoparticles; Sol-gel synthesis; Ciprofloxacin removal

## $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}/\text{Bi}_2\text{MoO}_6$ heterostructure for Rhodamine B photodegradation under visible light

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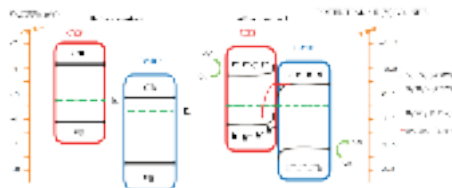
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The development of photocatalysts with strong reduction - oxidation capabilities for efficient degradation of pollutants in water is a grand challenge in the field of environmental remediation. Comparing to a single material, a composite of more than one semiconductor often yields enhanced photocatalytic performance. Herein, a novel  $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}/\text{Bi}_2\text{MoO}_6$  heterostructure photocatalysts for pollutant photodegradation were synthesized by a two-step solvothermal method. The crystal structure, electronic structure and morphologies of the samples were analyzed using several characterization tools such as X-Ray Diffraction (XRD), X-ray Photoelectron Spectroscopy (XPS), Scanning Electron Microscopy (SEM), Transmission Electron Microscopy (TEM), High-Resolution Transmission Electron Microscopy (HR-TEM), Energy Dispersive Spectroscopy (EDS) and UV-vis DRS spectra.  $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}$  nanoparticles (NPs) were deposited onto the surface of  $\text{Bi}_2\text{MoO}_6$  nanoplates. The combination of  $\text{Bi}_2\text{MoO}_6$  and  $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}$  improves carrier separation and recombination, as evidenced by Photoluminescence Spectroscopy (PL). In addition, the composite shows improved generation of superoxide radicals ( $\bullet\text{O}_2^-$ ) and holes ( $\text{h}^+$ ), which are active species in the photodegradation of Rhodamine B (Rh B). Using the optimum ratio of  $\text{Bi}_2\text{MoO}_6$  to 5% by weight of  $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}$ , the Rh B photodegradation efficiency is enhanced by almost two times compared to pristine  $\text{Bi}_2\text{MoO}_6$  and  $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}$ . Finally, the decolorization pathway of Rh B photodegradation was proposed based on liquid chromatography-mass spectrometry (LC-MS).

**Keywords:**  $\text{Cd}_{0.5}\text{Zn}_{0.5}\text{S}/\text{Bi}_2\text{MoO}_6$ , heterostructure, photodegradation



# Catalytic Chemistry (CC)

## Poster Presentation

## Fabrication of metal-free g-C<sub>3</sub>N<sub>5</sub> photocatalyst for antibiotic removal in aqueous media

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Trung-Hieu Dinh, and Minh-Vien Le\*

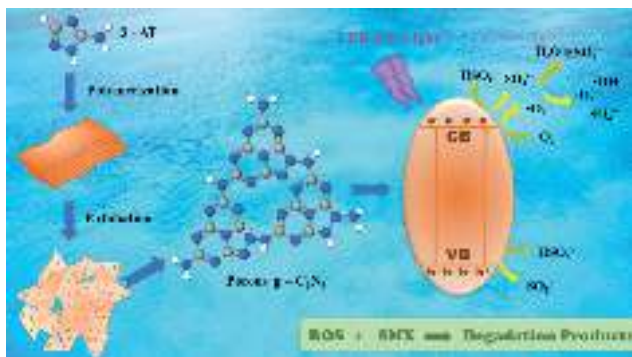
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Nitrogen-rich graphitic carbon nitride (g-C<sub>3</sub>N<sub>5</sub>) has emerged as a promising and fascinating photocatalyst for tackling problems related to antibiotic pollution. In this work, porous g-C<sub>3</sub>N<sub>5</sub> (pCN) was fabricated via facile two-step pyrolysis technique using 3-amino-1,2,4-triazole (3-AT) as precursor. The as-prepared samples were characterized by various analytical methods including XRD, SEM, TEM, BET, UV-Vis DRS, PL and photocurrent. The pCN sample exhibits a porous structure with a specific surface area of 90.2 m<sup>2</sup>·g<sup>-1</sup>, 6.9 times greater than that of bulk g-C<sub>3</sub>N<sub>5</sub> (bCN). In addition, pCN sample not only promotes charge transfer properties but also suppresses photogenerated electron-hole recombination. Photocatalytic experiments indicate that pCN sample displays the highest photocatalytic activity, which eliminates 74.2% sulfamethoxazole (SMX, 20 mg·L<sup>-1</sup>) after 60 min irradiation under UV 365nm light source. The addition of peroxydisulfate (PMS, HSO<sub>5</sub><sup>-</sup>) significantly accelerates SMX photodegradation rate as well as reduces the influence of pH solution during treatment process. The results of scavengers reveal that •O<sub>2</sub><sup>-</sup>, <sup>1</sup>O<sub>2</sub>, SO<sub>4</sub><sup>•-</sup>, •OH, h<sup>+</sup> are reactive oxygen species (ROS) contributing to SMX removal. Interestingly, the catalyst retains its high activity and stability even after four consecutive reuse cycles. This work provides a feasible strategy to design and modulate g-C<sub>3</sub>N<sub>5</sub> photocatalyst activated by PMS for antibiotic removal in wastewater.

**Keywords:** N-rich graphitic carbon nitride; g-C<sub>3</sub>N<sub>5</sub> –photocatalyst; Sulfamethoxazole degradation; Antibiotics; PMS activation.



## Synthesis of urea-derived Z-scheme photocatalyst $\text{LaFeO}_3/\text{g-C}_3\text{N}_4$ for tetracycline degradation under simulated natural irradiation

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In this work, perovskite  $\text{LaFeO}_3$  was prepared via citrate sol-gel method and simple calcination processes at different calcination temperatures ranging from 700 °C to 900 °C, and the non-metal material  $\text{g-C}_3\text{N}_4$  was synthesized via one-step thermal polymerization of urea. Besides, the urea-derived  $\text{LaFeO}_3/\text{g-C}_3\text{N}_4$  (LCN) composites with different contents of LFO were fabricated by facile ultrasonic dispersion and calcination methods. The samples LFO,  $\text{g-C}_3\text{N}_4$  and 30%LCN composite were characterized through X-ray diffraction (XRD), scanning electron microscopy (SEM), nitrogen adsorption/desorption, photoluminescence spectroscopy (PL), and DRS analysis. Additionally, the photocatalytic activities of as-prepared catalysts were evaluated through the degradation of tetracycline hydrochloride (TCH) under simulated natural light irradiation. The concentration of TCH was determined using the UV-Vis spectroscopy method with absorbance at 276 nm. XRD pattern of the composite 30%LCN shows that there are only peaks of  $\text{g-C}_3\text{N}_4$  and  $\text{LaFeO}_3$ , revealing that there are no impurity phases in this composite. Moreover, SEM-EDX analysis confirms that the composite LCN was formed and its composition content corresponds to the theoretical percentage. At equilibrium, the adsorption capacity of LFO700 sample was approximately 1.5 times and 2 times higher than that of the LFO800 and LFO900, respectively. In addition, 30%LCN composite possesses the best photodegradation efficiency of more than 80% TCH within 150 min. The superior photocatalytic activity of this composite was attributed to the formation of the Z-scheme heterojunction structure, effectively promoting the separation of photogenerated electron-hole pairs in agreement with the results of PL and the improvement on the adsorption. The radical trapping experiments also reveal that  $\text{O}_2^{\cdot-}$  is a dominant oxidative specie for TCH photodegradation with 30%LCN composite. The application of 30%LCN photocatalyst in industrial waste treatment is feasible given the high content of metal-free  $\text{g-C}_3\text{N}_4$  from urea as well as abundant, non-toxic, low-cost chemical with simple synthesizing methods.

**Keywords:**  $\text{g-C}_3\text{N}_4$ ;  $\text{LaFeO}_3$ ;  $\text{g-C}_3\text{N}_4/\text{LaFeO}_3$  photocatalyst; Z-scheme heterojunction; Tetracycline hydrochloride



## Preparation of $\text{BiVO}_4/\text{g-C}_3\text{N}_4$ composite with enhanced visible-light-driven photocatalytic activity

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In this work,  $\text{BiVO}_4$  was composited with  $\text{g-C}_3\text{N}_4$  at different mass ratios using an ultrasound-assisted method to fabricate BCN heterojunctions. The crystal structure, composition, morphology, optical, and electrochemical properties of the catalysts were comprehensively analyzed through some analytical techniques such as XRD, FESEM, XPS, BET, DRS, PL, transient photocurrent response. Additionally, their photocatalytic performances were determined by evaluating the degradation of tetracycline (TC) under visible light irradiation. The results indicates that the BCN sample with the mass ratio of  $\text{BiVO}_4$  and  $\text{g-C}_3\text{N}_4$  of (2:1) exhibits higher photocatalytic activity than that of the pure  $\text{g-C}_3\text{N}_4$  and pure  $\text{BiVO}_4$  and the performance achieves approximately 78.2% (within 60 min of irradiation). Moreover, the cyclic experiments proved that BCN (2:1) possesses good stability after five consecutive runs. The trapping experiments showed that  $\bullet\text{O}_2^-$  is the dominant radical in the degradation process on BCN (2:1). These findings also suggested evidence for the increased photocatalytic activity through the Z-scheme charge transformation system. Overall, this study demonstrated that the composite BCN appears to be a viable material for the development of future photocatalysts for the environmental degradation of organic pollutants.

**Keywords:**  $\text{BiVO}_4$ ;  $\text{g-C}_3\text{N}_4$ ; Tetracycline; Visible light irradiation; Z-scheme.

# Photocatalytic activity of N- and S-heteroatoms co-doped on graphene quantum dots under visible irradiation for degradation of organic dye

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The rapid industrialization and increased use of organic dyes for production in many industries have led to extensive environmental pollution concerns. In this research, we investigate the synthesis and applications of nitrogen and sulfur co-doped graphene quantum dots (N,S-GQDs) as photocatalysts for degradation of organic dyes. N,S-GQDs were prepared via hydrothermal method with incorporation of nitrogen and sulfur heteroatoms (ammonium sulfate was used as nitrogen and sulfur sources) into the GQDs structure, using glycine as the carbon precursor. Analyses of their structural and chemical properties were performed using various analytical techniques consisting of XRD, TEM, and SEM-EDX. Carbon, oxygen, nitrogen, and sulfur were discovered in N,S-GQDs by SEM-EDX measurement to confirm the formation of nitrogen and sulfur doping in N,S-GQDs. Methylene blue 10 ppm is a representative of organic dye solution that was used to evaluate the photocatalytic performance under visible light source that produced by xenon lamp with wavelengths from 100 to 1100 nm. The concentration of methylene blue was measured using UV-visible spectrophotometer at a wavelength of 665 nm, The results demonstrate that N,S-GQDs can contribute to highly efficient photodegradation of methylene blue during 2 h reaction time at room temperature with 77 % conversion.

**Keyword:** Photodegradation; Photocatalyst; Graphene quantum dots; GQDs; Dye degradation; Visible light; Methylene blue

## The study of nanostructured graphitic carbon material prepared from sugarcane bagasse for chemical sensor

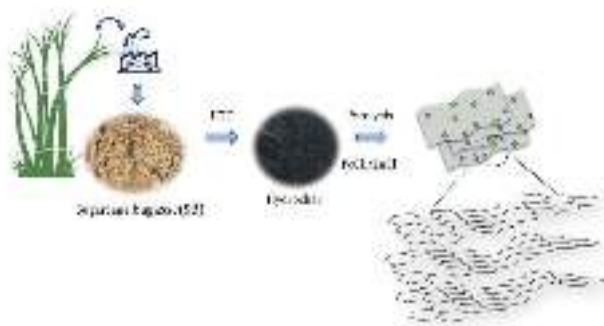
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Lignocellulosic biomass waste is considered as a renewable, low cost, and environmental-friendly carbon source to produce graphitic carbon materials. Herein, we report a simple route to transform sugarcane bagasse into graphitic nanostructured materials via two steps processes of a hydrothermal carbonization and pyrolysis with the presence of  $\text{FeCl}_3$  and  $\text{ZnCl}_2$  as activators. The obtained graphitic carbon nanostructure materials are then characterized using scanning electron microscopy (SEM), high-resolution transmission electron microscopy (HRTEM), X-ray diffraction (XRD) and Raman spectroscopy techniques. The results show that the graphitic carbon (SB-Fe) has the highest graphitic degree of  $I_G/I_D$  ratio (1.94) with the highest degree of graphitization of 68.47%. The formation of graphene-like structure of SB-Fe is seen by HRTEM observation as well-defined lattice fringes separated by an interplanar distance of 0.338 nm corresponding to the C(002) plane. The 0.338 nm d-spacing of the C(002) plane is confirmed by XRD analysis of 2theta peak at  $26.32^\circ$ . In addition, by combination of  $\text{FeCl}_3$  and  $\text{ZnCl}_2$  in graphitization process, the graphitic carbon (SB-FeZn) shows a lower degree of graphitization (50.92%) but exhibit higher BET surface area ( $715 \text{ m}^2/\text{g}$ ) than SB-Fe ( $194 \text{ m}^2/\text{g}$ ). The adsorption-desorption isotherm and pore size distribution of both samples exhibited a typical type-IV which an abundance of mesopores and micropores were present. The possible pore development was ascribed to the formation of molten  $\text{ZnCl}_2$  and Fe-species, which then act as templates inside the carbon to form pore structures and an ordered graphitic carbon structure resulting in porous graphitic carbon structure. In conclusion, this simple process successfully converts the sugarcane bagasse waste in to a higher value-added graphitic carbon nanomaterials. However, further studies are required for the development of a facile and highly efficient synthetic process.

**Keywords:** Sugarcane bagasse; Biomass; Graphitic carbon; Catalytic graphitization



# A nanocellulose template for the controllable synthesis of hollow mesoporous aluminosilicate nanomaterials

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We have developed an environmentally friendly method for synthesizing hollow mesoporous aluminosilicate nanomaterials, utilizing nanocellulose as a sustainable template. To achieve this, we initially derived cellulose nanocrystals and cellulose nanoparticles from sugarcane bagasse through a chemical treatment involving nitric acid, sodium hydroxide, and hydrogen peroxide. Cellulose nanocrystals were obtained through hydrolysis with sulfuric acid, while cellulose nanoparticles underwent further hydrolysis with  $\text{Fe}_3\text{O}_4$  nanoparticles. The synthesis of mesoporous nanomaterials was carried out using a sol-gel process with tetraethyl orthosilicate (TEOS) and sodium aluminate as precursors, maintaining a Si/Al ratio of 7.5. We systematically prepared a comprehensive series of samples by adjusting crucial parameters, such as the concentration of cetyltrimethyl ammonium bromide (CTAB) utilized as a co-template, types and contents of nanocelluloses, and water-to-ethanol ratios. As a result, we successfully prepared hollow spheres and hollow rods mesoporous aluminosilicates which contain non-ordered mesoporous shell structures featuring pore sizes of 2-3 nanometers. Additionally, wormlike pores were also observed. The resulting aluminosilicates exhibited high specific surface areas ranging from 500 to 1000 square meters per gram, while the sizes of the hollow structures could be fine-tuned between 2-4 nanometers by adjusting the size and quantity of the nanocellulose templates employed during the synthesis process.

**Keywords:** Nanocellulose; Green template; Hollow mesoporous nanomaterials; Aluminosilicate

## Solid acid catalyst development from rubber tire waste for biofuel and biochemical production

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The growth of vehicle industries increases the demand for rubber tires, resulting in high rubber tire waste affecting the environment. Using rubber tire waste is one of the methods to reduce environmental concerns as follows as Bio-Circular-Green-Economy (BCG). Many researchers have developed a way to utilize rubber tires in new applications, such as catalysts and adsorbents. To synthesize a rubber tire as a solid acid catalyst, the rubber tire is pyrolyzed at a high temperature to form carbon and further functionalized into a solid acid catalyst. Although this method seems promising, the process is complex and involves pyrolysis, leading to high energy consumption. This research aims to develop a solid acid catalyst from rubber tire waste using an uncomplex method and low energy consumption by sulfonation reaction of rubber tire. The effects of catalyst synthesis (temperature and acid concentration) were studied on the efficiency and catalyst stability (after recycling) through the esterification of levulinic acid and methanol as a probe reaction against a commercial solid acid catalyst (Amberlyst-15). The TW-SO<sub>3</sub>H synthesized under 150 °C and 98% H<sub>2</sub>SO<sub>4</sub> concentration showed high catalyst performance (98% conversion) with high product selectivity, which was higher than Amberlyst-15 up to 10% conversion. This research approach addresses the environmental impact of waste tires and contributes to sustainable catalyst development, paving the way for an eco-friendly waste management strategy.

**Keywords:** Rubber tire waste; Sulfonation; Solid acid catalyst; Levulinic acid; Esterification

## Bagasse heavy ash-derived Zn-loaded porous silica: Effects of bimodal mesopores on VOCs adsorption

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A novel and environmentally-friendly synthesis process using a single-template pH alteration process was applied to the synthesis of bimodal mesoporous silica (BPS) from bagasse heavy ash. The surface functional groups on the BPS products were then modified using a Zn precursor, and the obtained samples were examined for the adsorption of both polar (methanol and butanol) and non-polar (hexane and benzene) VOCs. Effects of hydrolysis–condensation rate controlled by varying sulfuric acid concentrations in the synthesis process on the formation of controllable bimodal mesopores were systematically investigated. The Zn-loaded bagasse ash-derived BPS products exhibited outstanding adsorption performances, especially for methanol and benzene adsorption over the BPS with medium to large pores, of approximately 4.10 and 7.51 times those over the monomodal mesoporous silica (MPS), due to the existence of large pores within the BPS products. This leads to the potential application of the bimodal mesoporous silica absorbents derived from bagasse heavy ash in adsorption—separation and catalytic processes.

**Keywords:** Bagasse heavy ash; Bimodal mesoporous silica; Zn modification; pH alteration process; VOCs adsorption

## Enhancing carbon capture efficiency: Optimization of ZIF-8 synthesis and integration into Advanced Adsorbent Systems

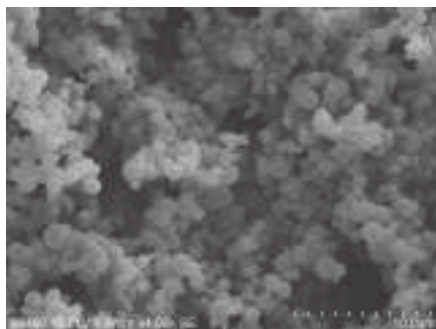
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The quest for mitigating CO<sub>2</sub> emissions has fueled research into innovative carbon capture technologies. ZIF-8 (Zeolitic Imidazolate Framework-8) a type of metal organic framework (MOF) is investigated as a CO<sub>2</sub> sorbent due to its anticipated qualities, including pore size, adjustable pore dimension and high surface area. Improving ZIF-8 to be more catalytically active and stable is still needed. The synthesis methods are one of the processes for developing and improving ZIF-8 to make it more physically efficient including morphology. ZIF-8 has been prepared by solvothermal synthesis using methanol as solvent, Zn(NO<sub>3</sub>)<sub>2</sub> · 6H<sub>2</sub>O as the source of metal and 2-methylimidazole as the organic linker. The reaction mixtures were stirred to yield a clear solution, which was subsequently transferred into a Teflon-lined autoclave for heating at various temperatures (120°C, 130°C and 140°C) over distinct time intervals (14h and 24h). The resultant material is then subjected to ethanol washing, centrifugation at 1,000 r/min for 5 min, overnight drying and calcination. Scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and Surface area and Pore size analyzer (BET) are used to characterize prepared adsorbents for surface area, pore size distribution, crystalline structure, and morphological attributes. The outcomes of our research represent a pivotal contribution to the ongoing efforts aimed at enhancing ZIF-8 materials, making them more robust and efficient for practical applications in carbon capture. These endeavors are essential in the global pursuit of reducing CO<sub>2</sub> emissions and addressing the challenges of climate change.

**Keywords:** CO<sub>2</sub> capture; Zeolitic imidazole frameworks-8; Solvothermal synthesis



SEM images of ZIF-8 from solvothermal synthesis at 140 °C 24h.

## Tuning selectivity of Ni/Al<sub>2</sub>O<sub>3</sub> catalysts in CO<sub>2</sub> Hydrogenation by incorporation of N, S-doped carbon

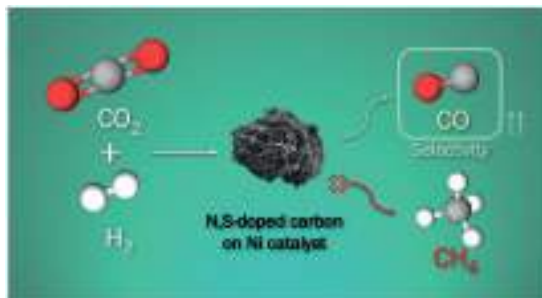
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In recent years, the continuously rising levels of CO<sub>2</sub> have become a primary concern. CO<sub>2</sub> hydrogenation is considered a promising approach to reduce the impact of CO<sub>2</sub>. Selective CO<sub>2</sub> hydrogenation towards CO over Ni catalysts is challenging but CO is an interesting intermediate for the synthesis of higher value liquid hydrocarbon and oxygenate products. The objective of this study was to study the effect of N- and S-doped carbon (1%, 3%, and 5% by weight) on Ni/Al<sub>2</sub>O<sub>3</sub> catalysts in the gas-phase CO<sub>2</sub> hydrogenation at 300-500 °C. All the catalysts were prepared by the incipient wetness impregnation method and then calcined at 550 °C for 5 h. The results show that increasing the N and S-doped carbon content significantly enhances the selectivity towards CO. The relationship between catalyst properties and activities was analyzed based on various characterization results, including SEM, TEM, XRD, FTIR, and CO<sub>2</sub>-TPD. Among the various catalysts studied, the 15Ni5GC86/Al<sub>2</sub>O<sub>3</sub> showed the best performances towards CO selectivity (99 percent CO selectivity with 30 percent conversion) at the reaction temperature 500 °C.

**Keywords:** Carbon dioxide; Hydrogenation; RWGS; Ni-based catalysts; Carbon catalysts



**Figure 1.** Graphitic abstract for CO<sub>2</sub> hydrogenation.

## Tuning the morphology of $\text{PbBiO}_2\text{Br}$ nanosheets for photodegradation of methyl orange under visible light

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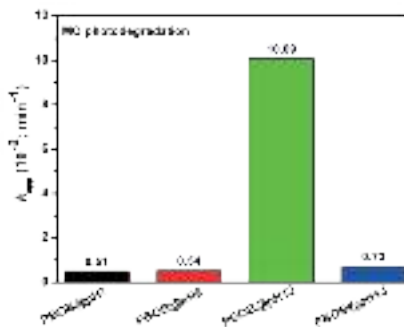
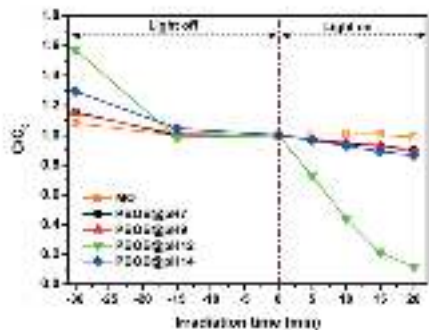
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Photocatalysts have ability to increase rate of redox reaction and thus have broad applications. Several semiconductors have potential to be photocatalysts. Among them,  $\text{PbBiO}_2\text{Br}$  have recently gained interests and it is the focus of this work.  $\text{PbBiO}_2\text{Br}$  photocatalysts were synthesized via a facile solvothermal method. The morphology of the samples is tuned by pH adjustment of precursor suspensions. Detailed structural and morphological characterization with X-Ray Diffraction Spectroscopy (XRD), Scanning Electron Microscopy (SEM), Transmission electron microscopy (TEM), Energy Dispersive Spectroscopy (EDS), UV-vis diffuse reflectance Spectroscopy and X-ray photoelectron Spectroscopy revealed that all  $\text{PbBiO}_2\text{Br}$  photocatalysts have rose like structure and nanosheet structure. The thickness of the samples increases at higher pH levels. Furthermore, differences in pH levels lead to variations in exposed facets. The obtained catalysts exhibit Methyl Orange (MO) photodegradation ability.  $\text{PbBiO}_2\text{Br}$  nanosheets prepared at pH 12 gives the highest efficiency with almost 100% MO degraded in 20 minutes under visible light. The kinetic constant of  $\text{PbBiO}_2\text{Br}$  at pH 12 is also the highest. All results suggest that pH is a valid choice to improve the efficiency of  $\text{PbBiO}_2\text{Br}$  and the obtained knowledge would benefit future design of similar photocatalysts.

**Keywords:**  $\text{PbBiO}_2\text{Br}$ , pH, morphology, exposed facet, photodegradation



## Catalytic LPG conversion over Ga/ZSM-5 zeolite catalyst: Effect of confined-space zeolite and external magnetic field

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In this work, green and efficient utilization concepts have been explored for the catalytic LPG conversion over Ga modified ZSM-5 zeolite through the application of confined-space molecular-sieve properties of ZSM-5 zeolite under an external magnetic field. The unique pore structure and suitable acidity of Ga modified ZSM-5 zeolite will provide the catalytic performance in aromatization reactions. In order to enhance the catalytic performance of BTX (benzene, toluene, and xylenes) production, 5 wt.% of Ga modified ZSM-5 zeolite was prepared and evaluated under an external magnetic field with a flux density of 27.7 mT in North-to-South orientation. The reaction was carried out at 500 °C under atmospheric pressure in a magnetic field-assisted packed-bed reactor system, using reactant flow rate of 30 mL/min. Under an external magnetic field, the LPG conversion increased from 62% to 68%, and the BTX yield increased from 35% to 40%, compared to those without an external magnetic field. These enhanced catalytic performances could be ascribed to the synergistic effects between external magnetic field and limited mass transfer within confined-space zeolite, which influence and enhance the mass transfer ability and reaction performance of reactant molecules. Consequently, this synergistic effect can potentially lead to green and sustainable innovations in chemical and separation processes in the future.

**Keywords:** ZSM-5 zeolite; Confined-space catalyst; External Magnetic Field; LPG conversion; BTX production

## The use of copper phyllosilicate as a supported template to prepare $\text{WO}_3/\text{SiO}_2$ catalyst for cross-metathesis of acetylene and ethylene

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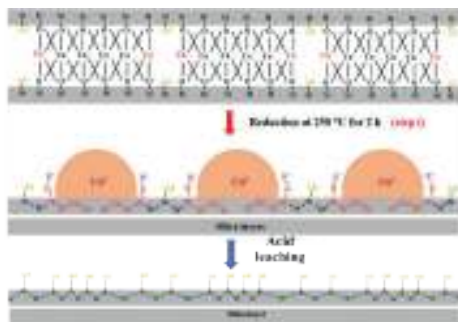
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Acetylene/Ethylene cross-metathesis was performed in continuous fixed-bed reactor at 450°C under atmospheric ethylene pressure using 8% $\text{WO}_3$  over fumed  $\text{SiO}_2$  (8% $\text{WO}_3/\text{SiO}_2$ ) and CuPS  $\text{SiO}_2$  template catalysts (8% $\text{WO}_3/\text{CuPS-Le}$ ). The CuPS  $\text{SiO}_2$  template was prepared from acid leaching of 30% Copper phyllosilicate (CuPS). The CuPS was synthesized from an ammonia evaporation-hydrothermal method. The  $\text{WO}_3$  species and dispersion were investigated by XRD, Raman spectroscopy, and DRUV-VIS spectroscopy. The catalysts were treated with ethylene at 600 °C for 2h to generate tungsten (IV) alkylidene species ( $\text{W}=\text{CH}_2$ ) as an active site prior to the reaction. The 8% $\text{WO}_3/\text{CuPS-Le}$  provide evidently higher both of activity of acetylene (87%) and selectivity of 1,3-butadiene (77%). While, 8% $\text{WO}_3/\text{SiO}_2$  performed lower activity and selectivity also(37% and 23%). Cause by the dispersion of 8% $\text{WO}_3/\text{SiO}_2$  lower than 8%  $\text{WO}_3/\text{CuPS-Le}$ .

**Keywords:** Cross-metathesis; Silica template; Tungsten oxide; Acetylene; Ethylene



**Figure 1.** The preparation of silica template from copper phyllosilicate [1].

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W. Prasanseang, K. Choojun, Y. Poo-arporn, A.-L. Huang, Y.-C. Lin, and T. Sooknoi, *Appl. Catal. Gen.*, 2022, 635, 118555.

## Effect of pH precipitation on ceria–zirconia supported Nibased catalyst via CO<sub>2</sub> reforming of CH<sub>4</sub> reaction

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Dry reforming is an interesting reaction to simultaneously reduce methane (CH<sub>4</sub>) and carbon dioxide (CO<sub>2</sub>) to produce hydrogen (H<sub>2</sub>) and carbon monoxide (CO), which are further converted to value-added hydrocarbon products via Fischer-Tropsch synthesis. This study explored the influence of nickel-supported ceria–zirconia (Ni/CZ) catalysts, prepared under different pH precipitation conditions, on the activity and stability of CO<sub>2</sub> reforming of CH<sub>4</sub> at 700°C. The CeO<sub>2</sub>–ZrO<sub>2</sub> support was synthesized using a soft template-assisted co-precipitation method, employing cetyltrimethylammonium chloride (CTAC) as a template under varying pH conditions (5, 7, 8.5, and 10)—denoted as CZ(x). Subsequently, nickel was loaded onto the support through the incipient wetness impregnation method. Results showed that pH precipitation levels influenced the quantity of CeO<sub>2</sub> and ZrO<sub>2</sub> formed, leading to differences in the CeO<sub>2</sub>–ZrO<sub>2</sub> ratios and associated chemical properties. Ni/CZ(8.5) catalyst exhibited the highest CH<sub>4</sub> and CO<sub>2</sub> conversions, as well as H<sub>2</sub>/CO ratio. The activity was also more stable during the reaction compared to the other catalysts. This can be attributed to the Ni/CZ(8.5) catalyst having a higher surface oxygen vacancy and increased basic sites on the CZ(8.5) surface. These properties enhanced CO<sub>2</sub> adsorption and dissociation, thereby reducing carbon accumulation on the catalyst during the reaction.

**Keywords:** Dry reforming; CeO<sub>2</sub>–ZrO<sub>2</sub>; Precipitation; Surface properties; Nickel catalyst

## The study of magnetic inducement on Ni catalyst on $\text{Gd}_2\text{O}_3$ - $\text{CeO}_2$ doped $\text{Al}_2\text{O}_3$ support for ethanol steam reforming

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Nickel is a common catalyst used in ethanol steam reforming due to its ability to break the C—C bond, but it easily deactivates from carbon deposition on the active sites. The use of support with oxygen vacancies, such as gadolinia-doped ceria, has been shown to reduce coke deposition on used catalysts. However, the dopant percentage is generally low which can cause poor distribution in the main support structure. Improving the distribution of gadolinia can affect its properties as an oxygen reservoir to reduce coking. It has been found that dopant distribution can be controlled by the application of a magnetic field during support synthesis in the case of ceria-doped alumina. In this study, two magnetic field patterns were applied during the synthesis of gadolinia-ceria-doped alumina support via ammonia precipitation method. The catalytic activity of the Ni catalysts loaded on the modified supports have been evaluated at 550, 575, and 600 °C. The surface area of the prepared supports are characterized using the BET method, and the amount of carbon deposition on used catalysts was analyzed using thermogravimetric analysis.

**Keywords:** Magnetic inducement; Ni catalyst;  $\text{Gd}_2\text{O}_3$ - $\text{CeO}_2$  doped  $\text{Al}_2\text{O}_3$  support; Ethanol steam reforming

## Development of CaO promoted Ni/Al<sub>2</sub>O<sub>3</sub> catalyst for direct methanation of biogas into biomethane

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In this study, the direct methanation of biogas to biomethane was performed via a CO<sub>2</sub> methanation reaction over Ni-based catalysts. The catalysts were prepared by a simple impregnation method using the evaporation-to-dryness technique. The catalytic enhancement of as-prepared catalysts in terms of CO<sub>2</sub> conversion and CH<sub>4</sub> yield was investigated in a fixed-bed reactor at 200-500°C, and atmospheric pressure. The variation of CaO loading on Al<sub>2</sub>O<sub>3</sub> support (10, 20, and 30 wt.% of total support) was studied, while the Ni loading of 10 wt.% was fixed. It was found that the 10%Ni/(10%CaO)-Al<sub>2</sub>O<sub>3</sub> catalyst exhibited the highest CO<sub>2</sub> conversion of 80.1% and CH<sub>4</sub> yield of 79.8 % at 325°C. In addition, the effect of nickel loading (10, 20, 30, and 40 wt.%) was optimized using the 10wt.%CaO-Al<sub>2</sub>O<sub>3</sub> support. As a result, the catalyst containing 30 wt.% Ni exhibited the optimal content, providing the highest CO<sub>2</sub> conversion of 86.3 % and CH<sub>4</sub> yield of 86.2 % at lower temperature of 275 °C. Furthermore, the sequence for loading Ni and CaO on Al<sub>2</sub>O<sub>3</sub> support was studied by using the optimum 30%Ni/(10%CaO)-Al<sub>2</sub>O<sub>3</sub> catalyst. It found that the loading sequence had a significant effect on the catalytic activity. At low temperature of 225°C, the CO<sub>2</sub> conversions were 11.1% to 76.2% for sequential-impregnation method and co-impregnation method, respectively. Various characterization techniques including BET, XRD, H<sub>2</sub>-TPR, CO<sub>2</sub>-TPD, and H<sub>2</sub> chemisorption were performed. The characterization results revealed that the promotion of CO<sub>2</sub> adsorption and H<sub>2</sub> dissociation active sites is necessary to carry out CO<sub>2</sub> methanation.

**Keywords:** Biogas; CO<sub>2</sub> methanation; Ni-based catalysts; Calcium oxide

## The production of fatty alcohol from methyl palmitate by selective hydrogenation over CuMgAl layered double hydroxide

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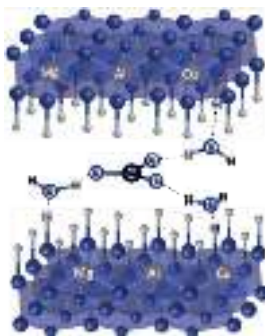
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The selective hydrogenation of methyl palmitate (MP) to hexadecanol over CuMgAl-Layered double hydroxides (Cu-LDH) was investigated in a continuous fixed-bed reactor at 250 °C atmospheric H<sub>2</sub> pressure. The catalysts were prepared by the co-precipitation and hydrothermal method and calcination at 550 and 750 for comparison. The crystal structure, reducibility, and Cu dispersion were examined by characterized by XRD, H<sub>2</sub>-TPR, and dissociative N<sub>2</sub>O adsorption using H<sub>2</sub>-TPR. The Cu dispersion of the catalysts depends on the calcination temperature. Cu/MgAlO calcined at 550 °C and 750 °C provides a similar MP conversion (54%). Nevertheless, the catalyst that calcined at 750 °C could provide a higher hexadecanol selectivity (91%) than calcined at 550°C (53%). In addition, the stability of the catalysts significantly relates to the Cu dispersion, which Cu/MgAlO calcined at 550 °C (100% Cu dispersion) shows a higher stability within 6 h. While Cu/MgAlO calcined at 750 °C with 67% Cu dispersion shows a severe deactivation. This could presumably be due to the presence of acid sites at the surface of the catalysts together with a relatively lower Cu dispersion.

**Keywords:** Hydrogenation; Copper LDHs; Methyl palmitate; Hexadecanol



CuMgAl-LDHs

## Transesterification of refined palm oil with methanol catalyzed by anion-exchange resin in rotating packed bed reactor

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The conventional method of producing biodiesel involves the transesterification of triglycerides with methanol to form fatty acid methyl esters (FAME). Commonly, homogeneous alkaline catalysts are used, but catalyst removal from the reaction mixture poses a problem. Additionally, methanol's extremely low solubility in the oil phase hampers the reaction, necessitating vigorous mixing for effective mass transfer between the two liquid phases. Anion-exchange resin is a less common catalyst for transesterification of oil/fat with alcohol. In this work, alkaline anion exchange resin, specifically the dense AmberLite™ IRA402 was used to catalyze transesterification. The resin was employed in a rotating packed bed reactor (RPB) attached to a magnetic stir bar for transesterification of refined palm oil with methanol. The reaction was conducted at 60 °C **in a jacketed glass reactor with a Graham condenser, lasting** for 4 h with a methanol-to-oil molar ratio of 9.5 to 1. In conventional transesterification with only a magnetic stir bar, two liquid phases persisted with large droplets of one phase in the other throughout and the resin beads agglomerated in lumps. In contrast, the reaction mixture after transesterification with resin packed in the RPB was transformed into a colloidal mixture, which significantly enhanced the yield compared to that from the conventional one. In the conventional setup, the FAME yield obtained was 5.39% at 1500 rpm and with 4 mL of IRA402, whereas in the RPB setup, a higher FAME yield of 9.71% was achieved with only 750 rpm and 3 mL of IRA402. The enhanced performance of the RPB could be attributed to improved inter-phase mass transfer. The rotational movement of the bed promoted better contact between the two phases, ultimately boosting the reaction rate.

**Keywords:** Biodiesel; Transesterification; Anion-exchange resin; Rotating packed bed reactor; Heterogeneous catalyst



Figure 1. Comparison of the reaction mixture in (a) a conventional reactor with a magnetic stir bar and (b) a rotating packed bed reactor.

## Effect of CH<sub>4</sub> impurity in flue gas feed on ethanol-assisted methanol synthesis from CO<sub>2</sub> hydrogenation over Cu-based catalyst

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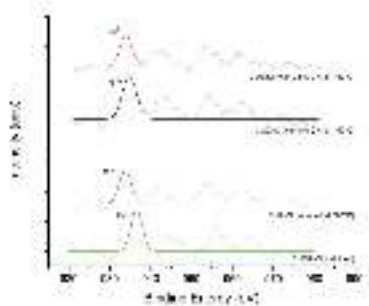
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Reusing CO<sub>2</sub> to produce methanol is one of the ways to deal with large CO<sub>2</sub> emissions issues. However, Flue gases emitted from industries not only contain CO<sub>2</sub> but also have various impurities, of which CH<sub>4</sub> is a common one. To minimize the cost of CO<sub>2</sub> capturing, implementing the flue gas without CH<sub>4</sub> separation was therefore to study the effect on the Cu/ZnO catalyst and methanol production efficiency. The experiments were tested by feeding a trace amount of CH<sub>4</sub> varied from 0% to 2.5% of total pressure together with CO<sub>2</sub> and H<sub>2</sub> to produce methanol in the batch reactor by the ethanol-assisted method in order to reduce the system temperature to favor the exothermic reaction. The effect of operating temperature was also studied by varying from 130°C to 170°C. From the results, the best condition with 1% CH<sub>4</sub> at 170°C could give 77% for CO<sub>2</sub> conversion and 34.67% of methanol yield. The CO<sub>2</sub> conversion and methanol yield of all the systems with CH<sub>4</sub> gave greater results when compared to the system without CH<sub>4</sub>. This is possibly due to the reducing ability of CH<sub>4</sub> and CO generated from CH<sub>4</sub> dry reforming reaction that could reduce the catalyst from Cu<sup>2+</sup> to Cu<sup>0</sup> which is better for methanol synthesis reaction and can be proved from XRD and XPS. After observing the physical characteristics of the used catalyst by TGA, SEM, and BET, it was found that the change was minimal when the CH<sub>4</sub> present in the system was less than 1.75%. The presence of a low amount of CH<sub>4</sub> not greater than 1% is thus beneficial in the CO<sub>2</sub>-to-methanol conversion reaction in terms of CO<sub>2</sub> conversion and methanol yield.

**Keywords:** Methanol; CO<sub>2</sub> utilization; CH<sub>4</sub> impurity; Cu/ZnO; Low-temperature methanol synthesis, Alcohol-assisted



**Figure 1.** XPS Patterns of fresh Cu/ZnO catalysts and used Cu/ZnO catalysts in the system with and without CH<sub>4</sub>

## Conversion of amine-captured CO<sub>2</sub> to CaCO<sub>3</sub> by electrodialysis

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The urgent need for efficient technology to reduce CO<sub>2</sub> emissions is increasingly highlighted to combat climate change. Currently, the most successfully commercialized technology for CO<sub>2</sub> capture is perhaps amine capture technology. CO<sub>2</sub>-containing waste gas is passed through an absorber with amine solution as an absorbent. More than 90 % of CO<sub>2</sub> can be absorbed chemically in the amine solution. One of the commonly used absorbents is aqueous monoethanolamine (MEA) solution. If MEA is used, carbamate and ammonium ions form from the reaction between MEA and CO<sub>2</sub> after absorption. This spent absorbent is regenerated in a reboiled stripper, which requires heat to operate, to reclaim the absorbent and release high-concentration CO<sub>2</sub> gas. This project studies electrodialysis as an alternative means for absorbent regeneration with co-conversion of CO<sub>2</sub> into fine CaCO<sub>3</sub> particles, converting waste into a potential product. 30 wt% monoethanolamine (MEA) presaturated with 1 atm CO<sub>2</sub> was used to imitate industrial spent absorbent. CaCl<sub>2</sub> solution was used as a calcium source. Our electrodialysis system offered a faradaic efficiency of 49% for CaCO<sub>3</sub> production at a current of 0.1 A. A key issue apart from this still low faradaic efficiency was precipitation of CaCO<sub>3</sub> directly on electrodialysis membrane. This study aims to improve both the faradaic efficiency and the membrane-precipitation issue. Process variables such as current density and additives in calcium solution will be studied to improve faradaic efficiency and minimize membrane precipitation.

**Keywords:** Amine-Captured CO<sub>2</sub>; Calcium carbonate; Ion-exchange membrane; Electrodialysis; Carbamate



Figure 1. Photograph of amine-captured CO<sub>2</sub> to CaCO<sub>3</sub> by electrodialysis at 0.1 A (left) and SEM image (right)

# Chemical Education (CE)

## Oral Presentation



## Diagnosis of fundamental concepts of chemical basis of life among high school students

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This research is a survey-based study aiming to diagnose the concepts of chemistry that underlie living organisms. Data was collected from 243 high school students from 3 schools, specifically targeting students who had never studied this topic. The research tool used was a closed-ended diagnostic test with four options. The distractors were developed based on misconceptions identified through interviews and literature reviews. The content covered atomic elements and compounds, water, and organic compounds in living organisms, including carbohydrates, proteins, lipids, nucleic acids, and chemical reactions within cells. Data analysis was conducted using descriptive statistics. The results revealed that most students hold misconceptions, especially at the molecular level and in symbolic representations, particularly regarding organic compounds and chemical reactions in cells. These findings are beneficial for designing learning experiences to help students develop accurate scientific concepts.

**Keywords:** High school students; Chemical basis of life; Diagnosis

## Promoting students' scientific explanation through the 6E STEM for BCG model on the topic of rate of reaction

Parinya Mutchā and Chatree Faikhamta\*

STEM plays important roles in developing students' science competency for sustainable development goals (SDGs). However, little is known about key features of STEM learning activities integrated with SDGs, particularly in chemistry class. The objective of this action research is to examine and develop students' scientific explanations during 6E STEM integrated the BCG economic model, one of the models leading to the SDGs, into the topic of rate of reaction. The participants were 40 grade 11 students in the first semester of the academic year 2023. Data were collected from a scientific explanation survey, classroom observations, students' reflections, and teachers' reflections. The data were analysed by an inductive process. The results indicated that STEM-BCG models using the theme of banana ripening and exporting bananas with packaging designed by students could promote their scientific explanations. Students were very engaged in real-life problem situations, such as the ripening of bananas. They did research about the factors affecting the reaction rate and used the data to solve problems. They designed innovation using the inquiry process and the engineering design process under the BCG economic model. They also developed their perspective on banana-related businesses to set goals or identify problems. They had a better understanding of the rate of chemical reactions, such as the nature of bananas as climacteric fruits and the temperature affecting the ripening of bananas. The implications of STEM-BCG for other chemistry topics are discussed.



## Entrepreneurial STEAM-BCG in a cup: The development of high school student's sensemaking practices through dialogical argumentation with chemistry concepts

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STEM education has been redefined several times as more suitable for different country contexts and distinct achievements. The new player in the STEM area, economy envisions learners using more scientific knowledge to solve real-world problems by gathering awareness to support the well-being of communities. This study aims to investigate the development of 24 high school students' sensemaking practices throughout an entrepreneurial STEAM-BCG chemistry learning activity. The data were collected from their worksheets and dialogs which were transcribed, then all data were analyzed by the combination of content analysis and inductive analysis underpinning of qualitative research design to describe their sensemaking practice around the concepts of solubility, colligative properties, and pH buffer. The results are presented in three sub-practices. Firstly, their modeling practices were elevated by the infusion of clients who require the visualization of what they would invest with chemistry ideas on the practical. Secondly, their explanation practices transferred the scientific concepts to easily communicate with local members in the given community, but they need to recall those messages by individual inquiring or collaborative problem-solving. Thirdly, their interpreting and using data practices showed a little growth through this lesson due to their lack of practice in turning the pain points into a marketing opportunity but they could embed the circular concepts to make more meaning in their pitching the solution. Further study around teaching STEAM-BCG or chemistry based on community-based chemistry could focus more on enhancing learners to use and interpret effectively while continuing the awareness of all stakeholders or partnerships for sustainable problem-solving.

**Keywords:** STEM; BCG; Sensemaking practice; Entrepreneurial skills

## Using an esterification activity to enhance advanced placement (AP) chemistry students' competency in higher-order thinking (HOT)

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Esterification is one of the most important concepts to introduce chemical reactions in organic chemistry for high school students and in many countries, including Thailand, it has been included as a learning outcome. This work objective is to illustrate using an Esterification activity to Enhance Students' Competency in HOT which is one of the five students' key competencies, according to the Basic Education Core Curriculum. Participants were 17 ninth graders who enrolled in an AP chemistry subject. The activity comprises 2 parts: In part 1, students play a card game to practice writing the structures of esters, carboxylic acids, and alcohols along with esterification equations. Then, utilizing the information in the clue, the students investigated a mystery cube and discovered how an ester is structured on its blank face. Finally, they designed their mysterious cubes. In part 2, students synthesized an ester as their perfume through esterification. Various carboxylic acids and alcohols were provided for them. Then, using Padlet software, they created infographics to present perfume. By analyzing data from observation, scoring rubric of HOT competency (critical and creative thinking were emphasized in this work), students' works, and self-assessment (mean=2.96, S.D.=0.19), students were able to apply the clue information as evidence to find out the ester structure on the blank face of the cube. In addition, students could create their mysterious cubes and infographics to present their work well. This indicated that students could apply critical and creative thinking throughout the activity.

**Keywords:** Esterification; Competency; Higher order thinking; Critical thinking; Creative thinking



**Figure** The esterification card game and the mysterious cube



## The effect of STEAM BCG through natural tie dye activities

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STEAM would enable students to learn and integrate scientific knowledge to hone problems- solving skills. The BCG Model is holistic economic development in which it is not only developing the economy but also promotes social development and the conservation of the environment to be balanced, stable, and sustainable. Both seem essential to integrate students into learning processes until they could develop their knowledge and abilities. Therefore, the researcher came up with the idea of utilizing studying the effect of STEAM BCG through natural tie dye activity to increase the value of local plant, especially mangosteen in their communication. The target of the study was grade-5 students. **Phase 1:** students analyzed the local plants and designed the unique pattern on the clothes by using scientific inquiry. Therefore, the natural tie dye activities consisted of “*What is the plant*” “*Let’s get to know the plant*” “*Plant extraction*” “*Tinting*” and “*Tie dye*”. This step is integrated science process. The students learned simple extraction, mathematics through design pattern on the clothes and how was the changing of color from plat after added Mordant. **Phase 2:** Problem-solving phase, students’ self-learning step. This step the researchers gave the task to students with the satiation “*What are the appropriate color and Mordant of designed pattern clothes?*”. It was found that students could explored, collected data, discussed, analyzed their local plants, and chose the appropriate color and Mordant of designed pattern clothes for increasing the value of plants in their community through natural tie-dye activity.

**Keywords:** STEAM BCG; Scientific inquiry; Natural tie dye activities

# Chemical Education (CE)

## Poster Presentation



## The study on the conceptual changes in chemical equilibrium of science high school students using experimental-based learning

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Chemical equilibrium is one of the fundamental topics to establish well understanding in other chemistry topics. However, many high school and undergraduate students were found to have several misconceptions on chemical equilibrium. It is therefore crucial to investigate misconceptions that students have on this topic and to help them improve their conceptual understanding through several learning activities. In this work, the conceptual changes in chemical equilibrium of Grade 11 students were studied after they had learned about chemical equilibrium using an experimental-based technique. Herein, 44 students did the two-tier diagnostic test (10 multiple-choice with open-ended questions) on the chemical equilibrium prior to learning and after finishing this topic. The 9-period learning activities included the ‘Determination of the Chemical Equilibrium Constant’ experiment in which students learned to calculate the equilibrium constant from the actual experiment, and the ‘Le Chatelier’s Principle Experiment’, where students had to predict, observe, and explain (POE) how each chemical equilibrium was affected when being disturbed. All these experiments were performed along with Q&A session and discussion to assess students’ understanding during learning process. The questions on the diagnostic test were designed to investigate students’ understanding on these major topics: Approach to equilibrium, Characteristics of equilibrium state, and Changing equilibrium conditions. It was found from the paired t-test that the average scores of the post-test were significantly higher than those of the pre-test ( $p\text{-value} < .05$ ) with the degree of freedom of 9 and the effect size as measured by Cohen’s  $d$ ,  $d = 3.37$ , indicating a large effect. In addition, the students gained the conceptual understanding in the level of ‘Sound conceptual understanding’ or ‘Partial conceptual understanding’ more on all questions after learning using the experimental-based technique.

**Keywords:** Chemical equilibrium; Conceptual changes; Experimental-based learning

## Intermolecular interactions that govern solute retention; thermodynamics learning in gas chromatography experiment

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Gas chromatography experiment usually involving analytical chemistry learning aspects by calculating parameters such as resolution, peak area and plate number from chromatogram. However, since the retention time and selectivity in gas chromatography (GC) were governed by the thermodynamics of the phase transition. In this installment, the basic thermodynamics underlying separation in GC were being cooperated with basic gas chromatography experiment. The molecular interaction thermodynamics between GC column HP-5 (intermediate polarity) and DB-Heavywax which considered highly polar column were used for separation of analog volatile chemicals such as toluene, ethylbenzene, hexane, heptane and octane. Variation of column temperatures and flow rate were explored. The results were not only investigation of analytical features but also calculation of standard free energy ( $\Delta G^\circ$ ), enthalpy ( $\Delta H^\circ$ ), and entropy ( $\Delta S^\circ$ ) by using retention time ( $t_m$ ), partition coefficient (K) and van't Hoff equation respectively. Working in this experiment the students were required to demonstrated how to operate the instrument and how to properly collect data from chromatogram. In order to evaluate the results in both analytical and physical chemistry aspects the students also must learned how to utilized spreadsheet program such as microsoft excel, libreoffice for facilitate all the calculations and displayed relationship between the obtained thermodynamics values and GC conditions.

**Keywords:** Interdisciplinary; Gas Chromatography; Thermodynamics

## An optimal representation of a small-scale chemistry experiment: A case of diffusion of substance lesson for 7th grade students

Pongsaton Panyanukit<sup>1\*</sup> and Chatree Faikhanta<sup>2</sup>

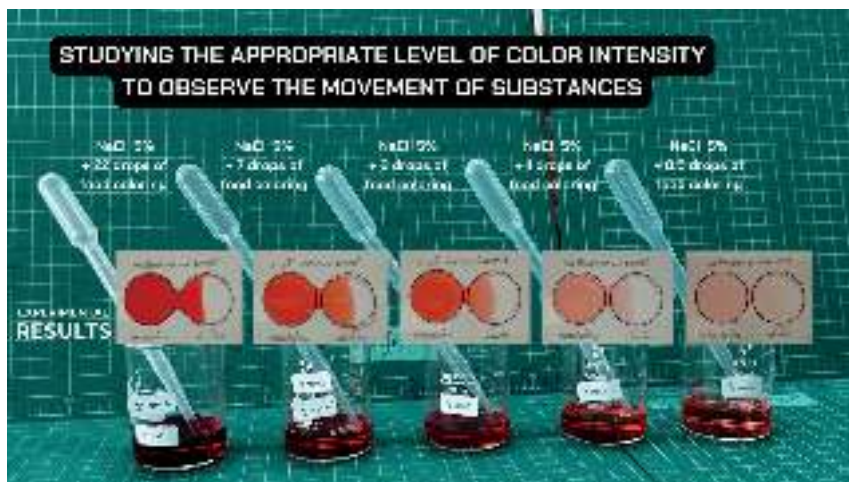
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In chemistry class, teaching and learning diffusion involves engaging students to observe the movement of potassium permanganate in water. However, this chemical tends to settle at the bottom of the beaker and diffuse very slowly, which makes it difficult to track its movement and reach diffusion equilibrium. Additionally, potassium permanganate can cause irritation. To address these issues, this study developed a simple and engaging small-scale chemistry experiment for middle school students studying diffusion. In this experiment, suitable substances for rapid, safe, and eco-friendly diffusion were investigated. A mixture of 10 ml of a 5% salt solution and 3 drops of 1.5% food coloring was found to achieve diffusion equilibrium within 30 seconds. This allowed students to comprehend the direction of substance movement, from areas of high concentration to areas of low concentration. They also learned that diffusion ends when the substance is evenly distributed, as observed by the consistent color intensity at equilibrium.

**Keywords:** Small-scale; Diffusion; Green chemistry



## Evaluating surface tension via smartphone-captured pendant drop method: enhancing accuracy in simplified experimental designs

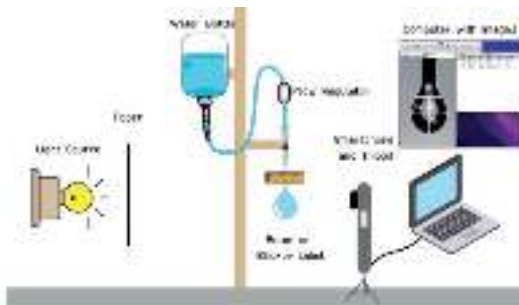
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Surface tension is a fluid property that reflects the force minimizing a liquid surface area. This force is vital in industrial applications such as detergents, oil recovery, paints, foods, and pharmaceuticals. Traditional surface tension measurement methods, including the capillary tube, Wilhelmy plate, and Du Nouy Ring, tend to be expensive, complicated, and require specialized equipment. This research introduces a simplified and cost-effective alternative: the pendant drop method using a smartphone for capture, making it accessible for high school and higher education lab settings. Optimized experimental parameters indicated that videos should be recorded at approximately two drops per second, capturing on drops exceeding half their full size. The drop width and height are processed using image software like ImageJ or Microsoft Paint. These measurements are carefully taken at the drop edge to maintain a misplacement of fewer than two pixels, thereby suppressing pixelation errors under 10%. For pixel-to-metric conversion, the reference scale in the image must be more than 80 pixel per mm, achievable with a standard ruler or sticker label. Straightforward experimental approach, under optimized conditions and with proper data analysis, measured the surface tension of distilled water to be 67.817 mN/m ( $n = 10$ ) at 27 °C, in accordance with the Young-Laplace equation. This closely matched the 69.790 mN/m ( $n = 10$ ) obtained from the Wilhelmy plate method. These results support our experimental design and analysis as appropriate for chemistry labs, ensuring precise results. Additionally, this technique could help determine the critical micelle concentration of surfactants.

**Keywords:** Surface tension; Pendant drop method; Pixelation





## Alcohol test kit: An integrated lesson in chemistry for high school students

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The alcohol-related content in high school chemistry covers chemical structures, nomenclature, and basic chemical reactions. To promote science competency in applying crosscutting concepts to solve real-world problems, we developed the learning module “Alcohol Test Kit.” The activity was implemented in the fundamental organic chemistry course for 240 Grade 11 students at Mahidol Wittayanusorn School. The first part comprised a regular lesson on the qualitative test for the hydroxy group using substitution and oxidation reactions. In the second part, students were introduced to the difference between qualitative and quantitative tests. Although methanol and ethanol could eventually turn permanganate solution into brown manganese oxide, the reaction rate in acidic conditions was differentiable. In the context of developing an alcohol test kit that is safe for household use, the class discussion led to a unanimous agreement on choosing a potassium permanganate test for further investigation. The third part involved a guided inquiry where students designed a small-scale experiment to test for factors that could affect the test results, such as the comparison between alcohol spray and alcohol gel. The average satisfaction with the course materials and the activity format was 4.29 on a 5-point Likert scale. One student commented that the experiment helped them see how chemical kinetics can affect functional group tests. Students’ self-assessment on science competency showed the highest score of 4.78 for the ability to formulate scientific questions and design an investigation under constraints.

**Keywords:** Alcohol; Oxidation; Integrated lesson

## Exploring betalain extraction from *Gomphrena globosa* L. as a green indicator in acid-base titration concepts

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This study introduces a straightforward approach to extracting Betalain from *Gomphrena globosa* L. using only hot water (90°C) as a natural pH indicator for acid-base titration. This novel indicator's performance was compared with the traditional phenolphthalein indicator in the context of titrating potassium hydrogen phthalate (KHP) and sodium hydroxide (NaOH), and the results were comparable. To further enhance the eco-friendliness and accessibility of acid-base titration, we developed a wax screen-printed microfluidic paper-based analytical device ( $\mu$ PAD). This  $\mu$ PAD offers numerous advantages, including cost-effectiveness, minimal chemical usage, low sample volume (in microliters), ease of operation, and portability, all in line with the principles of "Green Chemistry." With our proposed method, the endpoint of an acid-base titration can be easily determined by observing the indicator's color change with the naked eye. Notably, our method's performance closely aligns with conventional acid-base titration, affirming its reliability and accuracy. This innovative approach opens the door to more sustainable and accessible chemical analyses. This Greener acid-base titration on the  $\mu$ PAD utilizing Betalain extraction as a green indicator can be easily implemented as an alternative experiment to the conventional acid-base titration for both high school and undergraduate chemistry classrooms.

**Keywords:** Betalain; *Gomphrena globosa* L.; Green indicator; Acid-base titration; Microfluidic paper-based analytical device ( $\mu$ PAD)



## Enhancing physical chemistry education: Active learning strategies, student engagement, and assessment alignment for successful learning outcomes

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Teaching physical chemistry in line with curriculum learning outcomes involves utilizing active learning techniques such as Think-Pair-Share, collaborative learning, games, and video analysis. Students actively participate by creating tests, taking notes, and utilizing technology for learning through models and data analysis with Excel. This approach enhances the overall learning experience, promotes information-seeking, and encourages opinion expression. Results from these activities indicate improved understanding of physical chemistry principles among students. They exhibit a more assertive attitude, engaging in increased opinion exchange and demonstrating greater determination in presentations. Evaluation results, including exam scores, work pieces, and presentations, are consolidated into a score scale aligned with the program learning outcomes (PLO) of the curriculum, providing a clear reflection of each student's characteristics. This teaching information informs the organization of future teaching activities, ensuring alignment with curriculum goals and facilitating continuous improvement. The aim is to guarantee that students successfully achieve the curriculum's learning objectives.

**Keywords:** Active learning; Learning Outcome ; Activity ; Game ; Simulation



## Developing proficiency in applying exponential and logarithmic functions in the context of chemical kinetics for 11<sup>th</sup> grade students using the backward design teaching approach

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This research aims to enhance students' adeptness in utilizing exponential and logarithmic functions to comprehend and address challenges in chemical kinetics. The backward design approach is employed to efficiently structure the learning trajectory. The study involved a sample of 23 11<sup>th</sup> grade students of Mahidol Wittayanusorn School, selected through purposive sampling. A comparison was made between the math pretest and posttest to evaluate mathematical literacy before and after employing the backward design method, using a paired t-test. Furthermore, a paired t-test was utilized to compare the math posttest and chemistry posttest. The correlation between the math posttest and chemistry posttest was analyzed to determine the effectiveness of math learning for chemistry. Additionally, the sample was divided into two groups for interviews, one comprising students with high scores in both chemistry and math tests, and the other consisting of students with a high score in math but a low score in chemistry. The findings unveiled the following: 1) The average math scores of the student sample after the learning process significantly surpassed the scores before learning and also surpassed the 70% criterion at a significance level of 0.05. 2) The mean math scores of student sample after learning did not surpass the mean chemistry scores of the student sample after learning at a significance level of 0.05. And 3) There was no significant correlation between the math and chemistry scores ( $R^2=0.08$ ). In the interviews, it was observed that the high-scoring group comprehended and could demonstrate chemistry formulas, enabling them to tackle chemistry problems. Conversely, the low-scoring group only memorized the formulas without a deep understanding, hindering their ability to apply mathematical concepts to solve chemistry problems.

**Keywords:** Backward design; Chemical kinetics; Exponential function; Logarithmic function



## Environmental learning using problem-based learning and GLOBE protocol in the lotus field

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This study explores the fusion of Problem-Based Learning (PBL) and the Global Learning and Observations to Benefit the Environment (GLOBE) protocols within the lotus field ecosystem. The lotus field, in Salaya Subdistrict, Nakhon Pathom Province, Thailand, was a complex environmental challenge field for students to investigate the environment quality. Our study demonstrates how the combination of PBL and GLOBE protocols enriches student learning, encourages rigorous environmental data collection, and fosters community engagement for the betterment of lotus field conservation. Twenty-three students of Mahidol Wittayanusorn who enrolled in the Industrial and Environment Chemistry course were asked to implement their knowledge for evaluating the quality of water and soil of the lotus field. Students can collaborate in the real-world environment, promoting critical thinking and teamwork. The integration of GLOBE protocols provides a structured framework for collecting precise environmental data. These approaches allow students to immerse themselves in the lotus field environment, acquiring mini-project experience while using GLOBE protocol to investigate the environmental data. Students' mini-projects aim to determine the quality of water such as pH, temperature, DO, turbidity, and the quality of soil such as pH and humidity as well as small living things in the lotus field. After investigation teachers and students evaluated the efficacy of PBL- GLOBE integration in lotus field studies, assessing its impact on students' engagement and scientific acumen by presentation and discussion. In addition, students can see that the environmental quality assessment requires analysis of many elements. The information from a variety of sources was analyzed together. This activity can be used as a model for the larger environmental system.

**Keywords:** Environmental diversity; Lotus fields; Project-based learning; GLOBE protocol

## Determination of ethanol content in disinfectant spray by color photo intensity measuring on mobile phone

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Ethanol-based disinfectant spray is widely used in the COVID-19 pandemic and can help prevent bacteria and other viruses. The ethanol content of the disinfectant spray must be more than 70% v/v. Analytical methods for evaluating the ethanol content in the disinfectant spray should be simple, rapid, and reliable. In this study, the amount of ethanol in the disinfectant spray was determined by alcohol oxidation using a colorimetric method by color photo intensity measuring on a Mobile Phone. The chemical reagents used are potassium dichromate ( $K_2Cr_2O_7$ ) solution, ethanol standard, and ethanol spray samples. The color models (RGB) were used for monitoring a color change from orange ( $Cr^{6+}$ ) to green ( $Cr^{3+}$ ) in the reaction. For the quantitative analysis, the color of each sample was recorded in terms of the intensity of an RGB using the application on a mobile phone and further converted into absorbance, comparing it with the analysis of ethanol. The results showed a linear range of 50 - 90 %v/v ethanol and  $K_2Cr_2O_7$  solution ( $R^2 = 0.9893$ ). The concentration analysis of ethanol in the sample by measuring the color intensity from mobile phone camera results is similar to the analysis using NMR and UV-Vis spectrophotometry techniques. Furthermore, this experiment will help students develop practical and analytical skills in quantitatively analyzing ethanol levels in disinfectant spray. Designed for high school chemistry labs with limited equipment, it encourages students to explore digital imaging technology in basic chemistry analysis. Emphasizing portability, cost-effectiveness, and quick analysis, it offers a comprehensive learning experience.

**Keywords:** Ethanol spray; Colorimetric method; RGB color model; Mobile Phone

## A simple electrochemical experiment kit made from electrolyte gels

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In this work, the effect of the addition of hydrocolloid substances to  $\text{CuSO}_4$  and  $\text{ZnSO}_4$  electrolytes for creating electrolyte gels and gel batteries applied in electroplating experiment. To compare durable electric potential values of galvanic cells persisted for 6 hours, a various of hydrogels mixed with 1.0 M  $\text{CuSO}_4$  and  $\text{ZnSO}_4$  electrolytes, Zn-Cu (electrode) were tested. The result revealed that galvanic cell potential using carrageenan, agar-carrageenan and gelatin gel electrolytes displayed 0.989 V, 0.974 V, 0.954 V, respectively as compared with standard value 1.100 V. The effect of four concentrations of  $\text{CuSO}_4$  and  $\text{ZnSO}_4$  electrolyte solution (1.00, 0.50, 0.25, 0.10 M) on galvanic cell potential performed 6 hours using carrageenan gel as optimized choice were systemically studied. The electric potential cell was reported to 0.989 V (1.00 M), 0.978 (0.50 M) V, 0.964 V (0.25 M) and 0.948 V (0.10 M). A new prototype 6-cell gel battery fabricated from 0.10 M  $\text{CuSO}_4$  and  $\text{ZnSO}_4$  mixed with carrageenan as electrolyte gel using Zn and Cu electrode were applied to determine the efficiency of electroplating experiment. The electric potential of gel battery initially stood at 6.433 V and employed to study the electroplating of an iron nail with zinc performed 5 mins. A higher percentage yield was produced as compared with a normal 6-volt battery. This work indicated that 0.10 M electrolyte solution and carrageenan are suitable options for fabricating gel batteries for use in electroplating experiments in high-schools. High concentration metal-contaminated waste can be diluted and turned into electrolyte gels.

**Keywords:** Electrochemistry; Electrolyte gels; Hydrocolloid; Galvanic cells



# Environmental Chemistry and Renewable Energy (EE)

## Oral Presentation

## Microplastics and plastic additives in open dumping site soil from Thailand

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In Asian emerging countries, a large amount of plastic waste is discarded into open dumping sites without adequate management. In open dumping sites, plastic waste is expected to be deteriorated and fragmented into microplastics (MPs) by long-term exposure to UV light, and plastic additives would be released into the surrounding environment as well as MPs. However, few studies have investigated the pollution status and runoff behavior of MPs and plastic additives in Asian dumping sites, especially in Thailand. In this study, we collected 12 soil samples around an open dumping site in southern Thailand and analyzed MPs and organic plastic additives. As results, the huge numbers of MPs were detected in soil samples, and the maximum abundance was more than 150,000 items/kg dw. (Fig. A). A significant negative correlation between MP abundance and distance from the open dumping site in each sampling point were clearly observed. As for plastic additives, organic compounds including plasticizers, antioxidants, UV stabilizers, and flame retardants were detected in soil samples. Di(2-ethylhexyl) phthalate (DEHP: CAS#: 117-81-7) showed the highest concentration followed by di-*n*-butyl phthalate (DnBP: CAS#: 84-74-2) and tris(2-chloroisopropyl) phosphate (TCIPP: CAS#: 13674-84-5). The concentration of plastic additives was significantly correlated with the mass concentration of MPs in soil (Fig. B). These results suggest that open dumping site is a point source of MPs, and MPs act as a vector of harmful plastic additives into the environment.

**Keywords:** Open dumping site; Microplastic; Plastic additives; Point source; Thailand

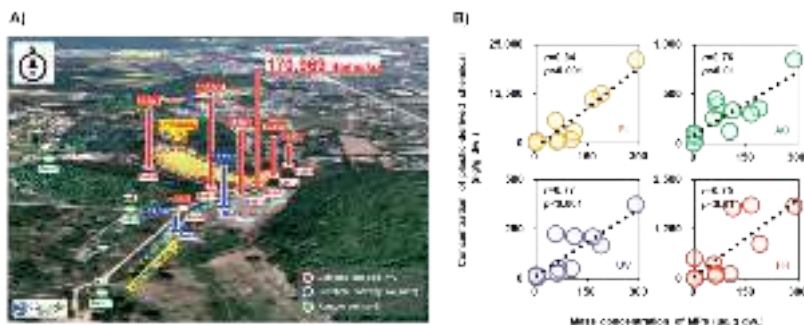


Figure A: Distribution of microplastics in soil around the open dumping site. Figure B: Correlation between mass concentration of MPs and concentration of plastic-derived chemicals in soil: DEHP, plasticizers; AOC, antioxidants; UV, UV stabilizers; TCIPP, flame retardant.

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## Preparation of porous biochar derived from avocado peel and its application on ciprofloxacin removal

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Highly efficient antibiotic adsorption was achieved using porous biochar derived from avocado peel (AvP-char). The material was prepared by carbonization of avocado peel and KOH activation. The porous structure of the adsorbent AvP-char, with a large surface area of  $878 \text{ m}^2 \cdot \text{g}^{-1}$  was confirmed using  $\text{N}_2$  sorption and scanning electron microscope. The effects of the pH solution and the time of the adsorption process were subsequently investigated. The adsorption kinetics for ciprofloxacin best fitted a pseudo-second-order model, while the adsorption isotherms best fitted the Langmuir model. At pH 2, the maximum adsorbed amount of ciprofloxacin is  $90 \text{ mg g}^{-1}$ ; the adsorption process reached equilibrium at 120 mins, and  $0.5 \text{ mg mL}^{-1}$  was the optimum dosage of AvP-char to remove ciprofloxacin. Thus, considering that the AvP-char showed high adsorption capacities and was derived from agricultural waste by a simple alkaline process, it seems highly suited for use as an efficient and environmentally friendly antibiotic adsorbent.

**Keywords:** Ciprofloxacin; Porous carbon; Avocado peel; Antibiotic; Adsorption



## Minimize residual formaldehyde content in melamine-formaldehyde PCM microcapsules

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Phase change materials (PCM) can be used as latent heat thermal storage (LHTS) systems. Due to the phase transition, encapsulation of PCMs is normally required to avoid leakage of liquid PCM to the surroundings. The material commonly used for microencapsulation shell is melamine formaldehyde (MF) due to its good thermal and mechanical stability, and chemical resistance. However, formaldehyde, one of MF raw materials, is a dangerous chemical compounds, affecting human health. Therefore, the residual formaldehyde that might be remained in the microencapsulated PCMs (microPCMs) should be minimized and removed. In this work, microPCMs were synthesized by in-situ polymerization using MF resin as a shell and n-Hexadecane as a PCM core. The MF prepolymer was prepared by varying the molar ratio of melamine (M) to formaldehyde (F). Residual formaldehyde content and properties of microPCMs were analyzed. The standard perforator method (EN 120) was used for the determination of residual formaldehyde, which exists in a ppm concentration range. Free formaldehyde in microPCMs is extracted with water and toluene and then derivatized by a 2,4-dinitrophenylhydrazine (DNPH) agent before being analyzed by high-performance liquid chromatography (HPLC). The molar ratio of 1:3 of M-F monomers showed the least residual formaldehyde content in microPCMs, while the encapsulation efficiency unaffected by varying molar ratios.

**Keywords:** Phase change material; Microcapsule; Melamine formaldehyde; Residual formaldehyde; Formaldehyde detection

## Conversion of fat and oil contaminant waste produced by stationary wastewater treatment plant into calcium soap for ruminant feed

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Urban wastewater containing fat, oil and grease often creates problems not only when collecting and transporting sewage to wastewater treatment plants (WWTPs) but also for their final management and treatment in WWTPs. Grease becomes a distinct waste when it undergoes a flotation process to separate it from the influent as an upper emulsion, defined as grease and oil mixture from oil/water separation (GOMOWS). This grease must be disposed of properly, or this can be a challenge, with the potential for environmental contamination. One efficient way to solve this problem is to transform this waste into a valuable product. In this research work, the utilization of this waste, GOMOWS, for the production of calcium soap was investigated. The reaction conditions relating to initial temperature, amount of calcium oxide and volume of water were optimized using response surface methodology (RSM) in order to achieve the maximum product yield within the acceptable acid value for commercialization purposes. Results showed that using 5g of brown grease, the optimized conditions were an initial temperature of 60, a stoichiometric mole ratio of CaO/g sample at 1.285, and water at 25%, resulting in a product yield of 6.63g with an acid value of 1 mgKOH/g sample. It can be concluded that GOMOWS can be used as a raw material to produce calcium soap for ruminant feed since the acid value of the final product is lower than permitted. However, the stability and characterization of the produced calcium soap should be assessed before commercialization.

**Keywords:** Brown grease; Calcium soap; Fusion method; RSM; Wastewater

# Exploring interphase instability in the LiTFSI-LiCl aqueous biphasic system through optical microscopy

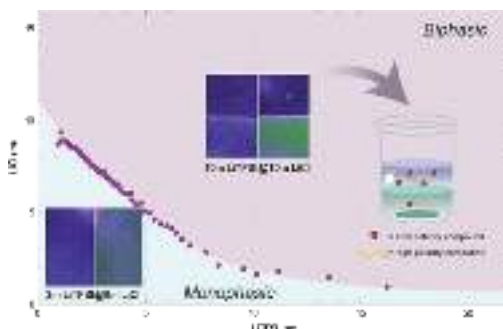
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Aqueous biphasic systems (ABSs) based on water-in-salt electrolytes (WISE) have garnered considerable attention in liquid-liquid interphases, especially in energy storage devices, due to the wide electrochemical stability window.<sup>(1, 2)</sup> In our study, we report the interfacial behavior of lithium bis(trifluoromethanesulfonyl)imide-lithium chloride (LiTFSI- LiCl) ABS using an optical microscope. Our observations reveal the liquid-liquid interphase at the microscale and instability phenomena at the interphase through high-resolution imaging. We also analyze the unwanted solid phase formation within ABS using Transmission Electron microscopy (TEM), ImageJ, and Mathematica programs to study the conditions that affect the formation of solid phases, such as salt concentrations and temperatures. This study not only contributes to fundamental knowledge in interfacial science but also holds significant implications for developing novel applications reliant on ABS stability.

**Keywords:** Aqueous biphasic systems, Water-in-salts electrolyte, ABS stability



**Figure** phase diagram and optical microscopy images of the LiCl-LiTFSI-H<sub>2</sub>O with the blue monophasic and purple biphasic regions at 298.15 K.

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# Nanostructured MoO<sub>2</sub>/MoS<sub>2</sub>/MoP heterojunction and N, S dual-doped reduced graphene oxide as high-performance electrode for supercapacitors

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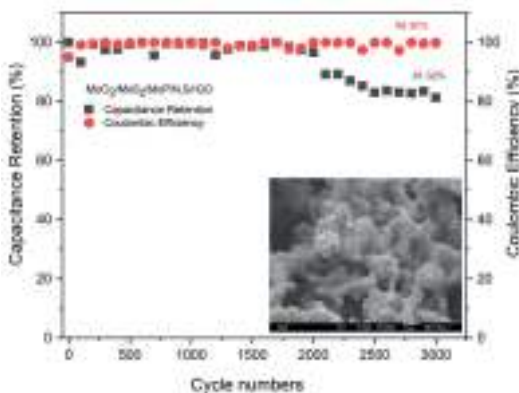
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Herein, a nitrogen, sulfur dual-doped reduced graphene oxide (N,S/rGO)-coated MoO<sub>2</sub>/MoS<sub>2</sub>/MoP heterojunction (MoO<sub>2</sub>/MoS<sub>2</sub>/MoP/N,S/rGO) architecture was developed, which exhibited favorable diffusion kinetics of electrolyte through an internal electric field built at heterointerfaces and alleviated the volume change through the core-shell structure, resulting in a MoO<sub>2</sub>/MoS<sub>2</sub>/MoP/N,S/rGO with the high adsorption of redox species, excellent electrical conductivity, and high reaction kinetics. This MoO<sub>2</sub>/MoS<sub>2</sub>/MoP/N,S/rGO can be used directly as a supercapacitor electrode with a high specific capacitance of 723.5 F g<sup>-1</sup> at 1 A g<sup>-1</sup> and an excellent rate capacitance (487.18 F g<sup>-1</sup>, 16 A g<sup>-1</sup>). The prepared MoO<sub>2</sub>/MoS<sub>2</sub>/MoP/N,S/rGO electrode exhibited excellent cycle stability with a coulombic efficiency of 99.30% at 16 A g<sup>-1</sup> after 3,000 cycles, highlighting the promising prospect of the electrode for supercapacitor application.

**Keyword:** Nanostructure; Heterojunction; Heteroatom dual doping; Reduced graphene oxide; Supercapacitor



## The fabrication of $\text{Ru}_2\text{P}$ nanoparticle decorated P-doped vegetable root-derived hierarchical porous carbon for supercapacitors with ultrahigh capacitance

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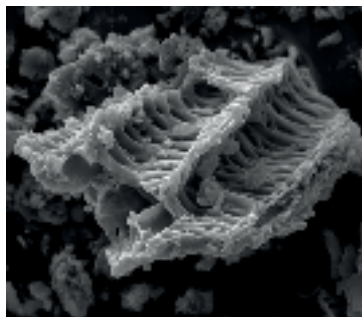
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The present work deals with the fabrication of electrode material, that is, ruthenium phosphide nanoparticle decorated phosphorous-rich hierarchical porous carbon ( $\text{Ru}_2\text{P}/\text{P-HPC}$ ) with a three-dimensional (3D) architecture by the facile carbonization of celery root followed by chemical activation. Celery roots are used as the precursor to prepare HPC due to extensively cultivated worldwide as human food and an abundant 3D structure, which remain unused and produce enormous pressure on the environment. HPC serves as both a support and a current collector. The inclusion of  $\text{Ru}_2\text{P}$  into the P-HPC backbone, that is  $\text{Ru}_2\text{P}/\text{P-HPC}$ , serves as the electrochemically active species. Several spectroscopic and microscopic methods are used to characterize the fabricated electrode material. The prepared material possesses pore volume of  $1.91 \text{ cm}^3 \text{ g}^{-1}$ . Scanning electron microscopy image of material shows a unique 3D hierarchical porosity. The formation of this 3D hierarchical morphology depicts stable architecture showing improved electrochemical performance. Cyclic voltammetry, galvanostatic charge-discharge measurement, and electrochemical impedance spectroscopy are used to evaluate the electrochemical performance of the prepared electrode material. The electrochemical study reveals a high specific capacitance of  $3,187 \text{ F g}^{-1}$  for  $\text{Ru}_2\text{P}/\text{P-HPC}$ . Finally, the strategy presented in this work provides valuable insights for designing electrode material for supercapacitors (SCs) with tunable specific capacitance that could be one among the future developments in flexible energy-storage systems.

**Keyword:** Supercapacitor; Hierarchical porous carbon; Transition metal phosphide; Biochar; Three-dimensional architecture



## Unveiling the potential of oxidative catalytic fractionation in spruce bark valorization

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In the quest for an economically competitive and environmentally responsible biorefinery, it becomes essential to harness the full potential of biomass, including the often overlooked bark component. Currently, bark, comprising 10% of timber and pulpwood, is predominantly incinerated, while the tops and branches, accounting for up to 50% of the bark, remain largely untapped. This study focuses on maximizing the potential of bark by extracting valuable aromatic compounds from the lignin in spruce bark using a “lignin-first” oxidative catalytic fractionation approach. This approach yielded monophenolic compounds with yields surpassing traditional nitrobenzene oxidation by a factor of 30. Additionally, we successfully isolated carbohydrate pulp, subsequently refined for the production of nanocellulose. These findings underscore the transformative potential of softwood bark, transcending its conventional role as a low-value fuel source and paving the way for a biorefinery that excels both economically and ecologically.

**Keywords:** Lignin-first; Spruce bark; Oxidative catalytic fractionation; Cellulose pulp

## Conversion of food waste to a valuable soil resource in a day

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More than 1,300 million tons of food waste have become organic waste per year. This waste inevitably brings about environmental pollution such as soil pollution, water pollution, and air pollution which probably results in greenhouse gases and global warming. The study aimed to reduce organic waste by composting which complied with the standards. Accordingly, the appropriate composter design was developed to cope with 5 kg of household waste. The mechanism of composters efficiently decomposed organic waste within 48 hours without making an odor. The decomposition process mainly focused on studying the impact of aeration, temperature, microorganisms, moisture, pH, and nutrients. In the initial fermentation step, the moisture of organic waste was operated at 40-95%. Concurrently, the decompose temperature was controlled at 40-60°C. The result of the experiments identified that the moisture was decreased in the range of 1-9% and the pH in the range of 6-7.7. The ratio of carbon to nitrogen (C: N) was explicit at 17:1 and the value of organic matter (OM) exhibited 38-59 % by weight. In addition, the total nitrogen content (total N), the total phosphate content (total  $P_2O_5$ ), and the total potassium contents (total  $K_2O$ ) were revealed contents at 1-4%, 0.5-1%, and 0.7-1.6%, respectively.

**Keywords:** Composting; Organic waste; Composting machine; Composting process

## Comparative study of torrefaction and pyrolysis behavior on rice straw using thermogravimetry-mass spectrometry (TG-MS) technique

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Rice straw is indeed regarded as one of the most abundant agricultural biomass resources in many rice-producing regions among Asia countries. Although, it is a potential feedstock for biocoal production, the selection of efficient conversion method must be considered in order to get a better quality of biocoal. It is shown that rice straw has carbon content around 39.73% and high heating value (HHV) about 15.28MJ/Kg. Torrefaction is a thermal treatment technique that involves heating biomass at 200-300°C in an inert environment to enhance its properties as a fuel or feedstock in a variety of applications such as power generation and other industrial processes. Pyrolysis is another technique that required higher temperature above 600°C in an oxygen-free condition. This study paid particular attention at both qualitative and quantitative analysis of gases generated throughout the thermal treatment process, utilizing the TG-MS technique for evaluating the torrefaction and pyrolysis behavior of rice straw biomass. The amount of gas products of pyrolysis condition upon weight loss decomposition was in the order of  $H_2 < CH_4 < CO < CO_2$ , whereas torrefaction produced only minor gases of CO and CO<sub>2</sub>. According to the findings of this research, torrefaction and pyrolysis provided varied solid, liquid, and gas yields of 79.30%, 16.95%, 4.04%, and 29.63%, 48.87, 21.50%, respectively.

**Keywords:** Torrefaction; Pyrolysis; Biomass; TG-MS

## Copper calcium hydroxide nitrate derived from chicken eggshell and their catalytic activity in the removal of aqueous methyl orange

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In this work, waste chicken eggshell was applied as precursors for the preparation of copper-calcium hydroxide nitrate (CuCa HDS), a wet air oxidation catalyst, in the removal of methyl orange (MO) dye from water. The eggshell was calcined for 4 hours at varying temperatures, 750°C -1050°C, to obtain bio-CaO. The CuCa HDS catalysts were hydrothermally heated in 30 minutes assisted with metal oxide method, at the control Cu: Ca molar ratio of 4:1. The physicochemical, structural and surface properties of bio-CaO and catalysts were investigated. The catalytic activity of the catalysts was evaluated in degradation of MO, through catalytic wet air oxidation process under ambient conditions, using 500 ppm of MO, and 2 g/L of catalyst loading. The results showed that the optimum calcination temperature of 900°C gave a relatively high specific surface area of bio-CaO (21.10 m<sup>2</sup>g<sup>-1</sup>). All CuCa HDS materials showed ~100% color removal efficiencies of MO and >90% COD removal efficiencies within 5 minutes. The waste chicken eggshell is of high potential to be utilized as a raw material to produce effective and reusable CuCa HDS catalysts for wastewater treatment.

**Keywords:** Bio-calcium oxide; Copper-calcium hydroxyl double salt; MO removal; Catalytic wet air oxidation process

## Photocatalytic degradation of organic dye and antibiotic by ZnO-based photocatalyst under natural solar light

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It is well accepted that high electron-hole recombination is the main problem affecting the photocatalytic performance of the sunlight-active photocatalyst. In the presentation, modification of ZnO photocatalyst by both silver decoration and creation of heterojunction with  $\text{BiVO}_4$  will be presented. Firstly, silver-decorated ZnO was prepared by photo-deposition method. The addition of 5 wt% silver is the optimal condition. The silver-decorated ZnO showed high photoactivity of 100% under natural sunlight toward degradation of reactive red 141 (RR141) dye and oxytetracycline (OTC) antibiotic. Secondly, the ZnO/ $\text{BiVO}_4$  heterostructure photocatalyst was synthesized by ultrasonic route. The heterojunction exhibited complete detoxification of RR141 dye and OTC antibiotic under natural solar irradiation. The removal of the pollutants by the prepared ZnO-based photocatalysts followed the first-order kinetics model. The structural stability of the photocatalyst was found after five times of use with excellent cycling ability. Photo-generated hydroxyl radicals play the major role in degradation of the pollutants. Improvement of the electron-hole separation efficiency is the key factor influencing the dramatic increase of the resultant photocatalytic activity. This work demonstrates the promising avenue for increasing the performance of the sunlight-responsive photocatalyst for environmental remediation.

**Keywords:** ZnO;  $\text{BiVO}_4$ ; Heterojunction photocatalyst; Silver decoration; Sunlight



## Performance evaluation of Phase Change Materials (PCMs) to improve energy saving potential of building

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Phase change materials (PCMs) have the potential to be used in building construction to reduce temperature fluctuations and reduce energy consumption, which helps to promote sustainability in the building sector. This research investigates the thermal performance and energy efficiency of PCMs integrated in a residential building located in Bangkok through energy transfer simulation. DesignBuilder software was used to model typical residential buildings and numerically analyze the efficiency of indoor temperature reduction and annual energy saving. Buildings with an integration of a 2.5 cm thick PCM layer in the wall were compared to those without PCM installation. PCM with different melting points ranging from 27 °C - 34 °C were studied. The energy savings were compared between two scenarios: a building that operates its HVAC air conditioning system for 24 hours, reflecting a work-from-home situation, and a 12-hour HVAC operation, indicating a scenario of normal stay-at-home throughout the night. The results found that PCM with a melting point of 28 °C was most suitable for use in buildings located in Bangkok due to the highest efficiency in annual energy savings of 157.7 kWh and saving occupants 697 baht in annual electricity bills. However, during the summer when outside temperatures are relatively high, PCM with a melting point of 29 °C was found to be the most effective to use in building. It potentially reduces the energy consumption for cooling by up to 43.4 kWh, which could save as much as 192 baht in March on electricity bills.

**Keywords:** Phase change material; DesignBuilder; Energy saving; Numerical simulation; HVAC

## One-dimensional simulation of an alkaline-acid direct glycerol fuel cell

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A one-dimensional model of an alkaline-acid direct glycerol fuel cell (AA-DGFC) was developed to study the influences of the operating parameters such as glycerol to sodium hydroxide ratio ( $C_3H_8O_3:NaOH$ ), glycerol concentration, and cell temperature on the AA-DGFC performance. A kinetic model of AA-DGFC was created by using a computational software. In setting up the model, mass transport and charge transfer equations were used to determine the concentration gradient and ohmic resistance, respectively. From the simulation results, it is evident that varying the concentration of NaOH has an impact on the anode concentration loss, while altering the  $C_3H_8O_3:NaOH$  ratio affects the anode activation loss. Similarly, variations in temperature influence the activation loss of this fuel cell. These parameters adjustment exert an influence on the voltage according to the cell voltage equation. The steady-state results from the simulation were validated with in-house experimental data which are polarization curves and product selectivity results. It was confirmed that the model not only can predict the cell performance but also can simulate the AA-DGFC behavior at various operating conditions.

**Keywords:** Alkaline-acid direct glycerol fuel cell (AA-DGFC); Mass transport; Charge transfer; Kinetic model; Steady-state condition



## Simulation of hydrogen production from water-hyacinth with equilibrium reactors

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The dependency on non-renewable resources, particularly fossil fuels, to produce chemical and energy to support daily needs has resulted in growing negative environmental impacts. Climate change is one of the most significant impacts of greenhouse gas emissions, especially carbon dioxide ( $\text{CO}_2$ ) from the combustion of fossil fuels. Currently, using renewable energy sources, hydrogen fuel ( $\text{H}_2$ ) is a more interesting way to reduce the effects of climate change. Utilizing biomass conversion is one of sustainable renewable methods for producing  $\text{H}_2$ . A potential process that combines steam reforming (SR),  $\text{CO}_2$  reforming (DR), and water gas shift (WS) reactions is called bi-reforming (BR). This process can be utilized for the generation of  $\text{H}_2$  while capturing  $\text{CO}_2$ . The process has been simulated with a series of equilibrium reactors on Aspen plus process simulator for hydrogen production from Water-Hyacinth. The bi-reforming process has been investigated on a single equilibrium reactor (SR+DR+WS), 2 equilibrium reactors in series (SR+DR separate WS, DR separate SR+WS, DR+WS separate SR and SR separate DR+WS), and 3 equilibrium reactors in series (DR to SR to WS). The investigated results have revealed that the equilibrium yields of  $\text{H}_2$ , CO, and  $\text{CO}_2$  products could be 0.28%, 0.08% and 0.11%, respectively, at 950 °C. Consequently, equilibrium reactor models could be employed for predicting equilibrium product distribution for well-defined catalytic reactions.

**Keywords:** Simulation; Equilibrium reactor; Hydrogen production; Water-Hyacinth; Bi-reformation

## Unveiling novel mechanisms in energy storage materials with mimic battery concept

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Dodzi Zigah<sup>2</sup>, and Olivier Fontaine<sup>1\*</sup>

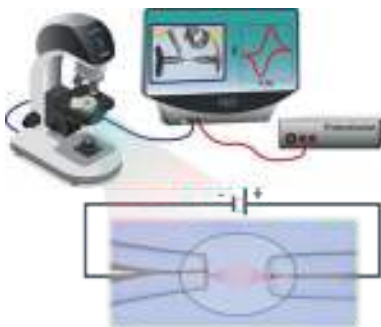
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In the presence day of the energy storage field the electrochemical communication between anode and cathode remains unknown. This work introduces the concept of the “Mimic Battery”, designed to closely imitate a real battery system. The key to the Mimic Battery lies in the potential observation of electrochemical phenomena through operando optical electrochemical measurements in the context of batteries and supercapacitors, such as the Li-ion battery and supercapacitor, using a high-resolution optical microscope. The Mimic Battery concept can operate at an exceptionally high scan-rate, due to the use of ultramicroelectrodes as the working electrode, requiring only a small quantity of electrolyte and electrode materials designed by our group. To demonstrate the novelty of our approach the mimic battery is applied to electroactive electrolyte for supercapacitors, associated to biredox ionic liquids (CITE my nature Materials). Shortly, using biredox ionic liquids the capacity of EDLC are increasing by 2. Unfortunately, the long self-discharge time unclear. The mimic battery systems is used to understand the present phenomena.

**Keywords:** Electrochemical energy storage; Operando optical measurement; Mimic battery concept.



**Figure** The concept of Mimic Battery analyzed by an operando optical electrochemical measurement.

## Efficient wastewater dye degradation using $\text{Fe}_3\text{O}_4\text{-CuS@SiO}_2$ photocatalyst: Mechanism and performance

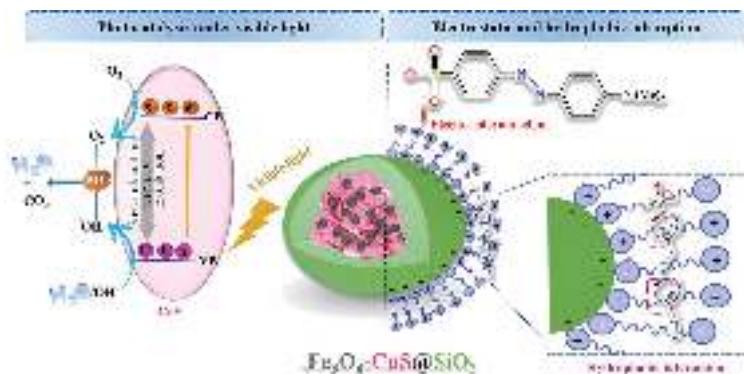
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The persistent presence of synthetic dyes in wastewater has become a critical environmental concern, demanding efficient remediation strategies. In response to this challenge, we have developed a novel  $\text{Fe}_3\text{O}_4\text{-CuS@SiO}_2$  photocatalyst through a multistep assembly technique, designed for the degradation of methyl orange (MO) dye in aqueous solutions under visible-light irradiation. The synthesis process involves the solvothermal generation of  $\text{Fe}_3\text{O}_4\text{-CuS}$  nanoflowers, followed by their encapsulation with silica ( $\text{SiO}_2$ ) shells using the sol-gel method to create the  $\text{Fe}_3\text{O}_4\text{-CuS@SiO}_2$  photocatalyst. This catalyst exhibits exceptional efficiency, achieving 94% degradation of MO within a remarkably short 20-minute timeframe, and demonstrates a notable sorption capacity of  $100.55 \text{ mg g}^{-1}$ , underscoring its potential to address dye pollutant removal from wastewater. The catalyst's superparamagnetic characteristics at room temperature facilitate the practical recovery of the adsorbent material, enhancing its usability. The study investigates the proposed MO degradation mechanism and assesses the impact of various parameters on sorption capacity, providing valuable insights for optimizing reaction conditions. Our work emphasizes the need for sustainable and effective solutions for environmental remediation in the face of dye pollutant challenges, and the  $\text{Fe}_3\text{O}_4\text{-CuS@SiO}_2$  photocatalyst stands as a promising avenue in this pursuit.

**Keywords:** Photocatalysis; Adsorption; Synergistic effect; Methyl orange degradation; Wastewater treatment



# Environmental Chemistry and Renewable Energy (EE)

## Poster Presentation

EE : Environmental Chemistry  
and  
Renewable Energy

## Dual-analyte fluorescent chemosensor based on carbazole-based oxime for determinations of chlorpyrifos and $\text{Fe}^{3+}$

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A new oxime-functionalized carbazole chemosensor was successfully synthesized and utilized as a dual-analyte sensor for detecting Chlorpyrifos and  $\text{Fe}^{3+}$  in different media and binding mechanisms. The sensor could provide selective and bifunctional determination of Chlorpyrifos in DMSO:PBS Buffer (4:1 v/v, 10 mM, pH 12) and  $\text{Fe}^{3+}$  in acetonitrile without interference from each other and other plausible interferences. In both media, the sensor demonstrated the selective ON–OFF fluorescence quenching at 370 nm and 375 nm toward Chlorpyrifos and  $\text{Fe}^{3+}$ , respectively. The mechanistic studies have unambiguously demonstrated that the sensor can detect Chlorpyrifos via nucleophilic substitution reactions. Unlike this, the sensor can detect  $\text{Fe}^{3+}$  by coordination with oxime moiety. The fluorescent limit of detections for Chlorpyrifos and  $\text{Fe}^{3+}$  are 0.26 ppm and 0.24 ppm, respectively. Importantly, both detection limits of the developed sensor were significantly lower than permitted Chlorpyrifos and  $\text{Fe}^{3+}$  concentrations in food and drinking water as indicated by the U.S. EPA and WHO.

**Keywords:** Fluorescent sensor; Carbazole; Oxime; Chlorpyrifos; Ferric cation

## Fluorescence-based detection by using green-synthesized rutin and quercetin-modified gold nanoparticles

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Rutin-AuNPs(Ru-AuNPs)andQuercetin-AuNPs(Qt-AuNPs)weresynthesizedthrough green methods, exhibiting an average size ranging from 19 to 25 nm and displaying a distinctive absorption peak at 528 nm in an aqueous solution. The fluorescence detection system involved a combination of Ru-AuNPs or Qt-AuNPs and 7-hydroxycoumarin, enabling the rapid and sensitive detection of etimicin. Upon excitation at 340 nm, the emission spectrum of 7-hydroxycoumarin at 458 nm coincided significantly with a substantial portion of the absorption spectrum of Ru-AuNPs at 528 nm. Consequently, Ru-AuNPs more effectively quenched the fluorescence of 7-hydroxycoumarin, than Qt-AuNPs. However, the introduction of etimicin led to a strong interaction with Ru-AuNPs, resulting in the restoration of fluorescence. The presumed mechanism of action involved the acidic and partially negatively charged phenolic hydroxyl groups in Rutin interacting with the amino groups in etimicin. Furthermore, specific sites on the surface of Ru-AuNPs, unoccupied by 7-hydroxycoumarin, facilitated the binding of etimicin. Ru-AuNPs acted as a potent fluorescent quencher, with a quenching percentage of 89.81%. However, etimicin, due to charge attraction, Au-N bond formation, and affinity with sugars, tightly bound to the surface of Ru-AuNPs, displacing 7-hydroxycoumarin. Additionally, one or more of these effects induced the aggregation of Ru-AuNPs, leading to rapid fluorescence recovery. A linear correlation between the fluorescence system and etimicin concentration was successfully established, with detection limits as low as 0.12  $\mu$ M. The developed system was effectively applied to the detection of etimicin in real samples.

**Keywords:** Rutin; AuNPs; Quercetin; Fluorescence sensor



## Study of the content of particulate matter in office and working unit of Muban Chombueng Rajabhat University

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The purpose of this study is to measure the particulate content and size in the offices or working units of Muban Chombueng Rajabhat University (MCRU), Rachaburi. The particulate matter measurements were taken from February to March 2023, during which there was a high PM<sub>2.5</sub> content, resulting in different levels of each particle. The Aerocet 381 is an automatic particle measuring device that measures 5 types of particulate matter: TSP, PM<sub>10</sub>, PM<sub>4</sub>, PM<sub>2.5</sub>, and PM<sub>1</sub>. The working units were divided into educational units, including the office of the Dean and the office of the director of the demonstration school, as well as supporting working units that were further divided into 1) stand-alone buildings and 2) office buildings with boundaries. The device was installed and collected particles during working hours (8 hours) for each working unit. The results show that PM<sub>2.5</sub> levels exceeded the Thai Air Quality standard (TQAS) in 10 working units, particularly in stand-alone buildings with windy areas or without buffer trees against the wind. Additionally, 3 working units had PM<sub>10</sub> levels that exceeded the TQAS. It is also worth noting that some working units had abnormally high levels of PM<sub>1</sub>, although the standard for PM<sub>1</sub> does not currently regulate its content in air quality. This study highlights the importance of identifying areas for prevention and control of particulate matter problems in the office to reduce health risks for employees.

**Keywords:** PM<sub>2.5</sub>; PM<sub>1</sub>; Particulate; Office; Working unit

## Synthesis of zeolite A from sugarcane bagasse ash and its application as a potential catalyst for amine solvent regeneration in CO<sub>2</sub> capture

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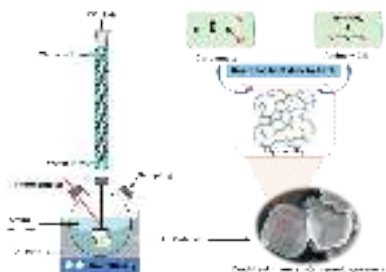
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Amine-based CO<sub>2</sub> capture is a promising option for suppressing CO<sub>2</sub> emissions from thermal power plants. However, the regeneration of a CO<sub>2</sub>-loaded amine stripper process requires a large energy consumption. To overcome this limitation, zeolite catalysts have been applied in amine regeneration process to decrease the energy requirement. In this work, a zeolite A catalyst was synthesized from an agricultural-waste sugarcane bagasse ash as a low-cost silicon source by a hydrothermal method. The process of amine regeneration were investigated in order to decrease heat duty. The NH<sub>3</sub>-TPD result showed that the synthesized zeolite A possessed a high acidity. The catalyst performance in amine regeneration at a low temperature of 86 °C showed that the synthesized zeolite A significantly improved the CO<sub>2</sub> desorption performance and reduced the heat duty by approximately 50 % compared to the noncatalytic system. These results indicated that the low-cost zeolite A derived from agricultural waste showed an excellent promising material to be applied in a desorption column for energy-efficient amine-based CO<sub>2</sub> capture.

**Keywords:** Zeolite A; Sugarcane bagasse ash; CO<sub>2</sub> capture; Amine regeneration; Hydrothermal

### Amine regeneration



## Synthesis of zeolite A from sugarcane bagasse ash and its application for adsorbent for removal of crystal violet dye

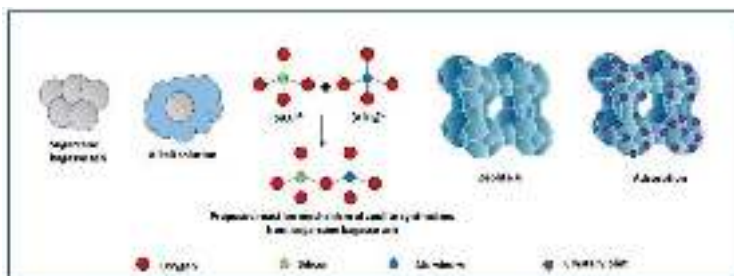
Jirawan Komuangmu<sup>1</sup>, Wassana Soila<sup>1</sup>, Patlada Boonsing<sup>1</sup>, Daranee Sukchit<sup>1</sup>,  
Saisamorn Lumlong<sup>1</sup>, Malee Prajuabsuk<sup>1</sup>, Jitlada Deshativong<sup>1</sup>, Prajakkit Rawee<sup>1</sup>,  
Pharit Kamsri<sup>2</sup>, Sasijuta Wattanarach<sup>3</sup>, Pajaree Thavorniti<sup>3</sup>, Bunjerd Jongsomjit<sup>4</sup> and  
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This research aims to utilize sugarcane bagasse ash from sugar mills for synthesis of zeolite A, as an adsorbent for crystal violet dye removal applications. The parameters for synthesis of zeolite A were evaluated, including ash:NaOH ratios ranging from 1:1 to 1:2, alkali fusion temperature varying from 500 to 650 °C, hydrothermal times ranging from 12 to 24 hours and hydrothermal temperatures varying from 80 to 110 °C. The optimum conditions for ash:NaOH ratios, alkali fusion temperature, hydrothermal times and hydrothermal temperatures were provided as following, 1:1.2, 500 °C, 12 hours and 90 °C, respectively. The synthesized zeolite A was characterized by X-ray fluorescence (XRF), X-ray diffraction (XRD), and Scanning Electron Microscope (SEM). The optimal parameters for the adsorption of crystal violet dye from aqueous solutions, including adsorbent dosage, contact time, adsorption kinetics, and adsorption isotherm were investigated. The results showed adsorption efficiency of 96% for crystal violet dye at a concentration of 100.0 mg/L. Based on the obtained results, the synthesized zeolite A from sugarcane bagasse ash could be successfully used as a highly effective adsorbent for treatment of crystal violet dye in wastewater because of its low cost and environmentally friendly.

**Keywords:** Zeolite A; Sugarcane bagasse ash; Adsorption; Crystal violet dye



## Synthesis of zeolite from industrial-waste coal fly ash for amine solution regeneration in CO<sub>2</sub> capture

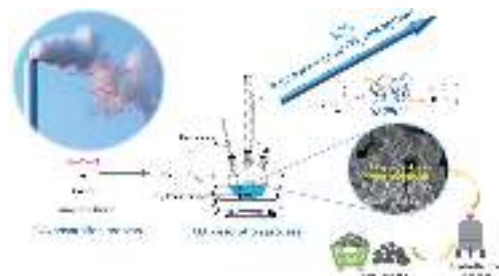
Natthawan Prasongthum<sup>1</sup>, Kritsakorn Janna<sup>2</sup>, Banluesak Butphan<sup>1</sup>, Darunee Sukchit<sup>3</sup>, Amornrat Suemanotham<sup>1</sup>, Lalita Attanatho<sup>1</sup>, Pornpan Pungpo<sup>3</sup> and Yoothana Thanmongkhon<sup>1\*</sup>

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Post-combustion CO<sub>2</sub> capture using amine solution has a great potential to reduce anthropogenic CO<sub>2</sub> emissions, but this process has the disadvantage of consuming a lot of energy for CO<sub>2</sub> stripping during solvent regeneration. To overcome this limitation, adding a solid acid catalyst such as zeolite to amine regeneration process has been investigated to decrease the energy requirement. However, the development of abundant and cost-effective materials is essential. In this work, the zeolite catalyst was synthesized by the hydrothermal method using an industrial-waste coal fly ash as a raw material and investigated its catalytic performance in the process of amine regeneration at a temperature of 100 °C. The experimental results showed that the prepared catalyst showed highly effective in amine regeneration process and could significantly improve the CO<sub>2</sub> desorption performance. Catalyst characterization results showed that the prepared catalyst possessed a high acidity, which can increase the CO<sub>2</sub> desorption rate to ultimately reduce the amount of heat required for amine regeneration by approximately 30%. The use of zeolite in the amine regeneration process improved the desorption performance by 2 times in comparison with the blank run. Results manifested that the low-cost zeolite catalyst showed high potential to be used in a stripper column for energy-efficient CO<sub>2</sub> capture processes.

**Keywords:** CO<sub>2</sub> capture; Amine regeneration; Catalyst; Zeolite



**Figure 1.** Schematic diagram of amine solution regeneration in CO<sub>2</sub> capture



## A prepared bio-sorbent from corn husk for the removal of crystal violet dye from aqueous solution

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In this work, the potential and efficiency of usage corn husks, obtained as an agricultural waste by-product from harvesting, as an affordable bio-sorbent for the removal of crystal violet (CV), a cationic dye used in dyeing of cotton, wood, and silk, from aqueous solution has been studied. The pre-treated bio-sorbents were prepared under the presence of three different concentration of sulfuric acid (98%, 75% and 50% by weight) and compared with untreated bio-sorbents as a reference. To investigate the surface morphology and potential interaction between the bio-sorbent and CV dye, the bio-sorbents were characterized by SEM and FT-IR spectroscopy techniques. The effects of contact time, initial dye concentration (10-50 mg L<sup>-1</sup>) and bio-sorbent dosage (0.10-0.30 g) on dye sorption tests were systemically carried out to determine the optimal conditions by batch experiments. The result showed that as the contact time and initial dye concentration increased, the adsorption capacity also increased, whereas an increasing in adsorbent dosage resulted to a decrease in adsorption capacity. The adsorption process could be well fitted by the pseudo second-order kinetic model with R<sup>2</sup> value of 0.999, reaching the equilibrium at 120 min, and the calculated activation energy was 46.45 kJ mol<sup>-1</sup>. The isotherm of the adsorption equilibrium data was found to be best followed by the Langmuir model. This research indicated that corn husk waste is an effective, low-cost, eco-friendly biological adsorbent, presenting a new sustainable alternative for crystal violet removal in industrial wastewater treatment.

**Keywords:** Corn husk; Bio-sorbent; Adsorption; Crystal violet

## Microplastic contamination in selected carbonated drinks in Thailand

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Microplastics (MPs) contamination in human food is an emerging issue. Recent studies have indicated that MPs have been found in various human tissues and organs, including the placenta, lungs, liver, and blood. This highlights the importance of investigating the presence and quantity of MPs in human food. This study investigates the number and characteristics of MP contamination in commercially available soft drinks in Thailand. Three soft drink brands namely S, F and C in Thailand with different packing types including plastic bottles, aluminum cans and glass bottles were investigated in this study. Soft drinks were purchased from a supermarket in Pathum Thani, with the consideration that each brand of soft drinks was from the same batch of production. The soft drinks were then filtered through cellulose nitrate (0.45  $\mu\text{m}$ ) membrane filters. For each brand, the filters were separated into two groups for analysis using fluorescent microscopy and Micro-FTIR analysis. Preliminary results indicated that all investigated soft drink brands, irrespective of packaging material, were contaminated with MPs, with MP concentrations varying from  $47 \pm 2$  to  $211 \pm 11$  particles per liter. Fragments were predominant, accounting for 90-98% of all samples. PE and PET were mainly found in the three studied soft drink brands. The presence of MPs in soft drinks raises concerns about potential impacts on human health due to their direct consumption.

**Keywords:** Microplastics; Carbonated soft drink; Human consumption; Contamination; Fluorescence microscopy; Packaging.



## Removal of chloride ions from wastewater through Friedel's salt chemical precipitation method

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Numerous industries, such as pickling, and water washing treatment for bottom ash, generate wastewater with elevated chloride ion levels. Discharging this wastewater into the environment can lead to various problems, including pipeline corrosion, soil salinization, harmful effects on plant growth and aquatic life. Consequently, there is a critical demand for the development of cost-effective technologies to effectively remove or control chloride ions before their discharge. This study aims to remove chloride ions from wastewater by chemical precipitation as Friedel's salt ( $\text{Ca}_2\text{Al}(\text{OH})_2\text{Cl}\cdot\text{H}_2\text{O}$ ). Calcium oxide (CaO) and aluminum hydroxide (Al) were employed as precipitating agents to react with chloride ions in wastewater, forming insoluble Friedel's salt and effectively eliminating chloride ions. A series of experiments with varying molar ratio of Ca:Al:Cl, reaction temperature, and reaction time were conducted to compare chloride removal efficiency to determine the optimal parameters. During the experiment process, sodium chloride (NaCl) at a concentration of 2600g/L was used as synthetic wastewater sample. Titration with as an indicator was performed to determine the sample's removal efficiency. Preliminary results indicated that increasing the Ca to Al ratio led to an improved removal efficiency of chloride. The highest chloride ion removal efficiency was achieved at a Ca:Al:Cl ratio of 2:2:1 at room temperature and time at 0.5 and 1.5 hr, reaching 40%. Study results showed no significant difference in removal observed when increasing the temperature of the reaction.

**Keywords:** Chloride ions; Friedel's salt; Wastewater; Precipitating reagents; Temperature; Molar ratio

## Decolorization and detoxification of Solvent Red 24 by *Bacillus* sp. FN1 producing laccase and lignin peroxidase

Peraya Buapho and Sinthuwat Ritthitham\*

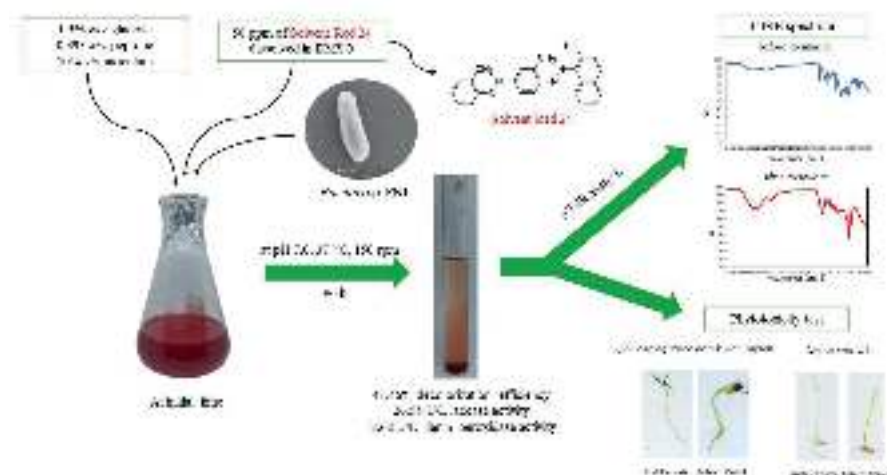
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*Bacillus* sp. FN1 isolated from textile effluent could decolorize the Solvent Red 24, a water-insoluble solvent dye obtained from drying processing of textile industry. In this study, the bacterium was cultivated at 37 °C under shaking condition in the medium containing 1.5% (w/v) glucose, 0.3% (w/v) peptone, and 50 ppm of dye. The decolorization efficiency of 41.46% was achieved at 96 h with the maximum laccase and lignin peroxidase activities of 26.55 U/L and 8.68 U/L; respectively. The FTIR spectrum of the Solvent Red 24 after biological treatment showed that the azo bonds and the aromatic rings were degraded. The biodegraded products metabolized by *Bacillus* sp. FN1 did not adversely affect the growth of *Ipomoea aquatica* Forsk and *Oryza sativa* L.

**Keywords:** Solvent Red 24; Decolorization; *Bacillus* sp. FN1; Laccase; Lignin peroxidase



## A demonstration process of high quality biomass pellet produced from sugarcane wastes

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Natthawan Prasongthum<sup>1</sup>, Amornrat Suemanotham<sup>1</sup>, Yoothana Thanmongkhon<sup>1</sup>,  
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This research aims to develop the production of high-quality biomass pellets derived from sugarcane leaves, employing an innovative torrefaction process. The investigation progresses through two sections. The first centers on the conversion of sugarcane leaves and scraps into biomass pellets through palletization techniques, with a comparative analysis between binder-infused and binder-free raw materials. The sugarcane leaves are crushed to achieve the requisite size and prepared to maintain moisture content of 15-30%wt. This feed is well-suited for the pelletization, resulting in a remarkable yield of 93-98%wt, while its properties consistently meet established standards. Notably, incorporating tapioca flour as a binder at a 3.5%wt ratio, along with approximately 30%wt moisture content prior to pelletization, yields biomass pellets of superior quality in terms of bulk density and pellet durability. For the second, the study investigates into the production of high-quality biomass pellets by utilizing the sugarcane leaf-based pellets as feedstock. The torrefaction process is explored using a reactor with 5-kg batch type capacity. The reactor, heated by LPG burners, is maintained a reaction temperature of around 260°C, for producing torrefied pellet. The product derived from both scraps and sugarcane leaves attains a yield of 70%wt, approximately. This study significantly contributes to the valorization of sugarcane leaf waste, presenting a sustainable solution for alleviating PM 2.5 emissions from the burning of sugarcane fields. Moreover, it could be served as an exemplar of a circular economy, inspiring farmers and sugar industries to turn agricultural residues into green resources for substitution on coal or fossil fuels.

**Keywords:** Sugarcane; Biomass; Torrefaction; Circular economy; PM 2.5

## A demonstration process of high quality biomass pellet produced from sugarcane wastes

Pathompat Khowattana<sup>1</sup>, Tosporn Phetyim<sup>2</sup>, Apichat Junsod<sup>1</sup>, Pathumrat Butniam<sup>1</sup>,  
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**Keywords:** Sugarcane; Biomass; Torrefaction; Circular economy; PM 2.5

## A machine learning approach to gasification process model for environmental sustainability

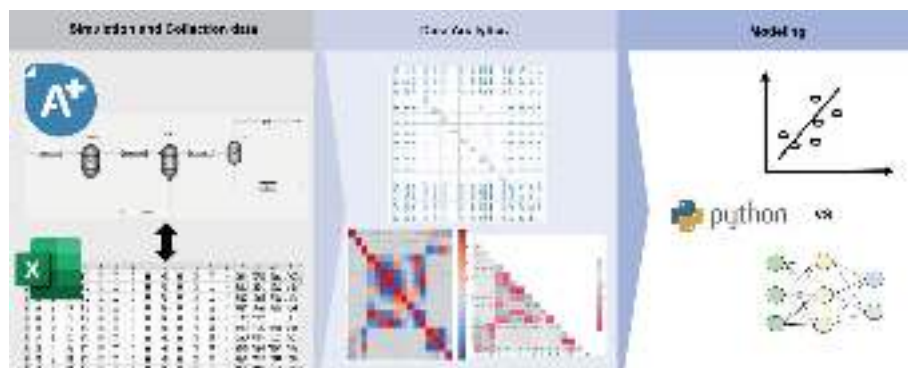
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Concerns over greenhouse gas emissions from fossil fuel usage have led to increased attention towards renewable and sustainable sources. Biomass/waste residues are regarded as viable resources for creating biofuels to replace petroleum-based goods in the transportation industry. Gasification is considered the most cost-effective and efficient method for biomass conversion to multiple energy/fuel vectors. However, there is a lack of accuracy and reliable simulation results in designing and optimizing the process. This study investigated the synergistic effect of operating conditions in biomass gasification using Aspen Plus software. Results showed that ER ratio and temperature are key parameters affecting the quality of syngas from biomass gasification. To measure the accuracy of the simulations, two machine learning models, multiple linear regression (MLR) and Artificial Neural Networks (ANN), were utilized. ANN showed a high accuracy of over 0.95 compared to MLR, as process behavior does not have a linear relationship, and ANN can learn by adjusting weight until the predicted value is close to the real target. Therefore, the simulation in this study would be a promising design tool to predict the syngas composition under the various operating conditions of an existing gasifier or a new gasifier. The model can be used in the scaling up of the process to reduce engineering costs and process development time from laboratory to pilot/industrial scales.

**Keywords:** Greenhouse gas emission; Gasification; Biomass; Artificial neural networks; Multiple linear regression



## Effect of fuel type on the characteristics and photocatalytic activity of ZnO nanoparticles synthesized via solution combustion method

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This research investigates the influence of organic fuels, including urea, citric acid, and agar, on the synthesis and photocatalytic performance of zinc oxide (ZnO) nanoparticles through the solution combustion method. Various analytical techniques, including X-ray diffraction (XRD), N<sub>2</sub> adsorption-desorption isotherms, scanning electron microscopy (SEM), UV-VIS diffuse reflectance spectroscopy (DRS), and photoluminescence spectroscopy (PL), were employed to characterize the synthesized ZnO nanoparticles. The photocatalytic activity of the synthesized nanoparticles was evaluated by degrading methyl orange under ultraviolet irradiation at ambient temperature. The results revealed that single-phase and well-crystalline ZnO nanoparticles with a wurtzite structure were formed regardless of fuel type. The ZnO nanopowders prepared with agar as a fuel had a foamy microstructure with the highest specific surface area of 8.58 m<sup>2</sup>/g compared to the others. The highest photodegradation of methyl orange under ultraviolet irradiation was also achieved by the ZnO powders prepared with agar due to their good crystallinity and higher specific surface area.

**Keywords:** Photodegradation; Organic fuels; Photocatalytic performance; ZnO nanoparticles; Solution combustion



## Purification of Biomethanol synthesized from biogas by three stages distillation

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Crude biomethanol obtained by varied ratio of CH<sub>4</sub> and CO<sub>2</sub> in range of 30/70, 50/50, 70/30 was methanol purity 95.98, 96.50 and 96.95 percent, contaminants (ppm) of water 50,500, 48,150 and 44,870, ethanol 2,000, 1,882 and 1,676, acetone 260, 183 and 120 and isopropanol 115, 103 and 80 respectively. The water in commercial requirement is lower 1,000 ppm. Biomethanol contained in ppm unit of water 58,919, ethanol 1,098, acetone 100 and isopropanol 635 was a representative for the purification study. A 2-meter height by 7.5 cm. of diameter of sieve column was tested in five steps that showed the decreasing of amount of water (ppm) from 58,919 to 12,403, 7,200, 4,300, 2,700 and 2,600. The water impurities were dropped 5 times at the first step, and slightly decreasing then stable at the last step. The number of steps would not solve for removing water contaminated. A 2-meter packed column filled with glass cylindrical Raschig ring was compared with 3- meter and 2-meter sieve columns by feeding methanol contaminated with 12,403 ppm of water, the result showed water (ppm) and reduction (%) 1,496 (12.06%), 5,600 (45.15 %) and 7,200 (58.05%). The packed column worked the best in low water contaminant. As a result, the three stages distillation combined column with the 2-meter (1<sup>st</sup>) and the 3-meter (2<sup>nd</sup>) sieve and the 2-meter packed column was studied by feeding the representative biomethanol and the reduction of contaminants (ppm) of water, ethanol, acetone and isopropanol 476 (58,919), 43(1,098), 30 (100) and 0 (635) respectively.

**Keywords:** Biomethanol; Commercial methanol; Purification; Packed column; Sieve distillation

## Flotation of surfactant-modified dispersive clay for the simultaneous removal of methyl orange and methylene blue from water

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A flotation method of surfactant-modified dispersive clay was developed for the rapid and simultaneous removal of a wide range of synthetic dyes from water. The dispersive clay was prepared by the soaking treatment of a layered clay mineral, montmorillonite, in NaF solution. Results of X-ray diffraction and surface area measurements indicated that the dispersive clay was free of layer-to-layer stacking and had a large surface area ( $263.4 \pm 0.8 \text{ m}^2/\text{g}$ ) comparable to the original montmorillonite ( $276.5 \pm 1.2 \text{ m}^2/\text{g}$ ). The dispersive clay was hardly separated from water because of its high dispersibility but it was readily collected at the water surface by adding the appropriate amount of a cationic surfactant, cetyltrimethylammonium chloride (CTAC), followed by feeding air bubbles to conduct flotation.

Fig. 1 shows time dependence on the removal of an acidic dye, methyl orange (MO), and a basic dye, methylene blue (MB). In water, both of dyes rapidly adsorbed on CTAC-modified dispersive clay and removal reached more than 90% within 10 mins.

Fig. 2 shows the effect of CTAC added on removing MB and MO. In the absence of CTAC, the removal rate was very low. However, the removal of MB increased with increasing the amount of CTAC added and then decreased when the amount of CTAC touched 0.5 mg. On the other hand, the removal rate of MO increased with increasing CTAC.

The optimal conditions were used for the simultaneous removal of different acidic dyes and basic dyes in water.

**Keywords:** Dispersive clay; Surfactant; Flotation; Wastewater treatment; Dyes

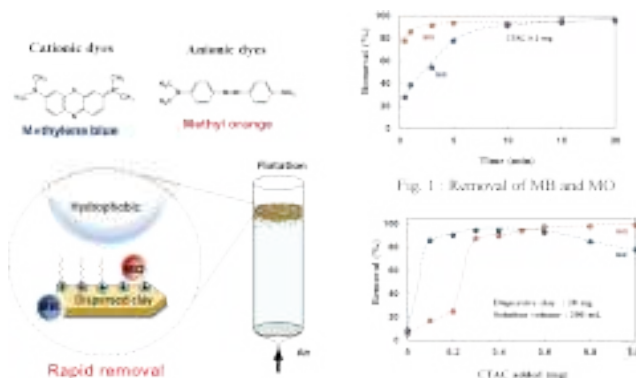


Fig. 2 Effect of the amount of CTAC on the removal of MB and MO



## High performance photodegradation of methyl orange with AgCl/Ag-impregnated glutaraldehyde-crosslinked alginate beads under sunlight irradiation

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In this paper, an AgCl/Ag photocatalyst was synthesized by a simple precipitation method, followed by impregnation with glutaraldehyde-crosslinked alginate to form beads (AGAB). The synthesized catalysts were characterized by XRD, FTIR and SEM-EDX. Their adsorption and photocatalytic activities were also investigated by the photodegradation of a methyl orange (MO) solution under sunlight irradiation. The results showed that AGAB exhibited excellent performance for the degradation of MO (99.4%) in 20 min, with activity higher than AgCl/Ag. It was shown that glutaraldehyde-crosslinked alginate could improve the photocatalytic activity by enabling more rapid and increased adsorption of MO. As a result, the photodegradation of AGAB increased. The kinetic analysis of AgCl/Ag and AGAB could be fitted with a first-order kinetic model. Moreover, The AGAB can maintain full photodegradation activity for at least four cycles. Consequently, AGAB is a promising material for the photocatalytic of dyes and similar organic contaminants in environmental pollution cleanup.

**Keywords:** AgCl/Ag; AGAB; Photodegradation; Glutaraldehyde-crosslinked alginate; Methyl orange

## Activated carbon derived from hemp core biowaste with a doped heteroatoms and large specific surface area for supercapacitor applications

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Energy consumption is growing exponentially these days, prompting the need for the development of energy storage systems. In this work, the synthesis of N, S-dual-doped activated carbon from hemp cores was developed for high-performance supercapacitors. Conversion of hemp core biomass into N, S-dual-doped activated carbon using thiourea as the nitrogen and sulfur sources via hydrothermal and activation processes was generated. Various thiourea ratios (wt%) were studied in both hydrothermal and activation methods. It was found that the N, S-dual-doped activated carbon exhibited a high surface area of  $2529 \text{ m}^2 \text{ g}^{-1}$ , which was 1.6 times higher than that of undoped activated carbon ( $1547 \text{ m}^2 \text{ g}^{-1}$ ). The electrochemical properties were then examined using cyclic voltammetry at a scan rate of  $30 \text{ mV s}^{-1}$  using a voltage region of  $-0.8$  to  $0.2 \text{ V}$ . The N, S-dual-doped activated carbon at 5%wt thiourea in both two-step processes exhibited outstanding electrochemical performance, which provided a specific capacitance as high as  $242 \text{ F g}^{-1}$  and high energy density of  $33.6 \text{ Wh kg}^{-1}$  and power density of  $3621.5 \text{ W kg}^{-1}$ . The evaluation of the electrochemical performance indicates that activated carbon generated from hemp cores could potentially be used as a promising electrode material in an electrochemical energy storage supercapacitor. The less expensive and more widely available hemp core materials, the simple chemical activation process, and high performance of the resulting carbon material indicate that it is achievable for commercial usage in supercapacitors.

**Keywords:** Supercapacitors; N, S-dual-doped activated carbon; Hemp cores biomass



## Development of pouch-cell Zn-ion battery using $\text{MnO}_2$ synthesized from spent alkaline battery as cathode material

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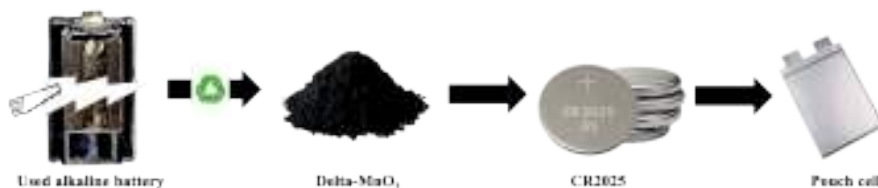
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Nowadays, the rising alkaline battery consumption results in a significant accumulation of spent battery waste which ends up in landfills. Therefore, this work focuses on the Mn recovery from the spent electrode of alkaline battery to form  $\delta\text{-MnO}_2$  as a final recycled product. The first step was the leaching process of spent electrode powder using 2 M sulfuric acid with the addition of 12 % (v/v) hydrogen peroxide as a reducing agent. The leaching solution was then mixed with potassium permanganate as precursors and produce  $\delta\text{-MnO}_2$  by the hydrothermal process at 160°C for 24 h. The recycled  $\delta\text{-MnO}_2$  was subsequently used as an active cathode material in the CR2025 and pouch-cell of Zn-ion battery (ZIB), which consisted of Zn foil as anode, filter paper as a separator and two types of electrolytes: 2M zinc sulfate solution and 0.25 M zinc triflate in dimethyl sulfoxide (DMSO). The CR2025 ZIBs using the recycled  $\delta\text{-MnO}_2$  cathode exhibited the high initial discharge capacities of 606.12 and 395.55 mAh/g at the current density of 0.05 A/g, while pouch-cell ZIBs exhibited the highest specific capacity at 303.23 and 231.11 mAh/g at the current density of 0.2 A/g using the above electrolytes, respectively. The result thus suggests ZIBs using zinc sulfate electrolyte show higher specific capacity but lower stability than zinc triflate in DMSO electrolyte.

**Keywords:** Zinc-ion batteries (ZIBs) ,  $\delta\text{-MnO}_2$  , ZIBs pouch-cell



**Figure 1.** Delta- $\text{MnO}_2$  from spent alkaline batteries upscale scheme.

## Preparation of composite polymer electrolytes based on poly (ethylene oxide) and cellulose nanofiber for solid-state zinc-ion batteries

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Recently, solid-state zinc-ion batteries (SSZIBs) based on polymer electrolytes have attracted increasing attention due to the fact that they would be able to overcome the challenges of aqueous zinc-ion batteries, e.g. Zn dendrite penetration and metallic Zn corrosion. The benefits of the polymer-based SSZIBs center on mechanical flexibility and acceptable ionic conductivity. Herein, composite solid polymer electrolytes (SPEs) are developed by incorporating polyethylene oxide (PEO) and zinc trifluoromethanesulfonate ( $\text{Zn}(\text{OTf})_2$ ) into a cellulose nanofiber (CNF) matrix derived from biological sources, acting as reinforcing phase. The PEO/ $\text{Zn}(\text{OTf})_2$ /CNF composite with a 10 wt% CNF filling gave a high mechanical strength as evidenced by the Young's modulus of 601.39 MPa and the tensile strength of 36.22 MPa, which could be attributed to the continuous nanofiber network and the unique strong morphological structure of CNF. Furthermore, the organic additive consisting of 0.5 M  $\text{Zn}(\text{OTf})_2$  salt and fume silica was introduced onto the PEO/ $\text{Zn}(\text{OTf})_2$ /10%CNF electrolyte to enhance the ionic conductivity of  $2.12 \times 10^{-4} \text{ S} \cdot \text{cm}^{-1}$ . After assembly of the symmetrical Zn/Zn cells using the composite polymer electrolyte, the constant-current cycling was performed and the resulting performance indicated that no short-circuiting was present as well as the zinc anode was favorable, ensuring sustained long-term stability (over 400 h) at a current density of  $0.5 \text{ mA} \cdot \text{cm}^{-1}$ . As for the full-cell testing:  $\text{Zn} | \text{PEO}/\text{Zn}(\text{OTf})_2/10\%\text{CNF} | \delta\text{-MnO}_2$ , it was achievable for a high reversible capacity of  $142 \text{ mAh} \cdot \text{g}^{-1}$  at a current density of  $10 \text{ mA} \cdot \text{g}^{-1}$  and a high coulombic efficiency of 97% after 50 cycles.

**Keywords:** Solid-state zinc-ion batteries; Composite solid polymer electrolytes; Cellulose nanofiber; Polyethylene oxide



## Fabrication of $\text{Sr}_2\text{Fe}_{0.9}\text{Ni}_{0.1}\text{MoO}_6$ anode supported solid oxide fuel cell by powder injection molding

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Solid oxide fuel cell (SOFC) is a well-known alternative power generator that can transform chemicals into electricity with high efficiency and no pollution. Materials used for electrode and electrolyte are mainly perovskite oxides or related structures.  $\text{Sr}_2\text{FeMoO}_6$  (SFMO) double perovskite structure has recently been proposed as a promising anode due to its excellent performance at low operating temperatures (600-800 °C). Apart from that, electrode design and cell fabrication are also very important for SOFC performance. In this study, we present the fabrication process and the effects of anode fabrication parameters, e.g. feedstock composition on moldability, sintering temperature on microstructure and porosity, of  $\text{Sr}_2\text{Fe}_{0.9}\text{Ni}_{0.1}\text{MoO}_6$  ( $\text{SFNi}_{0.1}\text{M}$ ) phase.  $\text{SFNi}_{0.1}\text{M}$  is prepared by a solid-state reaction and fabricated into anode-supported cell by powder injection molding (PIM) application using environmentally friendly chemicals and no pre-sintering requirement. The mixture of polyethylene glycol (PEG) and polyvinyl butyral (PVB) is used as a binder for feedstock preparation and the feedstock ratio between the  $\text{SFNi}_{0.1}\text{M}$  powder and binder are 45:55, 50:50, and 55:45 vol%. The sintering temperatures are 1250 °C and 1300 °C. The results show that optimal condition for PIM of anode support, of which the adequate strength and porosity achieved ensure gas transport on a fuel side, is the volume ratio of  $\text{SFNi}_{0.1}\text{M}$  powder to binder at 45:55, and the sintering temperature of 1250 °C. The obtained anode support cell already shows the potential PIM fabrication method for future upscale and cost-effective SOFC production.

**Keywords:** Solid oxide fuel cell; Powder injection molding; Anode support cell

## Applying supercapacitors in emergency lights to extend their useful life

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At the present, batteries are widely used and have been applied in a variety of applications, such as in cars that run on electric power instead of gasoline. However, batteries can only be used for a short period of time, cannot be used for a long time, and cannot supply power continuously for a long period of time. So we have developed supercapacitors for emergency light. The aim of this research was to compare brightness, charging time, and backup time between emergency lights that use batteries and supercapacitors. The results showed that the emergency lights that use battery backup had a backup time of about 120 minutes, but the emergency lights that use supercapacitor backup had a backup time of about 360 minutes. The brightness of emergency lights that use batteries is 50 lm; by the way, the ones that use supercapacitors are 48–60 lm. Emergency lights that use super capacitors take less time to charge but have backup time and more brightness than battery-powered emergency lights. Therefore, a supercapacitor in an emergency light is better than a battery. This work shows a promising application of supercapacitors for, but not limited to, emergency lights.

**Keywords:** Supercapacitor; Battery; Emergency light



## Preparation of bio-renewable corn starch-based electrolyte for a high performance, environmentally friendly supercapacitor

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In this work, a bio-renewable supercapacitor was fabricated using corn starch as natural host polymer for gel electrolyte with the addition of  $\text{H}_3\text{PO}_4$  as ion sources. To improve the capacitive behavior of the supercapacitor, hydroquinone (HQ), an organic redox additive, was also applied for enhancing the Faradaic reaction. The corn starch electrolyte was then assembled with the corn leaf-derived activated carbon as electrode materials for fabricating the supercapacitor. The electrochemical analysis revealed that the  $\text{H}_3\text{PO}_4$ -corn starch gel electrolyte with the presence of 0.0165 M HQ solution exhibited the highest specific capacitance of  $401 \text{ F g}^{-1}$  at a scan rate of  $10 \text{ mV s}^{-1}$  with a good cyclic stability of 90% after 10,000 charge-discharge cycles. The fabricated supercapacitors also demonstrated high capacitance retention under various environmental temperatures, indicating excellent thermal stability over a broad range of temperatures. This work not only suggested an efficient method to enhance the electrochemical performance of the natural-based polymer electrolyte for upcoming quasi-solid-state supercapacitors, but it also demonstrated a possible approach to employ sustainable, natural materials for energy storage applications.

**Keywords:** corn starch; gel electrolyte; hydroquinone; supercapacitor

## Biodiesel production via the electrocatalytic process from Pinari oil (*Sterculia foetida* L.)

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The conventional transesterification reaction of Pinari seed oil (*Sterculia foetida*) with methanol using natural fiber heterogeneous catalyst via electrocatalytic reactor was investigated. However, the cost is one of the main obstacles in commercializing in this process. Due to the multifaceted adversities of many of the catalysts, there is active consideration for an electrolysis process that does not require elevated temperature. In addition, an electrolysis by used heterogeneous catalyst is carried out the presence or absence of a catalyst or co-solvent. In this research, a various parameter such as electrolysis voltage, stirring rate, electrode type, water content, co-solvent, reaction temperature, molar ratio of oil to methanol and concentration of electrolyte. The chemical structure of biodiesel products was analyzed by nuclear magnetic resonance spectroscopy (NMR) and Fourier transform infrared Spectrometry (FTIR) techniques. The result showed our heterogeneous catalyst from natural fiber could be used as electrolysis transesterification catalyst to give a fatty acid methyl ester (FAMES) from Pinari and several seed oil in good yields.

**Keywords:** Biodiesel; Transesterification; Pinari oil; Electrolysis process; Heterogeneous catalyst

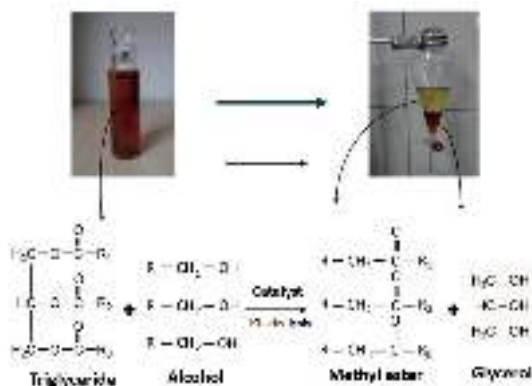


Figure 1 Transesterification process



## Simulating cyclic voltammetry at porous electrodes considering Faradaic and non-Faradaic currents

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Cyclic voltammetry (CV) is a commonly employed electroanalytical technique for characterizing the impact of electrode modification in electrochemical energy devices. Previous methods aimed to describe CV responses using models that relied on pore-scale data and assumed geometrical structures. In this study, we have developed a simpler and more efficient approach to model CV responses in porous electrodes by incorporating the Bruggeman correlation to account for the effects of porosity and tortuosity. Additionally, our developed model has been integrated with an equivalent circuit to simulate non-Faradaic currents using a constant phase element (CPE). The model's validity has been confirmed through comparisons with previous studies that assumed different geometrical structures, showing a reasonable level of agreement. Consequently, this developed model can be employed to simulate CV responses in porous electrodes without the need for detailed pore-scale information or assumed geometrical structures. Furthermore, we conducted a thorough investigation into the effects of various system parameters, including active surface area, reaction rate constant, porosity, Bruggeman exponent, and electrode thickness, to gain insights into how these parameters influence CV curves. This alternative approach to using CV responses for characterizing porous electrodes offers valuable opportunities for researchers to enhance their understanding of how to interpret CV curves in the context of porous electrode applications.

**Keywords:** Cyclic voltammetry; Porous electrodes; Bruggeman correlation; Non-Faradaic currents

## Topography optimized anode catalyst layer of polymer electrolyte membrane water electrolyzers under effects of gas coverage

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Currently, hydrogen serves as a globally recognized form of energy storage, providing benefits in the decentralization of energy resources and long-term storage. Recently, there has been a growing focus on green hydrogen, which is derived from renewable energy sources. One standout approach for the production of green hydrogen is the Polymer Exchange Membrane Water Electrolyzer (PEMWE). It exhibits remarkable performance due to its low operating temperature, rapid response to load changes, and compact design. However, a significant drawback of this technology is its cost-effectiveness, primarily because it relies on the use of iridium, a precious element, to fabricate the catalyst layer. The substantial use of this expensive material contributes to the high cost of the device. To address this cost issue, a numerical approach known as Topography Optimization (TO) has been applied. TO is employed to maximize the performance and systematically manipulate the distribution of material within the anode catalyst layer. This optimization method takes into consideration the effect of gas coverage generated by the electrochemical reactions on the active surface area. Comparing the results of the TO electrode with those of a uniform electrode, it is observed that the TO electrode performs less effectively in the low-voltage range (1.23-1.83V). However, in the high-voltage range (2.03-3.23V), the TO electrode demonstrates a remarkable performance enhancement, achieving a 3.5-fold increase compared to the homogeneous electrode. The current density achieved with this optimized structure offers significant economic advantages for this application.

**Keywords:** Topology optimization; PEMWE; Green hydrogen; Gas coverage; Catalyst layer

## Effect of the hydroxyl groups in passivating molecules on the electronic quality of TiO<sub>2</sub> films

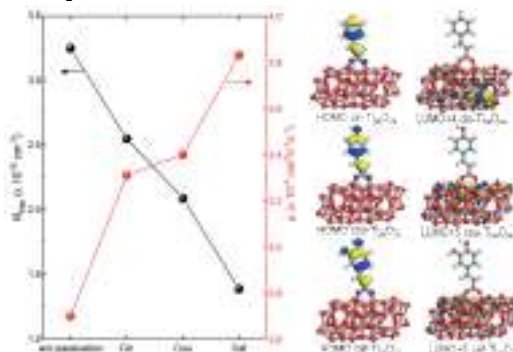
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Due to their superior optical and electronic properties, TiO<sub>2</sub> films are widely used as the electron transport materials in hybrid halide perovskite solar cells (PSCs). However, the existence of ionic defects, which act as trap states for charge carriers in TiO<sub>2</sub> films severely impacts the charge separation at the TiO<sub>2</sub>/perovskite interfaces. Therefore, in this work, we improve the electronic quality of the TiO<sub>2</sub> films by passivating their defects via a chemical treatment process. The films are chemically modified with small passivating molecules containing the carboxylate (-COO<sup>-</sup>) anchoring group, which include cinnamic acid (Cin), coumaric acid (Cou), and caffeic acid (Caf), exhibiting different numbers of the hydroxyl (-OH) groups in their structures. The trap density ( $N_{\text{trap}}$ ) and charge mobility ( $\mu$ ) of the devices fabricated from the modified TiO<sub>2</sub> and perovskite films are evaluated using a space-charge limited current (SCLC) method. The SCLC results reveal that the  $N_{\text{trap}}$  at the TiO<sub>2</sub>/perovskite interfaces is sensitively dependent on the numbers of the -OH groups in the passivating molecules. When the -OH content increases, the  $N_{\text{trap}}$  and  $\mu$  decreases and increases, respectively. Hence, the Caf-modified TiO<sub>2</sub> shows the best electronic quality. Moreover, as shown by density functional theory (DFT) calculations, the electron transfer occurs in the direction from the passivating molecules to the Ti<sub>38</sub>O<sub>76</sub> cluster (a model of TiO<sub>2</sub>), suggesting the appropriate energy level alignment of the passivating molecules anchored on the TiO<sub>2</sub> surface. This work demonstrates an effective approach for improving the electronic quality of TiO<sub>2</sub> films, which is beneficial for optoelectronic applications.

**Keywords:** Modified TiO<sub>2</sub>; Perovskite; defect; Charge carrier; Thin film



## Improved hydrogen electrolysis in sodium hydroxide solution by stainless steel electrodes optimization

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Optimum resistance by gas bubbles, size and type of stainless electrodes in Alkali Hydrogen Electrolysis (AHE) is important to minimize the power consumption per hydrogen produced. The resistance of gas bubbles was studied by installing Anodes (A) and Cathodes (C) in equally numbers and represented by AxC with 4x4, 8x8 and 12x12 of Stainless steel (SS) type 304 which dimension is 8 mm. diameter and 14 cm. length operated in 20 % by weight of Sodium hydroxide solution. The hydrogen was increased corresponding with increasing numbers of electrodes 4x4, 8x8 and 12x12 which resulted rate of H<sub>2</sub> (ml./min.) 35.00, 66.22 and 88.33, but the energy consumption (kWh/kg.H<sub>2</sub>) was raised 132.09, 224.21 and 366.50 respectively. It was found that increasing numbers of electrodes per AHE volume raising density of gas bubbles produced and reflected to increasing bubble resistance that effected to electron transferring from anodes to cathodes which caused of much power consumption. The resistance of electrode size was performed by varying diameters 4, 8 and 9.5 mm., the result showed rate of H<sub>2</sub> (ml./min) 39.36, 35.00 and 29.10 which consumed energy (kWh/kg.H<sub>2</sub>) 107.37, 132.09 and 141.48. The smallest diameter of electrodes showed the lowest resistance and reflected to the least energy consumption. The last is the resistance of metal by comparing stainless steel type 4 mm. of 4X4 SS316 with SS304 electrodes. The SS316 generated lower 4.48 % in energy consumption (kWh/kg.H<sub>2</sub>) of 102.56 (107.37 for SS304) as a result it was describing that SS316 was lower resistance than SS304.

**Keywords:** Alkali electrolysis; Electrode; Hydrogen; Energy consumption; Stainless steel



## ***In vivo* assessment and *in silico* prediction of estrogenic potency of endocrine disrupting chemicals using zebrafish (*Danio rerio*)**

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Estrogenic endocrine-disrupting chemicals (E-EDCs) are a group of natural or synthetic hormonally active xenobiotic compounds that can mimic endogenous hormones, altering endocrine functions, and consequently causing some adverse health effects. The present study aimed to evaluate the estrogenic potency of a wide array of E-EDCs via *in vivo* and *in silico* approaches using zebrafish. Zebrafish embryos were exposed to E-EDCs to investigate the effect on the estrogen-responsive *CYP19A1b* gene expression. Tested chemicals include bisphenol A and its analogs (BPs), equine estrogens (EEs), and zearalenone and its metabolites (ZENs), as well as 17 $\beta$ -estradiol (E2). We also performed *in silico* screening of estrogenic potency by constructing 3D homology models of ligand binding domains (LBDs) for three zebrafish ER (zfER) subtypes and subsequently simulating interactions between each of E-EDCs and zfER subtype LBDs. Exposure of embryos to E-EDCs resulted in the induction of *CYP19A1b* expression in a concentration-dependent manner by many tested chemicals. Based on the half maximal effective concentration (EC<sub>50</sub>), the estrogenic potencies were basically ranked as EEs (0.8-79 nM) > ZENs (24-163 nM) > BPs (290-35,000 nM). *In silico* docking simulations revealed that three amino acids (e.g., Glu321, Leu355, and His492 in zfER $\alpha$  LBD) were important for hydrogen bonding with those E-EDCs. The interaction energy of E-EDCs to each of zfER subtypes showed positive correlations with EC<sub>50</sub> for *in vivo* *CYP19A1b* induction by those compounds. The *in silico* simulations of interactions between ligands and zfER subtypes may help predict *in vivo* estrogenic potencies of untested chemicals.

**Keywords:** Endocrine disrupting chemicals; Estrogen receptors; Docking simulation; *CYP19A1b*; Zebrafish

# Food, Agriculture and Cosmetics (FA)

## Oral Presentation



## Development of coffee silver skin into food beverage and testing antioxidant activity

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Coffee silver skin (CS) is an outer layer of coffee beans. The conversion of CS into a higher-value product offers a promising approach to managing waste because of its rich antioxidant contents. Cinnamon powder (CP) is abundant in antioxidants but does not contribute to a pleasant aroma, whereas Bael powder possesses a sweet scent. This study aims to optimize the combination of CS with Bael powder (BP), Cinnamon powder and assess their antioxidant capacity using brewing (100ml of water) and tea bag using (100ml, 100°C, 3mins). Combination ranging from 100%, 75%, 50%, 25% of CS were studied. The results of the sensory evaluation shows that the most favorable ratio was 25% CS with 75% BP, yielding a total phenolic content (TPC) of 43.85 mg GAE/100 mL and antioxidants of 14.39 mgAAE/100mL for brewing, while 41.45 mg GAE/100 mL with antioxidant at 10.82 mgAAE/100mL for tea bags. For CS and CP combination, the highest sensory scores is optimal with ratio of 75% CS and 25% CP for brewing and 50% CS and 50% CP for tea bags. This resulting in TPC of 17.81 mg GAE/100 mL with antioxidants of 19.39 mgAAE/100ml for brewing, and a TPC of 16.82mgGAE/100mL with antioxidants of 17.60 mgAAE/100 mL for teabag. The study highlights that blending CS with BP or CP at specific ratios produces antioxidant-rich beverages with maintained sensory acceptability. A combination of CS below 50% shows promise for developing a sustainable beverage for waste management.

**Keywords:** Antioxidants; Beverage; Bael powder; Cinamon powder; Coffee silver skin.

## Characteristics of pomelo cellulopectin and its application in plant-based chicken nugget

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Agricultural waste is usually disposed of in landfill, but it can be a potential source of functional food ingredients. In this work, cellulopectin that is originated from pomelo albedo and a by-product from the pectin extraction process (pectin is a main product) is of our research interest. Its characteristics and rheological properties were studied. The results showed that cellulopectin contained soluble ( $23.06 \pm 1.68\%$ ) and insoluble ( $69.69 \pm 7.02\%$ ) dietary fibers which are mainly attributed to natural cellulose containing the remained pectin, respectively. In addition, its water and oil holding capacities were  $5.26 \pm 0.04$  g water/g sample and  $1.33 \pm 0.01$  g oil/g sample, respectively. The viscoelasticity of cellulopectin samples at varying concentration between 4 – 10% w/w revealed weak-gel characteristic with the storage modulus,  $G'$ , increasing with the concentration following the power-law relationship. Furthermore, all cellulopectin gels exhibited a shear thinning behavior that can be described by a power law model. Based on these results, cellulopectin gels at concentrations between 6 – 10% w/w were applied to plant-based chicken nuggets as a texture modifier. The texture properties of nuggets were evaluated using texture profile analysis (TPA) compared with commercial plant-based chicken nuggets. The results showed that hardness, cohesion, gumminess and chewiness increased with increasing cellulopectin concentrations. In addition, the measured TPA results were within the range of the commercial nuggets. Overall, the study highlights the potential use of cellulopectin from pomelo albedo as a binding and texturizing agent for plant-based chicken nuggets.

**Keywords:** Cellulopectin; Pomelo albedo; Characteristics; Rheology properties; Plant-based chicken nugget

## The application of coffee silver skin extract in pomegranate juice and study for its bioactivities

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Coffee silver skin (CS) is the main by-product of coffee roasting production. It consists of various valuable chemical compositions; therefore, it is highly interesting to valorize and study for its bioactivity and potential application. For further application, it is much easier to use the extracted product, so the CS was extracted by a subcritical water extraction process and freeze-dried to obtain the coffee silver skin crude extract powder (CSE). This study aimed to combine CSE with pomegranate juice and quantify the bioactive compounds in the juice. The Pomegranate juice was made from pomegranate powder and pomegranate syrup. The total phenolic content (TPC), antioxidant activity (AA), total caffeoquinic acid (T-CQA), caffeine, anti-hyaluronidase, and anti-glucosidase were studied to confirm the beneficial bioactivities of the combined juice. It was found that the CSE-permanganate juice contained TPC=439.20 mg GAE/100 mL, AA=62.22 (mg TE/100 mL), T-CQA=12.63 (mg/100 mL), and caffeine=30.49 (mg/100 mL). The percent inhibition of hyaluronidase was 52.73%, and the percent inhibition of glucosidase was 58.15%. These results indicate that coffee silver skin dried crude extract adds more benefits to the permanganate juice. Therefore, coffee silver skin Extract (CSE) is a valuable industrial ingredient source of antioxidative materials.

**Keywords:** Coffee silver skin extract; Pomegranate juice; Bioactivities; Anti-hyaluronidase; Anti-glucosidase

## Construction and application of digital platform for predicting metabolism and toxicity of pesticides

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Pesticides are chemical agents used to control pests and regulate plant growth, which play an important role in agricultural production. The effects of pesticides were not only caused by themselves, but also possibly by their metabolites. Of course, metabolites may also have adverse effects on the environment and human health. In recent years, people have realized the close relationship between the environment and human health, and the importance of protecting the environment. Therefore, effects of pesticide metabolites were focused. The identification of metabolites and their toxicity assessment are time-consuming and labor-intensive. In order to improve work efficiency, digital technology will be one of the objects worth paying attention to.

Digital platform is a “Digital Complex” composed of a series of digital technologies such as big data, artificial intelligence and the Internet. The digital platform of pesticide metabolism and toxicity prediction can be used to retrieve information about metabolites, metabolic pathway, to predict toxicity of metabolites. The digital platform can provide technical support and data for metabolite detection, assessment of environmental pollution possibility, and formulation of rational pesticide use program.

Herein, metabolism database and the prediction system as well as relevant application examples will be introduced.

**Keywords:** Pesticide; Digital platform; Prediction of metabolism; Prediction of toxicity

## The effect of ion exchange of clinoptilolite as a soil on the physiological response of radish

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The colonization of planets other than the Earth is not simple and there are many obstacles to overcome. One of the major issues is the food availability. There is continuously increasing interest in “soil-based” space agriculture. Spectral analysis suggested that components of the martian regolith are more likely zeolites, and clinoptilolite is considered one of the most widespread zeolites on Mars.

The aim of the work is to investigate the effect of particle size and ion exchange of clinoptilolite on growth, development, and physiological and biochemical characteristics of radish. The following scenarios were used: clinoptilolite with granulous size 0.9-2.5 mm and 2.5-5.0 mm and modified clinoptilolite with ammonium and potassium ions. Our findings contribute to the development of formulations that meet specific chemical, biological and agronomic requirements.

The germinability was investigated in three consecutive plantings. It was higher for  $C_{NH_4}$ -2.5 compared to C-2.5 and  $C_K$ -2.5 during the first run. It is interesting to note that the weakest germination showed seeds on  $C_K$ -2.5. Dramatic reduction in seed germination was established only in  $C_{NH_4}$ -5.0, while the germination was similar  $C_{NH_4}$ -2.5 during the second and third run.  $C_K$ -2.5 had positive effect on seed germination with the timing of the experiment, being higher during the third run. The small clinoptilolite fraction was more favorable for root crop production compared to bigger one, reaching the maximal values in  $C_K$ -2.5 plants during the first run. Dry samples preventively powdered in liquid nitrogen were used to determine the total proteins, carbohydrates and polyphenol content.

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**Keywords:** Soil; Natural zeolites; Clinoptilolite; Ion exchange; Physiological response

## Extracting bioactive protein from fish head using enzymatic hydrolysis

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The fish heads, which are leftover scraps from the fish processing industry, can be converted into high-value-added products, such as fish protein hydrolysates containing bioactive peptides. The objective of this study is to investigate the effects of enzymatic hydrolysis times and enzyme concentrations with alcalase on the extraction yield, protein content, and antioxidant properties of fish protein hydrolysates. The findings indicated that elevating the enzyme concentration and extending the hydrolysis time led to improvements in both protein extraction yield and antioxidant activities. Fish head protein hydrolysate has shown good nutritional value with high protein content, and all samples exhibited antioxidant activity. Considering the biological activities, these fish head protein hydrolysates are potential natural additives for functional foods.

**Keywords:** Hydrolysate protein; Fish head scraps; Enzymatic digestion



**Figure1.** hydrolysate protein from fish head scarps

# Food, Agriculture and Cosmetics (FA)

## Poster Presentation



## Effect of solutions on retrogradation of cooked sticky rice

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To increase the shelf life and keep texture of Khao Tom Mud (cooked sticky rice mixed with coconut milk), the effect of solutions on retrogradation of cooked sticky rice was studied. The sticky rice was soaked in sodium chloride (6 %w/v) and glycerol (1% v/v) solutions compared with filtered water for 8 hours at a room temperature. The ratio of sticky rice and soaking solutions was 1:10. The cooked sticky rice was mixed with the coconut milk, packed with banana leaves and vacuum plastic bags. All samples were stored in the refrigerator at 4 °C for 7, 21 and 28 days. The percentage of retaining water content was studied. The chemical structure of sticky rice was studied by Fourier transform infrared spectroscopy (FTIR). The hardness was studied by texture analyzer technique. The result showed that the highest rate of water content percentage was found for sticky rice soaked in sodium chloride solution. The chemical structure of all samples, observed from FTIR spectra, was similar and no significant changes in amylose and amylopectin structure. The short-range order of amylose and amylopectin, examined from the ratio of absorbance at 1047 and 1022 cm<sup>-1</sup>, indicated that the retrogradation was started at storage time for 7 days and the lowest retrogradation rate was found for sticky rice soaked in sodium chloride solution. The lowest rate of retrogradation from the hardness property was found for sticky rice soaked in sodium chloride and highest for that soaked in glycerol solutions. Sodium chloride solution can delay the rate of retrogradation.

**Keywords:** Retrogradation; Sticky rice; Khao Tom Mud; Amylose; Amylopectin

## Antioxidant activity of spent coffee ground and its extracts

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Spent coffee ground (SCG) is a by-product from coffee brewing process. SCG contains a considerable amount of organic compounds and is a great source of antioxidants. The objectives of this work were to evaluate the antioxidant activity of SCG and SCG extracts by different solvents ethanol (60 - 90% w/w) and hexane, as well as to determine oxidative stability by peroxide value, conjugated diene value, iodine value and acid value. The results showed that total phenolic content (TPC) of SCG was 16.49 mg GAE/g. The 2, 2-diphenyl-1-picrylhydrazyl (DPPH) radical scavenging activity and ferric reducing antioxidant power (FRAP) were 32.57  $\mu\text{mol TE/g}$  and 140.9  $\mu\text{mol Fe(II)/g}$ , respectively. For SCG extracts, 60% w/w ethanol extract contained the highest TPC and the strongest DPPH radical scavenging activity. The 80% ethanol extract had the highest FRAP value and the lowest conjugated diene value. The 90% ethanol extract had the lowest peroxide value and hexane extract has the lowest acid value. This study shows that the 60%w/w ethanol extract had the strongest antioxidant activity. Therefore, spent coffee ground can be considered as an antioxidant source for use in food products.

**Keywords:** Spent coffee ground; Antioxidant; Phenolic Compound; Extraction



## Fractionation of maltooligosaccharides from partial digested Hommali, Homnil and Sangyod rice starchs

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In this study, narrow ranges of maltooligosaccharides (MOS) were prepared without using MOS forming amylase. Three rice starchs were prepared from Hommali, Homnil and Sangyod rices and were partially digested with a heatstable  $\alpha$ -amylase (KLEISTASE T) at 90 °C, 3 hour. Maltopolysaccharides, degree of polymerisation (DP) >10, and undigested starchs were removed by precipitation in 76% ethanol. The liquid phase which contained maltooligosaccharides (DP 3-10) were further fractionated by column chromatography using microcrystalline cellulose (MC) as stationary phase and step-gradient aqueous-ethanol (90%, 85%, 80%, 75% and 70% ethanol) as mobile phase. Maltooligosaccharide components of each elution fractions were analysed by thin layer chromatography. The fractionation patterns from three rice starchs were similar. By using 3.2 g rice starch as starting material, typical yield (solid content) for 90% ethanol fraction (glucose, maltose, maltotriose) was 68-75 mg, 85% ethanol fraction (maltotriose, maltotetraose) was 35-51 mg, 80% ethanol fraction (maltotetraose, maltopentaose) was 24-31 mg, 75% ethanol fraction (maltopentaose, maltohexaose) was 19-33 mg and 70% ethanol fraction (maltohexaose, maltoheptaose) was 16-24 mg. The information in this preliminary study will be used for upscale preparation of higher specific maltooligosaccharides.

**Keywords:** Hommali rice starch; Homnil rice starch; Sangyod rice starch; maltooligosaccharides; Microcrystalline cellulose (MC) chromatography

## Pesticide residues in chilies collected from chili farms in southern Thailand

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The major chili production areas in southern Thailand are found in Songkhla, Phatthalung and Nakhon Si Thammarat provinces. In these areas, pesticides are applied to chili plants to control pests such as chili thrips and cotton bollworm, and viral or bacterial diseases such as anthracnose disease, powdery mildew, and leaf roll. Information on pesticide contamination of chilies from these provinces is limited. Therefore, this study will focus on the determination of pesticide residues in chilies (*Capsicum annuum* L.) collected from farms in Ranot district of Songkhla province (32 samples), Lampam district of Phatthalung province (18 samples), and Hau Sai district of Nakhon Si Thammarat province (20 samples). These sampling sites have been chosen since they are in main chili production areas where 3500-11000 chili plants are planted per area of about 2–5 rai. Some pesticides, e.g. chlorpyrifos, carbaryl, carbofuran, cypermethrin,  $\lambda$ -cyhalothrin and deltamethrin are of interest due to being the pesticide frequently used by farmers in the last 15 years. Chilies were extracted with hexane/acetone (1:1, v/v), and dichloromethane for testing (i) chlorpyrifos, carbaryl, carbofuran and (ii) cypermethrin,  $\lambda$ -cyhalothrin and deltamethrin contaminations, respectively. The extracts were purified using Florisil and C<sub>18</sub> solid phase extraction (SPE). After concentrating the extracts, final residues were analyzed in solution by gas chromatography (GC). Differences in the mean value were analyzed by one-way ANOVA. Most samples were not contaminated with the pesticides of interest. Two samples collected from Hau Sai district contained  $\lambda$ -cyhalothrin concentrations at 4.39 and 3.57  $\mu\text{g/kg}$  which do not exceed the maximum residue limit (MRL) of 10  $\mu\text{g/kg}$  for spices and 300  $\mu\text{g/kg}$  for chilies established by the Commission Regulation (EU) and the Thai Agricultural Standard, respectively.

**Keywords:** Pesticide; Chili; Gas chromatography; Contamination; SPE

## Separation and Partial Purification of Polysaccharides from Mung Bean Meal Using Liquid Extraction and Non-Chromatographic Techniques

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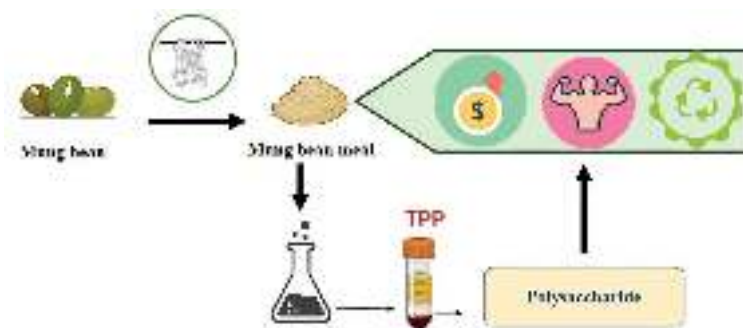
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Mung bean meal is a byproduct of the vermicelli processing industry which remains value of compounds. The exploitation of potential biological functional material is important to improve its valued product. Polysaccharide is one of the attractive polymers which are found in mung bean meal. Thus, the aim of this study was to develop a way to extract and separate polysaccharides from mung bean meal through an alternative approach involving liquid and extraction and enzymatic-assisted three-phase partitioning (TPP) for partial purification. Two distinct polysaccharides were extracted using hot water extraction (HWPE) and alkaline extraction (APE) methods under various conditions. The optimum extraction to obtain crude polysaccharides were found to be at 100°C and duration time 90 min for HWPE while under APE, the polysaccharides were successfully obtained at 2%KOH duration time 180 min. The APE resulted in a lower extraction yield (0.33%) than HWPE (0.56%). The enzymatic-assisted three-phase partitioning (TPP) process (5% amylase and followed by (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> and *t*-butanol) successfully eliminated approximately 85% of impurities, particularly proteins, from both HWPE and APE extracts. Furthermore, the microstructure analysis using SEM revealed a rod-like structure for HWPE and a flake-like structure for APE. Notably, both polysaccharides demonstrated the ability to stimulate nitric oxide (NO) production in macrophage cells (RAW264.7) than those of the non-treated group, indicating their potential in functional food applications. This study represents a significant step for the development of separation of polysaccharides and proteins, paving the way for their utilization in functional food.

**Keywords:** Alkaline extraction; Hot water extraction; Mung bean meal; Polysaccharide; Three phase partitioning



## Sensomic approach characterization of odorants in fried chicken

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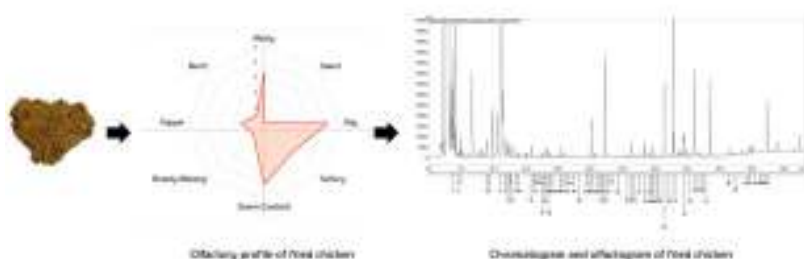
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Herein, we studied odorants in fried chicken (thigh) for quality control in food industry using sensomic approach. In this work, fried chicken was orthonasally evaluated using olfactory profiling to generate odor profiles of fried chicken for process follow-up. Fried chicken was initially extracted by dichloromethane, in which the volatile components were concentrated by solvent associated flavor extraction (SAFE) and fractional distillate. Analysis of volatile components by gas chromatography-olfactometry resulted in identification of odorants mainly responsible for meaty, oily and steam (cooked) perception. Moreover, 65 odorants detected by trained panelists were mainly categorized into pyrazine, hydrocarbon, and thiazole classes. This is the first report using sensomic approach to identify active odorants, through aroma extract dilution analysis (AEDA), in fried chicken.

**Keywords:** Fried chicken; Sensomic approach; Olfactory profiling; Solvent associated flavor extraction (SAFE); Gas chromatography-olfactometry (GC-O);





## Sensory attributes and antioxidant capacity of tomato meal extracts: A comparative analysis of enzymatic and ultrasonic extraction methods

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This research explored the sensory and antioxidant properties of tomato meal extracts by enzymatic and ultrasonic extraction. Based on sensory attributes and antioxidant activity. Tomato meal was treated with bromelain at 0, 5, 10 and 15% (w/w) for 0, 15, 30 and 45 min which compared to ultrasonic extraction at 50 °C for 0, 15, 30 and 45 min. Results showed that 15% of bromelain for 45 min was the optimum condition for enzymatic extraction while 30 min with ultrasonic wave was the optimum condition for ultrasonic extraction. The sensory scores were measured by semi-trained panelists using quantitative descriptive analysis with a 5-point scoring test (0-4). The umami and overall acceptance of tomato meal extract derived from 15% of bromelain for 45 min were higher than tomato meal while ultrasonic extraction played a crucial role in imparting distinct characteristics, demonstrating a significant increase in sourness. In addition, tomato meal extracts from enzymatic extraction exhibited DPPH and ABTS radical scavenging activity with 55.12 and 73.78 mmol TE/100g, respectively. Ultrasonic extraction could enhance DPPH and ABTS radical scavenging activity as well which were 52.04 and 79.26 mmol TE/100g, respectively. The chemical structure of glutamic acid was detected by Fourier Transform Infrared Spectroscopy (FTIR). The observed peak at 1407 cm<sup>-1</sup> and 1622 cm<sup>-1</sup> which was assigned to amino group structure and carboxylic group were detected. The tomato meal extracts exhibited a significant potential as a functional flavor enhancer with different characteristics which could be a viable alternative to synthetic flavor enhancers.

**Keywords:** Ultrasonic extraction; Enzymatic extraction; Umami; Antioxidant; Tomato meal

## Improvement of sensory attribute and antioxidant property of mungbean peptides by Maillard reaction

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At present, plant-based proteins are rising in popularity in food protein consumption. The high protein content of 70% in mungbean meal renders it a compelling protein source for a flavoring agent. This study aimed to improve sensory attributes and antioxidant activity of mungbean peptides. Mungbean peptides were separated based on different molecular weights (P1 = >10 kDa, P2 = 5-10 kDa, P3 = 1-5 kDa, and P4 = <1 kDa) and were reacted with reducing sugar as glucose and ribose under a thermal process (Maillard reaction). The sensory characteristics of all samples were determined by quantitative descriptive analysis (QDA) with 5-point scoring (1-5). Results showed that Maillard reaction products from P4 peptides reacting with ribose (R-P4) contributed to a higher score of sensory perception than its original peptides and all peptides reacting with glucose. The flavor characteristics of R-P4 possessed a high intensity of overall acceptance (3.6), meaty flavor (3.4), sweet flavor (4.2), and umami (3.2). In addition, R-P4 inhibited DPPH and hydroxyl radical scavenging activity with 290  $\mu\text{mol TE/g}$  and 79.80%, respectively. The chemical structure change of Maillard reaction products was explored by Fourier Transform Infrared Spectroscopy (FTIR). The functional group of ribose and amino acid bonding was detected after the reaction. The absorption peak of the amino groups of peptide bound to the carbonyl groups of reducing sugar was found in the observed peak at  $1646\text{ cm}^{-1}$ . Therefore, the Maillard reaction product of mungbean meal peptide might be an alternative to a plant-based flavoring agent.

**Keywords:** Mungbean meal; Peptide; Maillard reaction; Flavor enhancer; Antioxidant



## Immobilization of transglucosidase enzyme via polymer-inorganic hybrid for isomaltooligosaccharide production

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Isomaltooligosaccharides (IMOs) are relatively new functional food as prebiotic ingredients and have been utilized as dietary fibers that can be produced from carbohydrate raw materials by transglucosylation using transglucosidase enzyme (TGE). Normally, using free enzymes in the process of IMOs always denatured enzymes by the high temperature of heating wasted time and could not be reused or recycled enzymes. Thus, immobilized TGE is interesting for IMOs production because of many advantages such as high production efficiency and reusability. This work proposes to use cationic biopolymers hybridization with  $\text{Ca}_3(\text{PO}_4)_2$  nanoparticles (CP-NPs) for immobilization of transglucosidase at concentrations of 10% and 25% w/v that were fabricated by beads gelation of alginate (SA) and chitosan (CS) under salt solution for formatting CP-NPs and adding PEG to improve pore density and hydrophilicity of the immobilized enzyme. All samples were analyzed by scanning electron microscopy (SEM), X-ray diffraction (XRD), Fourier transform infrared (FTIR), DC (detergent compatible) protein assay, and thin layer chromatography (TLC). The results showed that the optimized ratio of SA/CS is 1:2 and the concentration of salts was at 100 mM for completing spherical beads as increase of salts affected on breaking bead surface. Addition of PEG enhanced immobilization efficiency of SA/CS/CP-NPs transglucosidase due to surface roughness and reduction of CP particle sizes. Hydrogen bonds form between PEG and SA and the addition of CS can form polyelectrolytic wall beads which support the reducing the decomposition and improving the stability of the beads. Moreover, the TLC analysis revealed that using 10% TGE-SA/CS/PEG/CP-NPs could produce IMOs better than that of using 25%TGE immobilized beads.

**Keywords:** Enzyme immobilization; Transglucosidase; Polymer-inorganic hybrid; Isomaltooligosaccharide

## Encapsulation of turmeric extracts via complex emulsion-coacervation for active ingredients in dietary supplement foods

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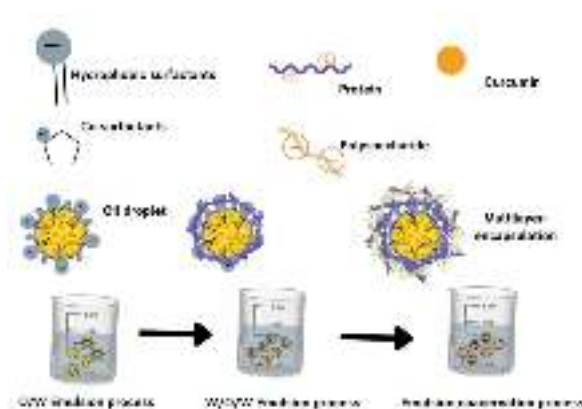
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Turmeric extract (TME) contains more than 95% curcuminoids, which is commonly used in foods, beverages, nutraceuticals, and functional foods. In the food industry, TME is added to dry powder dietary supplements. Tends to be difficult to dissolve in water and has low bioavailability. The objective of this research is to develop a curcumin extract delivery system using emulsion-coacervation that has better permeability than free extract for health food and nutraceuticals. Research has shown that the ternary phase diagram of the emulsion shows the best conditions: 50% for water, 20%-30% for coconut oil. A 1:1 mixture of lecithin and Tween80 was smooth and the droplet size was approximately 399 nm and less than 3  $\mu\text{m}$ . The particles were coacervated with a core emulsion. 70:30/1%wall\_CCO was 50% for water, 30 % for lecithin and Tween80, and 20% for oil. Functional group confirmation samples on coacervate particles coated with TME emulsion revealed that the CH stretching peak, CH stretching peak value, CH stretching value, NH and OH peaks can be concluded that the best formula is 70:30 core/wall\_CCO. This is an optimized TME encapsulation due to the particle size of 378 nm.

**Keywords:** Encapsulation; Emulsion; Complex coacervation; Turmeric extract



**Figure 1.** schematic drawing of encapsulated turmeric extracts by emulsion-coacervation

## Optimized production of isomaltooligosaccharide prebiotics from homnin and sangyod rice flours by enzymatic hydrolysis processes

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Prebiotics are non-digestible and non-absorbable foods that support the growth and/or activity of the beneficial probiotic bacteria in the large intestine, promoting good digestive health. Isomaltooligosaccharides (IMOs) are considered as potential prebiotics and are reported to stimulate the growth of organisms in rats and humans. They can be produced from carbohydrate sources, especially rice flour by enzymatic reactions. Homnin (HN) and Sangyod (SY) rice flours consist of amylose and amylopectin which are suitable for IMOs production. IMOs including 1,6 glycosidic bonds ((DP=2-20) were prepared by enzyme-catalyzed hydrolysis with  $\alpha$ -amylase and  $\beta$ -amylase and transglycosylation by transglucosidase (TGE). The resulting hydrolysate was evaluated by DNS method, thin layer chromatography (TLC), and nuclear magnetic resonance (NMR). For liquefaction (L) of HN and SY, the optimized condition should have maltodextrin at 12 dextrose equivalents (DE) for suitable maltose syrup production obtained from the conditions of 1%w/w  $\alpha$ -amylase (activity 200,000 U/g and activated pH 6.5, 95 °C) of 30%w/v HN for 20 min and 0.3%w/w  $\alpha$ -amylase of 10%w/v SY for 20 min. Sample L was optimized maltose syrup by  $\beta$ -amylase saccharification (S) which is 1.5% w/w  $\beta$ -amylase (activity 40,000 U/ml and activated pH 5.5, 55 °C) of HN and 0.1%w/w  $\beta$ -amylase of SY for 10 min because of high maltose. Finally, sample S was added 0.1%v/v TGE (activity 300,000 U/ml activated pH 5.5, 55 °C) into high and low maltose syrup for comparing transglycosylation ability of TGE confirmed by TLC and NMR having 1,4 glycosidic links (found in maltose and panose) and 1,6 glycosidic links on IMOs presented in NMR peaks at 5.4 and 5.0 ppm, respectively. This work focuses on the qualitative identification of IMOs molecules with a long chain containing more 1,6 glycosidic links than 1,4 glycosidic links. Thus, it can be concluded that the best IMOs optimization for IMOs syrup was 0.1%v/v TGE\_HN\_high maltose for 1 h showing the high peak of 1,6 glycosidic links.

**Keywords:** Isomaltooligosaccharide; Transglycosylation; Enzymatic Hydrolysis; Homnin rice; Sangyod rice

## Evaluation of total phenolic contents and *in-vitro* antioxidant activity of hemp (*Cannabis sativa L.*) leaves extracts for its application in cosmetic product

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Hemp (*Cannabis sativa L.*) contains cannabidiol (CBD) with lower amount of  $\Delta^9$ -tetrahydrocannabinol compared to cannabis. It also contains terpenoid, flavonoids, and other. These phytochemical compounds have therapeutic effects. Hemp has been utilized for various purposes, including ingredients in cosmetics formulations. Hemp leaves are the main waste of industrial hemp plantation. This study aimed to produce ethanolic extract from hemp leaves using a plant to solvent ratio of 1:10. Ethanolic extract of hemp leaves was investigated and evaluated for its *in-vitro* biological activity focusing on antioxidant activity using 1,1-diphenyl-2-picrylhydrazyl (DPPH) radical-scavenging capacity and hydrogen peroxide ( $H_2O_2$ ) scavenging method. In addition, total phenolic content expressed as total flavonoids content (TFC) and total tannin content (TTC) of the extracts were studied. The total flavonoids and total tannin amounts were analyzed by Folin-Ciocalteu's assay and aluminum chloride colorimetry, respectively. The result showed that hemp extract showed antioxidant activity with the  $IC_{50}$  value in DPPH scavenging assay at  $0.31 \pm 0.05$  mg/mL, while Trolox (standard) showed at  $IC_{50}$   $0.003 \pm 0.21$  mg/mL. The  $H_2O_2$  scavenging method showed the hemp extracts  $IC_{50}$  value at  $0.258 \pm 0.034$  mg/mL while ascorbic acid (standard) showed  $0.131 \pm 0.006$  mg/mL. Flavonoids and tannin content were found at  $129.90 \pm 14.73$  mg quercetin equivalent/g and  $65.12 \pm 9.89$  mg tannic acid equivalent/g extract, respectively. Phenolic compounds influence antioxidant activity that can minimize damages of skin cells from oxidative stress. All these results suggested that ethanolic hemp leaves extract can be used as active ingredients in skin care products and as an alternative source of antioxidant compounds in the cosmetics industry.

**Keywords:** Hemp leaves extracts; *Cannabis sativa L.*; Antioxidant activity; Total phenolic content; Cosmetic product

## Evaluate the green tea quality through post-fermentation utilizing *Eurotium cristatum*, MFUTB001

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Green tea is known for its rich content of polyphenols such as catechin and gallic acid. Epigallocatechin-3-gallate (EGCG) is the most common group of catechin found in green tea and is associated with numerous health benefits. However, EGCG is considered to increase the bitterness and astringency of green tea. *Eurotium cristatum* is commonly used in Fuzhuan brick tea and plays a significant role in the post-fermentation process of dark tea. Thus, this study aims to improve the flavor and aroma of green tea from Chiang Rai, Thailand, through post-fermentation of green tea with *E. cristatum*. The *E. cristatum*, MFUTB001 was isolated from a briquette of Fuzhuan brick tea. The species identification was done based on morphological and molecular phylogenetic analysis. Green tea was packed into a brick shape with a density of 0.3 g/cm<sup>3</sup> using a compression molding technique before being sprayed with a spore suspension of *E. cristatum*, MFUTB001. The quality of tea was evaluated after two weeks of incubation at 28 °C. Catechin and gallic acid content slightly decreased from 3.825±0.135 and 11.578±0.171 mg/g in non-treated (control) to 3.023±0.289 and 10.879±0.82 mg/g in *E. cristatum*, MFUTB001 treatment. Moreover, the principal component analysis revealed a significant difference in overall organic and volatile compounds between the two treatments. The sensory test also confirmed that *E. cristatum*, MFUTB001 had a beneficial effect on the quality of green tea as less bitterness and strong honey test notes were present in tea that post-fermented with this fungus strain.

**Keywords:** Quality of tea; *Eurotium. cristatum*; Fuzhuan brick tea; Fermentation; Polyphenols



## Evaluation of the chemical contents of avocado oil extracted with coconut oils for cosmetic application

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Avocados are one of the most essential commercial tropical fruits with many varieties. It is a good source of unsaturated fatty acids, which are monounsaturated and long-chain saturated fatty acid. Moreover, avocado contains high contents of vitamin E, carotenoids, and several antioxidants. Coconut oil is a natural oil that is edible and used in many skin care products. This research aims to evaluate the avocado oil extracted with coconut oil for the cosmetic application. The dried avocado pulp was macerated in coconut oil in 1:1, 1:2, and 1:3 ratios for 3-7 days. The chemical contents, oil properties, and antioxidant capacity of the obtained avocado oil were evaluated. The avocado oils were subjected to fatty acid methyl esters (FAMES) derivatization before the GC-MS analysis. 6-octadecenoic acid, methyl ester (omega-6), and 9-octadecenoic acid, methyl ester (omega-9), were among the fatty acids found in the avocado oil. The avocado oil prepared with the pulp to coconut oil with a ratio of 1:2 for 3 days showed the highest chemical contents. Its acid values, saponification values, and peroxide values were  $0.77 \pm 0.02$ ,  $145.30 \pm 5.89$ , and  $10.56 \pm 0.95$  mg/g respectively. Moreover, percentage inhibition in the DPPH scavenging assay of extract at 100  $\mu\text{g/mL}$  was  $43.52 \pm 0.96$ , Trolox as a standard showed  $\text{IC}_{50}$  at  $0.003 \pm 0.21$  mg/mL. These results suggest that avocado oil from the dried avocado pulp extracted with coconut oil has good antioxidation properties similar to the previous reported avocado seed oil ( $\text{IC}_{50}$  on ABTS assay is 62.99  $\mu\text{g/mL}$ ) and potential for cosmetic use.

**Keywords:** Avocado oil; Coconut oil; Unsaturated fatty acids; Antioxidant; Cosmetics



## Development and optimization of spray-dried kaffir lime peel essential oil microparticles using emulsion stabilized by modified Cassava Starch

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Thailand is recognized as the world leader in cassava production and there has been a campaign to encourage the use of cassava in a range of industries in order to increase the value of cassava starch. Consequently, in this work, cassava starch was modified and stabilized with kaffir lime peel essential oil through pickering emulsification for use in personal care products. Modified cassava starch, as a pickering emulsion stabilizer, was developed by using 1.58 M sulfuric acid and hydrophobic modification, which was altered by chemical and physical methods. Octenyl succinic anhydride was employed in the chemical process, while tetrafluoroethane and helium gas were used in the physical process (cold plasma process). To archive the dried powder, the emulsion was dried by a spray dryer with an inlet temperature of 160 °C, a sample flow rate of 9 ml/min, and an air flow rate of 600 L/h. The hydrophobic properties and encapsulation efficiencies were analyzed by contact angle measurements and GC-FID. The results demonstrated that the essential oil was successfully encapsulated in the emulsion stabilized with the chemical technique, which has  $3.71 \pm 0.78\%$  encapsulation efficiency. However, the modified casava starch using the physical technique effectively eliminated bacteria (*Epidermidis* ATCC 14990) and fungus (*Candida albicans* ATCC 10231). Though both procedures still cause skin irritation. Therefore, more research is required to establish the dose that may be applied without affecting consumer safety.

**Keywords:** Cassava starch; Kaffir lime peel essential oil; Cold plasma; Spray dryer; Emulsion

## Method validation of QuEChERS-GC- $\mu$ ECD method for pyrethroid pesticides analysis in mango

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Method validation for the analysis of pyrethroid pesticides in mango using GC- $\mu$ ECD is essential for laboratories to ensure accurate and reliable test results. Laboratories are required to validate parameters and criteria in accordance with SANTE/11312/2021, including linearity of analytical curves, instrument and method limits of detection and quantification, accuracy, and precision. The QuEChERS method (Quick, Easy, Cheap, Effective, Rugged, and Safe) was used to extract pyrethroid pesticides. The Calibration curves for the pesticides were linear in the range of 10–180  $\mu\text{g/kg}$ , with correlation coefficients exceeding 0.995. The limits of detection (LOD) and quantification (LOQ) were 5  $\mu\text{g/kg}$  and 10  $\mu\text{g/kg}$ , respectively. Recovery and precision were evaluated by spiking blank mango samples with 10, 50, and 100  $\mu\text{g/kg}$  of each pesticide, with five replicates at each concentration level plus a blank sample. The average recovery rates obtained for each pesticide ranged from 74.55% to 113.17%, with relative standard deviations ranging from 2.77% to 13.55% for all evaluated concentrations. This demonstrates the excellent repeatability of the method. Overall, the method validation results demonstrate that the GC- $\mu$ ECD method can be used to analyze pyrethroid pesticides remaining in mango.

**Keywords:** Method validation; QuEChERS; Mango; Pyrethroid; GC- $\mu$ ECD

## Exploration approach to differentiate Khao Dawk Mali 105 rice located in the northern and northeastern region of Thailand based on Rb, Sr, Mo, Mg, P, K analyzed by ICP-MS.

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High value of Thai Hom Mali rice in the global trade caused a potential problem of adulteration by suppliers mislabeling or adding inferior rice to make more profit. To reduce this risk, indication of geographical origin on rice packaging has been initiated. In this study, identification of authentic geographical origin of rice has been investigated using its compositional elements which were transferred from soil in which the rice is grown. To map the composition database of Khao Dawk Mali 105, samples of rice cultivated in the northern and northeastern regions of Thailand (164 samples) were collected. Six elemental data (Rb, Sr, Mo, Mg, P, K) were measured using inductively coupled plasma mass spectrometry (ICP-MS). Analyse-it program was used for statistical analyses. The strongest correlation was found in Mg-P (0.868) and the most negative correlation was K-Rb (-0.394). Elements with the highest uniqueness were Sr and K, with uniqueness values of 0.901 and 0.348, respectively. Scatter plots among elemental compositions at 90% density matrix revealed both negative and positive correlation patterns. The 2D correlation monoplots, which shows the relationships of the six variables, accounts for 64.0% variance. The most positive correlation coefficient was P-Mg with 0.745 and the most negative one was Rb-K with -0.394. The three most unique variables that could be used to discriminate the dataset based on geographical sources were Sr Mo, and Rb with uniqueness 0.996, 0.935 and 0.817, respectively. This model showed a possible approach to discriminate rice cultivated in the north and northeast region with p-values of elemental pairs Rb-Mo, Mg-P, Mg-K, and P-K being less than 0.0001 at 5% significance level.

**Keywords:** Khao Dawk Mali 105; Thai Hom Mali rice; Elemental composition; PCA; ICP-MS



**Figure 1.** Scatter plot and monoplots of elemental composition of K P Mg Rb Sr and Mo

## Unveiling MUS-7: A promising domain antibody for combating *Klebsiella pneumoniae* infections

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In response to the increasing prevalence of multidrug-resistant *Klebsiella pneumoniae*, a promising alternative strategy for combating bacterial infections is the use of antibody fragments. In this study, domain antibodies targeting mid-log phase *Klebsiella pneumoniae* were selected from a phage library through three rounds of successful bio-panning. Among the 11 positive clones identified by colony PCR, five exhibited the highest binding capacity to *Klebsiella pneumoniae* compared to control antibodies. MUS-7, in particular, showed great promise in terms of binding ability and bactericidal activity. Kill curve analysis demonstrated that MUS-7 could slightly delay the growth of *Klebsiella pneumoniae* under agitation conditions. Furthermore, to gain insights into its inhibitory mechanism, we performed protein target identification. Using far-western blotting, we found that MUS-7 interacted with a ~90 kDa protein. Subsequent analysis through mass spectrometry identified BamA as a potential target of MUS-7. BamA is a key player in multiple essential cellular functions, including nutrient uptake, protein secretion, and adhesion. This discovery highlights the potential of MUS-7 as a domain antibody for therapeutic antibody development, particularly in the context of combating *K. pneumoniae* infections. As multidrug resistance continues to pose a significant threat, novel approaches like MUS-7 become a promising molecule to combat bacterial infection.

**Keywords:** Domain antibody; *K. pneumoniae*; Phage display; ELISA; MUS-7

## Analysis of manganese, cobalt, copper and arsenic in unpolished rice (*Oryza sativa* L.) using inductively coupled plasma mass spectrometry (ICP-MS)

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Rice (*Oryza sativa* L.) is one of the economic crops of Thailand and is considered a staple food for Thai people. This study aimed to investigate the determination of some heavy metals (Mn, Co, Cu and As) in unpolished rice using inductively coupled plasma mass spectrometry (ICP-MS) with on-line internal standard method. The rice samples were digested in 4 mL of  $\text{HNO}_3$  and 0.5 mL of  $\text{H}_2\text{O}_2$  using microwave digestion at 1200 W for 30 min. The digested samples were adjusted to 25 mL with DI water and then filtered by 0.45  $\mu\text{m}$  before ICP-MS analysis. The method was validated using certified reference material, SRM 1568b rice flour. The percent recoveries of Mn, Co, Cu and As were  $97.6 \pm 4.3$ ,  $88.3 \pm 2.9$ ,  $91.0 \pm 3.9$  and  $82.2 \pm 4.9$ , respectively. The linearity ranges of Mn, Co, Cu, and As were 0.05-50, 0.0025-0.25, 0.25-50, and 0.025-0.5  $\mu\text{g L}^{-1}$ , respectively. The coefficient of determination was greater than 0.999. Limits of detection (LODs) and limits of quantitation (LOQs) were in the ranges of 0.055-7.656 and 0.062-8.101  $\mu\text{g kg}^{-1}$ , respectively. The concentrations of Mn, Co, Cu and As in unpolished rice samples were obtained in the ranges of 33.412-40.799, 0.021-0.027, 1.166-1.663 and 0.256-0.324  $\text{mg kg}^{-1}$ , respectively. As concentration in some rice samples were higher than the maximum level (ML). Results indicate that this proposed method could be used in the laboratory for the routine determination of these 4 heavy metals in rice with acceptable analytical performance.

**Keywords:** Heavy metals; Unpolished rice; Microwave digestion; ICP-MS

## Determination of heavy metals in honey using inductively coupled plasma mass spectrometry (ICP-MS)

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Arsenic (As), Cadmium (Cd), and Lead (Pb) contents in Thai honey samples were analyzed using inductively coupled plasma mass spectrometry (ICP-MS). The samples were digested with HNO<sub>3</sub> at 160 °C using closed-vessel microwave digestion. After digestion, appropriate dilution was performed prior to analysis by ICP-MS. Accuracy of the proposed method was examined by spiking standard solution into honey samples (n=3). The %recoveries of As, Cd, and Pb were 95.96±1.68, 94.51±2.57, 100.45±1.22, respectively, obtained within the acceptance criteria (80-110%). Linear calibrations were obtained in the ranges of 0.1-1 mg L<sup>-1</sup>, 0.025-1 mg L<sup>-1</sup>, 0.1-50 mg L<sup>-1</sup> for As, Cd, and Pb, respectively. The correlation coefficients for determination of As, Cd and Pb were higher than 0.9995. Limits of detection (LODs) for As, Cd, and Pb were 0.0016 mg/kg, 0.00012 mg/kg, and 0.0039 mg/kg, respectively. Limits of detection (LOQs) for As, Cd, and Pb were 0.0038 mg/kg, 0.00015 mg/kg, and 0.0041 mg/kg, respectively. The precision of the method was less than 10%. The determination of As, Cd, and Pb in 10 honey samples was also investigated. The obtained results confirmed that the proposed method can be a reliable method for the determination of the heavy metals in Thai honey.

**Keywords:** Honey; Heavy metals; ICP-MS; Method validation



## Optimization of lignin-loaded nanostructured lipid carrier using box-behnken design

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Lignin is a natural polymer that has UV protection potential for sunscreen. However, lignin can cause irritation to the skin if applied at high concentration. Therefore, nanostructured lipid carriers (NLCs) were used in this work to reduce the irritation and prolong the UV protection efficiency. This study focuses on the optimization of lignin-loaded NLCs by using experimental designs including plackett–burman (PBD) and box-behnken design (BBD). PBD was studied first to investigate three significant variables among five variables in which affected the quality of NLCs. Then, BBD was applied to find the optimum condition for producing NLCs formulation. The results showed that the most affected variables were sonication time, amplitude of sonication, and lipid concentration, whereas surfactant to lipid and solid to liquid lipid ratio had less effect on the particle size of the NLCs compared to the others. These three variables were used as independent variables for BBD. A 50:50 ratio of cetyl palmitate and caprylic/capric triglyceride and a 50:50 ratio of tween 80 and span 40 were used as solid to liquid lipid ratio and co-surfactants, respectively. The optimum condition showed the smallest NLCs particle size of  $95.9 \pm 1.3$  nm at time of 5 min 48 seconds, amplitude of 56%, and lipid concentration of 1.2%. The size was slightly decreased to  $85.3 \pm 0.86$  nm after loading lignin in the NLCs. In conclusion, PKD and BBD are significant tools for the experimental design to find the optimal condition by reducing the number of experiments.

**Keywords:** Nanostructured lipid carriers; Box-behnken design; Co-surfactant; Optimization; Lignin

## Fungal endophyte isolated from nibung palm (*Oncosperma* sp.) enhances the growth rate of red coral lettuce (*Lactuca sativa* L.)

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The combination of producing phytohormones and the ability in nutrient solubilization of fungal endophytes make endophytic fungi potential allies in promoting plant growth in sustainable agriculture. The fungal endophyte *Daldinia eschsholtzii*, MFLUCC20-0215 isolated from nibung palm (*Oncosperma* sp.) produced a significantly high amount of indole-3-acetic acid (IAA:  $120.30 \pm 3.15$  ug/mL) with the ability to solubilize phosphate ( $3.56 \pm 0.04$ ). This strain of endophytic fungi was cultured in sterile rice grains. After incubation at 28 °C for 2 weeks, those inoculated rice grains were combined with charcoal and rice husks and processed through fertilizer compacter. All growth indexes indicate that our biofertilizer and chemical fertilizer have an equal level of efficacy in promoting growth of red coral lettuce (*Lactuca sativa* L.). The length of shoot, fresh and dry weight of both shoot and root were significantly higher ( $p < 0.01$ ) in the pot with biofertilizer and chemical fertilizer (positive control) than those of two negative control treatments. Interestingly, the root length in biofertilizer treatment ( $15.74 \pm 2.63$ ) is significantly higher than other treatments including chemical fertilizer ( $13.12 \pm 2.64$ b), un-inoculate rice grain ( $12.7 \pm 1.79$ 1b), and no fertilizer ( $11.57 \pm 28.48$ b). This can be attributed to the ability of IAA production of *D. eschsholtzii* MFLUCC20-0215. Although, future experiment is required to determine the effects of biofertilizer from *D. eschsholtzii* MFLUCC20-0215 on other plant species; however, this study demonstrated that this fungus strain holds promise as a valuable biofertilizer for enhancing sustainable crop production systems.

**Keywords:** Fungal endophyte; Biofertilizer; Red coral lettuce; Indole-3-acetic acid; Phosphate solubilization



**Figure 1** A) Biofertilizer prototype; B) Red coral lettuce in biofertilizer treatment, and C) Red coral lettuce in control treatment (no fertilizer).



## Preparation and properties of wet wipes from water hyacinth

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Using plastic wet wipes made from petroleum that is single-use and disposable too much affects the natural environment due to its product's inherent resistance to decay in nature. One way to solve this problem is to develop environmentally friendly materials that are biodegradable after use. The researcher is therefore interested in applying water hyacinth into wet wipes to solve the problem. The mechanical properties of wet wipes by adding silica from rice husks. The chemical structure of the cellulose, silica and pectin was confirmed by ATR-FTIR. The hydroxyl of these sample decreased after the addition of silica. The thickness of the sample was around  $0.12 \pm 0.05$  mm after adding silica (0-1.5 g). The moisture content and moisture absorption of the sample decreased after the addition of silica. The water absorption of the sample was about 100% when using 1% silica. In the case of ethanol medium, the ethanol absorption was about 30% at 1%w/w silica. Moreover, the resulting wet wipes showed fungi resistance when observing digital camera and optical microscopy. The sample was easily decomposed in nature after use.

**Keywords:** Cellulose; Modification; Filler; Paper; Starch

## Preservation of plums (*Prunus salicina*) via the application of edible packaging films developed from tapioca starch/gelatin incorporating Hass avocado extract

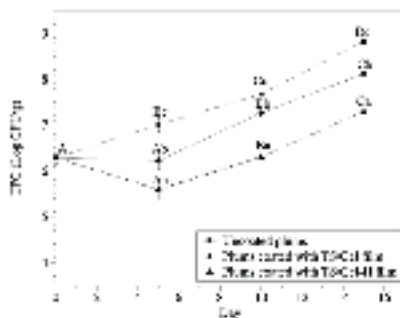
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The antibacterial properties of avocado extract are abundant, yet it has received little attention from researchers. Tapioca starch/gelatin (1/2 v/v) incorporating Hass avocado extract (5% v/v) (TS/Gel-H) was utilized to effectively synthesize an edible film with enhanced swelling, mechanical strength, and water stability in this study. Three group of plums (*Prunus salicina*) were implemented in the experiment: uncoated plums, plums coated with TS/Gel film, and plums coated with TS/Gel-H film. During the 15-day storage period at 4°C, a total plate count (TPC, log CFU/g) and sensory examination of the samples were performed with three replicates. The result showed that the plum coated with TS/Gel-H film exhibited the most effective control of aerobic microbial density. Following 15 days, the uncoated sample demonstrated a fruit structure that had become less rigid, while the TS/Gel-H film-coated sample retained its original appearance and structure without any noticeable changes. The findings acquired substantially improved the applicability of the edible film containing avocado extract for food preservation purposes.

**Keywords:** Active packaing film; Antibacterial activity; Edible packaging film; Fruit Presevation; Plums



**Figure.** Changes in total plate count (TPC, log CFU/g) of plums uncoated and coated by different films during 15 days of storage

(Notes: The different capital letters indicated significant differences ( $p < 0.05$ ) in TPC at various times within the same group of plums, while the different lowercase letters indicated significant differences ( $p < 0.05$ ) in TPC across different samples on the same day)



## Preparation of complex carrier from aloe vera mucilage/gelatin for kaempfer essential oil

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Kaempfer essential oil (KEO) has various properties such as antioxidant, anti-inflammatory, antibacterial, and antiviral properties, but KEO active compounds, whose major compound is kaempferol, easily deteriorate. So, microencapsulation techniques were used to increase stability. Therefore, the optimal ratio of encapsulated complexes was studied by using Aloe Vera (AV) and Gelatin (GE) as emulsifiers and cellulose nanocrystals (CNCs) as stabilizers. The optimum ratio of AV:GE:CNCs was 6:3:1, then processed into powder using Spray drying techniques for easy application, transportation, and storage. The physical characterizations were performed by Fourier Transform Infrared Spectrometer (FTIR), Scanning electron microscope (SEM), X-ray diffraction (XRD), Dynamic light scattering (DLS), Thermogravimetric analysis (TGA), Optical microscopes, Laser diffraction particle size analyzer, and Rheometer. Consequently, the FTIR spectrum of the KEO-complex proved that in the complex was presented the formation of KEO-loaded emulsion of AV, GE, CNCs, coconut oil, and Kaempfer essential oil (KEO). The particle size of the KEO-complex is  $266.2 \pm 24.3$  nm in the nanoscale range, with an increase in thermal stability. In addition, the rheological property of the KEO-complex indicates a non-Newtonian and shear-thinning flow behavior that shows a storage modulus  $G'$  higher than the loss modulus  $G''$ . This study can be applied to a variety of applications, such as synthetic preservatives.

**Keywords:** Kaempfer essential oil; Aloe vera; Cellulose nanocrystals; Emulsion; Spray dryin

## Effect of cooking process on physicochemical and biological properties of resistant starch content in Jasmine rice cultivated in saline soil area

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The production process of ready-to-eat resistant starch of Jasmine rice for commercial development in Nong Saeng Sub-district, Wapi Pathum District, Maha Sarakham province was investigated. The production process of resistant starch; briefly, the raw rice was cleaned, cooked with rice cooker and adding the oil vegetable (5 mL). After that cooked rice was stored in room temperature for 15 minutes, chilled in a refrigerator at 4 °C for 12 h. The ready-to-eat rice was reheated with the microwave for 3 minutes. Seven types of vegetable oils were used in the experimental such as bean oil, coconut oil, canola oil, olive oil, rice bran oil, palm oil, and sunflower seed oil. The physicochemical properties, mineral, amylose contents, total sugar and antioxidant activities of raw rice the ready-to-eat rice (vegetable oil) and the control rice (without adding vegetable oil) were studied and compared. The results the cooked process (cleaned and cooked) decrease the total sugar, amylose and carbohydrate content when compared with raw rice. Based on this research data, it could be used the production process to produce the resistant starch for further food business.

**Keywords:** Resistant starch; saline soil; Jasmin rice; Total sugar



**Figure 1** Ready-to-eat the resistant starch of Jasmine rice

## $\alpha$ -Glucosidase inhibitory activity of *Cyperus rotundus* rhizome extracts

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*Cyperus rotundus* L. or Ya Haew Moo is commonly named nutgrass and belongs to the Cyperaceae family. This plant displays various biological activities such as antidiabetic, antibacterial, antioxidant, and anti-inflammatory. Therefore, the present study extended to assess its utility for the enzyme inhibitory potential against  $\alpha$ -glucosidase, tyrosinase, and acetylcholinesterase. The dried powder of *C. rotundus* rhizomes was produced using sequential extraction over 7 days with hexane, dichloromethane, ethyl acetate, and methanol, respectively, by maceration at room temperature. The extracts were preliminarily screened for their potential to inhibit enzymes at a concentration of 500 ppm. The results found that the methanol extract exhibited the highest  $\alpha$ -glucosidase inhibition with  $93.36 \pm 0.62\%$ . This extract was more potent than acarbose as a positive control with an  $IC_{50}$  value of  $4.49 \pm 0.56$  ppm. However, the extracts of *C. rotundus* rhizomes showed no inhibition against tyrosinase and acetylcholinesterase.

**Keywords:** *Cyperus rotundus* rhizomes; enzyme inhibitory activity;  $\alpha$ -glucosidase; tyrosinase; acetylcholinesterase.



## Evaluation of enzyme inhibitory activity of *Ganoderma lucidum* (antler shaped lingzhi fruiting body) extracts

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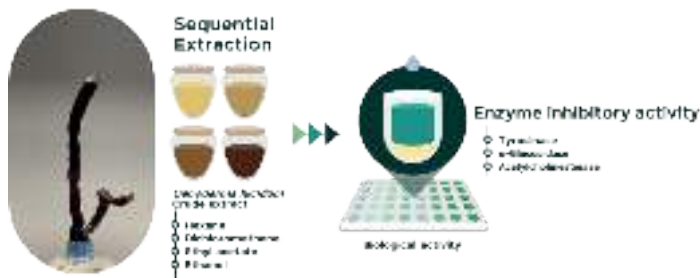
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In recent times, there has been a rising demand for supplementary food made from natural extracts and organic cosmetic items that contain bioactive compounds as part of their ingredients. Consequently, the extracts and bioactive compounds from Lingzhi (*G. lucidum*) stand out as particularly interesting ingredients due to their rich bioactive profile. In the present work, dried *G. lucidum* (antler shaped lingzhi fruiting body) was sequentially extracted using hexane, dichloromethane, ethyl acetate, and ethanol. All extracts were preliminarily screened for their  $\alpha$ -glucosidase, tyrosinase, and acetylcholinesterase inhibitory activities at a concentration of 50 ppm. As a result, the hexane extract possessed good potential for tyrosinase with  $37.09 \pm 0.43\%$  inhibition, whereas the ethanol extract showed the most potent against  $\alpha$ -glucosidase with  $24.45 \pm 1.68\%$  inhibition. However, no inhibition of the extracts was obtained for acetylcholinesterase. The results indicated that the mushroom extracts could be incorporated into the future development of skincare and dietary supplements.

**Keywords:** *Ganoderma lucidum*; Enzyme inhibitory activity; Tyrosinase; Acetylcholinesterase;  $\alpha$ -Glucosidase



## Algal-based protein: tempeh produced from *Cladophora glomerata* (Sarai-Kai: สาหร่ายโก)

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*Cladophora glomerata*, a common freshwater alga found in northern Thailand, is edible and high in protein content. The aim of this study was to propose an algae-based protein as a supplement for protein-rich tempeh production. The nutrition content based on dry weight of the algae extract was identified to be  $19.00 \pm 0.20\%$ ,  $17.50 \pm 0.30\%$ ,  $6.79 \pm 0.30\%$ ,  $17.50 \pm 0.60\%$ ,  $22.10 \pm 0.60\%$ , and  $30.20 \pm 0.50\%$  for protein, fat, moisture, ash, fiber, and carbohydrate, respectively. The optimum ratio of sterile algae in tempeh production was 20% in cooked soybean with 0.2% of *Rhizopus oligosporus* as a starter inoculum. The fungal mycelium showed a complete penetration into the algae tempeh (AT) with a mixture of soybean. The total protein content (TPC) of the algal-based tempeh was  $14.8582 \pm 0.17\%$  with a soluble protein content of  $294.37 \pm 0.01 \mu\text{g}/100\text{g}$  tempeh, and a pH of  $6.16 \pm 0.04$ . For the incubation duration, the AT incubated for 48 h exhibited the acceptable odors similar to soybean tempeh (control), with the TPC of  $19.6513 \pm 0.80\%$ . The essential amino acids (AA) composition was estimated to be in the range of 0.4–9.0% in the AT with major AAs as glutamate, asparagine, and leucine. Among the total of 18 amino acids composing the product, the AT comprises of umami amino acid (glutamate and asparagine) in the range of 5.5–9.0%, and sweet amino acids (alanine, glycine, serine, threonine, and proline) in the range of 2.1–2.6%. Additionally, we produced a freeze-dried algal protein powder from these tempeh products, opening up further possibilities for innovative food applications.

**Keywords:** Algae; *Cladophora glomerata*; Tempeh; Protein; Umami



**Figure 1** Tempeh and its powder (right) produced from *Cladophora glomerata*

(Sarai-Kai; สาหร่ายโก) (left) and dried algae (middle)

## The effect of ethanol and water ratios of star fruit (*Averrhoa carambola*) extract on total phenolic, total flavonoid, tartaric acid contents and an inhibitory of tyrosinase activity

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The research aimed to investigate the effects of different ethanol and water ratios on extracting phenolic, flavonoid compounds, as well as tartaric acid from star fruit, evaluating their inhibitory effect on tyrosinase activity. The ripe star fruit (*Averrhoa carambola*) puree was macerated for eight hours with various ethanol and water ratios of 0:100, 20:80, 50:50, 80:20, and 100:0. Different ratios yielded varied contents of total phenolic (TPC), flavonoid (TFC), and tartaric acid (TAC). The result showed contents of 8.48-101.50 mg GAE/g FW, 2.33-46.66 mg CE/g FW and 0.04-0.09 mg/g FW, respectively. The 50:50 ratio showed the highest TPC and TFC, whereas the 0:100 ratio had the highest TAC. The efficacy of the extracts on tyrosinase inhibition, using L-DOPA as a substrate, yielded the IC<sub>50</sub> value (54.90-210.37 mg/L). All extracts exhibited a significant IC<sub>50</sub> value ( $p \leq .05$ ). The 80:20 ratio demonstrated the most significant inhibitory activity, showing moderate inhibition of tyrosinase activity. These findings suggest *A. carambola* extracts could be valuable in cosmeceuticals for enhancing efficiency.

**Keywords:** *Averrhoa carambola*; Star fruit; Tyrosinase; Tartaric acid; Antioxidant

## Analysis of carnosine and anserine from the black chicken Nin-Kaset by high performance liquid chromatography

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Nin-Kaset black-boned chicken bred and developed by Kasetsart University was reported to show high level of carnosine (CAR) and anserine (ANS) dipeptides, but no specific amount was examined. These compounds are key bioactive compounds showing a wide range of therapeutic properties. However, it is difficult to quantify their exact amount because they are analogs. Specific and sensitive condition is required. Thus, in this work, the quantitative strategies and conditions were studied to analyze CAR and ANS contents in white feather (WF) and black feather (BF) in comparison to Baytong chicken (BC) using High Performance Liquid Chromatography (HPLC) at ambient temperature. The more convenient and simplified techniques were discovered. Asahipak NH<sub>2</sub>P-50 4E (4.6 x 250 mm) column where NaH<sub>2</sub>PO<sub>4</sub>/ACN: 45/55 acts as mobile phase was used. The photodiode array detector was set at 210 nm. The CAR and ANS compounds were extracted in acidic solution at pH 5.0. The CAR and ANS concentrations in all breeds were identified using our conditions at ambient temperature. The highest CAR and ANS concentrations of 3.0 and 8.4 mg/g were found in BF, whereas WF shows the lowest content of carnosine and anserine (2.1 and 6.2 mg/g). In this work, not only CAR and ANS contents of native Nin-Kaset chicken was revealed in comparison to local chickens, but the more convenient quantitative methods and conditions to identify CAR and ANS concentrations were reported here.

**Keywords:** Black chicken; Carnosine; Anserine; HPLC; Healthy food

## Efficiency of commercial tea against *Escherichia coli* and *Staphylococcus aureus*

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Commercial tea has been consumed widely because of its flavor and unique fragrance. The phenolic compounds in tea, especially catechin, are known as antibacterial substances. The chemical substances of tea differ in manufacturing processes. The research aims to extract one commercial tea with ethyl acetate and determine the antimicrobial effect of crude extract against *Escherichia coli* and *Staphylococcus aureus*. The ethyl acetate, the medium polar solvent, is suitable for extracting phenolic compounds by liquid-liquid extraction. After evaporation, the 0.2 g of crude extract was dissolved in 1 ml of ethyl acetate. The crude solution was minimized the insoluble substances by being left to stand for 30 min, and only the soluble fraction was evaluated for antimicrobial properties by the agar well diffusion technique. The results showed that the inhibition zone diameter was  $27.5 \pm 1.3$  mm against *S. aureus*, whereas no inhibition zone was found against *E. coli*. The ethyl acetate was used as a negative control, and no inhibition zone was found against both bacteria. The soluble fraction was also performed two-fold dilution with ethyl acetate before testing against *S. aureus* by liquid growth inhibition. The  $\frac{1}{2}$  fold soluble fraction showed growth inhibition and killing of *S. aureus*. The results show this commercial has an antibacterial effect against *S. aureus*. However, the amount of phenolic compound must be further determined, and the different commercial products must be tested more.

**Keywords:** Commercial tea; Crude extract; Bacterial gastroenteritis; Bacterial inhibition; Bactericidal activity

## Preparation and physical properties of cassava starch/poly (vinyl alcohol)/clay nanocomposite films

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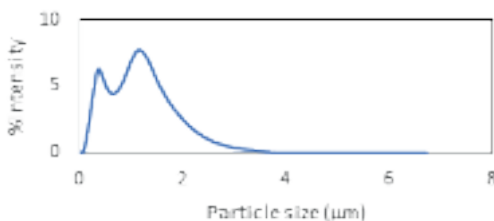
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Cassava starch (CS) is a complex carbohydrate, also known as a polysaccharide, commonly found in nature. The disadvantages of the CS are poor water resistance and mechanical properties. This problem was solved by the addition of poly(vinyl alcohol) (PVA) which is water soluble polymer and kaolin clay (KC). The CS/PVA/KC nanocomposite films with high mechanical and barrier properties were prepared by casting film. The CS (10% w/v) solution was blended with 10% PVA solution at ratio of 50/50 CS/PVA blend and the glycerol was added in the CS/PVA blend at 15% (w/w) based on with respect to CS. The various KC contents (1,2,3 and 5%w/w based on CS/PVA blend) was added in CS/PVA blend at constant stirring until it was homogenized entirely with the CS solution. After the sonication process, the polymer solutions were poured into plastic molds and dried in a convection oven at 65 °C for 5 h. Based on the CS/PVA matrix, the effects of KC content on the CS/PVA/KC nanocomposite films were investigated. X-ray diffraction results demonstrated that the CS/PVA/clay nanocomposite films exhibited KC good dispersion in the polymer matrix. FTIR spectra showed that the molecular interactions were enhanced in the CS/PVA/KC films with higher PVA content. The maximum tensile strength and elongation at break for the CS/PVA/KC nanocomposite films were 18 MPa and 330%, respectively. The CS/PVA/KC composite was applied to extend the shelf-life of banana and results showed that the good shelf-life of banana was accepted. The CS/PVA/KC nanocomposite film is a promising material for high barrier food packaging.

**Keywords:** PVA; Modification; Blend; Film; Cassava starch



**Figure 1** Particle size of the KD suspensions in water observed by digital camera

# Inorganic Chemistry (IC)

## Oral Presentation

## Highly dispersed and stable Palladium(II) species anchoring on ethylenediamine-grafted-MIL-101(Cr) for styrene oxidation

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The incorporation of palladium acetate over ethylenediamine-grafted on MIL-101(Cr) led to a highly stable Pd(II) species for the oxidation reaction. MIL-101(Cr) was first grafted by ethylenediamine (0.5-1.2 mmol/g) and followed by the addition of Pd(II) (0.03-0.2 mmol Pd/g) via double-solvent adsorption. The interaction between one amino moiety of ethylenediamine coordinated with the Cr<sup>3+</sup> nodes of MIL-101(Cr) was confirmed by X-ray photoelectron and Raman spectroscopy. While the other amino moiety of ethylenediamine is the anchoring site for the incorporated Pd(II) species. *In situ* X-ray absorption near-edge structure analysis showed that the strong interaction between Pd<sup>2+</sup> and ethylenediamine, within the confinement of MIL-101(Cr) structure, effectively prevented reduction to Pd<sup>0</sup>, even in the presence of H<sub>2</sub> at 150 °C. The catalysts with ethylenediamine:Pd(II) molar ratios of 3–16 provided a high activity for styrene oxidation (TOF ~28 h<sup>-1</sup>). Furthermore, the ethylenediamine ligand inhibited the reduction of Pd<sup>2+</sup> by the styrene and prevented the leaching of the active Pd<sup>2+</sup> species under oxidizing and acidic conditions.

**Keywords:** Ethylenediamine; MIL-101(Cr); Stability; Anchoring; Palladium(II)

## Biodegradable polyester composites, containing various metal oxide particles: A model study as shelf-life extendable packaging for bananas

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Utilization of food packaging allows the extension of food shelf-life and significantly slows down the deterioration rate of food – this leads to a reduction in food waste. Traditional food packaging can be obtained from conventional polymers such as polyolefin which is produced from non-renewable resources and is almost impossible to decompose. The use of metal oxide particles as additives in food packaging has provoked much interest in the last decades due to their abilities to scavenge ethylene gas and inhibit bacterial growth, the major sources of food spoilage. In this presentation, we will describe the preparation of biodegradable polymer composite based on polylactide (PLA)/poly(ethylene adipate-co-terephthalate) (PBAT) blends and various metal oxide particles. A model study for the utilization of the developed biodegradable polymer composites as active packaging for foods will be discussed. The effects of metal oxide particles on thermal and mechanical properties as well as the efficiency in pro-long food shelf-life of the prepared biodegradable polymer composite films will be explained.

IC

**Keywords:** Active packaging; Biodegradable polymer composites; Metal oxide particles; Ethylene scavengers; Aliphatic polyester

## A low-cost SFX-based hole transporting material for perovskite solar cells

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A low-cost hole transporting material (HTM), **C-SFX**, was designed for high-performance perovskite solar cells (PSCs). **C-SFX**, composed of a spiro[fluorene-9,9'-xanthene] (SFX) core with peripheral carbazole units, was synthesized using two palladium-catalyzed Buchwald–Hartwig amination reactions starting from *p*-anisidine and 2Br-SFX in an overall yield of 38%. According to cyclic voltammetry and ultraviolet photoelectron spectroscopy (UPS) results, the highest-occupied molecular orbital (HOMO) level of the new HTM is positioned above the valence band maximum of the perovskite, ensuring efficient hole extraction at the perovskite/HTM interface. The device with FTO/SnO<sub>2</sub>/perovskite/**C-SFX**/C configuration exhibited a power conversion efficiency (PCE) of 12.8%, comparable to that of spiro-OMeTAD (12.3%). Remarkably, **C-SFX** showed a slightly higher mobility ( $2.67 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) than spiro-OMeTAD ( $2.55 \times 10^{-3} \text{ cm}^2 \text{ V}^{-1} \text{ s}^{-1}$ ) indicating potentials of **C-SFX** as spiro-OMeTAD HTM alternative. Future examination includes the investigation of charge recombination loss and the study of long-term stability of the devices.

**Keywords:** Perovskite solar cell; Hole transporting material; Spiro[fluorene-9,9'-xanthene]; Carbazole; Hole mobility

## Switchable metal-ion selectivity in sulfur-functionalised pillar[5]arenes and their host-guest complexes

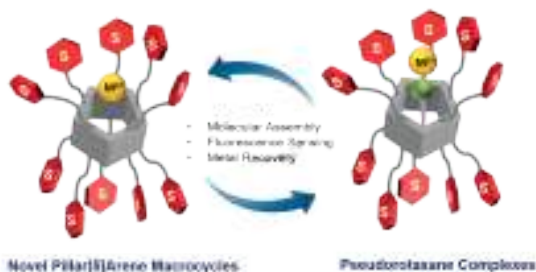
Bunyaporn Toddee,<sup>1</sup> Patharaporn Sanae,<sup>1</sup> Araya Ruengsuk,<sup>1</sup> Pattarapapa Janthakit,<sup>2</sup>  
Vinich Promarak,<sup>2</sup> Jonggol Tantirungrotechai,<sup>1</sup> Mongkol Sukwattanasinitt,<sup>3</sup>  
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Nucleophilic substitution of pertosylated pillar[5]arene (P-OTs) with commercially available sulfur containing nucleophiles (KSCN, KSAC, and thiophenol), yields a series of sulfur-functionalised pillar[5]arenes. DLS results and SEM images imply that these pillararene macrocycles self-assemble in acetonitrile solution, while X-ray crystallographic evidence suggests solvent-dependent assembly in the solid state. The nature of the sulfur substituents decorating the rim of the pillararene controls binding affinities towards organic guest encapsulations within the cavity and dictates metal-ion binding properties through the formation of favorable S–M<sup>2+</sup> coordination bonds outside the cavity, as determined by <sup>1</sup>H NMR and fluorescence spectroscopic experiments. Addition of a dinitrile guest containing a bis-triazole benzene spacer (**btn**) induced formation of pseudorotaxane host-guest complexes. Fluorescence emission signals from these discrete macrocycles were significantly attenuated in the presence of either Hg<sup>2+</sup> or Cu<sup>2+</sup> in solution. Analogous titrations utilizing the corresponding pseudorotaxanes alter the binding selectivity and improve fluorescence sensing sensitivity. In addition, preliminary liquid-liquid extraction studies indicate that the macrocycles facilitate the transfer of Cu<sup>2+</sup> from the aqueous to the organic phase in comparison to extraction without pillar[5]arene ligands.

**Keywords:** Sulfur-functionalised pillar[5]arenes; Host-guest complexes; Metal-ion selectivity



## Pillararene supramolecular assembly in supramolecular organic frameworks (SOFs) and mechanically interlocked molecules (MIMs)

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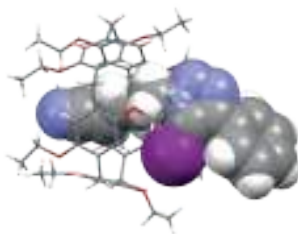
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For the past few years, supramolecular chemistry has advanced in broad research fields including material, sensing, and drug delivery. The design of macrocyclic hosts capable of forming strong and selective host-guest complexes is the key to manipulating interactions that are used in molecular organization. Pillararene is a pillar-shaped macrocycle that has electron-rich aromatic cavities and properties to construct host-guest complementary. In this work, we aim to investigate host-guest complexation properties of ethoxy pillar[5]arene (EtP5A) with a series of triazole-nitrile threads, a common organic linking motif for molecular assembly. Substituents at the 3, 4, and 5 of triazole significantly mediate binding affinities with EtP5A. X-ray crystallographic analysis of suitable crystals revealed a successful encapsulation of the thread with EtP5A which is stabilized by hydrogen bonds. These results are important information for designing other complex supramolecular architecture in advanced material applications.

**Keywords:** Mechanically interlocked molecules (MIMs); Supramolecular Organic Frameworks (SOFs)



**Figure 1.** Crystal structure of triazole-nitrile@EtP5A complex

## Synthetic studies and the applications of BINOL coordinated metalloporphyrins

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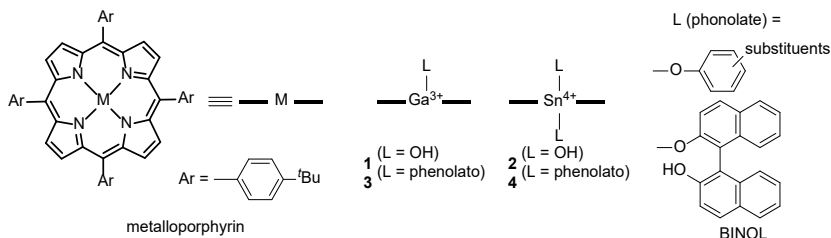
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Synthesis and characterization of metalloporphyrins have been attracting much attention over the past century. Although various modifications have been made to the porphyrin ligand, the field of coordination chemistry has increasingly embraced supramolecular and biomimetic strategies using weakly binding ligands. Introducing stable axial ligands to the metalloporphyrins could offer the promise for further chemical modifications. In this work, we utilized gallium(III)- and tin(IV)-porphyrins ([GaPor] and [SnPor]) due to their cationic hard-acid nature as ideal platforms for axial ligation such as phenolatos, *i.e.*, hard-base. We investigated their interactions with a variety of axial ligands on these Ga/Sn porphyrins.

The axial ligation was achieved by dehydration reactions of [GaPor](OH) (**1**) or [SnPor](OH)<sub>2</sub> (**2**) with various phenols, resulting in the formation of the desired complexes (**3**) or (**4**), respectively. As expected, all the products exhibited stability but display slight lability when exposure to acids. Several products were further subjected to structural analysis using single crystal diffraction studies. The ligations were extended to more complex phenolatos, *e.g.*, BINOL and naturally occurring tyrosine derivatives.

In this presentation, the details of the synthesis, structural characterization, and photophysical and electrochemical properties of **3** and **4** will be discussed.

**Keywords:** Metalloporphyrin; Gallium; Tin; BINOL; Axial coordination



## Neutral isocyanide-templated assembly of pillar[5]arene [2] and [3]pseudorotaxanes

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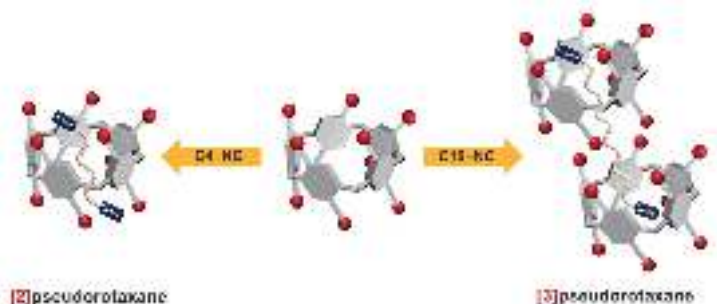
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Unprecedented pillar[5]arene–isocyanide pseudorotaxane complexes are reported. Extensive <sup>1</sup>H-NMR experiments reveal remarkably strong binding affinities of alkyl diisocyanide guests ( $K_a > 10^5 \text{ M}^{-1}$  in CDCl<sub>3</sub>) by pillar[5]arenes. Characterised by multinuclear <sup>1</sup>H and <sup>13</sup>C-NMR spectroscopy and single crystal X-ray diffraction, it is demonstrated that pillar[5]arenes are capable of binding a series of alkyl diisocyanides wherein either [2] or [3] pseudorotaxanes can be formed by varying alkyl chain length. Moreover, electron deficient aryl isocyanides, despite modest binding affinities in solution, are demonstrated to form inclusion complexes within the cavities of pillar[5]arenes stabilised by multiple C–H--- $\pi$  interactions. Furthermore, the pseudorotaxanes are locked by the multicomponent reactions. The mechanically interlocked architectures affect the intramolecular charge transfer of the pillar[5]arene ring.

**Keywords:** Pillar[5]arene; Pseudorotaxanes; Isocyanide; Host–guest; Rotaxane



## Development of chiral metal complexes coordinated by axial chiral ligands exhibiting circularly polarized luminescence

Daiki Tauchi<sup>1</sup>, Masashi Hasegawa<sup>2</sup>, Yasuhiro Mazaki<sup>2</sup>, Kazunori Tsubaki<sup>3</sup>, Ken-ichi-Sugiura<sup>4</sup> and Hiroyuki Nishikawa<sup>1\*</sup>

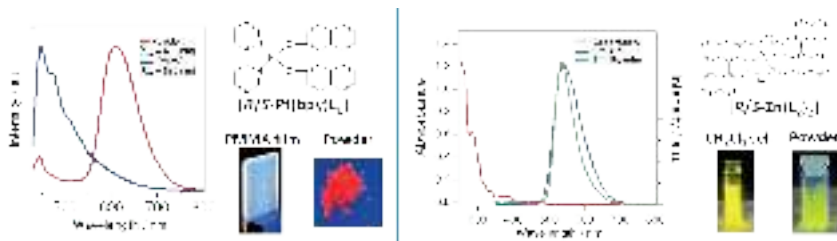
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Recently, there has been an active exploration in the research of development of circular polarized light-emitting devices utilizing chiral organic luminescent materials. In this presentation, we elucidate the syntheses of novel chiral platinum(II) ( $[R/S\text{-Pt}(\text{bpy})\text{L}_1]$ ) and zinc(II) ( $[R/S\text{-Zn}(\text{L}_2)_2]$ ) complexes coordinated by BINOL (2,2'-binaphthol) derivatives, and a comprehensive investigation of their structural characteristics and chiroptical properties.

While  $[R/S\text{-Pt}(\text{bpy})\text{L}_1]$  displayed no discernible emission in dilute solutions, distinct phosphorescence was observed in the forms of dispersed thin films in PMMA (polymethyl methacrylate) and powder states. The CPL (circularly polarized luminescence) spectra of the PMMA films and powder samples exhibited a g-value on the order of  $10^{-3}$ . These results indicated that both enantiomeric Pt complexes exhibited aggregation-induced circularly polarized phosphorescence. On the contrary,  $[R/S\text{-Zn}(\text{L}_2)_2]$  exhibited emission properties in both solutions and powder samples with relatively high photoluminescence quantum efficiencies ( $\Phi$ ) of 12% and 26%, respectively. The enhancement of  $\Phi$  in the solid state indicates aggregation-induced enhanced emission (AIEE), involving the suppression of molecular motion through rigid intermolecular interactions. The solution and powder samples of Zn complexes exhibited CPL with the g-value ranging from  $10^{-4}$  to  $10^{-3}$ , accompanied by a reversal in the sign of CPL signals between solution and powder states.

**Keywords:** CPL; Axial chirality ; Luminescent metal complexes; Schiff-base



**Figure** Molecular structure of  $[R/S\text{-Pt}(\text{bpy})\text{L}_1]$  (left) and  $[R/S\text{-Zn}(\text{L}_2)_2]$  (right), emission spectra and photograph of each emissions.

# Inorganic Chemistry (IC)

## Poster Presentation

## Effect of solutions on retrogradation of cooked sticky rice

On-on Chanprasartsuk<sup>1</sup>, Kamolwan Jantranon<sup>2</sup>, and Pornpen Atorngitjawat<sup>2\*</sup>

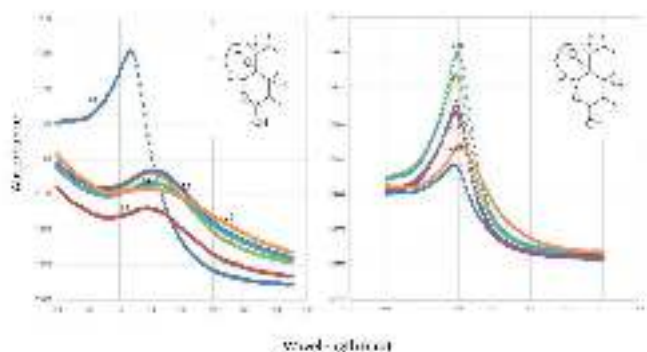
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To increase the shelf life and keep texture of Khao Tom Mud (cooked sticky rice mixed with coconut milk), the effect of solutions on retrogradation of cooked sticky rice was studied. The sticky rice was soaked in sodium chloride (6 %w/v) and glycerol (1% v/v) solutions compared with filtered water for 8 hours at a room temperature. The ratio of sticky rice and soaking solutions was 1:10. The cooked sticky rice was mixed with the coconut milk, packed with banana leaves and vacuum plastic bags. All samples were stored in the refrigerator at 4 °C for 7, 21 and 28 days. The percentage of retaining water content was studied. The chemical structure of sticky rice was studied by Fourier transform infrared spectroscopy (FTIR). The hardness was studied by texture analyzer technique. The result showed that the highest rate of water content percentage was found for sticky rice soaked in sodium chloride solution. The chemical structure of all samples, observed from FTIR spectra, was similar and no significant changes in amylose and amylopectin structure. The short-range order of amylose and amylopectin, examined from the ratio of absorbance at 1047 and 1022 cm<sup>-1</sup>, indicated that the retrogradation was started at storage time for 7 days and the lowest retrogradation rate was found for sticky rice soaked in sodium chloride solution. The lowest rate of retrogradation from the hardness property was found for sticky rice soaked in sodium chloride and highest for that soaked in glycerol solutions. Sodium chloride solution can delay the rate of retrogradation.

**Keywords:** Retrogradation; Sticky rice; Khao Tom Mud; Amylose; Amylopectin



**Figure 1.** UV-visible spectra of heme and heme-antimalarial drugs at different molar ratio

## The adsorption efficiency of composited magnetic biochar for tetracycline adsorption in an aqueous solution

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This work focused on adsorption capacity of tetracycline (TC) by magnetic biochar from corncob. Biochar was prepared by slow pyrolysis, then the biochar surface was improved using ferric oxide ( $\text{Fe}_3\text{O}_4$ ) for easily remove biochar from waste water treatment system and enhancement of adsorption efficiency. To increase highly effective removal of TC, the cobalt oxide (Co-O) was loaded on magnetic biochar using ultrasonication method. The interaction of Co-O@biochar composite was characterize by fourier-transform infrared spectroscopy (FTIR), which exhibited Co-O binding at the wavelength number 500-1000 nm. The adsorption efficiency of Co-O@biochar was investigated by adsorption TC solution in various concentration (0, 5, 10, 20, 30 and 50 mg/L). The adsorption performance of TC on Co-O@biochar was estimated by Inductively coupled plasma optical emission spectrometer (ICPOES). The result was found that the adsorption capacity by Co-O@biochar was higher than that of other sample.

**Keywords:** Tetracycline; Biochar; Adsorption; Magnetic; Nanoparticles



## Hydrothermal preparation of heteroatoms doped mangosteen peel carbon dots and their sensing abilities

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Carbon dots (CDs) are attractive nanomaterials because of their facile synthesis, biocompatibility, and low cost of their precursor. Compared to the traditional precursors, waste biomass was also seen as carbon source. In this work, a simple and cost-efficient single-step hydrothermal strategy has been used to synthesize CDs from agricultural biomass, mangosteen-derived carbon quantum dots (MCDs). Ethylenediamine ( $C_2H_8N_2$ ), sodium triphosphate ( $Na_5P_3O_{10}$ ) and sodium thiosulfate ( $Na_2S_2O_3$ ) were used as nitrogen, phosphorous and sulfur source, to fabricate heteroatom-doped MCDs. The structures of the synthesized doped-MCDs were characterized through X-ray photoelectron spectroscopy (XPS), transmission electron microscope (TEM) and Fourier transform infrared spectroscopy (FTIR). TEM results revealed that heteroatoms-doped MCDs have a spherical shape with the average size around 10 nm. The optical properties of heteroatoms-doped MCDs compared to MCDs have been studied using fluorescence spectroscopy. It was found that heteroatoms-doped MCDs showed a higher quantum yield than MCDs. Moreover, the fluorescence sensing abilities of heteroatoms-doped MCDs towards metal ions have been investigated.

**Keywords:** Carbon dots; Mangosteen peel; Biomass; Fluorescence sensing; Metal ion sensor

## Titanium complexes of phenoxy-azo and phenoxy-imine ligands: A comparative study for the ring-opening polymerization of *rac*-lactide and $\epsilon$ -caprolactone

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Two series of titanium complexes, bis(phenoxy-azo)titanium(IV) complexes (**1–6**) and bis(phenoxy-imine)titanium(IV) complexes (**7–9**), were prepared by the reactions between one equivalent of  $\text{Ti}(\text{O}^i\text{Pr})_4$  precursor and two equivalents of the corresponding ligand in hexane at room temperature. Complexes **1–6** were obtained as orange solids (48–75%), while complexes **7–9** were afforded as yellow solids (75–78%). The synthesized titanium complexes were characterized by  $^1\text{H}$  and  $^{13}\text{C}\{^1\text{H}\}$  NMR spectroscopy and X-ray crystallography. The X-ray structures of **1** and **4** revealed that the two ligands were  $\kappa^2$ -coordinated to the titanium center with the two phenoxy groups in *trans* positions and the two nitrogen atoms in *cis* positions. All complexes were active initiators for the ring-opening polymerization (ROP) of *rac*-lactide (*rac*-LA) and  $\epsilon$ -caprolactone ( $\epsilon$ -CL) with living fashions. The results revealed that complex **1**, having the least bulky *p*-methyl phenoxy substituents, displayed the highest catalytic activity. The polymerizations mediated by all titanium complexes were well-controlled, affording polymers with predetermined molar mass and narrow dispersity values. Kinetic studies demonstrated that polymerization was first-order kinetics with respect to monomer concentration. The bis(phenoxy-azo) titanium complexes exhibited higher catalytic activity than their bis(phenoxy-imine) titanium counterparts.

**Keywords:** Titanium complexes; Phenoxy-azo ligand; Phenoxy-imine ligand; Ring-opening polymerization

## Controlled and effective ring-opening (co)polymerization of *rac*-lactide, $\epsilon$ -caprolactone and $\epsilon$ -decalactone by $\beta$ -pyrimidyl enolate aluminum complexes

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This work describes a series of  $\beta$ -pyrimidyl enolate aluminum complexes with the general formula  $\text{LAlMe}_2$  (**1–6**) { $\text{L} = [(2\text{-C}_4\text{H}_2\text{N}_2\text{Cl})\text{-CH}=\text{C}(\text{O})\text{C}_6\text{H}_4\text{R}]$ ,  $\text{R} = \text{H}$  (**1**),  $\text{Me}$  (**2**),  $\text{OMe}$  (**3**),  $\text{CF}_3$  (**4**),  $\text{CN}$  (**5**),  $\text{Ph}$  (**6**)} that efficiently produce PLA, PCL, and PDL with controlled molar masses and narrow dispersity values. While the electronic characteristics of the ancillary ligands had no substantial influence on the catalytic activity for the *rac*-LA polymerization, the catalytic activity of the  $\epsilon$ -CL and the  $\epsilon$ -DL polymerizations was affected by the ligand substituent ( $\text{R}$ ), with complex **4** exhibiting the highest catalytic performance in both cases. In addition, six different types of well-defined block copolymer between *rac*-LA,  $\epsilon$ -CL, and  $\epsilon$ -DL were successfully prepared *via* a sequential-feed approach and the second monomer could be polymerized to complete conversion regardless of the order of the first monomer. The results unveiled that the order of monomer addition was not crucial in this catalytic system, which was advantageous for synthesizing triblock copolymers. Remarkably, the perfect random copolymer between  $\epsilon$ -CL and L-LA,  $\text{poly}(\text{L-LA-}r\text{-CL})$ , with a strict Bernoullian distribution, was successfully produced by complex **3** *via* a single-feed polymerization without transesterification side reactions. This is the first time that the random copolymer can be produced by utilizing sterically unhindered aluminum complexes with a strong electron-withdrawing character. The electronic influence from the pyrimidine ring of the ligand framework was believed to play an important role in the formation of the random copolymer. The success of this aluminum-based catalyst system allows for the future development of other bio-derived lactones and copolymers with varying properties.

**Keywords:** Aluminum catalyst; Ring-opening polymerization; Polylactide; Polycaprolactone; Polydecalactone

## Enhanced aerobic alcohol oxidation activity of multinuclear copper catalysts featuring amine-bis(triazoyl) ligands

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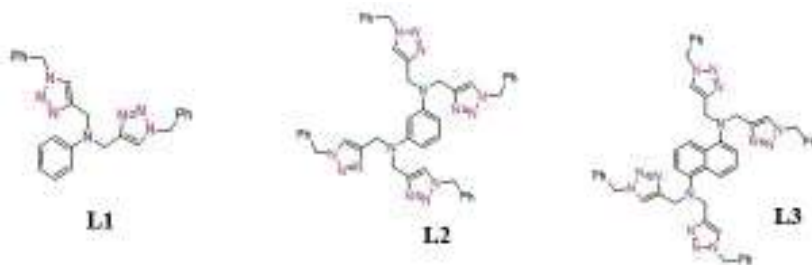
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Multinuclear copper catalysts are known to facilitate multi-electron transfer oxidation reactions in various oxidase enzymes. Similarly, multinuclear copper catalysts with nitroxyl radicals as co-catalysts also show improved catalytic activities towards aerobic alcohol oxidation to aldehydes, compared to their related mononuclear analogues. However, despite extensive studies, the effect of ligand structures on the catalytic oxidation performances of multinuclear copper complexes has not been reported. In this work, a class of amine-bis(triazoyl) ligands with single (**L1**) and dual amine-bis(triazole) chelates (**L2** with 1,3-phenylene linker and **L3** with a 1,5-naphthalene linker) were prepared. The catalytic activities of the *in-situ* generated CuBr/Ln/TEMPO/NMI (TEMPO = 2,2,6,6-tetramethylpiperidin-1-yl)oxyl, NMI = *N*-methylimidazole) toward aerobic oxidation of benzyl alcohol were evaluated and compared. Single crystal X-ray analyses and cyclic voltammetry were employed to rationalize their catalytic performances.

**Keywords:** Multinuclear copper complexes; Aerobic Alcohol oxidation; Amine-bis(triazole); Catalysis



**Figure 1.** Amine bis(triazoyl) ligands L1-L3

## Preparation of lead tree wood composite with zeolite NaA, NaX, NaP

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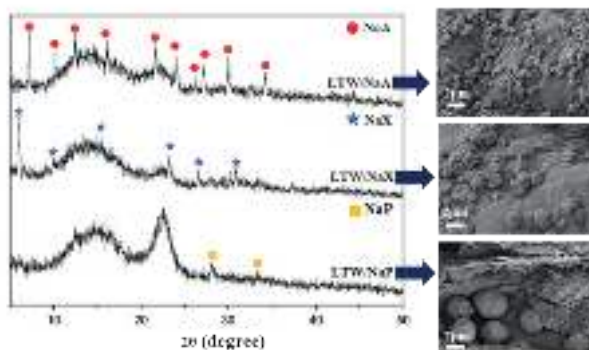
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Zeolites play a crucial role in various industrial applications, such as catalysis, separation, and adsorption, typically in powder form. However, the conventional separation process is time-consuming and generates considerable waste, including filter papers and syringe filters. To address this issue, an alternative approach involves producing larger-size zeolites. This study focuses on the synthesis of Lead Tree Wood (LTW) composites with zeolite NaA, NaX, and NaY. The selected wood, Lead tree (*Leucaena leucocephala*), is a fast-growing plant widely available in Thailand, with a wood structure that can potentially serve as zeolite support due to its larger xylem and phloem diameter. X-ray diffraction and scanning electron microscopy confirm the successful synthesis of wood composites with zeolite NaA and NaX using the standard synthesis method with the addition of Lead tree wood. However, the synthesis of the composite with zeolite NaP required a modified approach using the NaY zeolite synthesis method.

**Keywords:** Wood-zeolite composite; Lead tree wood; Zeolite NaA; Zeolite NaX; Zeolite NaP



## Aluminum complexes of tridentate [ONN]-phenolate ligands the ring-opening polymerization of *rac*-lactide and $\epsilon$ -caprolactone

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A series of aluminum complexes supported by [ONN]-phenolate ligands were successfully synthesized and characterized using NMR spectroscopy. In the presence of benzyl alcohol, all aluminum complexes effectively initiated the ring-opening polymerization (ROP) of *rac*-lactide (LA) and  $\epsilon$ -caprolactone ( $\epsilon$ -CL) in toluene at 70 °C. All polymerizations proceeded in a controlled manner, as evidenced by a good agreement between the experimental and theoretical molar masses and the observed narrow dispersity values. Kinetic studies revealed first-order kinetics in the monomer for both *rac*-LA and  $\epsilon$ -CL polymerizations. The effects of ligand structure on the catalytic activity and stereoselectivity were discussed. A good isoselectivity control was achieved for the polymerizations, with a  $P_m$  value up to 0.72.

**Keywords:** Aluminum complex; Single-site catalyst; Ring-opening polymerization; Polylactide; Polycaprolactone

## Synthesis of silver nanoparticles using carboxymethyl cellulose from water hyacinth biomass for the colorimetric detection sensor of Hg (II) ions

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Mercury ion ( $\text{Hg}^{2+}$ ) is one of the most hazardous heavy metal contaminants that can affects human life and ecosystem. In this work, the colorimetric sensors have been developed to detect mercury ions from natural water sources using silver nanoparticles (AgNPs). The AgNPs were synthesized using carboxymethyl cellulose (CMC) obtained from water hyacinth biomass. The successful formation of CMC-AgNPs was confirmed by UV-vis spectroscopy with a surface plasmon resonance band at 410 nm. CMC-AgNPs were also characterized using X-ray diffraction (XRD), flourier transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDX), and zeta potential analysis. The yellow color of the CMC-AgNPs solution changed to colorless when exposed to  $\text{Hg}^{2+}$  due to redox reactions between  $\text{Hg}^{2+}$  and CMC-AgNPs. The effects of different parameters such as CMC-AgNPs concentration, reaction time, and pH for detecting  $\text{Hg}^{2+}$  were studied. This sensor is aimed to use with artificial intelligence or AI colorimetric detection.

**Keywords:** Biomass; Silver nanoparticles; Mercury sensors; Colorimetric sensors

## Titanium complexes bearing tridentate [ONN]-phenolate ligands for the ring-opening polymerization of cyclic ester monomers

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In this work, twelve titanium complexes supported by tridentate [ONN]-phenolate ligands were synthesized and characterized by NMR spectroscopy. All titanium complexes were active initiators for the ring-opening polymerization of *rac*-lactide (*rac*-LA) and  $\epsilon$ -caprolactone ( $\epsilon$ -CL) in toluene at 70 °C. The polymerization of  $\epsilon$ -CL was found to be faster than that of *rac*-LA. All polymerizations exhibited living characteristics, as evidenced by narrow dispersity values. The theoretical molar mass values were in good agreement with the theoretical values calculated based on three initiating groups per titanium center. It was discovered that no significant stereocontrol was achieved for the *rac*-LA polymerizations, i.e., all complexes produced atactic PLAs ( $P_m = 0.50$ – $0.52$ ). The effects of electronic and steric from ligand substituents were found to have a significant impact on the polymerization activities. Kinetic investigations revealed that the zeroth-order and first-order kinetics in monomer concentration were exhibited for the ROP of *rac*-LA and  $\epsilon$ -CL, respectively.

**Keywords:** Titanium complexes; Ring-opening polymerization; Polylactide; Polycaprolactone; *rac*-Lactide;  $\epsilon$ -Caprolactone



## A study of N-heterocyclic imidazolium-functionalized cage-like silsesquioxane on transition metals as a catalyst

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Cage-like silsesquioxanes (SQ) or polyhedral oligomeric silsesquioxanes (POSS) have been paid attention to wide-range of applications (e.g. catalysis, sensing, electronics, etc.) because cage-like SQ show properties like organic-inorganic hybrid compounds. In other words, cage-like SQ bearing organic functional groups show ability to develop chemical compounds with various properties such as nano size, chemical inertness, and high thermal stability. One class of interesting organic functional groups is N-heterocyclic carbenes (NHC), which have been highly modified as support in particular transition metals to serve as catalysts. Interestingly, in earlier work, our group successfully investigated that cage-like SQ bearing NHC/imidazolium salt on palladium nanoparticles show as a highly active catalyst. However, palladium element provides some drawbacks such as toxicity, high price, and low abundance. Therefore, in this work, we are inspired to investigate the composite between copper(II) acetate and 1-methylimidazole functionalized octakis(3-chloropropyl)octasilsesquioxane (POSS-Cl) to directly catalyze alkyne-azide cycloaddition (CuAAC) reactions with follow on recent trends, including green and sustainable materials processing and catalytic performance.

**Keywords:** Silsesquioxanes; N-heterocyclic carbenes; Catalyst; Copper

## Facile synthesis of silsesquioxane appended with 1,8-naphthalimide benzo-15-crown-5 chemosensor

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Polyhedral oligomeric silsesquioxane (POSS) is a hybrid inorganic-organic material, which finds extensive demand across various applications, particularly as functional materials for sensors. This work designs and synthesizes a novel POSS chemosensor utilizing a heteroditopic concept. The incorporation of cation receptor, benzo-15-crown-5, within the POSS structure was achieved using low cost catalysts and conducting reactions at low temperatures. In particular, the synthesis involved the use of copper-catalyzed azide-alkyne cycloaddition (CuAAC) to construct a silsesquioxane chemosensor based on 1,8-naphthalimide benzo crown ether. The “click” reaction allowed the reaction to proceed at room temperature while providing a good product yield. The resulting product was characterized by  $^1\text{H}$ ,  $^{13}\text{C}$ ,  $^{29}\text{Si}$ , COSY, HMQC nuclear magnetic resonance spectroscopy (NMR), and mass spectrometry to confirm that the substituent *N*-(benzo-15-crown-5)-4-(1,2,3-triazole)-1,8-naphthalimide (PNC) was incorporated into the POSS structure.

**Keywords:** Silsesquioxane; 1,8-Naphthalimide; benzo-15-crown-5; Click chemistry; Sensor

## Synthesis of zeolite sodium A, X, Y from silica gel bead

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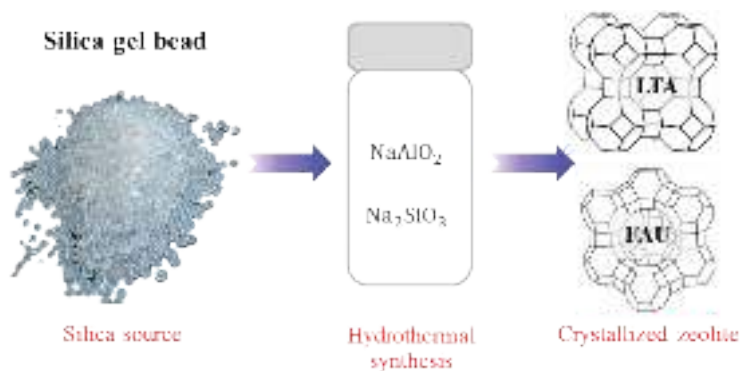
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Accumulation of industrial or agricultural solid waste leads to increased environmental concern. Some solid waste should be recycled or converted to value-added products. The interest of this research is silica gel, commonly used as a desiccant in packaging and discarded as solid waste. Silica gel has a high percentage of silica which can be used as a precursor in zeolite synthesis. This work aims to use silica gel waste as a silica source to synthesize zeolite A, X and Y. The zeolite products were characterized by X-ray diffraction and scanning electron microscopy. The phase-pure of zeolites A, X, and Y in sodium forms are successfully synthesized from silica gel waste by the conventional hydrothermal method.

**Keywords:** Silica gel bead; Zeolite A; Zeolite X; Zeolite Y



## Electrochemical self-coupling of benzyl halides catalyzed by cobalt complex with pincer based ligand

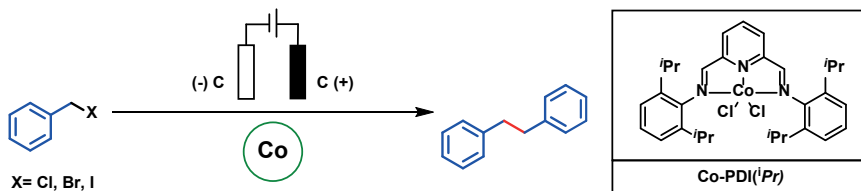
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Metal-catalyzed cross-coupling is a key reaction to access valuable organic molecules by C—C bond formations. Several transition metals have been utilized to catalyze the cross-coupling reaction, particularly the second-row and third-row transition metal, which are costly and less abundant. Methodologies for C—C bond coupling reaction catalyzed by first-row transition metal are being developed. In this report, we described a cobalt complex supported by pyridine diimine pincer which exhibited their ability in the electrochemical homo-coupling of organohalides. According to the cyclic voltammetry results, the addition of benzyl halides to the cobalt complex under argon atmosphere resulted in the current enhancement, leading to the presence of the homo-coupling reaction. The reactions proceeded through radical intermediates, generated by electricity. This reaction can be further developed as a greener methodology, as it reduces the by-product from the chemical reductant which is harmful to both humans and the environment. Benzyl halides were electrolyzed under argon to demonstrate the formation of C—C bond between the radical intermediates, providing bibenzyl as a desirable product.

**Keywords:** Electrosynthesis; C-C bond formation; Self-coupling; Pyridine diimine; Cobalt(II) catalyst



## The effect of polyethylene glycol chain length of nickel bis(aminomethyl)pyridine on hydrogen evolution reaction

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The proximal charge as the secondary coordination sphere in enzyme cofactor shows a crucial role for small molecule activation. This concept has been used to design various chemical catalyst by incorporating pendent polyether chain for hosting redox-inactive cation as a second coordination sphere. Herein, we report the Ni complexes with different chain length of polyethylene glycol (NiBAP<sub>n</sub>). The NiBAP<sub>n</sub> complexes were characterized by IR, UV-vis spectroscopy and their electronic properties were studied by cyclic voltammetry. The synthesized Ni complexes are able to perform electrochemical hydrogen evolution in organic media. The addition of redox-inactive cation to NiBAP<sub>n</sub> complexes, to generate heterobimetallic Ni complexes *in situ*, show the enhancement of hydrogen production, compared to the absence of the redox-inactive cation, showing that the binding of redox-inactive cation to the polyethylene glycol chain can affect the reactivity of the catalyst. The different chain length also imparted different binding ability and therefore, exhibited different hydrogen evolution reaction reactivity.

**Keywords:** Nickel heterobimetallic Complex; Redox-inactive cation; Secondary coordination sphere; Hydrogen evolution



# Industrial and Engineering Chemistry (IE)

## Oral Presentation



## Synthesis of silicon carbide by using rice husk ash from power plant wastes

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This research aimed to investigate the synthesis of silicon carbide (SiC) using silica extracted from rice husk ash and carbon black as the reactants. Magnesium was used as a catalyst during the synthesis process. The reactions were carried out in an alumina crucible, encapsulated in an Argon atmosphere at a temperature of 1200°C. The research focused on exploring various molecular ratios between SiO<sub>2</sub> and Mg to determine their impact on the formation and composition of SiC. To characterize the resulting structures and compositions, X-ray fluorescence (XRF) and X-ray diffraction (XRD) were utilized.

**Keywords:** Silicon carbide, Rice husk ash, Power plant wastes

## Development of neural network architectures for prediction of energy consumption and carbon dioxide emission in natural gas separation process

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Predictive models play an important role in enhancing energy efficiency and reducing greenhouse gas emission in various industrial processes. This study explores the utilization of network architectures including artificial neural network (ANN), convolutional neural network (CNN), and extreme learning machine (ELM) to predict energy consumption and carbon dioxide emission of natural gas separation process. Three neural network architectures are systematically trained and tested to examine the impact of different node numbers and hidden layer configurations on predictive performance. The findings reveal that each neural network architecture exhibits varying strength and weakness in predicting energy consumption and carbon dioxide emission. By identifying the optimal architecture and configuration, this study contributes to the ongoing efforts to enhance sustainability and reduce the environmental footprint of industrial operations for a cleaner and greener production.

**Keywords:** Neural network; Energy consumption; Carbon dioxide emission; Natural gas separation; Sustainable production

## Heat transfer analysis of a microwave reactor using computational fluid dynamics for polymer recycling

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Microwave heating has emerged as an attractive source of heat for polymer recycling processes such as alcoholysis. The rapid localized heating allows for the reaction time for alcoholysis to be decreased from hours to minutes. Despite this, microwave heating does suffer from a shortcoming which is also present in conventional heating i.e., nonuniformity of the temperature distribution. In order to optimize the design on the microwave reactor for large-scale polymer recycling via alcoholysis, it is essential to understand and predict the temperature distribution inside the reactor. This can be achieved through numerical simulations of microwave heating and the hydrodynamics of the system. In this study, a microwave heating model is developed by one-way coupling high frequency electromagnetism, heat transfer and fluid dynamics utilizing the finite element and finite volume methods by conducting two commercial packages i.e., ANSYS HFSS, and Fluent. The focus will be on analyzing the heat transfer mechanisms within the reactor using computational fluid dynamics simulations to accurately capture temperature distribution. Different operating conditions will be used to assess their impact on the temperature uniformity given a microwave heat source.

**Keywords:** Microwave heating; Computational fluid dynamics; Heat transfer analysis

## Beyond the extraction limit – molecular cages as membranes for chemical separations

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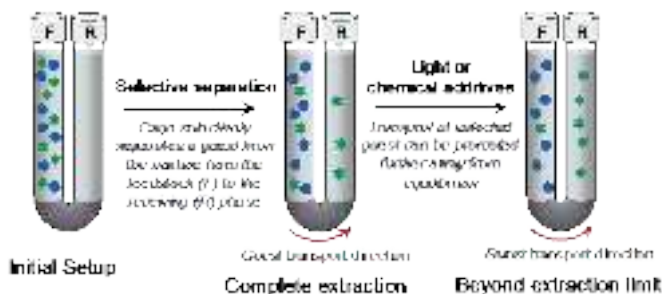
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Chemical separation is essential for several industrial processes such as wastewater treatment, air purification, and drug synthesis. To address contemporary challenges like global warming and limited oil resources, there is a need for more environmentally friendly, energy-efficient, and economically viable separation strategies. In this study, we introduce a water-soluble metal-organic molecular cage as a liquid membrane in a triphasic U-shaped tube system to separate two organic phases: the feedstock and receiving phases. This cage effectively encapsulates specific guest compounds from the feedstock phase and releases them into the receiving phase at ambient temperature. The transport of compounds was monitored by NMR, GCMS and UV-Vis spectroscopy. We demonstrate the use of light or chemical additives to enhance the transport of selected compounds beyond their equilibrium concentrations. Under light stimulation, *o*-fluoroazobenzene is pumped unidirectionally between the arms of a U-tube apparatus, in a realization of “Maxwell’s Demon” on the macroscale. The concentration gradient thus obtained could be further harnessed to drive naphthalene transport in the opposite direction. We have also developed a kinetic model to explain these observations. Furthermore, to expedite transport for industrial applications, we have designed and optimized a slug flow system. This continuous flow system provides improved extraction efficiency by creating more extensive phase contact areas and enhanced mixing through internal circulation within the flow. As a result, we achieve faster transport (within hours), reduce solvent usage, and minimize energy consumption. These findings hold significant industrial relevance, enabling selective separations under environmentally favorable conditions.

**Keywords:** Chemical separation; Host-guest chemistry; Metal-organic cages; Chemical pump; Continuous flow system



# Industrial and Engineering Chemistry (IE)

## Poster Presentation

## Investigation of dyeing polyester with disperse dyes in an oil/water dual-phase system

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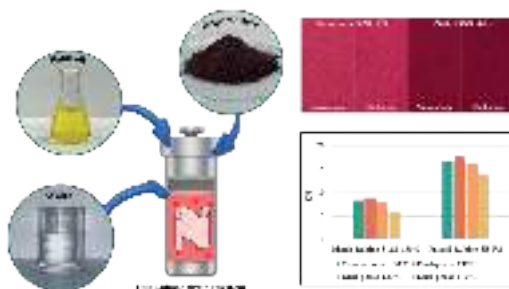
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This study aims to investigate the feasibility of dyeing polyester with disperse dyes in an oil/water dual-phase system. Conventional exhaust dyeing of polyester with disperse dyes is typically conducted in an aqueous medium at a dyeing temperature of 130°C for 30 min, using a dispersing agent as a dyeing auxiliary. In this dual-phase system, palm oil served as a non-aqueous phase with various oil-to-water ratios, and no dispersing agent was added. This investigation employed two disperse dyes: Dianix Rubine S-2G150%, representing a high-energy disperse dye, and Palanil Rubine SE-FG, representing a medium-energy disperse dye. The dyebath's pH was adjusted to 4 using acetic acid, and polyester was dyed with 1% owf disperse dyes at temperatures of 110, 120 and 130°C for 30 min. The color yields (K/S values) of the dyed polyester fabrics were assessed and compared between the two dyeing systems. The results demonstrated that dyeing polyester in a dual-phase system with both dye types, even at 120°C, yielded similar K/S values compared to the conventional dyeing process. The optimal oil-to-water ratios were found to be 1:30 for Dianix Rubine S-2G150% and 1:90 for Palanil Rubine SE-FG. Color yield could be built-up in the dual-phase system, comparable to conventional dyeing. Additionally, the fastness to washing and rubbing, both dry and wet, were similar for both dyeing systems. Hence, an oil/water dual-phase dyeing system was successfully applied for polyester dyeing at lower temperatures without the inclusion of a dispersing agent in the dyebath for both high and medium-energy disperse dyes.

**Keywords:** Polyester; Disperse dye; Dyeing; Oil/water dual-phase system



## Effect of fly ash to alkali activator ratios on pore properties of porous fly ash-based geopolymer under curing by microwave irradiation

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Porous geopolymers have become one of the most promising inorganic porous materials due to their cost-effectiveness and eco-friendliness, as well as their thermal and chemical stabilities, and multiple applications. In addition, porous geopolymers can be utilized to purify the hydrogen gas as CO<sub>2</sub> adsorbents in hydrogen production. This research aimed to study the effect of fly ash (FA) on the alkali activator ratio under curing by microwave irradiation on the pore properties and specific surface area of porous geopolymers. The alkali activator was prepared by mixing Na<sub>2</sub>SiO<sub>3</sub> solution with 10M NaOH solution by 2.5 in mass ratio. The ratios of FA to the alkali activator were 60:40, 50:50, and 40:60 by weight. After that, the fly ash and alkali activators were mixed thoroughly by the Hobart mixer for 10 minutes, and then the slurry was cast to mold before curing in a microwave oven for 10 minutes at an output power of 800 W. The amount of alkali activators affected the structural and physical appearance of porous fly ash-based geopolymer under microwave curing. Microstructure characterized by SEM revealed that a significant amount of alkali activators led to the development of the porous structure for the geopolymers. Moreover, the specific surface area was determined by BET. The phase composition, chemical bonding, and thermal properties were investigated by XRD, FTIR, and DSC analysis, respectively. In conclusion, the formulation with a 40:60 FA to alkali activator ratio presents a high surface area, showcasing enhanced structural characteristics and potential for CO<sub>2</sub> adsorption in hydrogen production.

**Keywords:** Geopolymer; Microwave; Alkali activator; Fly ash; Foams

## Amino acid fertilizer derived from poultry bio-waste

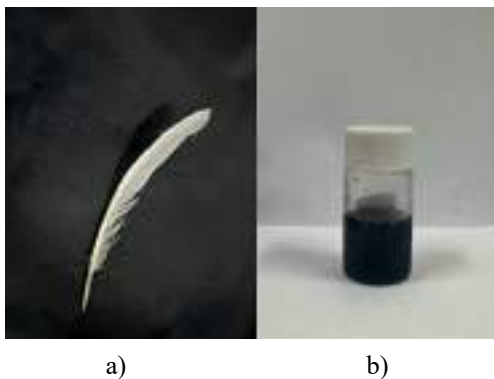
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Rapid growth in food industry has resulted in increasing bio-waste causing problem to surrounding environment. One of the bio-wastes are chicken feathers from poultry processing industries which are generally disposal in landfills. In this study, chicken feathers were hydrolyzed with 6M  $\text{H}_2\text{SO}_4$  for 5 hours in order to produce amino acid fertilizer. The hydrolysate is analyzed by CHN analyzer resulting in an approximate amino acid content in the feather hydrolysate. Furthermore, amino acid analyzer is employed to identify amino acid in the chicken feather hydrolysate. The result show cystine, glutamic, serine, proline and leucine are major amino acids with concentration higher than 5% by wt by weight in the chicken feathers. After hydrolysis, significant amount of amino acids are reduced due to strong hydrolysis conditions. Tomato, as test plants, is given 10ppm and 5 ppm hydrolysate solution to study its effect on plant growth. This liquid fertilizer may be used to generate valued added product from bio-waste, promoting zero waste economy.

**Keywords:** Chicken feather; Amino acid; Fertilizer; Bio-waste; Zero waste



**Figure 1.** a) chicken feather b) feather hydrolysate

## Ion exchange capacity and ionic conductivity of polyvinyl alcohol and nanocellulose based anion exchange membranes

Piyamad Kaewkoon<sup>1</sup>, Supatta Midpanon<sup>1</sup>, and Pinsuda Viravathana<sup>1,2\*</sup>

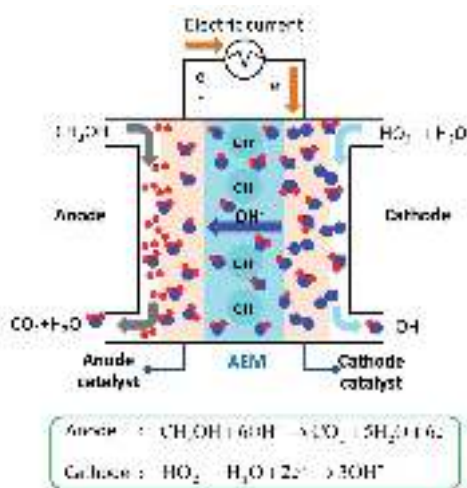
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This research is focused on a facile way of preparing anion exchange membranes (AEMs) based on polyvinyl alcohol (PVA) and nanocellulose (NC) from oil palm empty fruit bunch for anion exchange membrane fuel cells (AEMFCs). Both PVA and NC were modified by the addition of poly (propylene glycol) diglycidyl ether (PPGDGE) (at 5-30%PPGDGE). Then, the modified PVA and NC were mixed and casted to form a modified PVA/NC composited membrane. By increasing NC in the composited membrane, degree of swelling and water uptake properties were investigated. Besides, the alkaline stability, the methanol permeability, and the transport properties were studied. For the transport properties, ion exchange capacity (IEC) was determined using Mohr's titration method and ionic conductivity (IC) was measured using two-probe alternative current electrochemical impedance spectroscopy.

**Keywords:** Anion exchange membrane fuel cells; Nanocellulose; Polyvinyl alcohol; Ion exchange capacity; Ionic conductivity



## The opinion of citizens on governance management of the very small solid waste power plant in Thailand

Suwannee Missita and Wisakha Phoochinda

This study aimed to investigate the opinion of community leaders and citizens towards the Very Small Power Producer (VSPP) using municipal solid waste in Thailand. The questionnaire was employed to community leaders and citizens around the Very Small Municipal Solid Waste Power Plants (VSMSWPPS) by available technologies (stoke incineration technology, gasification technology, anaerobic digestion technology, landfill gas to energy technology), with a totaling of 610 samples by convenient sampling. Descriptive statistics were used to analyze data, including frequency and percentage.

The survey results found that most respondents were citizens, lived in the community more than five years before the power plant was developed, and were merchants. The citizens around the solid waste power plant were slightly aware of the management, with the most coming news from their friends. The average opinion on the governance of the power plant was at a low level, with the highest approval on the issue of the solid waste power plant having effective use of land in the community for electricity generation at a moderate level. In addition, the average opinion on the governance of the public section was at a moderate level, with the highest approval on the issue of the relevant government agencies involved in solving environmental problems arising from the operation of the solid waste power plant at a moderate level. While the average opinion on governance of people was at a low level, with the highest approval on the issue the citizens separated the type of waste for reuse at a moderate level and the least consensus on the issue of people taking part in the decision-making on the solid waste power plant project in the community at a low level.

**Keywords:** Community leaders and citizens; Solid waste; Environmental; Very small power producer; Very small municipal solid waste power plants

## Synthesis of biphasic calcium phosphate porous ceramic from fish scales

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Recently, the circular economy model concept has gained increasing attention for sustainable ecosystems. This model aims to reduce waste and promote reusing and recycling materials to make a new product. Fish scales are seafood industrial waste that has been used as natural raw material for synthesized hydroxyapatite (HA) in many applications. In this research, fish scales were utilized as natural raw material for fabricating biphasic ceramics of hydroxyapatite (HA) and tricalcium phosphate (TCP). Biphasic calcium phosphate powders were synthesized from fish scales via alkaline treatment and calcination at 1000 and 1200 °C. X-ray diffraction (XRD) and X-ray fluorescence (XRF) techniques were used to investigate the crystallinity and chemical composition of synthesized materials respectively. Then, the biphasic calcium phosphate was fabricated to porous granule and sintered at 1300 °C. The morphology of biphasic calcium phosphate granule was observed by scanning electron microscope (SEM). The characterization of the pore size and their porosity was also investigated by the mercury porosimetry technique. The biphasic calcium phosphate fabricated from fish scales presents a porous structure with approximately 60 % porosity.

**Keywords:** Biphasic calcium phosphate; Porous ceramic; Fish scale; Hydroxyapatite (HA); Tricalcium phosphate (TCP)



## Preparation and characterization of oil palm fibers from oil palm trunks for industrial applications

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Thailand is the third-place country in the world that exports palm oil, even though it was only 3.8% of the global total of palm oil producers in 2021. The country's palm oil production is mainly in the southern area. However, the central, northeastern, and northern regions also find harvested oil palm areas. Usually, the commercial lifespan of the oil palm tree is 25 years after decreasing its fruit production. Then, the new palms are planted for the next cycle of cultivation, leaving a large amount of oil palm trunks as biomass waste on the plantation. However, these oil palm fibers have value and can be utilized as raw materials in the paper and construction industries. Therefore, this work focuses on the chemical, physical, and mechanical properties of the oil palm trunk fibers treated under various conditions. The fibers were treated with 0% to 5% sodium hydroxide (NaOH) solutions for different reaction times. Then, the TAPPI standard was used to investigate the chemical components of treated fibers, including cellulose, hemicellulose, lignin, and ash contents. The crystallinity of the fibers was measured using X-ray diffraction (XRD). Fibers' length, morphology, and microstructure were analyzed using an optical microscope and a Scanning Electron Microscope (SEM). Furthermore, the mechanical properties of the treated fibers, such as tensile strength, tear resistance, and burst strength, were determined.

**Keywords:** Oil palm; Industry; Biomass; Waste material; Chemical treatment

# Material Chemistry and Nanotechnology (MN)

## Oral Presentation



## Asymmetric D-A-D' type hybridized local and charge transfer fluorophores as deep-red/near-infrared emitters for efficient non-doped OLEDs

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Recently, deep-red/NIR OLEDs have recently received more and more attention. However, efficient non-doped deep-red/near-infrared (NIR) emitters are limited owing to their intrinsic narrow band gap that affects low fluorescence emission efficiency giving rise to low device performance. The asymmetric D-A-D' type deep-red fluorophore of **TNZPPI** comprising of naphthothiadiazole (NZ) as an acceptor (A) core functionalized with two donor (D) units of 1-phenyl-1H-phenanthro[9,10-d]imidazole (PPI) as D and triphenylamine (TPA) as D' has been reported as the one of the good non-doped deep-red hybridized local and charge transfer (HLCT) emitter to realize OLED with deep-red emission (690 nm) and EQE<sub>max</sub> of 2.48%. Herin, to further improve the performance and red-shift the emission to NIR of such fluorophore, two new asymmetric D-A-D' type HLCT emitters, **DPANZPPI** and **DMANZPPI** are designed and synthesized. As compared to TPA in **TNZPPI**, **DPANZPPI** and **DMANZPPI** employ stronger donor units of N,N-diphenylnaphthalen-1-amine (DPA) and N,N-dimethylaniline (DMA) as D', respectively. The experimental studies and the DFT calculations indicate that both molecules possessed HLCT characteristics with high thermal and electrochemical stabilities and decent hole mobility. **DPANZPPI** and **DMANZPPI** show deep red and NIR emissions with PLQY of 40% and 32% in neat films, respectively. They are successfully applied as non-doped emitters (EML) in the OLEDs (ITO/HATCN (6 nm)/TAPC (30 nm)/TCTA (10 nm)/EML (60 nm)/B3PymPm (40 nm)/LiF (1 nm)/Al (100 nm). The **DPANZPPI**-based device achieves deep red EL emission (692 nm) with an improved EL performance ( $V_{on} = 2.5$  V and EQE<sub>max</sub> = 4.9%) compared to the **TNZPPI**-based device ( $V_{on} = 2.8$  V and EQE<sub>max</sub> = 3.2%). Pointedly, the **DMANZPPI**-based device shows NIR emission (731 nm) with a high EQE<sub>max</sub> of 1.92%, which is among the best-reported non-doped NIR OLEDs.

**Keywords:** Deep-red emitter; NIR emitter; Organic light-emitting diode; Hybridized local and charge transfer; Naphthothiadiazole

## Boosting OLEDs performance via hot exciton mechanism: The study of heteroatom and different the number of donor unit effects on D- $\pi$ -A type emitters

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The enhancement of singlet exciton utilization efficiency through reversed intersystem crossing (RISC) process has received more attention and developed for highly efficient OLEDs. In this work, six compounds of donor- $\pi$ -acceptor (D- $\pi$ -A) type fluorescent materials, namely **IDL-1**, **IDL-2**, and **IDL-3** for **IDL-TAZ** series, **BTI-1**, **BTI-2** and **BTI-3** for **BTI-TAZ** series using 5,10-dihydroindolo[3,2-*b*] indole (**IDL**) and 10*H*-benzo[4,5]thieno[3,2-*b*]indole (**BTI**) as an donor group and 2,4,6-triphenyl-1,3,5-triazine (**TAZ**) derivative as an acceptor unit were designed, synthesized, characterized. All compounds exhibited good thermal stability. A large bathochromic effect due to the intramolecular charge transfer (ICT) and the aggregation induced emission (AIE) were observed. Their doped OLEDs with mCP as a host material were successfully fabricated. The doped devices of **IDL-TAZ** series showed green emission with high luminance and exceeding maximum quantum efficiency (EQE) over 5%. Among them, the emitter **IDL-3** showed the highest EQE value of 7.50%. In case of **BTI-TAZ** series, sky-blue emission was observed. The emitter **BTI-3** provided maximum EQE value of 3.62%. Interestingly, the doped devices of all emitters exhibited high exciton unitization efficiency ( $\eta_s$ ) of 69, 60, 71, 41, 40 and 86% for **IDL-1**, **IDL-2**, **IDL-3** **BTI-1**, **BTI-2** and **BTI-3**, respectively. According to the Lipper-Mataga plot, the study of the first ten singlet ( $S_1$ - $S_{10}$ ) and triplet ( $T_1$ - $T_{10}$ ) excited states, and natural transition orbitals (NTOs) analysis, are solid evidence that the reverse intersystem crossing (RISC) process occurred in high-lying triplet excited state through "hot exciton" channel.

**Keywords:** Hot exciton; Exciton utilization efficiency; OLEDs

## Development of near-infrared phosphorescent organoiridium(III) complexes bearing 2-arylquinoxaline-based cyclometalated ligands

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Since near-infrared (NIR) light is invisible to the naked eyes and penetrates living tissues, NIR light-emitting devices are applicable as light sources in the fields of medical science and security technology. In the case of organic light-emitting diodes (OLEDs), phosphorescent materials are superior to traditional fluorescent ones in terms of exciton generation efficiency. However, due to the energy gap law, few examples have so far been reported for practical NIR phosphorescent materials with high photoluminescence (PL) quantum yields ( $\Phi_{\text{PL}}$ ). Here we report synthesis and NIR PL properties of bis-cyclometalated iridium(III) complexes bearing 2-arylquinoxaline-based cyclometalated ligands, namely, **Ir-1-Me** ( $-\text{CF}_3$ ) and **Ir-2-Me** ( $-\text{CF}_3$ ) (Fig. 1), especially focusing on the impact of the 3-trifluoromethyl group on the PL characteristics.

As shown in Fig. 2, **Ir-1-Me** exhibited deep red emission with a  $\Phi_{\text{PL}}$  of 0.60 in toluene (PL maximum  $\lambda_{\text{PL}}$ ; 662 nm), whereas the 3-trifluoromethyl analogue **Ir-1-CF<sub>3</sub>** showed NIR emission with a  $\Phi_{\text{PL}}$  of 0.14 under the same conditions ( $\lambda_{\text{PL}}$ ; 713 nm). This indicates that introduction of the 3-trifluoromethyl group in place of the 3-methyl group led to an effective red shift of PL to the NIR region, although the  $\Phi_{\text{PL}}$  is somewhat reduced. We successfully fabricated OLEDs using the developed complexes, and the NIR electroluminescence was obtained from the devices upon application of electric voltage.

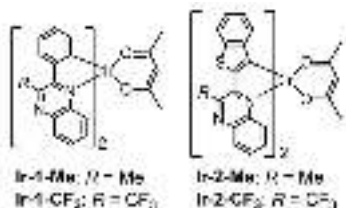


Fig. 1. Structures of Ir-1-Me ( $-\text{CF}_3$ ) and Ir-2-Me ( $-\text{CF}_3$ ).

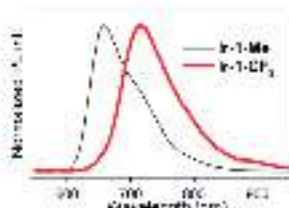


Fig. 2. PL spectra of Ir-1-Me and Ir-1-CF<sub>3</sub> in deaerated toluene at rt.

**Keywords:** Iridium complex; Phosphorescence; Near-infrared emission; Electroluminescence; Organic light-emitting diode

## Facile synthesis of highly active and durable carbon composite as a non-precious metal oxygen reduction reaction electrocatalyst in alkaline media

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Designing high performance and durable non-precious metal oxygen reduction reaction (ORR) catalyst is the key strategy to push the high energy conversion efficiency and zero-carbon dioxide emission fuel cell technology to global market. The carbon composite catalyst is simply fabricated by pyrolyzing the solid mixture of iron (II) acetate, 2-methyl imidazole, and carbon powder at 900 °C under a nitrogen atmosphere. The ORR performance for the synthesized non-precious metal catalyst against the precious Pt/C catalyst is electrochemically investigated using cyclic voltammetry (CV) and linear sweep voltammetry (LSV) techniques under alkaline solution. CV result indicates the fabricated carbon composite catalyst is thermodynamically ORR active. The ORR kinetic ( $E_{1/2}$ ) evaluated by LSV technique for the carbon composite catalyst is found to be 0.850V vs RHE, while the Pt/C catalyst generates  $E_{1/2}$  value of 0.853 V vs RHE under O<sub>2</sub>-saturated 0.1 M KOH solution. The fabricated non-precious metal catalyst exhibits 10 mV more efficient to facilitate ORR under alkaline media as compared to the precious Pt/C catalyst. Furthermore, the synthesized carbon composite catalyst undergoes ORR process with a direct 4-electron transfer number and exceptionally low HO<sub>2</sub><sup>-</sup> intermediate concentration. The effect of iron, nitrogen and carbon precursors on the ORR performance will be discussed. The phase and surface area of the catalyst is physically examined using XRD and BET techniques. On the other hand, accelerated durability test (ADT) over 5000 ORR cycles for the carbonized catalyst in comparison to the precious Pt/C catalyst will also be presented.

**Keywords:** Oxygen reduction reaction; Carbon composite; Electrocatalyst; Fuel Cell

## Preparation and characterization of MoS<sub>2</sub>/lignin-based carbon nanocomposite fibers for supercapacitor electrodes

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Carbon nanofibers derived from renewable resources such as lignin have gained much attention for the use as supercapacitor electrodes due to their excellent properties including high specific surface area, high porosity, good chemical and thermal stability, and high electrical conductivity. However, in practical, carbon materials do not meet the rising need for high specific capacitance. To improve their capacitive performance, the integration of the carbon nanofibers with transition metal sulfide is proposed. In this study, molybdenum disulfide/lignin-based carbon nanocomposite fibers (MoS<sub>2</sub>/CNFs) are explored for their use as free-sanding supercapacitor electrodes. Lignin-based carbon nanofibers are prepared via a facile technique of electrospinning while MoS<sub>2</sub> is synthesized via a hydrothermal process. The electrochemical performance of the MoS<sub>2</sub>/CNFs electrodes is investigated by cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), and electrochemical impedance spectroscopy (EIS), in comparison to that of the CNFs electrodes. The addition of MoS<sub>2</sub> increases specific capacitance of the CNFs more than 2 times. The MoS<sub>2</sub>/CNFs is therefore a promising material for supercapacitor electrodes.

**Keywords:** Carbon nanofibers; Molybdenum disulfide; Lignin; Supercapacitor; Nanocomposite

# Solution plasma-assisted integration of Mxene nanosheets with iron and nitrogen-doped carbons as electrocatalysts for oxygen reduction reaction

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The oxygen reduction reaction (ORR) occurring at the cathode is pivotal in determining the overall performance of hydrogen fuel cells. Among various proposed catalysts, iron–nitrogen-doped carbon (Fe–N–C) catalysts have demonstrated outstanding ORR activity and stability, which has the potential to rival commercially available Pt-based catalysts. Integrating Fe–N–C catalysts with highly conductive materials (e.g., CNT, graphene, or Mxene) has emerged as an effective approach to enhance their ORR activity. Herein, we synthesized Fe–N–C from acrylonitrile (C<sub>3</sub>H<sub>3.5</sub>N) with the dispersion of Mxene nanosheets using Fe as electrodes via a solution plasma process. During the plasma process, Fe–N–C was formed and self-attached on MXene. Subsequently, the Fe–N–C/Mxene composites were post-treated at 700 °C under Ar flow. The X-ray diffraction (XRD) patterns revealed the diffraction peaks corresponding to the amorphous phase of Fe–N–C and the Mxene phase. The scanning electron microscopy (SEM) image confirmed the presence of Fe–N–C on the Mxene surface. For the electrochemical measurements for ORR activity, a three-electrode system equipped with a rotating disk electrode (RDE) in O<sub>2</sub>/N<sub>2</sub>-saturated 0.1 M KOH solution was employed. The cyclic voltammetry (CV) and linear sweep voltammetry (LSV) curves demonstrated that the ORR activity of Fe–N–C/Mxene composite, including onset potential, current density, and half-wave potential, was enhanced when compared to single Mxene and Fe–N–C.

**Keywords:** Fe–N–C; MXene; Electrocatalyst; Solution plasma process; Oxygen reduction reaction

## Parameter optimization for the synthesis of hybrid gold nanoparticle-carbon dot colloids and their luminescent properties alteration

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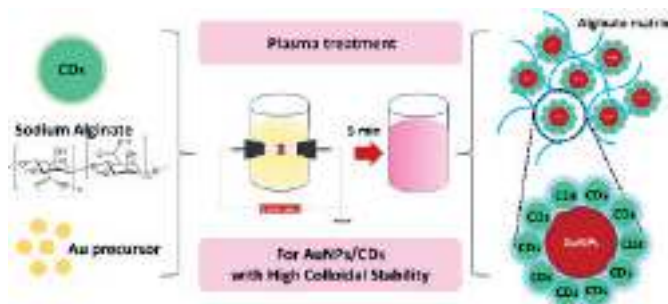
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In this study, we present the synthesis of hybrid nanoparticles composed of gold nanoparticles (AuNPs) and green-light-emitting carbon dots (CDs) via a two-step process. Firstly, green-light-emitting CDs were synthesized through a hydrothermal method. Subsequently, we generated plasma in a mixed solution of a gold precursor (i.e., gold (III) chloride trihydrate) and CDs to create the hybrid AuNPs/CDs. Our research focused on investigating the influence of critical parameters on the synthesis process. We explored the impact of adding a stabilizer, sodium alginate, on the colloidal stability of the AuNPs/CDs. The effects of varying plasma discharge times and the ratio between gold precursor and CDs were examined. Our findings demonstrated that including sodium alginate is critical in achieving stable AuNPs/CDs colloidal suspensions. Furthermore, the plasma treatment duration and the ratio between gold precursor and CDs significantly influenced the colloidal stability, shedding light on fine-tuning these parameters for precise control over the synthesis process. Notably, the synthesized AuNPs/CDs exhibited a pronounced blue shift in luminescence compared to the pristine CDs. This research offers valuable insights into the controlled synthesis of AuNPs/CDs. It highlights the importance of tailoring experimental conditions to achieve the desired properties, opening doors to various nanotechnology and materials science applications.

**Keywords:** Carbon dots; Gold nanoparticles; The plasma treatment



## Development of colloidal cellulose nanocrystal suspensions as a sprayable PM<sub>2.5</sub> remover

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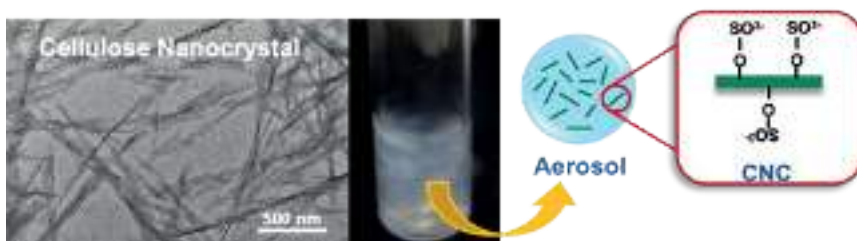
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Particulate materials with an average aerodynamic diameter less than 2.5  $\mu\text{m}$  or PM<sub>2.5</sub> has been increasingly posing critical risks to human health and environmental problems. Apart from conventional dry method, such as air filtration and electrostatic air treatment for alleviating particulate matter problem, we proposed a wet scrubbing method utilizing colloidal cellulose nanocrystal (CNC) suspensions for suppressing PM<sub>2.5</sub> pollution. CNCs were extracted from nata de coco by sulfuric acid hydrolysis. The extracted CNCs were characterized by dynamic light scattering, transmission electron microscopy, FT-IR spectroscopy, and X-ray diffraction. The PM<sub>2.5</sub> capture efficiency of the purified colloidal CNC suspensions was evaluated and compared with distilled water microdroplets by the specifically designed device. We found that the PM<sub>2.5</sub> removal efficiency tested with the designed device were 73.1% and 17.1% when the polluted air was sprayed with 1% (w/w) colloidal cellulose nanocrystal suspension and distilled water, respectively. The mechanism of enhanced PM removal efficiency was also proposed.

**Keywords:** Cellulose nanocrystal, Particulate materials, Wet scrubber, Dust suppression



**Figure 1.** Overview of cellulose nanocrystalline suspensions for use as sprays.

## Colorimetric sensing of polymers by using polydiacetylene/zinc (II) ion/zinc oxide nanocomposites: Effects of solvents and cationic surfactant

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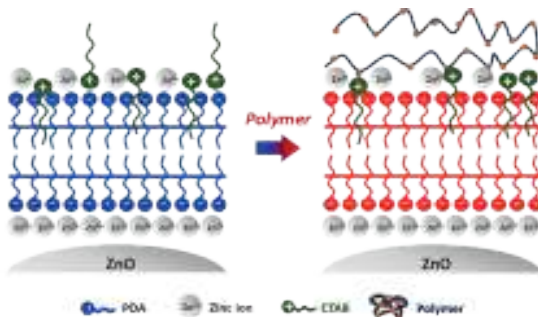
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Polymers are widely used materials for products in everyday life. To identify polymers, several methods such as Raman spectroscopy, Fourier-transform infrared spectroscopy (FT-IR), and Differential scanning calorimetry (DSC) are employed with high accuracy. However, these techniques are expensive and time consuming. Colorimetric sensors are alternative methods, which are simple and cost-effective. Polydiacetylene (PDA)-based sensors are color-responsive upon exposure to different types of stimuli. This unique optical property allows for applications such as thermosensors, chemosensors, and photosensors. This study expands the utilization of PDA-based colorimetric sensors for detecting various types of polymers. PDA/zinc (II) ion/zinc oxide nanocomposites are synthesized in organic solvents. A cationic surfactant, cetyltrimethylammonium bromide (CTAB) is added. The PDA/zinc (II) ion/zinc oxide-CTAB sensors exhibit colorimetric response to polymers with partially negative charge due to the interaction between the functional group of polymer and the CTAB headgroup. The types of organic solvent and CTAB concentrations are important parameters for tuning the sensitivity. Our discovery extends the utilization of PDA-based materials in polymer sensing applications.

**Keywords:** Polydiacetylene; Nanocomposite; Colorimetric sensing; Solvent effect; Cationic surfactant



## Polydiacetylene-based materials for colorimetric sensing of fatty acids

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Oleic acid, a monounsaturated fatty acid, is the most plentiful fatty acid that causes adipose tissue in the human body. Although it has positive impacts on various tissues, it may affect the cardiovascular system. For example, it decreases the myocardial infarction rate and reduces systolic blood pressure. Therefore, it is important to explore a rapid method for detecting oleic acid. In this study, we introduce polydiacetylene/zinc(II) ion/zinc oxide nanocomposites as colorimetric sensors for detecting oleic acid. It was found that the nanocomposites dispersed in ethanol exhibited blue-to-red color transition when exposed to oleic acid. The use of other solvents such as butanol, hexanol, octanol, 1,4-dioxane and toluene affected the sensitivity of nanocomposites. Furthermore, the incorporation of cetyltrimethylammonium bromide (CTAB) into the structure of the nanocomposites resulted in an increase of sensitivity. The paper-based sensor can be fabricated and utilized as a mobile test kit. Our study extends the utilization of PDA-based materials as sensors in the food industry.

**Keywords:** Polydiacetylene; Sensor; Smart materials; Fatty acids

## Quercetin mediated Ag@Au core-shell nanoparticles: Synthesis, characterization and applications

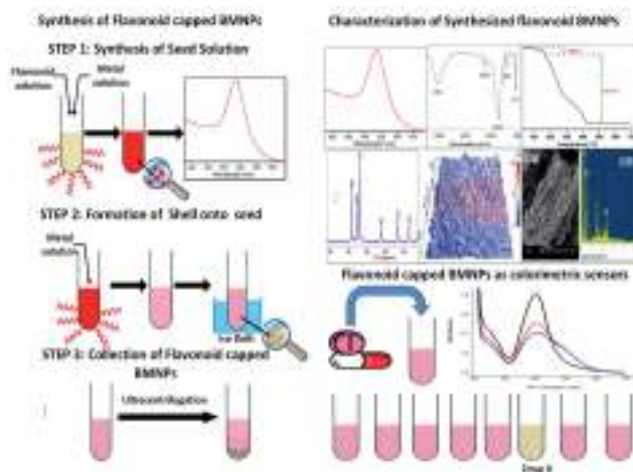
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In this study, quercetin mediated Ag@Au core-shell nanoparticles (Querc-Ag@Au NPs) were synthesized by stepwise chemical reduction. UV-visible spectra of quercetin mediated AgNPs based core appeared at 416 nm. On reacting synthesized silver nanoparticles with gold solution, shift of uv-visible absorbance to 528 nm confirmed the formation of gold nanoshell. Querc-Ag@Au NPs were mixed with solutions of various active pharmaceutical ingredients (APIs). Only Levofloxacin was positively sensed by Querc-Ag@Au NPs. Increase in the concentration of API and decrease in absorbance of quercetin capped Ag@Au nanoparticles were found to be directly proportional to each other. Particle size analysis and poly dispersity index (PDI) of Querc-Ag@Au NPs indicated that average particle size i.e. 75.61 nm with good uniformity (PDI: 0.293). Antibacterial activities of Querc-Ag@Au NPs with and without the presence of levofloxacin were evaluated. Combined effect of both levofloxacin and synthesized Ag@Au NPs showed good inhibition in E.coli (ATCC 25922) and significant inhibition for other organism.

**Keywords:** Quercetin; Core-shell ;Ag@Au; Levofloxacin; Nanosensor



## Synthesis of gold nanoparticles supported on carbon nanomaterials via solution plasma sputtering as electrochemical sensors for mercury(II) ion detection

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Gold nanoparticles (AuNPs) supported on graphene-mixed activated carbon (AuNPs-SGP+AC) nanocomposites have been developed as an electrochemical sensor material for highly sensitive and selective detection of  $\text{Hg}^{2+}$  ions in aqueous solution. The synthesis of AuNPs-SGP+AC nanocomposites involved solution plasma sputtering (SPS) of gold electrodes in different media, with the presence and absence of acetic acid. The resulting AuNPs on SGP+AC exhibited a spherical shape with a particle size ranging from 14 to 27 nm, depending on the conditions of the solution medium. The introduction of acetic acid led to a reduction in particle size, size distribution, and agglomeration of AuNPs. Moreover, the content of AuNPs supported on the SGP+AC increased from 12.0 to 17.7 wt%, thereby enhancing the sensitivity performances of AuNPs-SGP+AC for mercury(II) ion detection. Under the optimum conditions, the Hg oxidation peak current intensity from differential pulse voltammograms (DPVs) of the probe exhibited a linear relationship with the concentrations of  $\text{Hg}^{2+}$  ions over the range of 0.5–37  $\mu\text{M}$ . The sensor demonstrated good selectivity for  $\text{Hg}^{2+}$  ions over several metal ions, including  $\text{Pb}^{2+}$ ,  $\text{Cd}^{3+}$ ,  $\text{Cr}^{3+}$ ,  $\text{Mn}^{2+}$ ,  $\text{Zn}^{2+}$ ,  $\text{Ni}^{2+}$ , and  $\text{Cu}^{2+}$  ions. However, the oxidation peak intensity in the presence of a mixture of all metal ions decreased by 29.3% compared to the condition with pure  $\text{Hg}^{2+}$  ions.

**Keywords:** Carbon nanomaterials; Electrochemical sensors; Gold nanoparticles; Mercury(II) ion detection; Solution plasma process

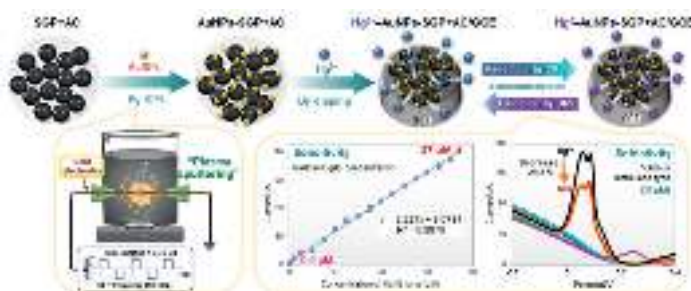


Figure 1 Graphical abstract of this study

## Synthesis and characterization of nitrogen-doped carbon dots from bird's nest for heavy metal detection

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Carbon dots (CDs) are biocompatible nanoparticles easily derived from natural carbon-containing materials. This study focuses on utilizing bird's nests, often discarded as waste, which still retain valuable amino acids and minerals for CD synthesis. Furthermore, we introduce hetero atom of nitrogen (N) doping with CDs with the help of amines (primary, secondary, and tertiary) to enhance the fluorescence properties of these carbon dots. The nitrogen-doped carbon particles derived from the microwave (750 watts, 12 minutes and water solvent) and hydrothermal (180 °C, 15 hours and water solvent) processes were examined for their optical properties using a fluorescence spectrophotometer (Fluorescence and Absorbance Spectrometer, Horiba.). When activated at 350 nm, carbon dots exhibit luminescence, emitting light at 540 nm. Subsequently, we investigate optical properties of these particles change in the presence of different types of ions at varying concentrations (ranging from 10 to 1000 ppm), including Cd<sup>2+</sup>, Pb<sup>2+</sup>, Hg<sup>2+</sup>, Co<sup>3+</sup>, Fe<sup>3+</sup>, Cu<sup>2+</sup>, and Ni<sup>2+</sup>. The high-resolution transmission electron microscopy (HRTEM) analysis helps in determining the size of the CDs within the range of 5-8 nm. Moreover, these carbon dots demonstrate effective quenching with Fe<sup>3+</sup> solutions, suggesting their potential application as sensors for heavy metals, including environmental monitoring. Our endeavors lay the foundation for an eco-friendly and streamlined large-scale production of high-performance heteroatom-doped materials

**Keywords:** Carbon dots; Glycoprotein; Metal ion; Bird nest.



**Figure 1.** Nitrogen-Doped Carbon Dots from Bird's Nest

## Voltammetry of paraquat-based bismuth nanoparticles screen-printed electrodes for environmental surveillance

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In Thailand, paraquat is used for pre-planting weed control in the fields of sugar cane, corn, cassava, and rubber trees. Since the toxic chemical has been used for a long time, Paraquat sensors need to be used to monitor environmental safety. Paraquat (PQ) is a nonselective and high toxicity of weed attraction. The residue paraquat has remained in soil, water, and food chains. Here, we are interested in using the disposable screen-printed electrode to detect paraquat. We also study the electrochemical behavior of bismuth nanoparticles mixing into the carbon ink to fabricate in mass production, namely BiNPs-SPCE. The BiNPs exhibited a good property of an abundance of active sites when the oxidation number of Bi(III) was changed to Bi<sup>0</sup> by the potential applied to SPCE. This attractive analyst occurs in the reversible reaction on BiNPs-SPCEs. The morphology of nanoparticles on the electrode was characterized by scanning electron microscopy (SEM) and energy-dispersive X-ray spectroscopy (EDS). The results show that Bi nanoparticles (BiNPs) are uniformly dispersed on the surface of the screen-printed electrode (SPCE). The voltammetry of BiNPs-SPCEs and SPCEs was investigated using cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS). Differential pulse voltammetry (DPV) was investigated on BiNPs-SPCEs, and SPCEs via mixed-mode chromatography (sorbent of magnetic Microcomposites). The results found that the BiNPs-SPEs show multiples of reduction peaks, and two oxidation peaks show the predominated PQ<sub>1</sub> and PQ<sub>2</sub>, respectively. The comparison of electrochemical sensors between SPCE, BiNPs-SPCEs, and MMCs-BiSPCEs at PQ<sub>2</sub> shows the performance resulting in linearity range, sensitivities, and LOD of the current response, using differential pulse voltammetry (DPV). The mass production of BiNPs-SPCE was successfully fabricated and can potentially be used for environmental surveillance.

**Keywords:** Paraquat; Electrochemical sensors; Disposable screen-printed electrodes; Bismuth nanoparticles; Environmental safety.

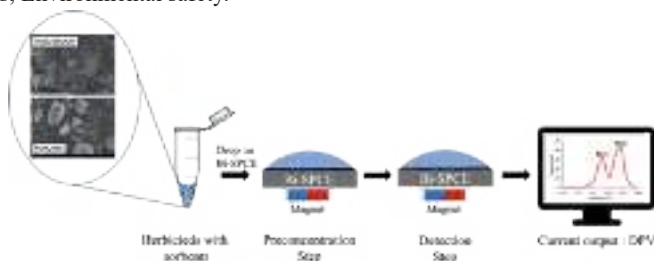


Figure 1. The paraquat detected based BiNPs-SPCE including micro-composites.

## pH-Responsive polymer as a new stable solid electrolyte interphase for water-in-salt battery

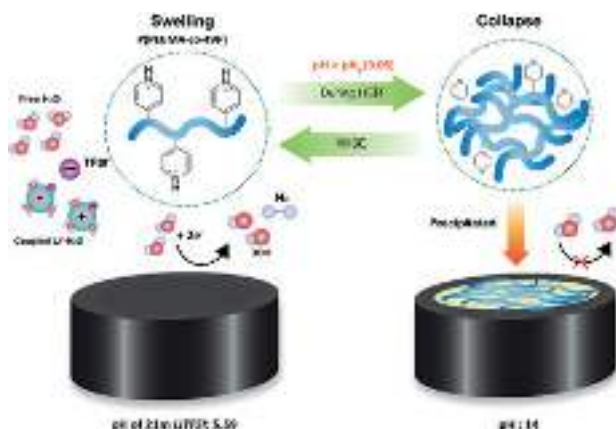
Rossukon Jommongkol<sup>1</sup>, Nantawat Kaekratok<sup>2</sup>, Yachao Zhu<sup>3</sup>, Tobias Burton<sup>1</sup>, Siraprapha Deebansok<sup>1</sup>, Daniel Crespy<sup>2\*</sup>, and Olivier Fontaine<sup>1\*</sup>

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Overcoming the cathodic limits of water -in-salt electrolyte (WiSE ) and developing new active materials is a key for producing aqueous Li-ion batteries (ALIBs) with higher voltage and higher energy. In particular, using additives to improve the performance of Li-ion batteries by stabilizing the solid-electrolyte interphase (SEI) is expected to improve the performance of WiSE. A polymer was designed to display pH-responsive properties in alkaline conditions and to be soluble in WiSE. The addition of the polymer in WiSE allows to expand the window of stability of ALIBs. The polymer prevents water reduction and coprecipitates with LiTFSI salt in alkaline conditions , resulting in a stable SEI layer. The formation of the composite SEI layer is investigated by X-ray photoelectron spectroscopy and electron microscopy. Finally, the addition of the polymer in Mo<sub>6</sub>S<sub>8</sub>/LiFePO<sub>4</sub> full cells subjected to conducting charge/discharge testing improved the Coulombic efficiency up to 96% at 0.5C rate in 10 cycles and with no capacity fading after 10 h discharge.

**Keywords:** Water-in-salt electrolyte; pH-Responsive polymer; Solid electrolyte interphase



**Figure** schematic of the SEI formation with the pH-responsive polymer additives P(PEGMA-co-4VP).

## Preparation and characterization of silver nanowires/cellulose nanofibrils-based conductive paper

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The growing awareness of environmental and health hazards associated with electronic waste (e-waste) has spurred a focus on developing green electronics made from biodegradable materials. In this regard, nanocellulose serves as an eco-friendly substrate for producing conductive paper by incorporating metal nanoparticles, particularly silver nanowires (AgNWs), into cellulose nanofibrils (CNFs) matrices. The synthesis process involves pretreating durian peel waste to obtain CNFs, controlling the synthesis of AgNWs using a polyol method, and blending these components to create composite paper. Material characterization entails scanning electron microscopy (SEM), transmission electron microscopy (TEM), and Fourier-transform infrared (FTIR) spectroscopy to assess the morphologies and surface properties of CNFs, AgNWs and composite paper. Additionally, X-ray diffraction (XRD) analysis is employed to examine the crystalline structures of CNFs, AgNWs, and composite paper. The resulting paper has a thickness of approximately 160  $\mu\text{m}$ . Its electrical conductivity varies with different AgNWs loading percentages (ranging from 2.5% to 55% w/w). The optimal combination is achieved with 45% w/w AgNWs, resulting in conductive paper exhibiting low sheet resistance (2.49  $\Omega\cdot\text{m}$ ) and surface conductivity (0.40 S/m). Furthermore, these papers effectively shield electromagnetic signals in the context of mobile phone communication.

**Keywords:** Durian peel; Cellulose nanofibril; Conductive paper; Silver nanowires



## Plasmon enhancement of photodetectors based on CsPbBr<sub>3</sub> quantum dots

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In-organic perovskite quantum dots (CsPbBr<sub>3</sub>) show great potential for optical sensing applications that have excellent optic properties such as high carrier mobility, long carrier diffusion length, excellent visible light absorption. The absorption spectrum well overlaps with localized surface plasma resonance (LSPR) of noble Au nanocrystals (Au NCs). Currently, the state-of-art photocurrent of CsPbBr<sub>3</sub> is within the nanoampere range, limiting further practical application. Therefore, we would like to enhance the photocurrent of CsPbBr<sub>3</sub> quantum dots and improve the device's stability. With the nature of energy level alignment between Au nanoparticle and CsPbBr<sub>3</sub> quantum dot, significant photocurrent enhancement was demonstrated.

In this study, CsPbBr<sub>3</sub> perovskite quantum dots have been synthesized and used to fabricate the photodetector onto the gold finger electrode. Under laser excitement with wavelength at 520 nm, it has been observed that CsPbBr<sub>3</sub> quantum dots alone could obtain the photocurrent to 100 nA. By introducing with the Au Nanoparticles, the net photocurrent has been increased nearly 1 μA. Therefore, it could be said that Au nanoparticles can assist the photocurrent generation of CsPbBr<sub>3</sub> quantum dot more sufficiently with better stability. This allows the further device system integration of such CsPbBr<sub>3</sub> quantum dot with Au nanoparticles.

**Keywords:** CsPbBr<sub>3</sub>; Photodetector; Plasmon; Electrodes; Perovskite

# Influence of chemical surface-treatment agent on mechanical and neutron-shielding properties of recycled high-density polyethylene (r-HDPE)/gadolinium oxide ( $Gd_2O_3$ ) composites

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Despite the great benefits of radiation and nuclear technologies, excessive exposure to ionizing radiation, especially neutrons, can cause both acute and long-term effects to users. In order to reduce risks from exposure, this research aimed to develop neutron-shielding materials based on recycled high-density polyethylene (r-HDPE) and gadolinium oxide ( $Gd_2O_3$ ) composites. Furthermore, to improve surface compatibility between  $Gd_2O_3$  and the r-HDPE matrix, a silane coupling agent (KBE903) with varying contents from 0 to 5, 10, 15, and 20 pph was used to treat the surfaces of  $Gd_2O_3$  particles prior to sample preparation. The results showed that the chemical surface treatment of  $Gd_2O_3$  particles with 5 pph KBE903 led to greater enhancements in mechanical properties and neutron-shielding properties of the 20 wt%  $Gd_2O_3$ /r-HDPE. Moreover, the investigation on the composites containing varying surface-treated- $Gd_2O_3$  contents from 0 – 20 wt% indicated that the r-HDPE composites with the addition of 5 wt% surface-modified ( $Gd_2O_3$ ) exhibited the most preferable properties among all filler contents. In addition, the current results were compared with commercial neutron shielding products based on borated polyethylene (PE) containing 5 wt% and 15 wt% of boron, for which the result confirmed the superiority of our work, as seen by higher values of macroscopic cross-section ( $\Sigma_t$ ) and the tensile strength. In summary, the surface-modified ( $Gd_2O_3$ )/r-HDPE composites presented great potential to be used as effective neutron-shielding materials that can be applied in various applications, especially those related to radiation protection.

**Keywords:** r-HDPE;  $Gd_2O_3$ ; KBE903; Neutron shielding; Mechanical

## Metal-organic chalcogenolates – An emerging family of low-dimensional hybrid semiconductors

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Metal-organic chalcogenolates (MOCs) are an emerging family of low-dimensional hybrid organic-inorganic semiconductors that combine the robustness of inorganic materials with the fabrication convenience and tunability of organic semiconductors. Silver phenylselenolate (AgSePh), a prototypical member of the MOC family, is a 2D semiconductor that features multiple exciting properties including narrow blue luminescence, in-plane anisotropy, large exciton binding energy, robust stability, non-toxic chemical composition, and scalable synthesis methods that are compatible with modern thin-film microelectronics manufacturing. Compared to other 2D semiconductors like layered perovskites and transition metal dichalcogenides, MOCs are distinguished by the presence of organic ligands covalently bound to their inorganic cores, which provides a unique handle to control their structures and electronic properties.

In this presentation, I will present advancement in the synthesis of MOCs, show the impacts of organic modification on their optoelectronic properties, provide examples of their applications in light emission and sensing, and discuss the insights into the exciton physics of this novel semiconductor family.

**Keywords:** Metal-organic chalcogenolates; Semiconductors; Optoelectronics; 2D materials

## Bio-CaCO<sub>3</sub> from *Perna viridis* shells for plant coating

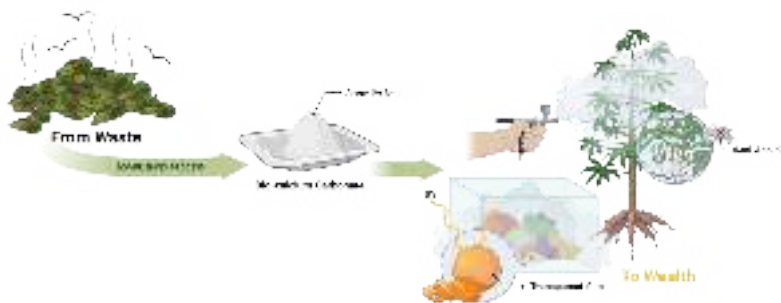
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Thailand generates approximately 42,000 tons of green mussel (*Perna viridis*) shell waste as a result of its extensive consumption. This study focuses on upcycling calcium carbonate (CaCO<sub>3</sub>) extracted from green mussel shell waste as plant sunscreen for protecting sun damage. Based on the thermal gravimetric analysis technique, a green mussel shell is composed of 95–97% (w/w) CaCO<sub>3</sub> and 3–5% (w/w) organic matrix. The CaCO<sub>3</sub> extraction process mainly consists of two steps, including eco-friendly process of eliminating the organic matrix and physically disintegrating the hierarchical CaCO<sub>3</sub> structures. The extracted CaCO<sub>3</sub> has plate shapes with a bisector length of 3–5 microns and a thickness of 200–500 nm as observed in optical and SEM micrographs. X-ray diffraction patterns reveals that extracted CaCO<sub>3</sub> platelets possess aragonite crystal structures. Molecular information of the extracted CaCO<sub>3</sub> is investigated by FT-IR and Raman spectroscopies. Primary aragonite CaCO<sub>3</sub> platelets are stacked into layer structures that selectively reflect UV radiation and blue light with wavelengths ranging from 290 to 400 nm as revealed by UV-visible absorption test. The extracted CaCO<sub>3</sub> could be dispersed in aqueous media containing cellulose nanocrystals (CNCs) and cellulose nanofibers (CNFs). The CaCO<sub>3</sub>-CNC-CNF aqueous mixture could be sprayed on various part of plants and the resulting CaCO<sub>3</sub>-CNC-CNF composite film could prevent water loss and sun damage. This environmentally friendly process transforms worthless shell waste into valuable biomaterials and offers sustainable alternatives to conventional landfilling. Furthermore, the applications of the extracted CaCO<sub>3</sub> as plant sunscreen effectively address fresh produce quality and food sustainability.

**Keywords:** Calcium carbonate; *Perna viridis*; Aragonite; Sun damage; Green mussel



The processed calcium carbonate from waste green mussel shells is used as a coating for plants.

## Microstructural modification of nickel aluminium bronze against erosion corrosion

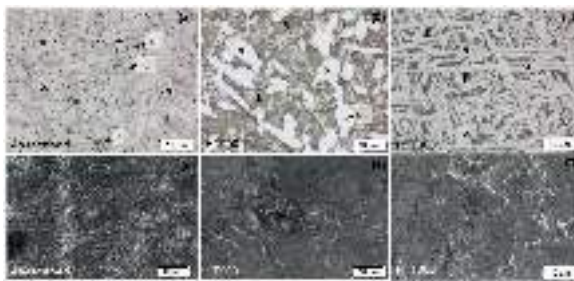
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Nickel aluminum bronze (NAB) is widely used in marine applications e.g. seawater impellers and ship propellers. During service, it is exposed to seawater containing sand. This condition causes erosion-corrosion deterioration. Heat treatment is used to modify microstructure of metal for life extension. In this work, the as-received NAB, comprising of  $\alpha$ ,  $\beta'$  phases and  $\kappa_I$ ,  $\kappa_{II}$ ,  $\kappa_{III}$ ,  $\kappa_{IV}$  precipitates, was hardened by heat treatment at 900 and 1000°C for 2 hours then water quenching to homogenize microstructure. The erosion-corrosion was tested in a chamber containing 30 g/L of 300-500  $\mu\text{m}$  sand particles suspended in 3.5 wt.% NaCl solution. The samples were rotated at a rotational speed of 1500 rpm for 6 hours. This test method allowed sand particles erode and NaCl solution corrode the sample simultaneously. After hardening at 900°C, the  $\alpha$  phase still remained in a matrix of  $\beta$  phase; while, most of  $\kappa$  precipitates were dissolved. Hardening at 1000°C all of the  $\kappa$  precipitates were dissolved, only the needle-shaped of  $\alpha$  phase in a matrix of  $\beta$  phase was observed. Modification of microstructure after hardening enhanced hardness over the as-received sample, especially hardening at 1000°C. The XRD results of heat-treated samples showed additional peaks of  $\text{Al}_7\text{Cu}_4\text{Ni}$  and  $\text{Al}_5\text{FeNi}$  phases compared with the as-received sample as they were the hard phases obtained after hardening. The erosion corrosion resistance corresponded to hardness of samples. SEM investigation also indicated the slightest damage in the hardest sample, hardening at 1000 °C, after erosion corrosion test as shown in the Figure.

**Keywords:** Nickel aluminium bronze; Erosion-corrosion; Slurry corrosion; Heat treatment; Hardening



**Figure 1.** Microstructure of (a) as-received (b) 900 °C heat-treated and (c) 1000 °C heat-treated samples, SEM surface morphology of (d) as-received (e) 900 °C heat-treated and (f) 1000 °C heat-treated samples after erosion-corrosion test

## Synthesis of RGB fluorescent helical network polymers in chiral liquid crystals and evaluation of their circularly polarized luminescence

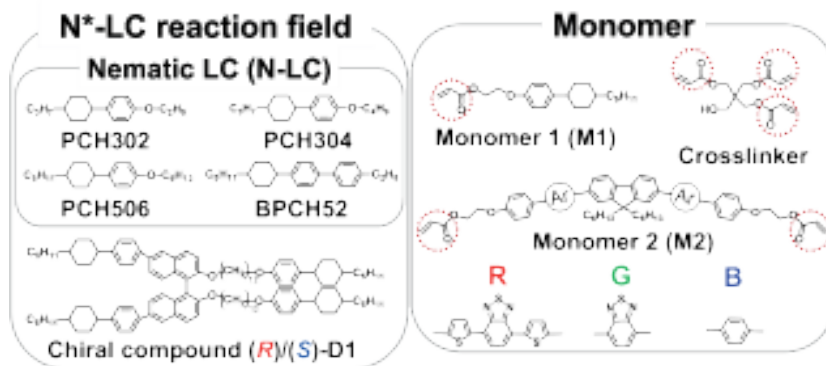
Hiromasa Yamamoto<sup>1</sup>, Satoru Yoshida<sup>1</sup>, Keita Horie<sup>2</sup>, Kosuke Kaneko<sup>1</sup>, Tomonori Hanasaki<sup>1</sup>, and Kazuo Akagi<sup>2\*</sup>

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Recently, helical network polymers were synthesized by photo-radical polymerization of acrylate derivatives in chiral nematic liquid crystals (N\*-LC) and chiral smectic liquid crystals (S<sub>c</sub>\*-LC). The polymers exhibited blue circularly polarized luminescence (CPL) due to their helical structures and fluorescence properties. In this work, three novel acrylate derivatives exhibiting red, green, and blue (RGB) fluorescence were synthesized. Then, RGB fluorescent helical network polymers were synthesized by the photo-radical polymerizations of acrylate derivatives in N\*-LC. The polymers not only exhibited fingerprint optical textures similar to those of N\*-LCs, but also CPL with RGB colors.

**Keywords:** Chiral liquid crystal; Circularly polarized luminescence; Photo-radical polymerization; RGB fluorescence; Helical network polymer



**Figure 1.** Molecular structures of the host N-LCs, the chiral compound, and the monomers.

# Synthesis of achiral fluorene derivatives exhibiting circularly polarized luminescence induced in chiral nematic liquid crystal medium

Yuki Fujita<sup>1</sup>, Keita Horie<sup>2</sup>, Kosuke Kaneko<sup>1</sup>, Tomonori Hanasaki<sup>1</sup>, and Kazuo Akagi<sup>2</sup>

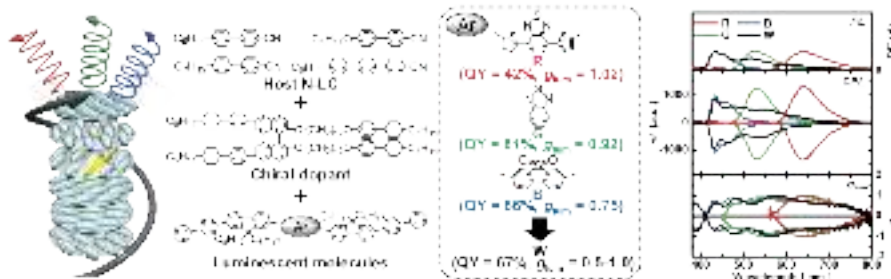
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Chiroptical materials bearing circularly polarized luminescence (CPL) are required to have desired emission wavelengths, high quantum yields (QY), and high luminescence dissymmetry factors (glum). The addition of achiral luminophores into chiral nematic liquid crystal (N\*-LC) is a promising way to generate CPLs. In this study, we aimed to generate red-green-blue (RGB) and white CPLs by adding three types of fluorene-based luminescent molecules and their mixture into N\*-LCs. First, achiral fluorene derivatives with RGB emission colors were synthesized and added to the N\*-LCs containing alkylcyanobiphenyl and alkylcyanoterphenyl-based nematic liquid crystals (N-LCs) and an axially chiral binaphthyl compound. The mixture of RGB fluorene derivatives was prepared in an appropriate mixing ratio and added to the N\*-LC. The N\*-LCs including the fluorene derivatives or the mixture were injected into liquid crystal cells and measured to evaluate the chiroptical properties. The fluorene derivatives dissolved in the N\*-LCs exhibited induced CPLs of RGB and white colors with QY of 60~90% and glum values of 0.6~1.0. In addition, the changes in CPL properties were investigated using different host liquid crystal systems and luminescent molecules. It is found that the host N-LCs containing highly linear dichroic luminescent molecules and highly birefringent 4-cyano-4'-pentyl-p-terphenyl (5CT) are suitable for inducing CPL with higher glum values.

**Keywords:** Circularly polarized luminescence; Chiral nematic liquid crystal



**Figure 1.** The structures of host N-LC, chiral dopant, luminescent molecules, and PL, CPL, and  $g_{\text{lum}}$  spectra of N\*-LC.

# Material Chemistry and Nanotechnology (MN)

## Poster Presentation

## Activated biocarbons prepared by chemical activation of cashew nut shells as potential electrode materials for supercapacitors

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In today's world, the imperative for sustainable energy production and storage is undeniable. Supercapacitors play a pivotal role in meeting this demand since they provide rapid charge-discharge capabilities, coupled with prolonged lifespans and high efficiency. The study focuses on the utilization of biocarbons derived from cashew nut shells as an electrode material for supercapacitors (SC). The process involved the pre-carbonization of cashew nut shells at 400 °C, followed by mechanical mixing with KOH at the mass ratio of 1:1. Subsequently, the mixture underwent activation at temperatures of 650, 750, and 850 °C. The resulting activated biocarbons exhibited an amorphous phase with high carbon purity. With increasing activation temperature increased from 650 to 850 °C, the specific surface area increased from 1,545 to 2,034 m<sup>2</sup>.g<sup>-1</sup> with the major proportion of micropores exceeding >85%. To assess the charge storage properties of activated biocarbons, electrochemical measurements were conducted using a three-electrode system in 1 M Na<sub>2</sub>SO<sub>4</sub> electrolyte. Notably, the biocarbon activated at 750 °C demonstrated the highest specific capacitance of 106 F.g<sup>-1</sup> at a current density of 0.5 A.g<sup>-1</sup>, attributed to the optimal ratio of micropores to meso/macropores. For practical applications, coin-cell symmetric supercapacitors were assembled using activated biocarbons (750 °C) as positive and negative electrodes. The specific capacitance of the coin cell was 18 F.g<sup>-1</sup> at a current density of 0.5 A.g<sup>-1</sup> within a 1.0 V potential window, exhibiting 70% capacitance retention at 2 A.g<sup>-1</sup> after 10,000 cycles. This underscores the potential of activated biocarbons from cashew nut shells as promising electrode materials for supercapacitors and related applications.

**Keywords:** Cashew nut shells; Activated biocarbons; Chemical activation; Supercapacitors

## Cobalt/nitrogen-doped carbons derived from teak sawdust as low-cost and stable electrocatalysts for oxygen reduction reaction in fuel cells

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The fuel cell is an electrochemical device that generates electrical energy by converting hydrogen and oxygen into electricity without combustion. Its key advantage lies in its environmentally friendly operation, as it produces no pollution. However, the use of platinum (Pt) as a catalyst for the oxygen reduction reaction (ORR) at the cathode poses a significant cost challenge. To tackle this issue, the development and exploration of efficient and low-cost catalysts to replace Pt is highly desirable for next-generation fuel cells. In this study, cobalt/nitrogen-doped carbons (Co/N-SC) were synthesized from teak sawdust, a byproduct of the wood furniture industry, as a potential cathode catalyst. The synthesis of the Co/N-SC catalyst involved pyrolysis of a mixture of cobalt (II) nitrate hexahydrate ( $\text{Co}(\text{NO}_3)_2 \cdot 6\text{H}_2\text{O}$ ), dicyandiamide ( $\text{C}_2\text{H}_4\text{N}_4$ ), and sawdust carbon (SC) at 700 °C under an argon gas atmosphere. Evaluation of the ORR activity was carried out using a three-electrode system by cyclic voltammetry (CV) and linear sweep voltammetry (LSV) in a 0.1 M potassium hydroxide (KOH) solution under oxygen and nitrogen saturation. Co/N-SC exhibited an enhanced ORR onset potential and current density compared to sawdust carbon and single cobalt or nitrogen-doped sawdust carbon. Further analysis using Koutecky–Levich analysis, derived from rotating disk electrode (RDE) data, revealed that the ORR occurring on Co/N-SC predominantly proceeded through a four-electron pathway. Additionally, stability testing through chronoamperometry at  $-0.3$  V for 8 h revealed Co/N-SC's superior stability in comparison to Pt/C. Although the ORR activity of the Co/N-SC catalyst remained lower than that of Pt/C, there existed potential for further improvement and development.

**Keywords:** Oxygen reduction reaction; Electrocatalysts; Fuel cells; Cobalt/nitrogen-doped carbons

# Synthesis of $\text{MnO}_2/\text{C}$ composite from spent alkaline battery by one-step hydrothermal process for rechargeable Zn-ion battery application

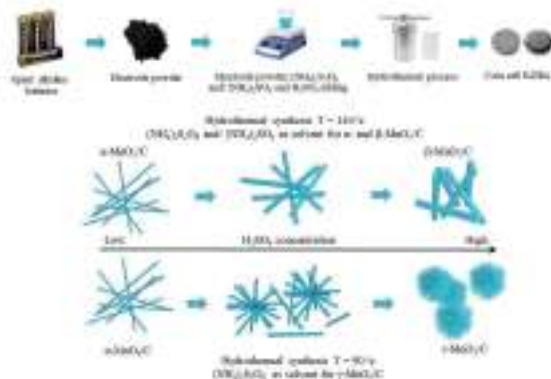
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Alkaline battery is one type of single-use energy storage devices that pose a significant waste issue and have a negative impact on the environment. Therefore, this research aims to recover Mn and C from the spent electrode powder in form of  $\text{MnO}_2/\text{C}$  composites and to utilize the recycled materials in the rechargeable zinc-ion battery (RZIB) application. The process began with the dismantling and sieving at 200 meshes of spent alkaline batteries to obtain spent electrode powder. The spent electrode powder and  $(\text{NH}_4)_2\text{S}_2\text{O}_8$  and/or  $(\text{NH}_4)_2\text{SO}_4$  were then used as precursors to synthesize various phases of  $\text{MnO}_2/\text{C}$  composite through a one-step hydrothermal process. The XRD and SEM results confirm the presence of  $\alpha$ -,  $\beta$ -, and  $\gamma$ - $\text{MnO}_2/\text{C}$  with nanofiber, nanorod, and nano-urchin morphologies, respectively. The SEM-EDS and XRF techniques were utilized to detect the chemical composition and to estimate the Mn recovery efficiencies. The results show that  $\alpha$ - $\text{MnO}_2/\text{C}$  has the highest Mn% recovery of 62.79%, followed by  $\beta$ - and  $\gamma$ - $\text{MnO}_2/\text{C}$  at 61.90% and 51.78%, respectively. Subsequently, the recycled  $\text{MnO}_2/\text{C}$  was utilized as active cathode materials in RZIB. The galvanostatic charge-discharge analysis at 0.1-0.5 A/g was performed to demonstrate the electrochemical performance of the batteries. The results show that the  $\beta$ - $\text{MnO}_2/\text{C}$  cathode has the highest specific capacity of 291.35 mAh/g at 0.1 A/g, followed by  $\alpha$ - and  $\gamma$ - $\text{MnO}_2/\text{C}$  at 263.84 and 175.76 mAh/g, respectively.

**Keywords:** Spent alkaline battery; Battery recycle process; Hydrothermal process;  $\text{MnO}_2/\text{C}$ ; Zinc-ion battery



Synthesis  $\alpha$ -,  $\beta$ - and  $\gamma$ - $\text{MnO}_2/\text{C}$  from spent alkaline batteries by one-step hydrothermal process and morphologic evolution simulation at different concentration of  $\text{H}_2\text{SO}_4$  and hydrothermal temperature

## Mesoporous carbons synthesized via solution plasma process: A potential electrode material for mesoscopic perovskite solar cells

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Perovskite solar cells represent a significant technological advancement in the realm of solar cell technologies, offering several advantages. Notably, these cells can be constructed through a straightforward method, making them cost-effective and easy to implement. In conventional perovskite solar cells, the counter electrode typically consists of precious metals such as gold or silver, requiring high-energy machining and expensive tools for fabrication. However, a comprehensive review of previous research revealed that more economically viable carbon materials could serve as substitutes for these precious metals. In this study, we present the synthesis of mesoporous carbons through the solution plasma process (SPP) for serving as electrode materials in mesoscopic perovskite solar cells. The resulting mesoporous carbons from SPP were optimally mixed with a specific quantity of graphite and  $\alpha$ -terpineol to prepare the carbon paste. The perovskite solar cells were subsequently fabricated by coating  $\text{TiO}_2$  and  $\text{ZrO}_2$  onto fluorine-doped tin oxide (FTO) coated glass substrates as electron transport and insulating layers, respectively. The carbon paste was then applied as the top electrode. The cells underwent exposure to a solar light simulator to evaluate their efficiency and performance. The fabrication of mesoscopic perovskite solar cells with carbon electrodes is not only simple and uncomplicated but also cost-effective compared to the utilization of metal electrodes.

**Keywords:** Carbon electrode; Mesoscopic Perovskite solar cell; Mesoporous carbon; Solution plasma process



## Improving photocatalytic efficiency of zinc oxide immobilized on glass slides by using plasma surface modification

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Photocatalytic oxidation is an effective method for removing organic pollution from wastewater. However, the transition from bench-scale operation to large-scale operation needs the development of heterogeneous catalysts that allow repeated use with low-cost recovery. This study aims to improve the efficiency of zinc oxide (ZnO) coated glass slides for photocatalytic oxidation by using air plasma to activate the glass surface. The glass slides were placed under low-pressure plasma power 20 W for 30 seconds. The plasma treatment increased the wettability of the surface, because of the formation of carboxyl and amide groups on the fibers' surface, which facilitated the spreading and deposition of ZnO precursor onto the rough surface of sandblasted glass slides. Scanning electron microscopy (SEM) displayed the ZnO nanoparticles (NP-ZnO) with average diameters of 48 nm and 70 nm on the glass slides treated with plasma and acid, respectively. In addition, the SEM images showed a more uniform distribution and better coverage of the NP-ZnO on the glass surface. The higher density and contact surface of NP-ZnO on the plasma-treated glass slide resulted in superior photocatalytic activity. Under UV-C germicidal lamp illumination, the plasma-treated glass slide led to 86% degradation of methylene blue in 60 mins which was higher than the 73% degradation when using the acid-treated glass slide. The plasma-treated glass slide exhibited high durability and could be reused more than five times without a decrease in catalytic efficiency.

**Keywords:** Zinc oxide; Photocatalytic oxidation; Plasma surface treatment

# Synthesis of chemically activated carbons from waste macadamia shells through potassium hydroxide activation for symmetric supercapacitors

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The Mae Fah Luang Foundation has successfully cultivated macadamia, thereby reducing dependence on imported products. This success has led to the utilization of macadamia kernels for the mass production of seasoned snacks and desserts in Thailand. However, the macadamia shells leftover from production were discarded as waste without any purpose. To enhance the value of macadamia waste, they were converted into porous carbons through potassium hydroxide (KOH) activation. The process involved mixing carbonized shells and KOH at weight ratios of 1:1, 1:2, and 1:3 until achieving homogeneity. Subsequently, the mixtures were pyrolyzed at 800 °C under Ar flow. Upon characterization, scanning electron microscopy (SEM) images revealed an increase in roughness and the development of a porous structure with higher KOH content. The broadening X-ray diffraction (XRD) pattern and Fourier-transform infrared spectroscopy (FTIR) results indicated that the activated carbons exhibited an amorphous phase and the decomposition of the lignocellulose, respectively. Additionally, the specific surface area of the carbon increased from 715 to 1024 m<sup>2</sup>/g as the KOH increased from 1:1 to 1:3. The activated carbons were then fabricated into symmetric coin cell supercapacitor electrodes for electrochemical testing. The cyclic voltammetry (CV) and galvanostatic charge-discharge (GCD) tests in 1 M Na<sub>2</sub>SO<sub>4</sub> electrolyte demonstrated an electric double-layer capacitor (EDLC) behavior with excellent rate capabilities and stability. Consequently, the chemically activated carbons derived from macadamia shells have the potential to be applied as electrode materials in symmetric supercapacitors for multipurpose everyday applications.

**Keywords:** Macadamia shells; Activated carbons; Symmetric supercapacitors; Chemical activation; Biomass conversion

## Formulation a catechol-based copolymer for the creation of MXene dispersible in organic solution

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MXene, a two-dimensional nanomaterial, consists of transition metals (M) linked by carbon or nitrogen atoms, with surface functional groups ( $T_x$ ) such as hydroxyl (-OH), oxide (-O), or fluorine (-F) groups. One specific MXene variant,  $Ti_3C_2T_x$ , is recognized for its superior electrical conductivity and surface functional groups. In aqueous environments, the surface functional groups of MXene enable it to disperse effectively. However, its propensity to oxidize and convert into titanium dioxide ( $TiO_2$ ) presents a challenge. To counter this, researchers are striving to enhance MXene's oxidation resistance by altering its surface functional groups. Concurrently, maintaining stable dispersion in organic solvents is vital for expanding its applications. In this study, the surface of MXene was modified through copolymerization using Controlled Radical Polymerization (CRP). This innovative approach opens up new possibilities for the use of MXene in various fields, including energy storage, sensors, and catalysis. The copolymerization process allows for precise control over the polymer structure, leading to improved performance and stability of the resulting MXene. Furthermore, the use of catechol-based copolymers provides additional benefits, such as enhanced adhesion and mechanical properties. This research represents a significant step forward in the development of MXene-based materials and their potential applications.

**Keywords:** MXene; Ligand; Copolymer; Controlled radical polymerization; Catechol

## Organic ligand enhanced MXene based water dispersible polymer composite as a source for hybrid aerogel fabrication

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MXene materials, which are 2D nanomaterials with high metal conductivity derived from metal carbides and nitrides, have attracted increasing attention for various applications. However, MXenes ( $M_{n+1}X_nT_x$ ) suffer from oxidation induced stability degradation and conductivity loss. To overcome this, organic ligands are used to modify the surface of  $Ti_3C_2T_x$  ( $T_x = -OH, -O, -F$ ) and improve its oxidation resistance and conductivity. Another method is to form a 3D structure in a water-dispersible polymer composite by freeze-drying and heat treatment, which shows high stress-strain performance, flexibility, lightness, and conductivity. This aerogel can be applied in electromagnetic interference, batteries, and water-in-oil emulsion separation.

**Keywords:** Aerogel; Surface modified MXene; Organic ligand; Water-dispersible polymer

## Organic processing and applications of MXenes: surface-modified ligand library

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MXenes, a type of 2D nanomaterial, are composed of transition metals (M), group III or IV elements (A), and either carbon or nitrogen (X), with termination groups ( $T_x$ ) such as -O, -OH, -F, etc. They are typically created by etching a transition metal carbide known as the MAX phase in a fluoride-containing acid medium. MXenes have been explored for use in a variety of fields, including electrochemical energy storage, sensors, and photocatalysis. However, their application has been limited due to their poor long-term storage stability as they can only be dispersed in aqueous media and are prone to oxidation when exposed to water and air. In this study, we address this issue by treating MXenes with a range of natural or synthetic ligands like catechol-based one, resulting in surface-functionalized MXenes. These modified MXenes exhibit enhanced oxidation stability, maintain high electrical conductivity, and show excellent compatibility in organic media. This makes them suitable for use in various industries as electrodes or interlayers that can be processed organically.

**Keywords:** MXenes; 2D nanomaterial; Surface functionalization; Organic-dispersion; Ligands

## Wireless preparation of Ni-Ag alloyed janus objects using bipolar electrochemistry

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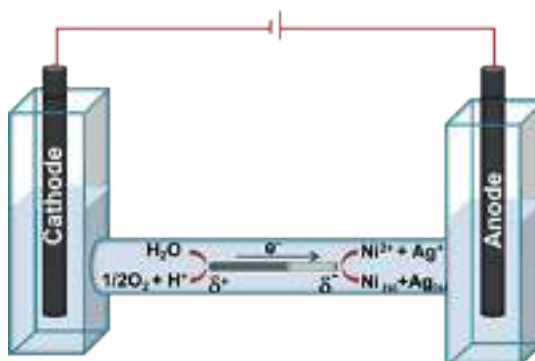
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The preparation of Ni-Ag Alloyed Janus particles by Bipolar Electrochemistry was studied. This technique allowed the development of new methods for controlling surface modification at the micro- and nanoscale. The optimum conditions for Ni deposition on 900  $\mu\text{m}$  of carbon rods were investigated with 0.01 M  $\text{NiSO}_4$  and electric field at 7 V/cm. Deposition time was 1 minute. While the optimum conditions for Ag deposition on carbon rods were determined by 0.005 M  $\text{AgNO}_3$ , electric field at 5 V/cm and deposition time of 1 minute. Furthermore, the alloyed deposition of Ni-Ag on 10  $\mu\text{m}$  of carbon microfiber (CMF) was created with this technique and characterized by SEM and EDS. The modified objects can be created with bipolar electrochemistry that could find applications as key components for drug delivery.

**Keywords:** Bipolar electrochemistry; Janus particles; Alloyed deposition



## Synthesis of mesoporous silica film from sodium silicate by electrochemically assisted self-assembly method

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Mesoporous silica film (MSF) synthesized by an electrochemically assisted self-assembly (EASA) method on various substrates is of interest for many applications. Tetraethoxysilane (TEOS) is commonly used as a silica source in the synthesis. However, it is relatively expensive and has low water solubility. The reaction also emits harmful methanol. To avoid the disadvantages of TEOS, in this work, sodium silicate ( $\text{Na}_2\text{SiO}_3$ ) is investigated as a silica source for the MSF synthesis. The EASA method was used to deposit MSF onto fluorine-doped tin oxide-coated glass (FTO glass). An electrochemical cell used in the synthesis consists of FTO glass, Ag/AgCl electrode, and stainless steel mesh as a working electrode, a reference electrode, and a counter electrode, respectively. The three electrodes were immersed in a sol solution containing  $\text{Na}_2\text{SiO}_3$  and cetyltrimethylammonium bromide (CTAB) as a surfactant template. Various cathodic potentials ranging from -1.1 V to -1.6 V were applied to the electrodes to initiate polycondensation of the reactants in the sol mixture. The ratio of CTAB/ $\text{Na}_2\text{SiO}_3$  was varied from 0.3 to 1.2, and the deposition time was varied from 15 s to 120 s. A transmission electron micrograph reveals that a film with a hexagonally packed mesopore structure was obtained at the applied potential of -1.3 V and the deposition time of 60 s. Characterization of the film by cyclic voltammetry also indicated that the as-synthesized MSF fully covered the FTO surface without cracks. The results clearly show that  $\text{Na}_2\text{SiO}_3$  can be used as the silica source to synthesize MSF.

**Keywords:** Mesoporous silica film; Sodium silicate; Electrochemically assisted self-assembly

## High surface area electrode for direct CO<sub>2</sub> capturing in air

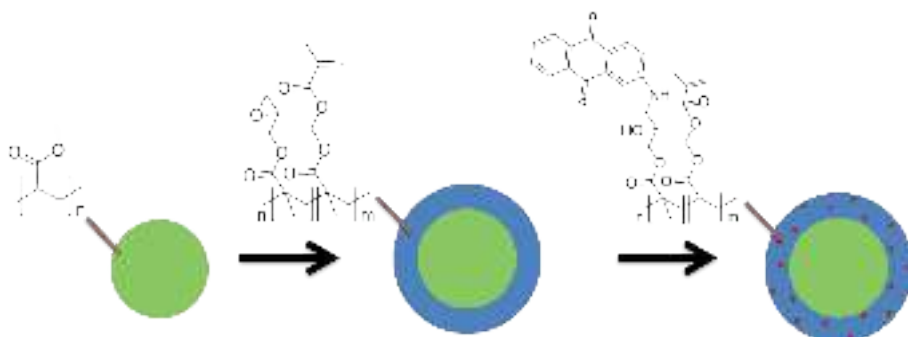
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Swing Adsorption technology for capturing carbon dioxide (CO<sub>2</sub>) in mixed gases, is a popular method for reducing CO<sub>2</sub> emissions. Continuous development is required to address issues related to excess energy consumption and to improve efficiency. Electro Swing Adsorption (ESA) employs redox molecule capable of CO<sub>2</sub> adsorption and releasing upon a change in applied potential. This technology offer a promising solution for cost-effective CO<sub>2</sub> capture and holds potential for practical field applications. In this study, we focus on enhancing the stability of redox molecules, which play pivotal roles in ESA. Routes to synthesize polymeric nanoparticles made from glycidyl methacrylate, designed to efficiently attach the redox molecule 2-amino anthraquinone (AAQ), were explored. Through AAQ loading efficiency by electrochemical measurement, the optimum synthesis path for producing polymeric nanoparticles encapsulating redox molecules was achieved. This could provide the possibility of incorporating other redox molecules, capable of CO<sub>2</sub> adsorption, even when susceptible to oxidation by other gases for the ESA process.

**Keywords:** Carbon dioxide; Polymer; Electro swing adsorption; High-surface-area; Redox molecule



## Surface modification of titanium with poly(amidoamine) dendrimer and its impact on bacterial adhesion and biofilm formation

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Titanium-based materials have been widely used as implants in various applications. However, bacterial infections associated with titanium implants remain a serious clinical problem. Development of functional materials to improve efficacy and prevent infection is a promising solution. Thus, the use of poly(amidoamine) (PAMAM) dendrimer for coating was proposed as an effective strategy to control bacterial infection and colonization on the device surface. In this study, we performed the surface coating or functionalization of titanium with PAMAM dendrimer at a concentration of 1.0 mM. The effects of incubation period and the number of coatings (layer-by-layer) with PAMAM dendrimer were evaluated for optimization of surface modification. Additionally, the coated titanium surface was tested its properties regarding bacterial adhesion and biofilm formation. Results showed that the PAMAM dendrimer adsorbed on the titanium, and the coated surface exhibited functionality. No noticeable discrimination was observed between the incubation of 1 hour with double coating (bilayers) and of 2 hours with single coating (a monolayer). Titanium coated with PAMAM dendrimer showed a reduction in the number of *Enterococcus faecalis* TISTR 379 attached to the surface of the material compared to non-coated titanium. The antimicrobial test of the treated surfaces indicated the log reduction value of  $0.157 \pm 0.049$  for 1-hour incubation and coating as bilayers and  $0.072 \pm 0.026$  for 2-hour incubation and coating as a monolayer. This alternative coating method has great potential for the preparation of titanium implants and prevention of infections.

**Keywords:** Titanium; PAMAM dendrimer; Surface modification; Bacterial adhesion; biofilm

## Green synthesis of ultrasound-assisted Fe<sub>3</sub>O<sub>4</sub>/berry extract nanocomposites for enhanced antibacterial activity and 4-NP reduction reaction

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Iron oxide nanoparticles (Fe<sub>3</sub>O<sub>4</sub> NPs) hold significant advantages for nanobiotechnologists and chemical industries, owing to their broad applications in biomedicine and catalysis. Fe<sub>3</sub>O<sub>4</sub> serves as an antibacterial agent, affecting bacterial cells by disrupting the cell membrane and generating reactive free radicals. Anthocyanins, potent antioxidants present in red, blue, and purple fruits and vegetables, offer valuable properties applicable in diverse biomedical scenarios. This study explores the application of various berry extracts in coating Fe<sub>3</sub>O<sub>4</sub> nanoparticles. Initially, Fe<sub>3</sub>O<sub>4</sub> nanoparticles were synthesized using a straightforward co-precipitation method. Subsequently, extracts from Raspberry, Strawberry, and Blueberry were employed. The appropriate amount of berry extract was applied to the surface of Fe<sub>3</sub>O<sub>4</sub> using an ultrasonication process. The magnetic Fe<sub>3</sub>O<sub>4</sub> nanoparticles coated with berry extract (BE), known as Fe<sub>3</sub>O<sub>4</sub>/BE nanocomposites, were characterized using X-ray diffraction (XRD), Fourier-transform Infrared spectroscopy (FTIR), and HRTEM analysis. XRD results revealed that the Fe<sub>3</sub>O<sub>4</sub>/BE nanocomposites adopted a face-centered cubic structure, with particle size determined using Debye-Scherrer's equation, yielding particles sized between 14-18 nm. Ultimately, the obtained Fe<sub>3</sub>O<sub>4</sub>/BE nanocomposites were utilized as antibacterial agents against Escherichia coli and Staphylococcus aureus-902. They exhibited potent antibacterial activity against both bacterial species. Additionally, the catalytic efficiency of the Fe<sub>3</sub>O<sub>4</sub>/BE nanocomposites was evaluated in the reduction of 4-nitrophenol to 4-aminophenol in the presence of sodium borohydride. The results demonstrated that all the berry extract-coated Fe<sub>3</sub>O<sub>4</sub>/BE nanocomposites displayed exceptional catalytic activity. In particular, the  $k_{obs}$  values indicated that the Fe<sub>3</sub>O<sub>4</sub>/blueberry nanocomposites exhibited better catalytic activity than Raspberry and Strawberry. This heightened activity can be attributed to blueberries containing a larger amount of flavonoids and anthocyanin in their extract, which reduces the particle size and enhances catalytic activity.

**Keywords:** Berry Extract; Magnetic Fe<sub>3</sub>O<sub>4</sub>; Antibacterial activity; 4-Nitrophenol reduction



## Green synthesis of gold nanoparticles from macadamia nut shell extracts and their antioxidant, antibacterial and catalytic activities

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Green synthesis methods like this have garnered attention for their potential to replace conventional chemical methods, which often involve hazardous chemicals. The use of waste macadamia nut shell extract as a stabilizing and self-reducing agent for the green synthesis of gold nanoparticles (AuNPs) represents a sustainable and environmentally-friendly approach in nanotechnology. This method likely involves harnessing the natural compounds present in the macadamia nut shells to reduce gold ions, ultimately leading to the formation of AuNPs. The formation of AuNPs was characterized by UV-visible spectrum, X-ray diffraction (XRD), transmission electron microscopy (TEM), and Fourier-transform infrared spectroscopy (FTIR). The UV-Visible absorption spectrum of the colloidal AuNPs showed a peak at 540 nm. X-ray diffraction (XRD) analysis revealed distinct peaks at angles ( $2\theta$ ) of  $38.25^\circ$ ,  $44.12^\circ$ ,  $64.32^\circ$ ,  $77.47^\circ$ , and  $80.175^\circ$ , corresponding to the (111), (200), (220), (311), and (222) crystallographic planes of the face-centered cubic (FCC) lattice of gold. The transmission electron microscopy (TEM) images depicted nearly spherical-shaped AuNPs, with a size range of 10 -16 nm. The green-synthesized AuNPs exhibited excellent antioxidant and antimicrobial properties against both gram-positive and gram-negative bacteria. Furthermore, catalytic efficiency was also assessed through the reduction of 4-nitrophenol (4-NP). The obtained results demonstrated that AuNPs derived from macadamia nut shell extracts displayed outstanding hydrogenation reaction properties. The newly developed green-synthesized AuNPs have proven to be simple, cost-effective, and environmentally-friendly nanoparticles suitable for various applications include food packing, bio-sensor, and catalysis in pharmaceuticals reactions.

**Keywords:** Gold nanoparticles (AuNPs); Macadamia nut shells; Antioxidant; Antibacterial; Hydrogenation reaction.

## Green preparation method of silver nanoparticles for cosmetic applications

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This study aimed on investigating the environmental-friendly method involving the generation of suspensions of silver nanoparticles (AgNPs) with the antibacterial activity suitable for the use in cosmetic applications such as antibacterial pads and sanitary napkins. The colloidal suspension of AgNPs was successfully synthesized via green synthesis routes using Gac fruit (*Momordica cochinchinensis* Spreng) as a reducing agent. The size of the obtained AgNPs determined via the dynamic light scattering (DLS) technique was found to be in the average of 44 nm. The presence of metallic nanoparticles was also observed and confirmed using UV–Visible spectroscopy (UV-Vis) and transmission electron microscopy (TEM). The results illustrated the formation of the uniform, well-dispersed spherical AgNPs. The prepared AgNPs were found to be effective against both gram-positive and negative bacteria. The antibacterial effect of nanosized silver solution was preliminary tested in the form of sanitary napkins. The personal satisfaction survey revealed the beneficial effect of the AgNPs on human skin after applying for 3 days.

**Keywords:** Silver nanoparticles; Green synthesis; Gac fruit





## Preparation of silver nanoparticles by orange peel extract for antibacterial paper packaging

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Fruits typically have a short shelf life after harvest, making them susceptible to spoilage, especially during transportation. The purpose of this research was to create antibacterial packaging to extend the shelf life of fruits by coating paper packaging with silver nanoparticles (AgNPs). These silver nanoparticles were synthesized using a green method that utilized orange peel extract as both a reducing agent and a stabilizer. The results from absorbance, particle size, and morphology analysis revealed that the AgNPs exhibited maximum absorption at 425 nm and had an average size of  $128.1 \pm 26.6$  nm, and showing good dispersion with spherical shape. Paper packaging coated with AgNPs effectively inhibited the growth of both gram-positive and gram-negative microorganisms, thereby reducing the risk of fruit spoilage during transportation. Furthermore, this research investigated the physical characteristics of tomatoes. The findings indicated that AgNPs-coated paper packaging extended the shelf life of tomatoes in comparison to uncoated paper packaging. This implies that the antibacterial properties of the AgNPs contributed to preserving the quality of tomatoes for a longer duration. In conclusion, the development of antibacterial packaging by coating paper with silver nanoparticles synthesized using green synthesized orange peel extract as a reducing agent has the potential to inhibit bacterial growth and prolong the fruit's shelf life.

**Keywords:** Silver nanoparticles; Green synthesis; Antibacterial

## Enhanced adsorption of Ceftriaxone antibiotic from hospital wastewater by modified granular activated carbon

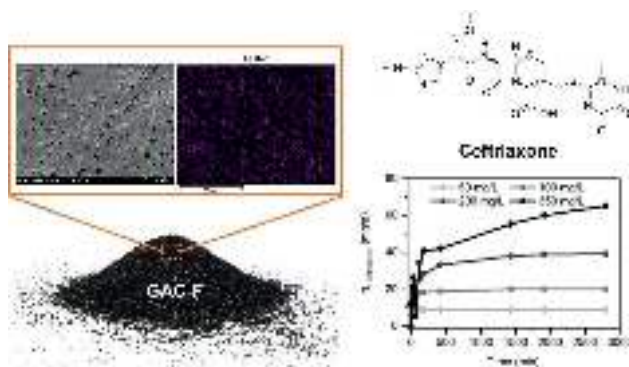
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Antibiotic residual in water and wastewater becomes a serious concern for sustainable ecosystems. Trace antibiotic residual has lethal effects on aquatic organisms and human health, particularly leading to antimicrobial resistance development. Ceftriaxone (CTX) is third generation cephalosporin family for the treatment of several bacterial infections. It is employed in the top five antibiotic groups in Thai hospitals, so it is mostly found in hospital wastewater as well. To remove antibiotics, adsorption has proved to be a safe, effective, and environmentally friendly method. Therefore, this study aims to develop a simple process for the modification of commercial granular activated carbon (GAC) as an adsorbent for CTX. SEM, FTIR, BET, and Zeta potential measurements were used to analyze surface morphological, pore textural, and chemical structural characteristics of the iron modified GAC (GAC-F). The CTX adsorption was carried out in batch experiments with both CTX containing solutions: synthetic CTX solutions and real hospital wastewater (collected at the sedimentation tank of the wastewater treatment plant). The adsorption results showed the maximum adsorption of GAC-F ( $q_{\max}$ ) was  $77.5 \text{ mg g}^{-1}$  which was higher than that of GAC ( $34.7 \text{ mg g}^{-1}$ ). The CTX adsorption isotherm was fitted with the Langmuir isotherm and the pseudo-second order kinetic models indicating favorable monolayer adsorption and chemisorption process, respectively. Furthermore, the rapid adsorption within 15 min (100% removal efficiency) of CTX in real hospital wastewater was observed by GAC-F. These results demonstrated the enhancement of CTX adsorption efficiency of GAC-F showing a potential adsorbent for antibiotic removal.

**Keywords:** Antibiotic adsorption; Activated carbon; Ceftriaxone; Simple modification; Hospital wastewater



**Figure 1** adsorption performance of ceftriaxone by GAC-F.



## Development of the cellulose microcrystalline as a potential carrier of biologics delivery

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Cellulose-based microscale materials could be used as biocarriers for biologics and drug delivery systems due to their biocompatible, biodegradable, and low-toxicity properties. Preparation of cellulose microcrystalline (CMC) from cotton through an acid hydrolysis process with two different durations (1 hour 30 minutes and 4 hours), followed by a 2,2,6,6-tetramethylpiperidine-1-oxyl (TEMPO) oxidation process. The results showed that the hydrolysis duration affected the size and morphology of CMC, with longer hydrolysis times resulting in smaller CMC with a short fibrous structure. TEMPO oxidation process introduced numerous carboxyl groups on the surface of CMC, rendering it more hydrophilic and allowing for easy conversion to other functional groups. In this study, chitosan was selected for surface modification of CMC due to its hydrophobic nature, compatibility, and efficient binding capabilities with biologics. To assess their effectiveness as carriers, we examined biologic loading using bovine serum albumin (BSA) as a representative protein. The chitosan-modified CMC (CMC/CHI) demonstrated superior BSA loading, measuring around 10.40-11.44% by weight. We also demonstrated that pattern of BSA releasing between the CMC and CMC/CHI appeared differently under various pH levels (3.4, 7.4, and 9) in a standard phosphate buffer and standard buffer without phosphate.

**Keywords:** Cellulose microcrystalline; Acid hydrolysis; TEMPO oxidation; Biocarriers; Biologics delivery

## Cationic chitosan-fluorescein tagged BSA nano-delivery system

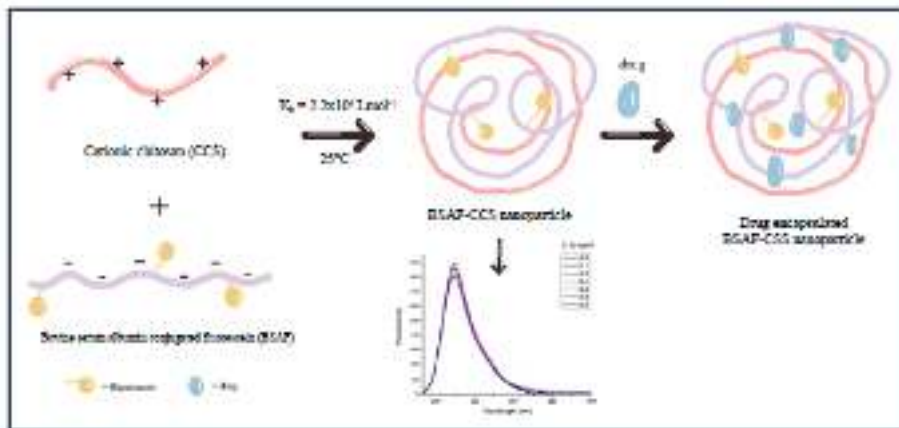
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In this work, the novel drug delivery system consisted of bovine serum albumin conjugated fluorescein (BSAF) and cationic chitosan (CCS) have been developed. The photophysical properties of BSAF-CCS have been studied by using UV-Vis and fluorescence spectroscopy. UV absorption spectra of BSAF in PBS buffer pH 7.4 in presence of CCS have not been changed. The fluorescence emission of BSAF was studied by excited at 460 nm and emission at 523 nm have been detected. The fluorescence intensity of BSAF decreased when the concentration of CCS increase indicated the interaction of BSAF and CCS was occurred. The binding constants ( $K_b$ ) of BSAF-CCS nanoparticles were  $2.2 \times 10^4 \text{ Lmol}^{-1}$  and  $7.1 \times 10^2 \text{ Lmol}^{-1}$  at  $25^\circ\text{C}$  and  $37^\circ\text{C}$ , respectively. The binding constants ( $K_b$ ) suggested that when the temperature increased the binding interaction of BSAF-CCS nanoparticles decreased. The particle size was studied by using DLS showed that increasing the CCS resulted the smaller size of nanoparticle. This BSAF-CCS nanoparticle system will be used as drug carrier in the further studied.

**Keywords:** Quercetin; nanoparticle; nano-delivery system; chitosan; bovine serum albumin



**Figure 1.** Scheme for the synthesis of BSAF-CCS nanoparticle.



## Microwave-assisted green synthesis of gold nanoparticles using amino acids and their antibacterial and catalytic activities

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The amino acid-stabilized nanoparticles have gained significant attention in recent years due to their potential applications in various fields, including medicine, catalysis, and materials science. This study explores the eco-friendly microwave-assisted synthesis of gold nanoparticles (AuNPs) employing a variety of amino acids (AAs). The synthesized AA-AuNPs nanoparticles were characterized by UV-Vis spectroscopy, FTIR, SEM/EDS, and TEM analysis. The surface Plasmon resonance (SPR) study indicates the formation of AuNPs. Based on the wavelength, the various types of amino acids were able to produce nanoparticles of different sizes. Furthermore, the size of the AuNPs was determined by TEM analysis, revealing that Alanine-AuNPs were between 5-8 nm, Tryptophan-AuNPs ranged from 10-14 nm, and Valine-AuNPs measured 9-13 nm, respectively. The biological efficiency test was conducted using the prepared AuNPs, and the results showed that the synthesized AuNPs were highly toxic against *Staphylococcus aureus* (*S. aureus*) and *Escherichia coli* (*E. Coli*) bacteria. Additionally, the catalytic efficiency of the prepared AA-AuNPs was studied for the reduction of 4-nitrophenol to 4-aminophenol in the presence of sodium borohydride. The progress of the reaction was monitored by observing the absorbance peak in UV-Vis spectroscopy. The study yielded positive results, demonstrating that Tryptophan-AuNPs exhibited catalytic activity. It was also observed that the gold nanoparticles remained stable for an extended period.

**Keywords:** Amino acids; AuNPs; Antibacterial activity; Reduction reaction.

## Carbon dots from latex using microwave-assisted pyrolysis for tyrosine detection

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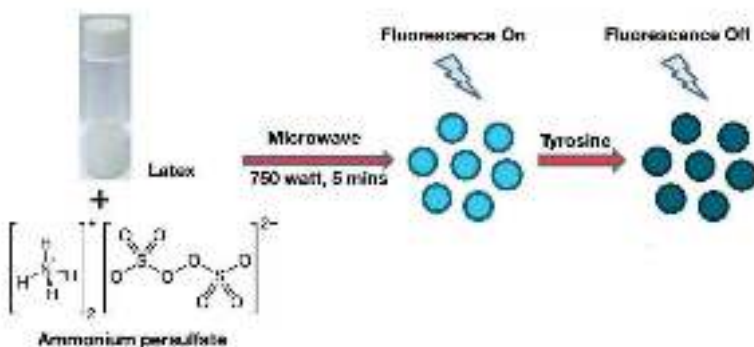
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In this study, the carbon dots (CDs) were prepared from the rubber latex (*Hevea brasiliensis*) as the carbon source and ammonium persulfate as the nitrogen source using “microwave-assisted pyrolysis”. Various instrumental techniques such as transmission electron microscopy, UV-visible spectrophotometry, fluorescent spectrophotometry and fourier-transform infrared spectroscopy were employed to characterize CDs. The particle size of synthesized CDs was less than 5 nm and CDs showed good optical properties and solubility in water. The optical properties of CDs were strongly influenced by several functional groups (-OH, -CHO, -COOH, -CO, -COO) formed on the CDs surface. Finally, the CDs were applied as a fluorescent probe for the selective and sensitive detection of tyrosine. Furthermore, to explain the quenching mechanism, the FI quenching was calculated by Stern-Volmer equation. On the whole, this work is a novel illustration of The CDs-based sensor application for the tyrosine detection.

**Keywords:** Carbon dot; *Hevea brasiliensis*; Tyrosine; Fluorescence; Detection



## Development of antibacterial and wound dressing hydrogels based natural biopolymer composite with curcumin stabilized gold nanoparticles-loaded nanoliposome

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This work describes the preparation of curcumin-stabilized gold nanoparticles loaded into nanoliposomes (CUR/AuNPs-nanoliposome). The formation of curcumin-stabilized gold nanoparticles was evaluated using UV-vis spectroscopy, and a surface plasmon resonance band at 524 nm clearly confirmed the formation of silver nanoparticles. In addition, the nanoliposomes prepared from lecithin and curcumin concentrations of 2.7 mmol were synthesized using the thin film technique with an evaporator. The nanoliposomes exhibit a maximum absorbance in the UV-vis spectrum at 202 nm, indicating the  $\pi$ - $\pi^*$  transition of curcumin nanoliposomes, and at 418 nm, indicating the curcumin derivatives. CUR/AuNPs-nanoliposome were characterized by UV-vis spectroscopy, Attenuated total Reflectance Fourier Transform Infrared Spectroscopy (ATR-FTIR), Transmission Electron Microscope (TEM), Dynamic Light Scattering (DLS), and Zeta potential. Interestingly. Notably, the efficiency of CUR/AuNPs-nanoliposome was tested for its antibacterial activity and applied to the synthesis of CUR/AuNPs-nanoliposome hydrogels to absorb fluid from wounds. This approach enhances the efficiency in healing and drying wounds, improves the efficiency of storing important substances, maximizes the efficiency of active ingredients, and ensures high stability, making it suitable for biomedical applications in the future.

**Keywords:** Curcumin nanoliposome; Gold nanoparticle; Hydrogel; Antibacterial activity

## Morphology-controlled microwave synthesis of tetragonal copper bismuth oxide with needle-like flower architecture

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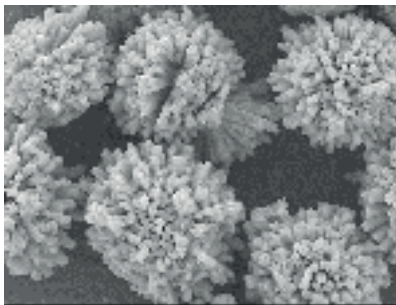
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Copper bismuth oxide ( $\text{CuBi}_2\text{O}_4$ ) with a needle-like flower morphology and a pure tetragonal structure has been successfully synthesized by a facile microwave-assisted method. This was achieved using a domestic microwave oven with a power of 300 W and a short reaction time of only 10 min. A single-step microwave synthesis of  $\text{CuBi}_2\text{O}_4$  produces high-purity material with the tetragonal phase, as confirmed by X-ray diffraction (XRD) analysis. The high BET surface area of the  $\text{CuBi}_2\text{O}_4$  flower-like sphere, assembled by  $\text{CuBi}_2\text{O}_4$  needles, could be attributed to its porous and hollow structure. This makes it suitable for a heterogeneous catalyst system. Ultraviolet-visible diffuse reflectance spectroscopy (UV-vis DRS) results exhibit an absorption edge in the visible range, and the band gap is estimated to be approximately 2.90 eV. Consequently, this synthesis technique addresses limitations in current photocatalytic nanomaterial production methods, particularly in scalability and energy efficiency. It accelerates reactions, enabling quick nanoparticle formation, and its energy-efficient direct heating minimizes heat loss, leading to cost-effective and eco-friendly production.

**Keywords:** Copper bismuth oxide;  $\text{CuBi}_2\text{O}_4$ ; Microwave synthesis; Flower-like structure



**Figure 1.** SEM image showing the morphological evolution of  $\text{CuBi}_2\text{O}_4$  prepared from Microwave-assisted method.

## Microwave synthesis of nitrogen and boron co-doped carbon dots from ascorbic acid

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In order to enhance optical performances and expand range of applications of carbon dots, doping with heteroatoms is one of the most interesting and effective approaches. In this work, nitrogen-doped carbon dots (N-CDs) and nitrogen/boron co-doped carbon dots (N/B-CDs) were successfully synthesized by facile microwave-assisted synthesis using ascorbic acid, urea, and boric acid as carbon, nitrogen, and boron sources, respectively. This method provides simplicity, rapid reaction rates, high efficiency in heating, environmental friendliness, and energy savings. Morphologies and optical properties of the synthesized N-CDs and N/B-CDs were characterized by transmission electron microscopy (TEM), UV-Visible spectroscopy, and fluorescence spectroscopy. The N-CDs showed maximum fluorescence emission at wavelength of 412 nm with an excitation wavelength of 338 nm, while the N/B-CDs showed maximum fluorescence emission at wavelength of 413 nm with an excitation at wavelength of 324 nm. Both of carbon dots exhibited blue fluorescence under black light irradiation at wavelength of 365 nm. These materials potentially offer excellent performances in sensing and imaging applications.

**Keywords:** Doped carbon dots; Microwave synthesis; Fluorescence; Ascorbic acid

## Effect of graphene quantum dots in enhancing plant growth and anti-oxidant activity of mung bean

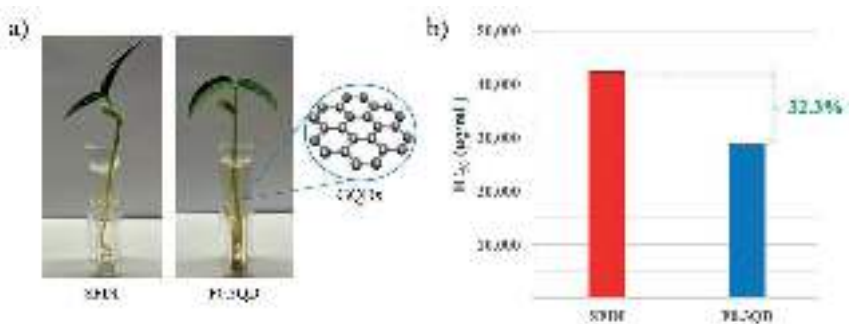
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Graphene quantum dots (GQDs) are carbon nanomaterials with excellent fluorescent properties resulting from quantum confinement effects. They also exhibit relatively high biocompatibility with living cells and low toxicity<sup>[1]</sup>. In this research, mung beans were grown by incorporating GQDs through three different methods. The first method involved soaking the mung bean seeds in GQDs for one night before planting. The second method included adding GQDs as a form of fertilizer. The third method combined the first and the second approaches. It was found that all three methods enhanced the antioxidant activity of mung bean plants compared to conventional cultivation. On the other hand, the addition of GQDs decreased the growth of mung bean in term of the total height. The best condition to obtain the highest antioxidant activity is using GQDs as fertilizer (0.3 mg/ml, F0.3QD), in which it enhances the activity by 32.3% compared to the one growing under water.

**Keywords:** Graphene quantum dots (GQDs); Anti-oxidant; DPPH; Mung bean; Soaking



**Figure 1.** a) Mung bean plants grown under water(left) and with 0.3 mg/ml GQDs(right) b) comparison of IC<sub>50</sub> of mung bean plants grown under water and 0.3 mg/ml GQDs.

# One-pot synthesis of magnetic activated carbon by consecutive hydrothermal pretreatment and pyrolysis of cassava rhizome for methylene blue adsorption

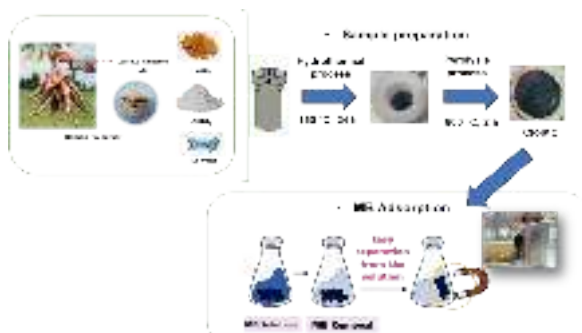
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Biomass derived magnetic activated carbons (MC) have been widely studied as low-cost adsorbents to remove the pollutants from water due to an abundance of carbon precursors, eco-friendly, variable textural properties, and magnetic separation capability. However, more research is needed for the development of a facile and an efficient synthesis process. The conventional preparation methods of MC involve multiple steps and require large energy input. In addition, the attachment of magnetic particles often leads to the clogging of existing pores, result in poor adsorption performance. In this work, MCs were prepared through the simultaneous pyrolysis, activation, and magnetization of the hydrothermally treated cassava rhizome (CR).  $\text{ZnCl}_2$  and  $\text{FeCl}_3$  were added into the reaction mixture as the activating agent and the magnetizer respectively during the hydrothermal treatment. As-synthesized CR-MC endows the highest  $S_{\text{BET}}$  (554  $\text{m}^2/\text{g}$ ) with 77% mesoporosity when addition of  $\text{FeCl}_3$  into the reaction mixture with the weight ratio of  $\text{FeCl}_3:\text{ZnCl}_2$  of 1(3MC-1). 3MC-1 was tested as the adsorbent to investigate the adsorption efficiency of methylene blue (MB) in water. The adsorption behavior of 3MC-1 towards MB was monolayer adsorption based on the Langmuir isotherm model with  $R^2$  of 0.9953 exhibiting a maximum adsorption capacity of 102  $\text{mg/g}$ . In addition, 3MC-1 with a saturation magnetization value of 3.343  $\text{emu/g}$  could be easily separated from the solution using an external magnet. The findings show that CR-MC can be successfully synthesized by using biomass as carbon precursors and simply functionalized the magnetic particles into the carbon to enable manipulations in industrial operations.

**Keywords:** magnetic activated carbon; cassava rhizome; hydrothermal treatment; methylene blue; adsorption



**Figure 1.** Schematic illustration for synthesis of CR derived MC and its adsorption test of MB

## Synthesis and characterization of cellulose aerogel composite from pineapple leaves and polyvinyl alcohol

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There are massive amounts of agricultural waste from discarded pineapple leaves after pineapple harvesting, which can cause environmental problems. To maximize agricultural waste utilization, pineapple leaves were used to synthesize the cellulose aerogel composite in this study. First, dry pineapple leaves were pretreated and bleached to obtain the pineapple leaf fiber (PF) and enrich the cellulose content. From the determination of the composition of PF, it was found that the cellulose content rose to 88%. Polyvinyl alcohol was used as a binder and cross-linker to synthesize the cellulose aerogel composite from PF via the freeze-dry method. The surface area and average pore diameter of the synthesized aerogels were characterized by nitrogen adsorption-desorption (BET) analysis. The density, thermal properties, morphologies, and chemical structure of the cellulose aerogels were investigated. The BET surface areas were between 188-207 m<sup>2</sup>g<sup>-1</sup> with an average pore diameter of 4.4-9.4 nm. The cellulose aerogels have low density and thermal conductivity of 0.03-0.04 g.cm<sup>-3</sup> and 0.056-0.064 Wm<sup>-1</sup>K<sup>-1</sup>. The cellulose aerogel composites from PF can be further developed as a good candidate for thermal insulation due to their low thermal conductivity.

**Keywords:** Aerogel; Cellulose; Pineapple leaves; Fiber; Insulation



## The study of rheological properties of silk fibroin in ionic liquids

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The Bombyx mori silk fibroin (SF) which obtained from different degumming process was prepared with different methods and dissolved in Ionic liquids (ILs) (AmimCl, BmimCl and EmimCl). All SF/ILs samples was dissolved in Ionic liquids with 0.1-15.0 %wt at 90 °C for 2 hr and 60 °C for 1 hr, respectively, and keep in oven until get uniform solution. The rheological properties of this sample were measured with Physica MCR-300 and MCR-301 Rheometer. For all oscillatory shear measurement was performed under stain-control model in the frequency,  $\omega$ , range 0.1-100 rad/s at various temperatures. The steady shearing behavior suggested that Ionic liquids is a good solvent for SF molecules. It was found that the modulus of SF/ILs obtained from precipitation procedure show higher modulus than both SF obtained by conventional procedure and regenerated SF with Ajisawa's reagent. These results were corresponded to the degradation of SF of which those methods. The viscosity of SF/ILs solutions were increased with increased concentrations and SF/EmimAc solution also exhibits lower viscosity than other with each concentration. Otherwise, the solutions of SF/ILs showed a typical plastic flow behavior which observed by the increasing of the moduli with  $\omega$  and tended to cross at high  $\omega$  except at the highest temperature, which is similar to the dynamic viscoelastic behavior of the native silk spinning dope at low temperature. The existence of plateau like behavior denotes the weak network in the solution.

**Keywords:** Silk fibroin; Ionic liquids; Moduli; Rheology; Degumming

## The Metal Nanoparticles Coupling with Carbon Quantum Dots via Solution Plasma Discharge and Embedding in Metal-Organic Frameworks for Dye Degradation

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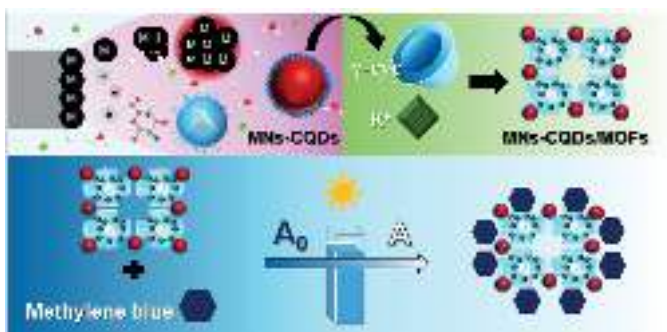
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Driven by water pollution, especially in the dye industry, metal nanomaterials are popular materials used in the catalytic field due to their high surface-to-volume ratio and rich active surface atoms. However, they are easily coalescent, leading to a reduction in the catalytic activity. Herein, we reported the facile synthesis of highly stable metal nanoparticles, including Au, Ag, and Cu, coupling with carbon quantum dots (CQDs) through one-step plasma discharge in solution. The photocatalysts were further embedded in cyclodextrin metal-organic frameworks (MOFs), a green-based, high-porous material, to enhance thermal stability and improve photocatalytic performance. The photocatalyst MOFs revealed cubic morphology in a nanosized range of 150–400 nm with a large specific surface area. The dye removal was completed after adding the photocatalyst into the dye solution and placing it in the dark for 30 minutes, then turning on a Hg lamp for 15 minutes. Among all composites, the Ag-CQDs/MOFs demonstrated the best catalytic activity in methylene blue degradation, achieving an impressive 92.78% efficiency and a reaction rate of  $0.08501 \text{ min}^{-1}$  in the first cycle. Furthermore, the composite maintained a substantial 78.64% degradation efficiency after three cycles, highlighting its enduring and robust catalytic performance.

**Keywords:** Metal Nanoparticles; Carbon Quantum Dots; Metal-Organic Frameworks; Solution Plasma Discharge; Dye degradation



## Fabrication and characterization of MOF-808/PVDF films

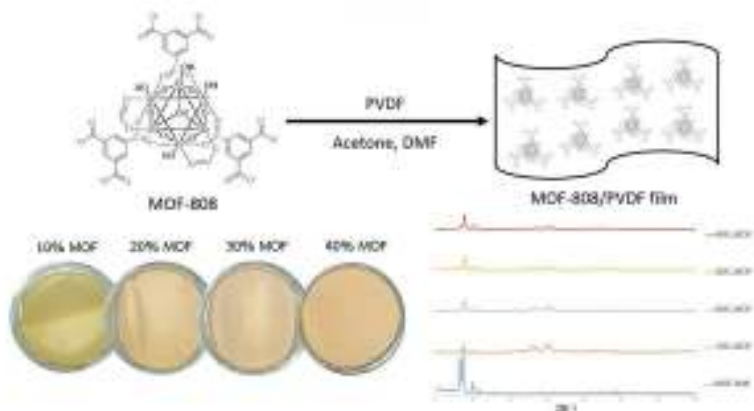
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Recently, metal–organic frameworks (MOFs) have attracted tremendous interest in preparing a MOF film, which could help expand their uses in a variety of technological applications such as catalysis or adsorption. Particularly, by employing MOFs as modifying agents, due to the benefits from their excellent functional designability, good compatibility with polymers, and customizable and regular pore structure, the film performance could be enhanced. In this study, MOF-808 film was created by anchoring MOF-808 within polyvinylidene fluoride (PVDF). The crystallinity, thermal stability, morphology, and functionality of MOF-808/PVDF films with varying MOF-808 content (10, 20, 30 and 40% by weight of MOF-808) were then thoroughly assessed. The MOF-808/PVDF films possessed good mechanical strength and flexibility. The films were characterized by FT-IR spectroscopy, XRD, and TGA measurements. XRD results reveal that the crystallinity of MOF-808 still retained after film fabrication. Characterization of the films showed MOF-808/PVDF films still have the crystallinity of MOF-808 while retained the flexibility and elasticity of PVDF.

**Keywords:** MOF-808; PVDF; MOF films



## ZIF-8 synthesis for oil removal from water surface

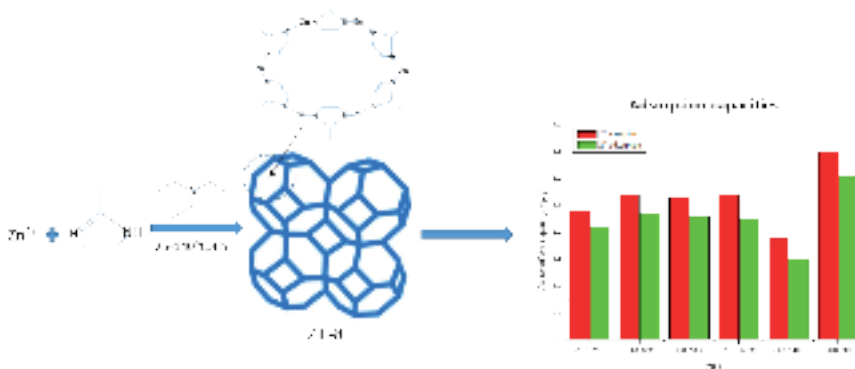
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ZIF-8 (Zeolite imidazole framework) has excellent properties that are useful in oil/water separator application such as thermally and chemically stability, high surface area, reusable and hydrophobic property. One-pot hydrothermal synthesis of ZIF-8 was prepared using TEA as a modulating agent for controlling the particle size. The reaction was conducted in temperature range from 25 °C to 140 °C. The synthesized ZIF-8 is consider as hydrophobic material which contact angle (CA) is 113°. This result confirms capability of oil/water separation. According to the XRD, FT-IR, SEM-EDS and adsorption capacity, ZIF8-80°C is the suitable condition for synthesis due to its high crystallinity, small particle size, and well disperse. It also shows highest adsorption efficiency (2.5 g/g). For practical application, ZIF-8 was made as a pellet and directly adsorbed oil from water surface. The result show that oil has been completely removed. Therefore, lab-synthesized ZIF-8 can be used for oil/water separation. However, compared the oil adsorption capacity with other commercial products, the efficiency of ZIF-8 is in the average range of other products. On the contrary, ZIF-8 has some advantages such as one-pot synthesis which suitable to large-scale production, high purity and reusable. Therefore, ZIF-8 will be further studied oil adsorption improvement.

**Keywords:** ZIF-8; oil removal; hydrothermal; modulating agent



**Figure** ZIF-8 synthesis and oil removal in wastewater treatment application.



## Trimethylamine adsorption and host-guest interaction within UiO-66-NH<sub>2</sub> framework

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Trimethylamine (TMA) is a volatile organic compound with a characteristic foul odor commonly associated with the decomposition of seafood and other organic matter. Development of efficient adsorption techniques and sensitive detection method for TMA can directly impact the quality control processes within the seafood supply chain. In this study, TMA adsorption by UiO-66-NH<sub>2</sub> was explored and the specific host-guest interactions between TMA and UiO-66-NH<sub>2</sub> were identified. Powder X-ray diffraction (PXRD) and Fourier transform infrared spectroscopy were employed to characterize the structure of TMA-loaded UiO-66-NH<sub>2</sub>, the identity of host sites within the framework, and perturbations induced by host-guest interactions. According to the results, UiO-66-NH<sub>2</sub> shows high stability toward TMA adsorption with retention of the structure and porosity. The activation of the framework by conventional heating and vacuum was found to remove solvent molecules from the framework and resulted in lower TMA adsorption compared to the framework activated by solvent-exchange. Reitveld refinements of the PXRD data demonstrated that the presence of ethanol molecules as guests in the framework caused an enhancement of TMA adsorption of UiO-66-NH<sub>2</sub> by providing binding sites for TMA molecules. This understanding is essential for the rational design and modification of materials to enhance their TMA adsorption capacity and selectivity.

**Keywords:** Trimethylamine; UiO-66-NH<sub>2</sub>; Adsorption; Host-guest

## Pomelo peel nanocellulose for pickering stabilization of oil-in-water emulsion

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Pomelo peel is a fiber-rich waste material that serves as a valuable source for cellulose utilization. This study aimed to increase the value of pomelo peel by extracting nanocellulose and utilizing it as a Pickering emulsion stabilizer. The process involved the mild pretreatment of pomelo peel with low sodium hydroxide and hydrogen peroxide, followed by hydrolysis with citric acid at different reaction times. The resulting nanocellulose was characterized using various techniques, including transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD) for cellulose crystallinity index ( $C_rI$ ), and zeta potential measurements. The characterization revealed cellulose nanofibrils (CNFs) with micro-scale lengths and diameters ranging from 2 to 5 nm, along with carboxyl functionalization of the surface. The charged surface groups of CNFs resulted in improved colloidal stability, with a  $\zeta$ -potential higher than -35 mV. The crystallinity index of nanocellulose exhibited values in the range of 50-70%. These CNFs were employed to stabilize oil-in-water Pickering emulsions at various concentrations. The emulsion droplet sizes ranged from 1 to 3  $\mu$ m. Furthermore, these Pickering emulsions displayed long-term storage stability against creaming for at least one month.

**Keywords:** Pickering emulsion; Pomelo peel; Nanocellulose



## Performance of lignin as eco-friendly reinforced filler in dental adhesives

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Fillers in dental adhesives have been developed throughout the years to increase the performance and other mechanical properties of dental adhesives. Natural polymers are one of the fillers that have attracted attention and developed as potential fillers in dental adhesives. This research purpose is to investigate the possibility and performance of incorporating the extraction of lignin from rice straw as a filler in dental adhesives with respect to their mechanical properties and cytotoxicity. The efficiency of the dental adhesives containing lignin fillers showed an increase in bond strength between dentin and composite resin. The hybrid layer and resin tags between dentin and resin adhesive were revealed as contributing to the improvement of bond strength. Furthermore, the dental adhesives containing lignin fillers was tested for cytotoxicity to confirm their non-toxic property toward human fibroblast cells.

**Keywords:** Dental adhesive; Lignin; Micro-tensile bond strength; Filler.

## Preparation of activated carbon from spent coffee grounds by radiation processing for methylene blue adsorption

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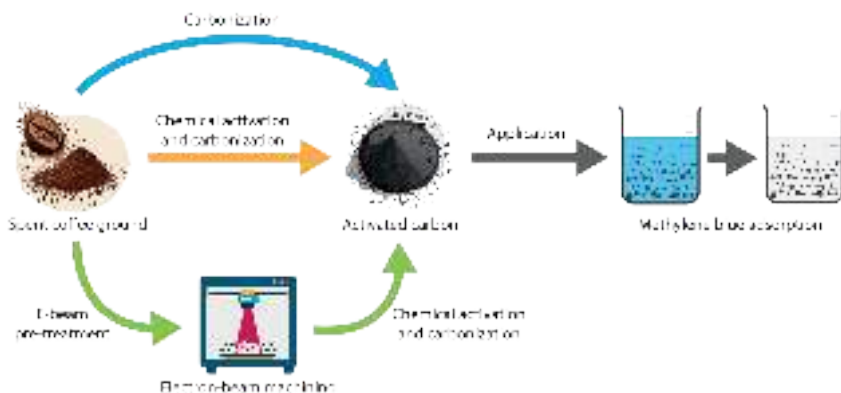
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Activated carbon is commonly used in water purification systems due to its high surface area and non-toxicity. One of the promising precursors for the preparation of activated carbon is spent coffee grounds because of their high carbon and low inorganic contents. In addition, pre-treatment of the carbon source is an important step to improve the properties of the activated carbon. Therefore, in this work, we proposed a pre-treatment method for the activated carbon using e-beam irradiation to decompose the lignocellulose chains of the spent coffee grounds. The samples pre-treated with e-beam irradiation were compared to those without pre-treatment. The physical characteristics of all activated carbon were investigated using x-ray powder diffraction (XRD), scanning electron microscopy (SEM), Fourier-transform infrared (FT-IR) spectroscopy, and specific surface area measurements. Furthermore, we tested all samples in the adsorption of methylene blue (MB). The results showed that the activated carbon pre-treated with e-beam exhibited porous surface and a larger surface area. Compared to the sample without pre-treatment, the surface area improved from 117.82 to 1,064.1 m<sup>2</sup>/g. Moreover, it demonstrated an adsorption capacity of 150 mg/g. The results illustrated that e-beam irradiation is an effective pre-treatment method for the preparation of activated carbon.

**Keywords:** Radiation processing; Spent coffee ground; Activated carbon; Chemical activation; Methylene blue adsorption



## Surface modification of porous titanium complex with bioactive RGD for bone tissue regeneration

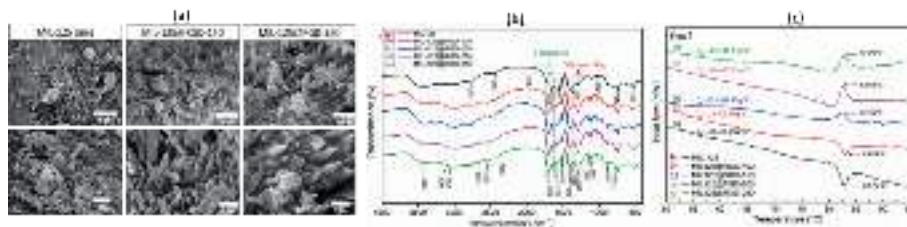
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One of orthopedic procedures to replace and regenerate lost bone cells in bony fractures is applying an artificial scaffold between two broken parts or around surgically implants to stimulate the new bone tissue formation. One way to develop an effective bone substitute is to grafting biomolecules on hard materials to obtain biomedical functions with osteoinductive effect and practical to use for orthopedic surgeons. Here, we focus on using *in vitro* tissue engineering techniques to design and develop a biocompatible scaffold that resembles the extracellular matrix found naturally in bones. We performed the fabrication of arginine-glycine-aspartate (RGD) peptides, an important bioactive molecule for cell regeneration, on a porous titanium oxide complex (MIL-125). Results from SEM show changes in surface morphologies of the MIL-125 with different amount of RGD. More needle-like structures were observed due to the more formation of grafted RGD crystals on the materials surface. We characterized the complex structures by FT-IR and micro-DSC techniques. Interestingly, a sharply flipped exothermic peak ( $T_{max}$ ) at 82.57°C which is the phase transition of the sample MIL125@RGD-150, indicating an optimum condition for the synthesis of this bone graft. These results can be useful for the development of porous bone scaffolds for specific purposes of bone fracture treatments.

**Keywords:** Tissue engineering; Bone scaffold; Fabrication; Bioactive molecule



**Figure 1.** Scanning electron microscopy (SEM) images (a), FT-IR spectra (b), and micro-DSC analysis (c) of the MIL125@RGD samples after solvent soaking for 36 hr

## The effect of calcination temperatures on NIR reflection of lateritic soil pigments

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The aim of this research is to develop pigments from lateritic soil to reflect near-infrared (NIR) radiation. The lateritic soils used in this research were received from Pha Khao district, Loei province, Thailand. The raw lateritic soils were ground to reduce the size to smaller than 45  $\mu\text{m}$  and were then calcined at 900-1300°C for 1 h. The calcined pigments were characterized by an X-ray diffractometer (XRD), a scanning electron microscope (SEM), and a UV-Vis-NIR Spectrophotometer. The experimental results showed that the highest NIR reflective pigments from lateritic soil could reflect more than 90% of infrared radiation at a calcined firing temperature of 1300°C for 1 h. It was found that quartz and  $\text{FeAl}_2\text{O}_4$  were the two main compositions. The highest NIR reflective pigments occupied particle sizes in the range of 1-20  $\mu\text{m}$ .

**Keywords:** lateritic soil; NIR reflective pigment; calcination; powder sedimentation; particle size

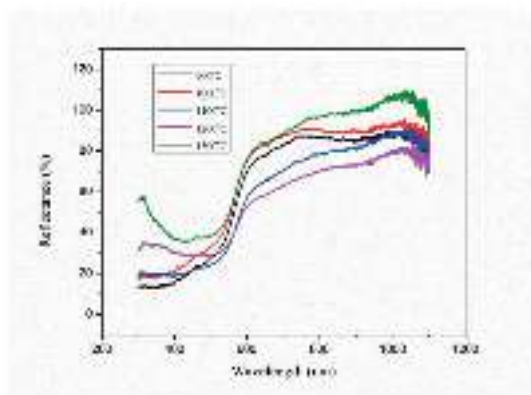


Figure 1. NIR Reflectance of calcined lateritic soil at different temperatures

## Optimizing color conversion and luminance enhancement in ultra-thin films through aerosol-deposited perovskite quantum dot/metal oxide composites

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In the past, displays employing down-converting color-changing media incorporated color filters as a crucial element in elucidating the balance between authentic colors and transmittance. In this study, we report the development of a novel, smart process for producing thin luminescent films that completely convert colors and enhance light intensity. Highly dense films are prepared by the co-deposition of perovskite quantum dots and metal oxide particles as color conversion layers and scattering agents, respectively. These layers can be directly deposited on blue organic light-emitting diodes using ultrasonic-assisted aerosol deposition (UAD). This method can allow displays using a down-conversion system to streamline the process due to absence of color filters. Using this method, films can be a minimum of 3  $\mu\text{m}$  thick for complete conversion of blue light, a quarter that of inkjet-printed films. We demonstrate 7,353  $\text{cd m}^{-2}$  in green and 411  $\text{cd m}^{-2}$  in red converted emissions with no blue light leakage. Furthermore, the developed technique was shown to be compatible with versatile patterning processes. For example, UAD may be combined with a fine-metal shadow mask to produce a pattern of 30- $\mu\text{m}$ -diameter dots. Even without using a mask, the method still produces a pattern of 13  $\mu\text{m}$  wide lines. This system provides a new approach that may serve as an alternative to inkjet printing.

**Keywords:** Perovskite quantum dots; Aerosol deposition; Color conversion; Scattering effect; OLED backlight

## White electroluminescence emission using perovskite nanocrystals and organic emitters

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In the present study, we report for the first time three color white-light emission with high brightness from white-emitting PeQD organic light-emitting diodes (WPeQD-OLEDs) fabricated using a PeQD material and organic emitters. A WPeQD-OLED bilayer was prepared by depositing a blue-emitting organic layer on top of a CsPb(Br/I)<sub>3</sub> QD layer mixed with N9,N10-Bis(4-(tert-butyl) phenyl)-N<sub>9</sub>,N<sub>10</sub>-Di-*o*-Tolylanthracene-9,10-Diamine (*p*-Tb-*o*-Me-TAD), which were spin-coated as red and green organic emitters, respectively. The WPeQD-OLED device was stable during operation and demonstrated emission of three primary colors. In the WPeQD-OLED device, charge carriers were distributed by an 9-(naphthalen-1-yl)-10- (naphthalen-2-yl)anthracene ( $\alpha,\beta$ -ADN) blue-emitting host material with a deep highest occupied molecular orbital (HOMO) level. The electroluminescence (EL) spectra of the WPeQD-OLEDs showed EL maximum peaks at 460, 527, and 640 nm; the CIE color coordinates of the emitted light were (0.33, 0.40). The EL results confirmed that the maximum luminance was 49,000 cd m<sup>-2</sup> and the maximum luminance efficiency and power efficiency were 4.48 cd A<sup>-1</sup> and 2.16 lm W<sup>-1</sup>, respectively.

**Keywords:** Perovskite quantum dots; White electroluminescence emission; Hybrid perovskite QD-organic emitters; Hybrid light emitting diodes



## **Hydrogels containing liquid crystal droplets for stretchable display applications**

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Producing flexible and stretchable displays based on organic light-emitting diodes or LED-backlit liquid crystals (LCs), which require minimal energy consumption during operation, is an important challenge. Non-emissive liquid crystal displays can be made flexible through the use of polymer-dispersed liquid crystal (PDLC). Hydrogels on the other hand can be designed to be stretchable and wearable device-compatible. Combining LCs with hydrogels remains a challenge due to the inherent incompatibility between hydrophobic LCs and hydrophilic hydrogel structures. Only a low amount of LCs, approximately 2 – 4 wt%, could be directly dispersed and stabilized in hydrogels.

Herein, we present a new strategy for embedding LC emulsion droplets into a hydrogel matrix with LC content of up to 20 – 40 wt%, i.e. ten times higher than previous reports. Droplets of the liquid crystal compound N-(4-methoxybenzylidene)-4-butaniline (MBBA) with sizes ranging from 670 to 840 nm were prepared via the miniemulsion technique. The behavior of MBBA LCs droplets embedded in polyacrylamide hydrogel was investigated. Differential scanning calorimetry (DSC) measurements revealed a significant shift in the nematic-isotropic phase transition temperature of the LCs. Further investigations of the electro-optical performance demonstrated that the LC cells was driven at a higher frequency, up to 1 MHz, in comparison to cells made from pure MBBA LCs, which requires a lower frequency, around 200 Hz, for a thickness of 125  $\mu\text{m}$ . Lastly, hydrogels embedding LCs exhibited flexibility and stretchability as demonstrated by rheological measurements. This study represents an important step towards stretchable displays based on non-emissive LCs for low-energy consumption devices.

**Keywords:** Liquid crystals; Emulsion; Hydrogel; Optical property; Rheological property

## Encapsulation of *Mitragyna speciosa* (Roxb.) korth. using coaxial electrospray technique

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Kratom is an herbal plant found mainly in Southeast Asia. Generally, people consume its leaves in order to be more productive at work and to be resistant under the hot weather. It is usually consumed in the form of an energy drink or by chewing fresh leaves. In the kratom plant, there are more than 25 kinds of alkaloids, such as Mitragynine, Speciogynine, Speciociliatine and Mitraciliatine, etc. However, alkaloids have low solubility in water. They are also unstable under light and heat. It's reported that there is good pharmacological activity when used at an optimized dosage. Overdosing should be avoided due to its unwanted side effects. To solve these problems control the dosage use and prevent alkaloids' decomposition, the researchers are using the Coaxial Electrospray Technique to encapsulate kratom extracts in boba form. This study is focusing on optimization to demonstrate conditions for preparing boba capsules of crude kratom extract. Encapsulation of crude kratom extract mixed with gelatin in sodium alginate with core-shell structures was conducted. The effects of parameters such as the applied electric voltages and the flow rates were studied. The identity of the boba capsules was investigated using FT-IR spectroscopy. It was found that crude kratom extract was encapsulated inside the capsule particles. Physical characteristics were studied by imaging and measuring the size of the boba capsule particles. The result showed that the boba capsules formed using Volt revealed more consistent capsules than the boba capsules formed without Volt. Notably, the size of both conditions is slightly different. This research could be applied in food and medical industries.

**Keywords:** Kratom; Boba; Coaxial electrospray; Encapsulation

## X-ray absorption studies on emerald and jade-like glass prepared from glass waste

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In this research, upcycling of glass waste was performed by re-melting and subsequent shaping into ornaments. The emerald and jade-like silicate glass was produced by mixing glass waste with chromium powder (a colorant). The base glass formula is composed of  $\text{SiO}_2$  (from colorless glass waste),  $\text{Na}_2\text{CO}_3$ ,  $\text{K}_2\text{CO}_3$ ,  $\text{ZnO}$ ,  $\text{H}_3\text{BO}_3$ ,  $\text{CaO}$  and  $\text{Al}_2\text{O}_3$ . All components including chromium powder were melted at  $1150^\circ\text{C}$  for 3 hrs. The glass melt was poured onto the metal mold, annealed at  $550^\circ\text{C}$  for 2 hour and left cool to room temperature to obtain a cylinder-shape glass sample. Varying amount of chromium powder was attempted leading to two types of green glass, emerald (clear) and jade-like (opaque) glass. The opaque glass was produced when higher amount of chromium powder was being used. The coefficient of expansion (COE) of opaque glass ( $15.23 \times 10^{-6} (^\circ\text{C}^{-1})$ ) is higher than that of the clear glass ( $14.47 \times 10^{-6} (^\circ\text{C}^{-1})$ ). However, both COE values are still in the common range of the silicate glass. The fingerprints of the bond vibrations obtained from IR absorption data in both clear and opaque glass are similar to those in other silicate glass. X-ray absorption near edge structure (XANES) data showed the existence of  $\text{Cr}^{3+}$  in clear glass and  $\text{Cr}^{6+}$  in opaque glass. While the extended near edge structure (EXAFS) showed the best fit results with the Cr-O bond lengths of 1.97 and 1.64 Å for clear and opaque glass samples respectively. The clear and opaque green glass samples were further shaped into pear cut and glass bead ornament respectively (see Figure 1).

**Keywords:** glass waste; upcycling; glass ornament; X-ray absorption



**Figure 1.** The pear cut of the clear green glass and Jade-like glass bead ornament made from glass waste

## Effect of flux treatment process on photocatalytic dye degradation of aluminium-doped strontium titanate

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This study aimed to investigate the photocatalytic efficiency for organic dye degradation of aluminum-doped strontium titanate (Al-doped SrTiO<sub>3</sub>) synthesized by the flux treatment method. The preparation process involves the solid-state synthesis of SrTiO<sub>3</sub> using SrCO<sub>3</sub> and TiO<sub>2</sub> as precursors at 900–1300 °C followed by flux treatment with SrCl<sub>2</sub> in an alumina crucible at 1150 °C for 10 hours. Al doping was performed by adding Al<sub>2</sub>O<sub>3</sub> powder during flux treatment process. To investigate the effect of flux-treatment, Al-doped SrTiO<sub>3</sub> was also prepared by solid state without fluxing process. The obtained products were characterized for phase, morphology, chemical composition, surface area and optical property using X-ray diffraction (XRD), Scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDS), Brunauer-Emmett-Teller (BET) analysis, and Fluorescence spectroscopy, respectively. It was found that the pure SrTiO<sub>3</sub> phase was formed after solid-state synthesis at 1300 °C and remained unchanged after treatment with SrCl<sub>2</sub> flux. SEM images obviously showed that the morphology of SrTiO<sub>3</sub> particles changed from an irregular shape to a cubic shape (200–700 nm) when it was treated with SrCl<sub>2</sub> flux. Additionally, the particle size of cubic SrTiO<sub>3</sub> was drastically increased (0.3–1.5 μm) after Al-doping. The photocatalytic efficiency was evaluated by photodegradation of rhodamine B solution under UV light irradiation for 60 minutes. The results showed that flux-treated Al-doped SrTiO<sub>3</sub> sample could degrade rhodamine B up to 21.66%, more efficient than flux-treated SrTiO<sub>3</sub> (10.24%), solid-stated SrTiO<sub>3</sub> (3.10%) and solid-stated Al-doped SrTiO<sub>3</sub> (0.64%), respectively. It can be suggested that flux treatment using SrCl<sub>2</sub> and Al doping played an essential role in enhancing photocatalytic activity for dye degradation of SrTiO<sub>3</sub> under UV light.

**Keywords:** Photocatalysis; Strontium titanate; Dye degradation; Flux treatment; Solid-state

## Effect of shape stabilizers on properties of calcium chloride hydrate composite phase change materials for solar cell cooling

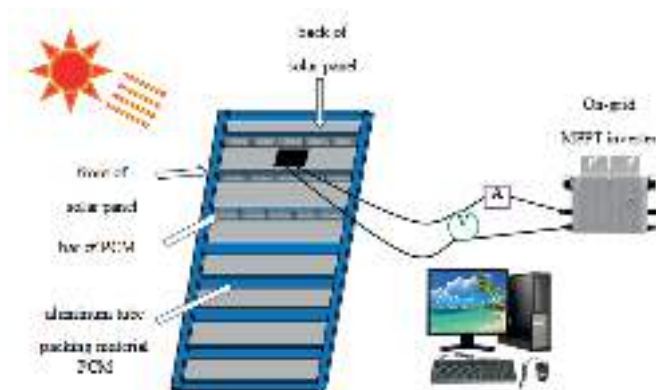
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This research aims to study the temperature reduction efficiency of photovoltaic solar panel using phase change materials (PCM). By containing a phase change material that is mixed with shape stabilizers, for example expanded graphite, expanded perlite and rice husk ash, mixed with calcium chloride hydrate. The PCM composites were then packed in a one-inch square aluminum tube and installed on the back of the solar panel. It was found that the addition of all three types of stabilizers gave similar performance when mixed at 20% by weight ratio. The 2.56 kg of phase change material reduces the temperature of solar panels by 5-10 °C and increases the conversion efficiency of solar energy by about 5%. To test the uniformity and stability of PCM materials, temperature fluctuations were simulated during 25-65 °C for a period of 5,000 cycles. Each cycle is equivalent to the temperature increasing and decreasing in each cycle of the day or equivalent to 13.5 years. When tested with DSC, it was found that the phase change material still works normally.

**Keywords:** Phase change materials, Solar panel



**Figure 1.** Solar panel installation model and data acquisition system

## Corrosion inhibition studies of tamarind shell tannins on mild steel in acidic medium

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The characterization of tamarind shell tannins for potential use in corrosion inhibition was studied. Fourier-transform infrared spectroscopy (FTIR), nuclear magnetic resonance (NMR), and thermal gravimetric analysis (TGA), were applied to examine tamarind shell tannins. The yield of extraction revealed that the water extract of tamarind shell (TWE) was rich in condensed tannins. Furthermore, the FTIR and NMR studies confirmed the presence of tannins. The corrosion inhibition studies were examined using electrochemical impedance spectroscopy (EIS), potentiodynamic polarisation (PD), and electrochemical noise measurement (ENM) analysis. The increase in concentration of the extracts increases the inhibition efficiency up to a maximum concentration of 1000 ppm. The inhibition efficiency was 82.43%. Potentiodynamic polarization analysis showed that extract was mixed type corrosion inhibitor with major impact of corrosion at cathodic sites. Nyquist plots showed that there was an increase in the resistance of charge transfer values and decrease in the constant phase element (CPE) as the concentrations of extract was increased. The extracts adsorption study followed the Langmuir isotherm. The extract molecules were physically adsorbed on the mild steel surface with a free energy absorption of  $\Delta G_{\text{ads}} \text{ TWE} = -20.03 \text{ kJ mol}^{-1}$ . Moreover, the surface morphology and elemental composition studies using SEM and EDX, confirmed the occurrence of extracts adsorption on the surface of mild steel.

**Keywords:** Tamarind shell; Tannins; Corrosion; Inhibition; Electrochemical

## NP : Natural Products, Biological Chemistry and Chemical Biology



## NMR-based stability evaluation of (*E*)-1-(3,4-dimethoxyphenyl)butadiene (DMPBD) from *Zingiber cassumunar* Roxb. rhizome

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(*E*)-1-(3,4-Dimethoxyphenyl)butadiene (DMPBD) isolated from *Zingiber cassumunar* Roxb. rhizome has been reported as a potent compound for anti-inflammatory and anticancer activities. Although DMPBD has an efficient potential for phytomedicines, its limited stability needs to be considered. The evaluation of chemical stability is critical for new drug development in order to keep its qualities within specified limits for the lifetime of product usage. Herein, we aim to evaluate the stability of DMPBD under various conditions, including solvents, temperatures, and light, to identify stability-affecting factors and define storage and handling conditions. The determination of the absolute quantity of DMPBD as a function of time and changes thereof over a month was monitored using an internal standard quantitative <sup>1</sup>H NMR (qHNMR) technique. The results suggested that DMPBD significantly decomposed in chloroform-*d*, while its content remained stable in methanol-*d*<sub>4</sub>. The content of DMPBD remained constant when stored at temperatures below 4 °C, both as a methanolic solution and the component in the crude extract. Light exposure had a slight effect on its content. Some degradation products were observed and might be influenced by O<sub>2</sub>-induced diene moiety cleavage. DMPBD should be stored as a crude extract or purified material in methanolic (or alcohol-water) solution for pharmacological and therapeutic applications. Ideally, the storage temperature should be below 4 °C, and O<sub>2</sub> should be excluded. Furthermore, the qHNMR technique was reliable for DMPBD quantification, confirmed by method validation.

**Keywords:** DMPBD; *Zingiber cassumunar*; Stability evaluation; NMR

## Molecular docking simulation tool CB-Dock2 confirmed high binding affinity between curcuminoids and I $\kappa$ B $\alpha$ /p50/p65 protein complex

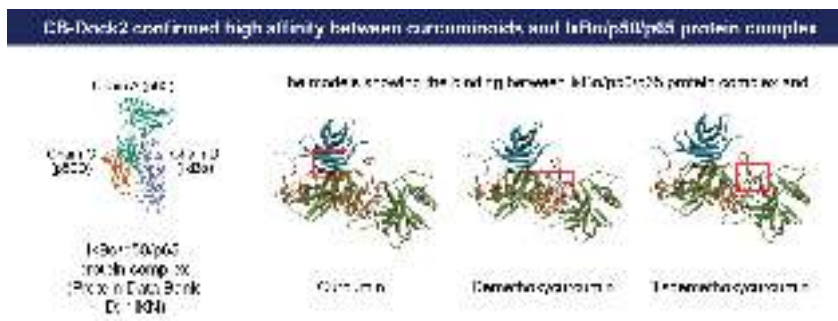
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*Curcuma longa* L. (turmeric) contains main active compounds termed curcuminoids, including curcumin, demethoxycurcumin, and bisdemethoxycurcumin. Many experimental data and molecular docking simulations have shown the biomolecular mechanism of curcuminoids in the canonical NF- $\kappa$ B signaling pathway, however, the interactions between curcuminoids and I $\kappa$ B $\alpha$ /p50/p65 protein complex (Protein Data Bank ID: 1IKN) in the pathway are not fully elucidated. To address it, we used a web-based blind docking simulation tool known as CB-Dock2. Regarding the five largest binding pockets of the protein complex identified from CB-Dock2, the resulting greatest negative Vina scores of curcumin, demethoxycurcumin, and bisdemethoxycurcumin were  $-8.0$ ,  $-9.2$ , and  $-8.8$  kcal/mol, respectively. There are many favorable intermolecular interactions between each curcuminoid and I $\kappa$ B $\alpha$  subunit of the protein complex. Curcumin binds to the specific contact residues of the dimerization sequence of p50 of the protein complex. Demethoxycurcumin and bisdemethoxycurcumin bind to the specific contact residues of the DNA-binding and dimerization sequences of p65 of the protein complex. Therefore, CB-Dock2 may substantiate the strong interactions between curcuminoids and the protein complex.

**Keywords:** Curcuminoid; CB-Dock2; Blind docking; Canonical NF- $\kappa$ B signaling pathway





## ***in silico* and *in vitro* studies on nucleoside-based inhibitors for pan-antiviral drug repurposing**

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Bunpote Siridechadilok<sup>1</sup>, Chanya Srisaowakarn<sup>2</sup>, Suwimon Manopwisedjaroen<sup>2</sup>,  
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The emergence of novel viruses underscores the demand for broad-spectrum antiviral drugs. The development of pan-antiviral drugs, capable of targeting multiple infectious agents, has gained prominence as a versatile approach to combat a wide range of human infectious diseases. Nucleoside-based inhibitors for pan-antiviral drug repurposing, highlighting their well-established pharmacological properties and conserved viral targets, have emerged as promising candidates for this purpose. In this study, experimental antiviral infectious assays were conducted on seventy-four FDA-approved nucleoside/nucleotide drugs targeting the RNA-directed RNA-dependent polymerase (RdRp) of dengue, influenza, and SARS-CoV-2. The results showed that gemcitabine, azacitidine, and  $\beta$ -D-N4-hydroxycytidine have relatively broad antiviral activity, and they have an antiviral effect by reducing virus infection by over 50% compared to the control. Computational studies of these pan-antivirals were conducted to elucidate shared attributes affecting binding interaction in different viruses. The findings have implications for the development of nucleoside-based pan-antiviral drugs targeting human virus RdRp and provide valuable guidance for future laboratory synthesis in upcoming studies.

**Keywords:** Drug repurposing; Nucleoside drug; Pan-antiviral drug; Molecular docking; Infectious assay; Viral RdRp

## Chemical constituents and their biological activities from the rhizomes and leaves of *Curculigo orchioides*

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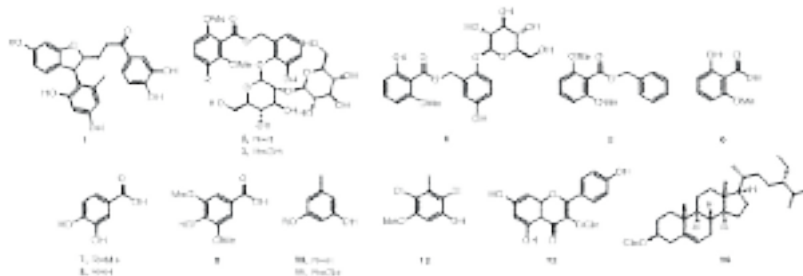
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<sup>2</sup>Integrated Nanotechnology Research Center, Department of Physics, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand.

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Phytochemical investigation of the rhizomes and leaves of *Curculigo orchioides* led to the isolation of fourteen compounds. They consist of one new dihydrobenzofuran (**1**), two new benzyl benzoate glycosides (**2–3**), and eleven known compounds: curculigoside B (**4**), benzyl 2,6-dimethoxybenzoate (**5**), 2-hydroxy-6-methoxybenzoic acid (**6**), isovanillic acid (**7**), 3,4-dihydroxybenzoic acid (**8**), syringic acid (**9**), orcinol (**10**), orcinol- $\beta$ -D-glucoside (**11**), 2,4-dichloro-5-methoxy-3-methylphenol (**12**), flavonoid- $\beta$ -D-glucoside (**13**) and daucosterol (**14**). The isolated compounds were identified by analysis of spectroscopic data (IR, 1D and 2D NMR, MS especially HRMS for identifying new compounds). Compound **1** belongs to a new dihydrobenzofuran. It displayed a broad range of antiproliferative activities: cervical cancer cells (HelaS3,  $IC_{50} = 3.6 \mu M$ ), lung cancer cells adenocarcinoma (A459,  $IC_{50} = 29.8 \mu M$ ), breast cancer cells (MCF-7,  $IC_{50} = 13.9 \mu M$ ), liver cancer cells (HepG2,  $IC_{50} = 56.3 \mu M$ ), and was non-toxic to Vero cells. It also inhibited the tyrosinase enzyme ( $IC_{50} = 120.8 \mu M$ ).

**Keywords:** *Curculigo orchioides*; Dihydrobenzofuran; Anti-proliferative activity



**Figure 1** Chemical structures of the isolated compounds from *Curculigo orchioides*.

## Immobilized chitinase as an effective biocatalytic platform for producing bioactive chitobiose from biomass-derived chitin

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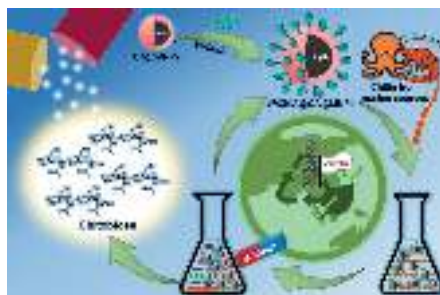
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This study describes the development of chitinase immobilization using magnetic nanoparticles (MNPs) as a biocompatible support for chitobiose production from chitin food wastes. The success of chitinase immobilization was validated by transmission electron microscopy (TEM), Fourier transform infrared spectroscopy (FTIR) and thermal gravimetry analysis (TGA). The immobilized chitinase from the marine bacterium *Vibrio harveyi* (*Vh*ChiA) exhibited an immobilization yield of  $89 \pm 2\%$  with  $98 \pm 2\%$  retention of activity and showed improved thermostability and storage stability compared to the free enzyme. The immobilized enzyme retained 49% of its activity after 16 reaction cycles and could be readily separated from the reaction mixture. Our system showed higher catalytic activity than the free enzyme in converting shrimp shell and squid pen chitins into chitobiose in a single-step reaction. The final yield of the purified compound was 37% from shrimp chitin and 61% from squid-pen chitin. In conclusion, we developed an efficient MNPs-based chitinase immobilization system that can be further tailored for large-scale production.

**Keywords:** Chitin; Chitinase; Chitoooligosaccharides; Enzyme immobilization; Magnetic nanoparticles



# Natural Products, Biological Chemistry and Chemical Biology (NP)

## Poster Presentation



## Effects of Mangosteen peel extract against *Staphylococcus aureus* and *Candida parapsilosis*

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The issue of skin disease infections caused by bacteria and fungi remains a public health concern. Prolonged antibiotic use can cause resistance to antibiotics in several pathogens leading to an ineffective treatment. Therefore, exploring natural extracts that can inhibit the causative agents causing skin infections presents an interesting pharmaceutical alternative. Mangosteen peels, a waste of mangosteen consumption, are increasingly discarded today. This research aims to investigate extraction methods providing the highest inhibition to *Staphylococcus aureus* and *Candida parapsilosis*, pathogens causing skin infection. The experiments involve extracting mangosteen peels using water, methanol, and ethanol as solvents. Mangosteen peel extract typically contains bioactive phenolic and flavonoid compounds. From the study compared to the standard graph, it was found that ethanol crude extract exhibited the highest phenolic content at  $439.104 \pm 7.501$  mg gallic acid eq per 1 g extract, followed by methanol, and water crude extracts. For flavonoids, water crude extract showed, the highest concentration at  $548.8 \pm 15.3$  mg catechin eq per 1 g extract, followed by methanol and ethanol crude extract. Subsequently, we evaluated the inhibitory properties of the extracts against representative pathogens using broth microdilution assay. The results from these experiments will contribute to the development of agricultural waste, thereby increasing its value and potentially serving as a valuable resource for future treatments of skin diseases.

**Keywords:** Dermatitis; Mangosteen peel extract; Proximate analysis; *Staphylococcus aureus*; *Candida parapsilosis*

## Antibacterial effect of *Syzygium aromaticum* essential oil against normal flora on the skin

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Central line associated bloodstream infection (CLABSI) is an infection that occurs after the insertion of central line into patients. Most two common microorganisms caused CLABSI are *Staphylococcus aureus* and *S. epidermidis* which represent as normal flora on human skin. To prevent this event, chlorhexidine gluconate (CHG) is used to inhibit the growth of normal flora bacteria around the insertion site. However, some patients are allergic to CHG, and cause rash and itching. Therefore, changing an antiseptic agent in the dressing from CHG to other antibacterial agents can be beneficial to patients who have an allergy to CHG. Clove oil is an essential oil from clove bud (*Syzygium aromaticum* (L.) Merr. & L.M. Perry) and has been reported about its antimicrobial activity. This research aimed to evaluate the antibacterial activity of clove oil against *S. aureus* ATCC 25923 and *S. epidermidis* ATCC 12228. Clove oil was obtained by hydrodistillation, and major composition was determined by using gas chromatography coupled with mass spectrometry. From the chromatogram, eugenol was found as major component (0.27mg%). Antibacterial activity was observed by using Kirby-Bauer disc diffusion assay, minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) determination. Clove oil demonstrated MIC value against *S. aureus* and *S. epidermidis* as 1% and 0.5% v/v respectively. For MBC value against *S. aureus* ATCC 25923 and *S. epidermidis* ATCC 12228 is 1% v/v. Time-kill analysis showed that there was a reduction after an exposure to clove oil at least 5 minutes. In conclusion, clove oil demonstrated the strong antibacterial activity against the normal flora. This result might be developed as antibacterial patch which use clove oil as disinfectant agent.

**Keywords:** Antibacterial activity; Clove oil; Normal flora; Chlorhexidine gluconate; Infection



## Selection of the membrane for centrifugal ultrafiltration and protein profile analysis of human primary keratinocyte secretome

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The potential of keratinocyte secretome as a cell-free regenerative medicine for wound healing necessitates the optimization of its concentration. This study aimed to select an appropriate molecular weight cutoff (MWCO) membrane for centrifugal ultrafiltration of the conditioned medium from human primary keratinocyte cell culture. Three membranes with MWCOs of 3, 10, and 30 kDa were tested at centrifugation speeds of 4,000×g and 14,000×g. The 30 kDa membrane was unsuitable as all the solution permeated, leaving no retentate. At the lower centrifugation speed, protein loss due to adsorption to the membrane was significant, resulting in suboptimal concentrations. In contrast, using the 10 kDa membrane at 14,000×g achieved a near two-fold increase in protein concentration. The concentrated secretome extracellular vesicles ranged between 20 - 200 nm. The protein profile analysis using mass spectrometry indicated the presence of essential growth factors for wound healing, including vascular endothelial growth factors (VEGF), fibroblast growth factors (FGF), and epidermal growth factors (EGF). Our findings demonstrate that a 10 kDa membrane is optimal for obtaining a concentrated secretome rich in vital wound-healing components. This membrane will be used for further study of the large-scale production of the keratinocyte secretome using tangential flow filtration.

**Keywords:** Keratinocyte conditioned medium; Keratinocyte secretome; Centrifugal ultrafiltration; Molecular weight cutoff (MWCO); Protein concentrations

## Live-cell imaging of intracellular esterases using a rhodol-based fluorescent ester surrogate substrate

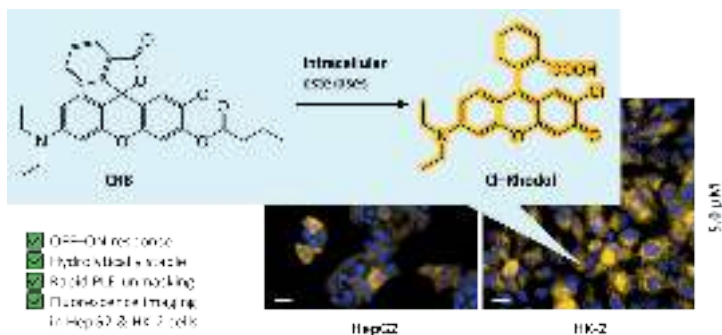
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Efforts to develop stable acyl-masked fluorescent probes for esterases are highly significant due to the susceptibility of ester linkages to spontaneous hydrolysis, which competes with enzyme activity. Previous reports have demonstrated that introducing a chlorine atom (–Cl) into phenolic fluorophores can insulate the acyl masking group from that of hydrolysis, making ester profluorophores suitable for practical applications. In this study, we present chlorinated rhodol butyrate (**CRB**) as a stable ester surrogate substrate for detecting esterase activity *in vitro* and *in cellulo*. Our results indicate that the interjection of the –Cl atom into the rhodol fluorophore, along with the hydrophobicity of the butyryl pendant, has enhanced the hydrolytic stability of **CRB**. Unmasking of **CRB** by porcine liver esterase occurs rapidly, with kinetic constants of  $k_{\text{cat}}/K_{\text{M}} \approx 1.85 \times 10^3 \text{ M}^{-1}\text{s}^{-1}$  and  $K_{\text{M}} \approx 66.55 \text{ }\mu\text{M}$ . Under microscopy, the diffuse yellow cytosolic fluorescence staining observed in unwashed HepG2 and HK-2 cells confirms both the cellular internalization of **CRB** and its subsequent activation by intracellular esterases. This work illustrates the utility of **CRB** for further basic research, including the identification of functional esterases from bioresources and the detection of mammalian cell viability.

**Keywords:** Esterases assay; Ester surrogate substrate; Profluorophore; Live-cell imaging



**Figure 1.** *In cellulo* assay of esterases, with confocal microscopic images of unwashed HepG2 & HK-2 cells, Hoechst-counterstained, and incubated with CRB at 5.0  $\mu\text{M}$  for 10 min. Scale bar = 20  $\mu\text{m}$ .

# Alpha-glucosidase inhibition of major cannabinoids from the leaves of *Cannabis sativa*: Preliminary results, isolation, bio-assay, and kinetic study

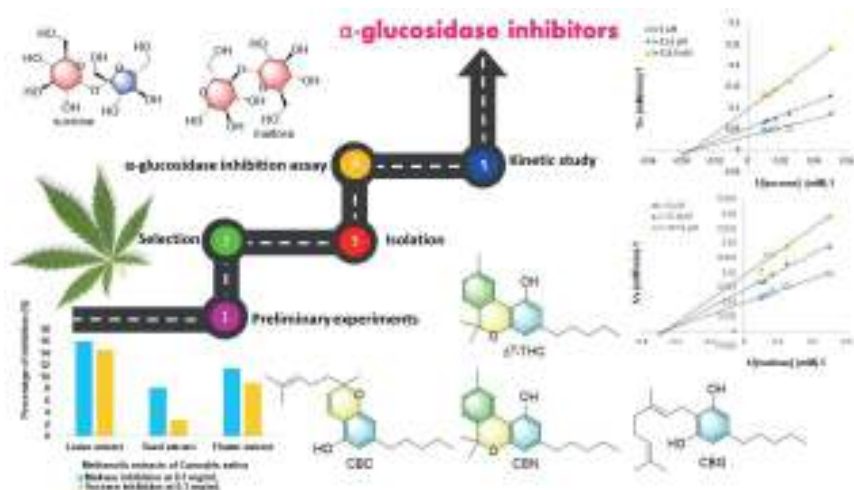
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Bioactive-guided phytochemical investigation of *Cannabis sativa* led to the isolation of four major cannabinoids including tetrahydrocannabinol ( $\Delta^9$ -THC), cannabinal (CBN), cannabichromene (CBC) and cannabigerol (CBG). Their chemical structures were determined by analysis of one-dimensional and two-dimensional nuclear magnetic resonance (NMR), as well as in comparison with literature data. Four isolated compounds were evaluated for  $\alpha$ -glucosidase inhibition. CBN and CBG showed the most active inhibition against sucrase, with  $IC_{50}$  values of 361.7 and 313.7  $\mu$ M, respectively. Additionally,  $\Delta^9$ -THC and CBN exhibited the most significant activity inhibition against maltase, with  $IC_{50}$  values of 268.3 and 211.8  $\mu$ M, respectively. Further study on mechanism underlying rat intestinal  $\alpha$ -glucosidase inhibition indicated that  $\Delta^9$ -THC, CBC and CBN could retard the maltase and sucrase function by non-competitive mechanism, while CBN was identified as an un-competitive inhibitor.

**Keywords:** Cannabinoid; Diabetes; Cannabis; Rat  $\alpha$ -glucosidase; Inhibitors



## Bacterial cellulose for wound dressing with preventing infection with Mangosteen peel (*Garcinia mangostana*) and Pa Thalai Chon (*Andrographis paniculata*) extracts

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When a fresh wound occurs and is not properly cleaned, bacteria can enter the skin, leading to infection. Wound dressings are frequently used for wound covering and healing. The ideal wound dressings should prevent bacterial infection, provide a moist environment for wounds and promote wound healing and skin recovery. Bacterial cellulose is a biopolymer synthesis by some bacteria. It has several unique properties such as high surface area, flexibility, biocompatibility, high absorption capacity and high porosity, permeability to liquid and gases. This study aims to develop wound dressing using bacterial cellulose supplemented with extracts from mangosteen peel (*Garcinia mangostana*) and Pa Thalai Chon (*Andrographis paniculata*) to prevent infections. Mangosteen peel extract contains xanthenes that inhibit the growth of bacteria and tannins which aid in wound healing. *Andrographis paniculata* extract also contains Andrographolides, known for their anti-inflammatory effects. Bacterial cellulose was produced from *Acetobacter xylinum* in coconut water medium containing 5% Sucrose 0.5% (NH<sub>4</sub>)<sub>2</sub>SO<sub>4</sub> and was adjusted to pH 4 using acetic acid to develop a wound dressing. The substances extracted from mangosteen peel and Pa Thalai Chon were added to the wound dressing along with alginate and glycerol in bacterial cellulose to form the wound dressing. Then the wound dressing was evaluated for its ability to inhibit the growth of *Staphylococcus aureus*. The concentration of extract substances used was 500 mg/mL by using disk diffusion method. Properties including absorption property and effectiveness of the wound cover were also assessed. This work could provide a new material for wound dressings that can inhibit the growth of bacteria and prevent infection.

**Keywords:** Bacterial cellulose; Wound dressing; *Acetobacter xylinum*; *Garcinia mangostana*; *Andrographis paniculata*

## First report of indole-3-carbinol in vegetables from local market, southern Thailand

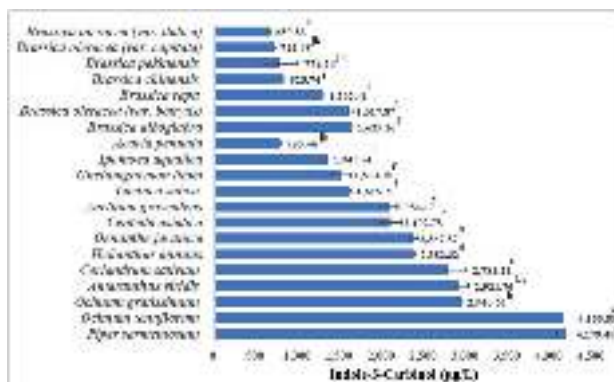
Supinya Tanyaros<sup>1\*</sup>, Pinyapat Petchpan<sup>1</sup>, Pimchana Rojanahasadin<sup>1</sup>, Kosin Teeparuksapun<sup>2</sup> and Nicha Prasongchan<sup>2</sup>

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Indole-3-carbinol (I3C), a secondary metabolite, has been found in plants of Brassica genus, exhibiting various interesting biological activities. In addition, the antioxidant activity exhibited a crucial role in anti-cancer properties and has been shown to inhibit carcinogenesis at the initiation stage of human, such as lung cancer, colon cancer, prostate cancer, and breast cancer. In this study, the researchers aimed to study the quantity of I3C in 20 species of vegetable collected from local market in Songkhla province, southern Thailand. A microplate spectrophotometric method using a chromogenic reagent was used to analyze the concentration of I3C in the samples. The concentration of I3C were statistically tested by the Games-Howell method. The results showed that the concentration of I3C in 7 species of Brassica genus (*Brassica oleracea* (var. *italica*), *B. oleracea* (var. *capitata*), *B. pekinensis*, *B. chinensis*, *B. rapa*, *B. oleracea* (var. *botrytis*) and *B. alboglabra*) were significantly lower than 9 species of vegetable plants including (*Piper sarmentosum*, *Ocimum tenuiflorum*, *O. gratissimum*, *Amaranthus viridis*, *Coriandrum sativum*, *Helianthus annuus*, *Oenanthe javanica*, *Centella asiatica*, and *Anethum graveolens*), respectively ( $p < 0.05$ ). The I3C concentration was the same between *B. alboglabra* and *B. oleracea* (var. *botrytis*) with *Lactuca sativa* and *Gnetum gnemon* ( $p > 0.05$ ), but significantly higher than vegetable plants (*Ipomoea aquatica* and *Acacia pennata*) ( $p < 0.05$ ). The highest concentration of I3C was found in *Piper sarmentosum* and *Ocimum tenuiflorum* whereas the lowest concentration of I3C in 3 species of Brassica genus (*B. oleracea* (var. *italica*), *B. oleracea* (var. *capitata*) and *B. pekinensis*) were shown in the present study.

**Keywords:** Indole-3-carbinol; antioxidant; anti-cancer; carcinogenesis; vegetable



**Figure 1.** The concentration of Indole-3-carbinol in 20 species of vegetable collected from local market in Songkhla province, southern Thailand.

## Total phenolic content and antioxidant activity of *Brassica napus* var. *pabularia* (Red Russian Kale)

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Kale is a popular leafy vegetable with high contents of health-promoting compounds and used to be a mainstay of the traditional diet. There are a few reports in the literature that mention about antioxidant and biological activities of *Brassica napus* var. *pabularia* (Red Russian Kale). The aim of this study was to determine the total phenolic content and antioxidant activity of *B. napus* var. *pabularia* leaf. The extracts were prepared by continuous maceration technique with different organic solvents; hexane, dichloromethane, and methanol. Crude extracts were investigated for total phenolic content based on the Folin–Ciocalteu colorimetric assay. Antioxidant activity was studied using 2,2-diphenyl-1-picrylhydrazyl (DPPH) and 2,2'-azino-bis-3-ethylbenzothiazoline-6-sulfonic acid cation (ABTS) radical scavenging capacity assays. The results showed that the methanol extract gave the highest percentage yields ( $6.10 \pm 0.37$  %w/w), followed by dichloromethane ( $1.78 \pm 0.02$  %w/w) and hexane extracts ( $0.95 \pm 0.04$  %w/w). The methanol extract contained the highest total phenolic content of  $68.05 \pm 0.48$  mg GAE/g extract and also showed the highest antioxidant activity on DPPH and ABTS radicals of  $32.71 \pm 0.74$  and  $32.47 \pm 0.25$  mg trolox/g extract, respectively. This study demonstrated that the polar solvent (methanol) extract has a better total phenolic content, DPPH, and ABTS radical scavenging activity than the nonpolar solvent extracts. These results indicate that the methanol extract of *B. napus* var. *pabularia* leaf may be a potential source of antioxidant agents and serves as an effective free radical scavenger. So, *B. napus* var. *pabularia* leaf could be developed as a promising and effective pharmaceutical product for several diseases caused by free radicals.

**Keywords:** *Brassica napus* var. *pabularia*; Red Russian Kale; Total phenolic; Antioxidant

## A novel organic fluorescent molecule for protease enzyme detection

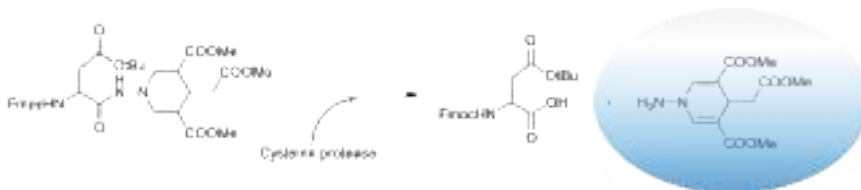
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Proteases are generally involved in various biological processes within living systems. Their primary function is to break the peptide bonds within numerous cellular and extracellular processes. Cysteine proteases are typically found in all organisms. Many proteases play important roles in cellular functions and implicate disease pathways such as cancer, neurodegenerative disorders, and diabetes. Furthermore, parasitic and pathogenic infections can also release proteases into host cells, which can cause diseases like AIDs, malaria, and immune-related diseases. Therefore, the tools for detecting or visualizing these proteases are valuable for gaining a better understanding of the enzymatic activity and their relevance to any disease. In this study, we applied our synthetically developed fluorescent molecule, 1,4-Dihydropyridine (1,4-DHP) derivative, as a biosensor for detecting protease enzymes, particularly, cysteine protease. The common cysteine proteases papain and bromelain were tested to demonstrate the peptide bond cleaving concept. The hydrolytic activity was measured by assessing the relative fluorescence enhancement using a fluorometer. The selectivity of the fluorescent biosensor towards the specific cysteine proteases will also be compared with similar function enzymes *in vitro*.

**Keywords:** Cysteine protease; Fluorescent biosensor; 1,4-DHP derivative; Enzymatic detection



Fluorescence on

## Chemical constituents from the roots of *Zygostelma benthamii*

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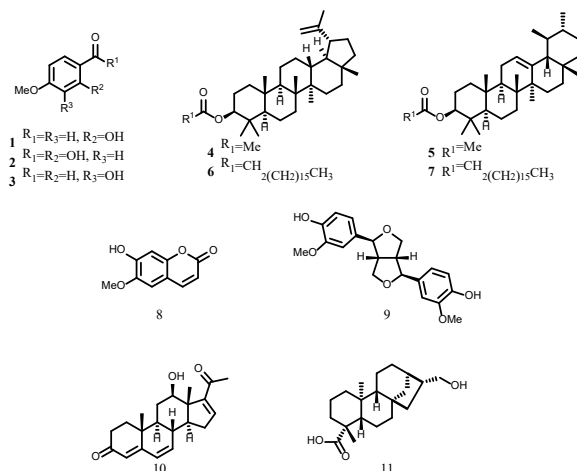
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Phytochemical investigation of the roots of *Zygostelma benthamii* led to the isolation of eleven known compounds. The isolated compounds were identified by analysis of physical and spectroscopic data. We report three phenolic compounds (**1–3**), four triterpenoids (**4–7**), one coumarin (**8**), one lignan (**9**), one pregnane terpenoid (**10**), and one diterpenoid (**11**). It is the first time that *Zygostelma benthamii* is investigated, and this is therefore the first study of the *Zygostelma* genus. In addition, compounds **7** and **11** are reported from the Apocynaceae family for the first time. Compounds **6**, **7**, **10** and **11** were evaluated against several cancer cell lines and *Vero* cells. Compound **10** showed strong anti-proliferative activity against all the selected cell lines, with IC<sub>50</sub> values in the range of 1.70–6.8 µg/mL.

**Keywords:** *Zygostelma benthamii*; Apocynaceae; triterpenoids; cholangio- carcinoma; anti-proliferative activity



**Figure 1.** The isolated compounds from the roots of *Zygostelma benthamii*.

## New chromone from the stems of *Harrisonia perforata*

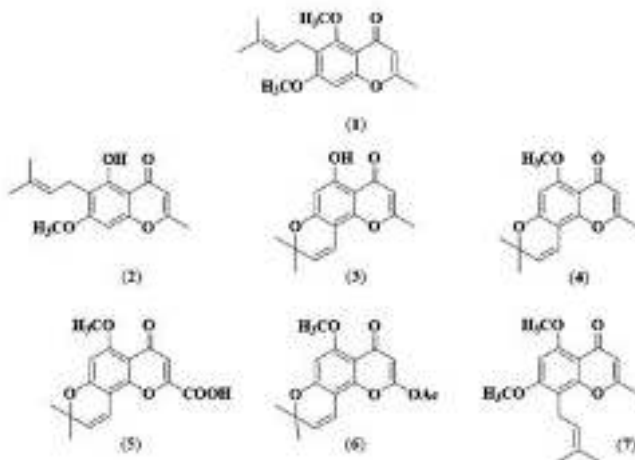
Thawatchai Sriwongsa, Waraluck Chaichompoo, Wachirachai Pabuprapap, and  
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Phytochemical investigation of the stems of *Harrisonia perforata* (Blanco) Merr. (Simaroubaceae) led to the isolation of one new chromone, peucenin-5-methoxy-7-methyl ether (1), together with six known chromones, peucenin-7-methyl ether (2), alloptaeroxylin (3), *O*-methylalloptaeroxylin (4), perforatic acid (5), perforatic acid methyl ester (6), and heteropeucenin-5-methoxy-7-methyl ether (7). The structure of the new compound was elucidated by spectroscopic data. The known compounds were identified by comparisons of their spectroscopic data and physical properties with those reported in the literature.

**Keywords:** *Harrisonia perforata*; Simaroubaceae; phytochemicals; chromones



## Antibiotic resistance progress and challenges among gram-negative and gram-positive pathogens in Southern Thailand: A retrospective 10-year study

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Multidrug-resistant bacteria pose a significant threat worldwide, including in Southern Thailand, where vancomycin-resistant enterococci (VRE) and *Pseudomonas aeruginosa* remain a public health concern. To investigate the epidemiology and antibiotic resistance patterns of these bacteria, a retrospective descriptive study was conducted on VRE and *P. aeruginosa* isolates from tertiary care hospitals, Southern Thailand over a 10-year period. Of the 304 isolates analyzed, 94 (30.9%) and 210 (69.1%) were found to be VRE and *P. aeruginosa*, respectively, with the highest rates of infection in 2014 and 2016. VRE infections were more common in men, while *P. aeruginosa* infections were more common in women. Most of the positive isolates were from sputum and the genitourinary tract, with the highest rates occurring in medical departments (81; 26.6%), followed by emergency room (42; 13.8%), surgical ward (40; 13.2%), and operation room (33; 10.9%). Resistance to commonly used antibiotics was high, particularly for carbapenems in *P. aeruginosa* and beta-lactamase inhibitors in VRE. Multidrug-resistant VRE patterns were found in all isolates, while *P. aeruginosa* showed a range of resistance patterns, with the carbapenem-resistant pattern being the most prevalent (CR; 121, 57.6%), followed by the carbapenem-resistant with multidrug-resistant pattern (CR-MDR; 72, 34.3%), and the multidrug-resistant pattern (MDR; 17, 8.1%). Therefore, it is important to monitor the distribution of bacteria and their antibiotic resistance to revise certain empirical criteria, and control may provide useful insights on disease epidemiology.

**Keywords:** Antibiotic resistance; Carbapenems; Enterococci; Epidemiology; Multidrug resistance; *Pseudomonas aeruginosa*



## Fabrication and releasing of anonaine encapsulated in sodium alginate beads

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In this study, the encapsulation of anonaine in sodium alginate beads was investigated. According to the previous research, an alkaloid, anonaine, was found in custard apple seeds. This compound exhibits high toxicity to insects, making it a potential insecticide. For this study, anonaine extract obtained from local custard apple seeds was used. Two solvents, water and ethanol, were used to compare the extraction process. The presence of anonaine was identified by an absorbance peak in the UV region (lambda max around 200-300 nm) using ultraviolet spectrophotometry. It was found that the anonaine absorbance peak appeared at different lambda maximum values depending on the solvent used, consistent with prior reports. The extract was then encapsulated in sodium alginate beads via basic and reverse spherification techniques for comparison. In this fabrication, the solution of calcium chloride was used as a crosslinking agent. The release of anonaine in aqueous solutions with different pH values as a function of time was monitored. The release mechanism was proposed. Furthermore, the release of anonaine in water containing the mosquito larvae was also investigated. In order to monitor larvicidal activity, mosquitoes were kept in the beaker containing distilled water and various concentrations of isolated anonaine in sodium alginate beads. As time passed, samples were taken from the beaker to measure absorbance peaks. Then number of dead larvae was then counted. Finally, the results from each experiment were compared to determine the encapsulation method with the highest entrapment efficiency.

**Keywords:** Encapsulation; Custard apple seeds; Anonaine; Sodium alginate beads; Larvicidal activity

## A comparison of TLC and HPLC methods for the quantitative analysis of mitragynine in Kratom products

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*Mitragyna speciosa*, a native plant of Thailand and Indonesia known as 'Kratom', is a plant of considerable interest. Although Kratom contains many alkaloids, mitragynine is a unique psychoactive biomarker of the species and is responsible for its psychoactive effects. Our study compared the suitability of chromatographic techniques, such as high-performance liquid chromatography (HPLC) and thin-layer chromatography (TLC), for the determination of the mitragynine content of ten Kratom plant items that were accessible as dried leaf powder. The recovery percent of the spiked samples was 91.0-101.2% and 95.5-102.3 % for HPLC versus 88.2-98.7 % and 89.0- 99.5 % for the recommended TLC, respectively. The study successfully employed the detection of mitragynine in the samples. This method is characterized as a rapid technique that allows naked eye detection of mitragynine. It has high sensitivity and high selectivity and is convenient for on-site mitragynine detection. This study suggests that the TLC method can be used to develop detection devices for mitragynine analysis in real samples. This indicates potential applications in regulatory compliance, quality control, or field testing of Kratom products.

**Keywords:** Kratom; *Mitragyna speciosa*; Mitragynine; Quantitative analysis

## Isolation and screening of antimicrobial properties of the actinobacteria isolated from Thailand

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Microbial natural products have played a very significant role in drug discovery and development during the last century. Thailand is endowed with natural resources inform of microbial natural products from various habitat which are yet to be fully explored. The aim of this study was to isolate actinobacteria using different media and evaluate the antimicrobial potential of the isolated actinobacteria against methicillin resistant *Staphylococcus aureus*, *Acinetobacter baumannii*, and *Klebsiella pneumonia* using agar overlay assay and microdilution bioassay technique. Additionally, the study focused on molecular identification of the isolated actinobacteria using the 16S rRNA sequencing technique and use of LC-MS data to identify the putative bioactive compounds present in the extract. The result from this study revealed that out of 165 strains isolated from various sources, 23 strains exhibited antimicrobial activities accounting for 14% of the isolated actinobacteria. The actinobacteria extracts from the 23 strains exhibited antimicrobial activities against the three tested pathogens with minimum inhibitory concentration of between 9.9 µg/mL-1250 µg/mL. The 16S rRNA sequencing revealed that all the isolated actinobacteria strains belong to the genus streptomycetes. Moreover, online dereplication via the GNPS showed the presences of (*E*)-5-(4-methoxy-5-methyl-6-oxopyran-2-yl)-3-methylhex-4-enoic acid, Picroside III, Desferrioxamine X3 and norlichexanthone among other compounds. This study will significantly contribute to the discovery of novel antimicrobial agents needed to combat the threat of antimicrobial resistance.

**Keywords:** Microbial natural products; Antibiotics; Actinobacteria; Antimicrobial resistance; Drug discovery



**Figure 1.** Agar overlay culture of methicillin resistant *Staphylococcus aureus* (MRSA, A) and actinobacteria (WU15) with MRSA (B)

## Inhibition of *Staphylococcus aureus* biofilm formation by natural coumarins

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Antibiotic resistance development in bacteria raise concerns worldwide. One of the most recognized pathogens that rapidly develop drug resistance is Gram-positive bacterium *Staphylococcus aureus*. The ability to form extracellular matrix called biofilm has been reported to strongly associate with drug resistance in *S. aureus*. Biofilm could shield bacteria from host's immune response and antibiotic treatment; therefore, a higher concentration of antibiotic is required to eradicate bacteria under biofilm state. This may attribute to drug resistance development. Here in, we searched for natural products that could inhibit *S. aureus* biofilm formation. Scopoletin and isofraxidin were isolated from *Mallotus sporocarpus* (Euphorbiaceae) plant. These coumarin adducts were first determined their ability to inhibit *S. aureus* growth using Kirby-Bauer disk diffusion susceptibility assay. The results indicated that these compounds could not interfere with bacterial growth. We further investigated their ability to inhibit *S. aureus* biofilm formation. Scopoletin and isofraxidin at concentration ranging from 0.5 to 500 µg/mL were tested. The biofilm developed by *S. aureus* ATCC 25923 in the presence of 1% sucrose was used as the positive control while the negative control was media without bacteria. Scopoletin and Isofraxidin exhibited moderate potency with IC<sub>50</sub> of 320.7 and 264.9 µg/mL, respectively.

**Keywords:** Antibiofilm; Coumarin; Isofraxidin; Scopoletin; *Staphylococcus aureus*

## Syntheses of curcumin derivatives and their biological activity against *Staphylococcus aureus*

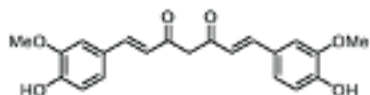
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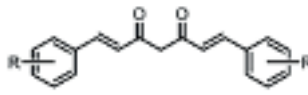
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Biofilm formation is considered one of the most serious health concerns. It could lead to an infection that could be lethal. In the biofilm state, biofilm provide a shelter to protects bacteria from being eradicated by antibiotics, leading to drug resistance development. Several anti-biofilm-forming strategies were established. Disruption of bacterial adhesion is one of the alternative methods to avoid biofilm formation at the beginning step, particularly during the initial step that planktonic cells need to attach to a surface. In this work, we investigate the antibacterial activity of curcumin and derivatives against the pathogenic bacteria *Staphylococcus aureus*, which has a cysteine transpeptidase enzyme that plays a significant role in the bacterial adhesion, formation and maintenance of biofilms. Due to the Michael addition of enone functional group of curcumin and derivatives that possibly irreversible covalent bond with sulphydryl group of cysteine, our hypothesis was that these substances might have antimicrobial properties. A total of four curcumin derivatives and one non-conjugated derivative were subjected to susceptibility assays and biofilm formation against *S. aureus*. We discovered that curcumin could inhibit bacterial growth activity against *S. aureus*, which shows a clear inhibition zone of  $8.64 \pm 0.18$  mm. Moreover, there are several derivatives that exhibited anti-biofilm activities with a higher potency than curcumin.

**Keywords:** Curcuminoids; Curcumin derivatives; *Staphylococcus aureus*; Sortase inhibitory activity; Antibacterial activity



Curcumin



Curcumin derivatives

R = m-OMe  
R = p-OMe  
R = p-OH  
R = H

- Inhibit Growth of *Staphylococcus aureus*
- Inhibit *S. aureus* Biofilm Formation

## Siamfuranones B and C, two new furanone derivatives from the flowers of *Uvaria siamensis*

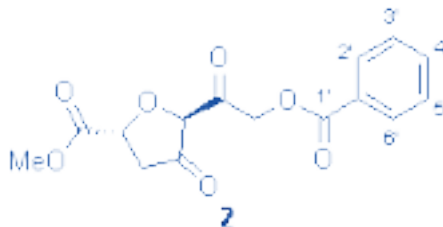
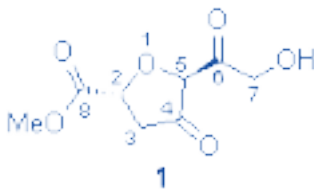
Awat Wisetsai<sup>1\*</sup>, Florian T. Schevenels<sup>2</sup>, Supachai Jadsadajerm<sup>1</sup>, Ratsami Lekphrom<sup>2</sup>, and Nuttapon Yodsin<sup>3</sup>

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Two previously undescribed furanone derivatives named siamfuranones B (**1**) and C (**2**), together with 7-benzoyloxy-6-oxo-2,4Z-heptadiene-1,4-olide (**3**), 7-benzoyloxy-6-oxo-2,4E-heptadiene-1,4-olide (**4**), (4Z)-6-acetoxy-7-benzoyloxy-2,4-heptadien-4-olide (**5**), (4E)-6-acetoxy-7-benzoyloxy-2,4-heptadien-4-olide (acetylmeiodorinol) (**6**), and isomelodrinol (**7**), were isolated from the flower extract of *Uvaria siamensis*. Their structures were determined through analysis of spectrometric and spectroscopic evidence, while electronic circular dichroism (ECD) calculations were used to determine their absolute configurations. In addition, gauge-including atomic orbitals (GIAO) NMR chemical shift calculation, supported by the advanced statistical method DP4 plus, was used to confirm the relative configuration of siamfuranone B (**1**). The skeleton of the two previously undescribed compounds is unprecedented, and their biosynthesis from the C<sub>7</sub>N-unit was proposed. This work expands the structural diversity of furanone natural products, as siamfuranones B and C belong to a new class of hydrofuranones.

**Keywords:** *Uvaria siamensis*; Hydrofuranones; Heptadienes



# Heterologous expression of *aristolochene synthase* and its site-directed mutagenized form from *Menisporopsis theobromae* BCC 4162 in *Aspergillus oryzae* NSAR1

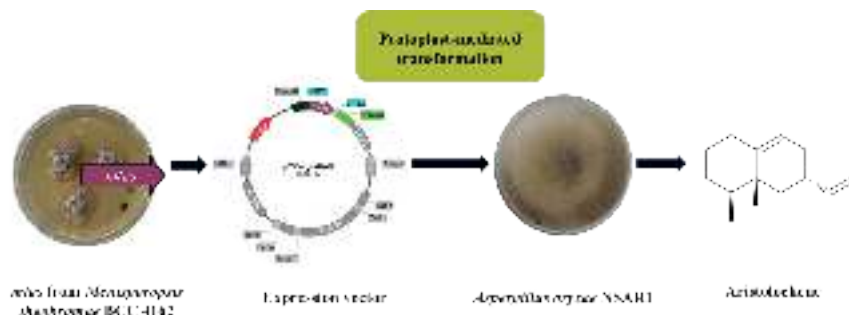
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*Menisporopsis theobromae* BCC 4162 is a seed fungus containing more than one hundred possible natural product biosynthetic gene clusters. Many gene clusters are cryptic or have low expression level including terpene synthase gene similar to that encoding aristolochene synthase. In this work, the *aristolochene synthase* (*mtas*) from *M. theobromae* BCC 4162 was cloned into an expression vector and then introduced into the heterologous host, *Aspergillus oryzae* NSAR1 for metabolite production. In addition, *mtas* mutants were constructed by site-directed mutagenesis (SDM) at aromatic amino acid residues around the active site of aristolochene synthase. The mutant variants of *mtas* were studied for their effects on the production of aristolochene. The transformants carrying wild-type *mtas* and its mutants were screened for metabolite production by using gas chromatography-mass spectrometer (GC-MS) technique. The GC-MS results showed that aristolochene was present in the crude extract of *A. oryzae* transformants carrying *mtas*, whilst its mutant variants can also produce other sesquiterpenes. The results from this work could provide a new biological platform for production of invaluable terpenes.

**Keywords:** Heterologous expression; Sesquiterpenes; Aristolochene; *Menisporopsis theobromae* BCC 4162; *Aspergillus oryzae* NSAR1



**Figure 1.** Overview of heterologous expression of *mtas* from *Menisporopsis theobromae* BCC 4162 in *Aspergillus oryzae* NSAR1

## Biosynthetic study of alternapyrone: A highly methylated polyene $\alpha$ -pyrone

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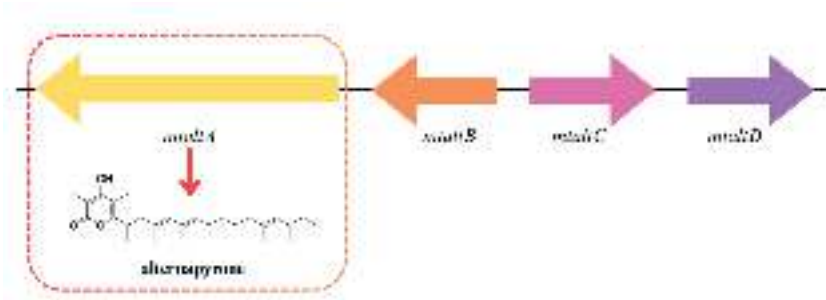
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Alternapyrone contains an  $\alpha$ -pyrone core structure with a long highly methylated alkenyl chain. The  $\alpha$ -pyrone core structure is present in many naturally occurring compounds such as rasfonin, tipranavir, viridepyrone. These compounds display a variety of biological activities such as anticancer, antiviral, and anti-fungal activities. In this work, the alternapyrone gene cluster from *Menisporopsis theobromae* BCC 4162 containing a polyketide synthase gene (*mtaltA*) and three auxiliary genes (*mtaltB-D*) was studied. The auxiliary genes are expected to encode enzymes involved in oxidations. Heterologous expression of these genes could result in the production of new metabolites by modification on the alkenyl side chain of alternapyrone. Although the alternapyrone biosynthesis has been previously reported but its methylation programming remains unknown. Therefore, the effect of C-methyltransferase and ketoreductase domains of MtAltA was investigated. The result revealed the importance of both domains for alternapyrone biosynthesis. The results from this work provide us a better understanding on the methylation programming of highly methylated  $\alpha$ -pyrone.

**Keywords:** Alternapyrone; Site-directed mutagenesis; *Menisporopsis theobromae* BCC 4162; C-methyltransferase domain; Keto-reductase domain



Biosynthetic gene cluster of alternapyrone found in *M. theobromae* BCC 4162

# Dicarboxylic acids as substrates for a new type III polyketide synthase from *Cavenderia subdiscoidea*

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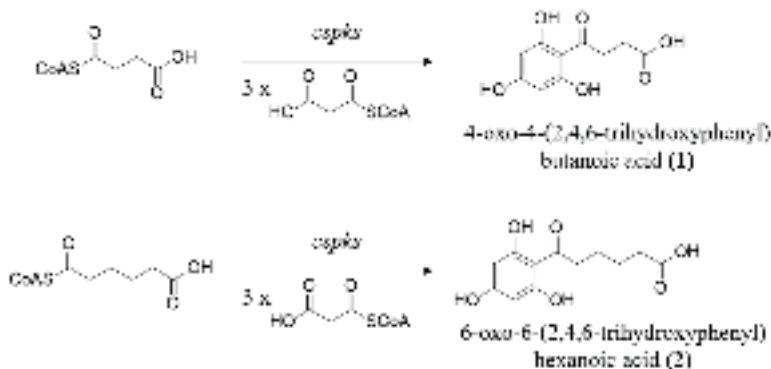
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*Cavenderia subdiscoidea* is a dictyostelid social amoeba found in Northern Thailand. Based on genomic data, this social amoeba contains several natural product genes including a type III polyketide synthase gene. In this work, a type III polyketide synthase gene from *C. subdiscoidea* (*cspks*) was cloned into expression vectors and introduced into *Aspergillus oryzae* NSAR1 and *Saccharomyces cerevisiae* BJ5464 for metabolite production. All crude extracts from both *A. oryzae* and *S. cerevisiae* transformants carrying *cspks* were analyzed by high-performance liquid chromatography (HPLC). The differences of HPLC chromatograms between crude extracts of transformants carrying *cspks* and control led to the isolation of two acylphloroglucinols, 4-oxo-4-(2,4,6-trihydroxyphenyl)butanoic acid (**1**) and 6-oxo-6-(2,4,6-trihydroxyphenyl)hexanoic acid (**2**). This is the first report for a type III PKS using dicarboxylic acids as substrates.

**Keywords:** *Cavenderia subdiscoidea*; Type III polyketide synthase; Acyl phloroglucinol; 4-oxo-4-(2,4,6-trihydroxyphenyl)butanoic acid; 6-oxo-6-(2,4,6-trihydroxyphenyl)hexanoic acid



Proposed biosynthetic pathways of compounds (1) and (2)

## Heterologous expression of the fungal reducing polyketide synthase genes in *Aspergillus oryzae*

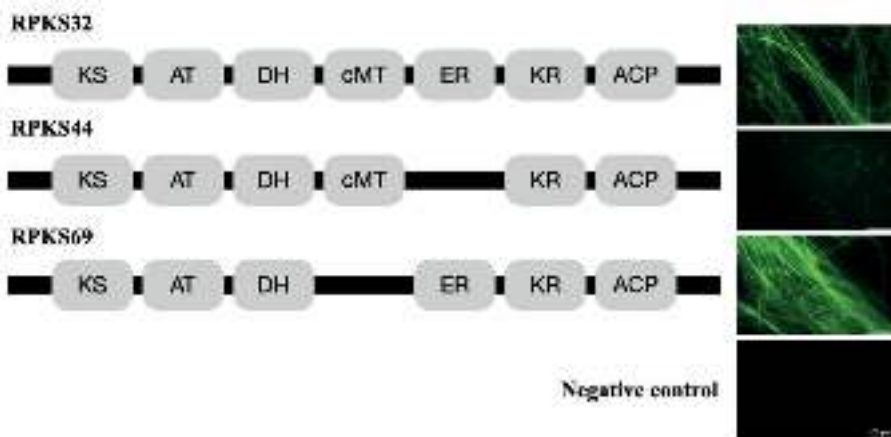
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With the increased number of antibiotic-resistant microbes and new infectious diseases, the discovery of novel drugs is extremely important. In this work, the heterologous expression approach was applied for production of novel metabolites by activating the expression of cryptic natural product genes. Three cryptic reducing polyketide synthase (R-PKS) genes, i.e., *rpks32*, *rpks44* and *rpks69* from a seed fungus, *Menisporopsis theobromae* BCC 4162, were cloned into an expression vector fused with a reporter gene, *egfp*. The resulting expression vectors were then introduced into *Aspergillus oryzae* NSAR1 by protoplast-mediated transformation. The transformants carrying these R-PKS genes were then analyzed for their expression by fluorescence microscopy (Figure 1). This work showed that *A. oryzae* NSAR1 can be utilized as the host for expression of the R-PKS genes from *M. theobromae* BCC 4162. The metabolites produced by all transformants carrying these R-PKS genes will be further investigated.

**Keywords:** *Menisporopsis theobromae*; *Aspergillus oryzae*; Heterologous expression; Polyketide



**Figure 1** Domain organizations of the R-PKSs and fluorescence microscopy analysis of eGFP



## LC-ESI-MS based structural elucidation of major chemical compounds in *Boesenbergia rotunda* (L.) Mansf. ethanol extract and its antioxidant activity

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The study aimed to examine chemical composition and antioxidant activity of the ethanolic extract of *Boesenbergia rotunda* (L.) Mansf., commonly called fingerroot. *B. rotunda* root powder was extracted with ethanol using sonication. The chemical composition of the extract was determined by using liquid chromatography and mass spectrometry. Flavones and prenylated flavonoids have been studied and identified. The major compounds which are alpinetin, pinocembrin, pinostrobin and panduratin A were identified by using the information from Electrospray ionization mass spectrometry (ESI-MS) comparing with known compounds previously reported in the literature. Mass spectra showed that molecular ions were corresponded to these major compounds. MS/MS fragmentation were also studied to investigate the compounds. In addition, the antioxidant activity was determined using 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay. The extract showed moderate activity with the  $IC_{50}$  of  $588.89 \pm 51.86 \mu\text{g/mL}$  comparing with gallic acid ( $IC_{50} = 3.10 \pm 0.38 \mu\text{g/mL}$ ) and rutin ( $IC_{50} = 36.42 \pm 7.03 \mu\text{g/mL}$ ).

**Keywords:** ESI-MS; *Boesenbergia rotunda*; Fingerroot; Flavone

## Inhibition effect of Cytochrome P4502A6 enzyme mutant alleles 7 (CYP2A6\*7) activity by Luteolin

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Nicotine, one of the major substances in cigarette smoke, has been previously reported as a key compound responsible for smoking addiction. Inhaled nicotine passes to the brain and stimulates dopamine secretion, resulting in pleasure feeling. Nicotine is metabolized by liver-specific cytochrome P4502A6 (CYP2A6) enzyme. This nicotine clearance mechanism, however, could lead to cigarette craving and smoking more frequently in order to maintain nicotine levels in the bloodstream. Thus, maintaining blood-nicotine level by inhibiting the CYP2A6 activity is an alternative approach to decrease cigarette smoking. Luteolin has been previously reported as one of flavonoid compounds that could effectively inhibit the wild-type CYP2A6 (wt-CYP2A6) mediated coumarin 7-hydroxylation activity *in vitro*. This study aims to determine the inhibitory effect of Luteolin against the polymorphic cytochrome P450 2A6 mutant 7 (CYP2A6\*7) that has been report in Thai population. Upon measuring the 7-hydroxy coumarin hydroxylation, the results indicated that Luteolin could inhibit wt-CYP2A6 and CYP2A6\*7 with IC<sub>50</sub> values of  $5.929 \pm 1.815 \mu\text{M}$  and  $8.810 \pm 0.432 \mu\text{M}$ , respectively. The molecular docking experiment indicated that wt-CYP2A6 and CYP2A6\*7 were bound to Luteolin with different non-covalent interactions.

**Keywords:** Cytochrome P4502A6; Nicotine; Inhibition; Luteolin

## Computational studies of inhibitory effect of brazilin and hematein from *Caesalpinia sappan* Linn. against *Cutibacterium acnes*

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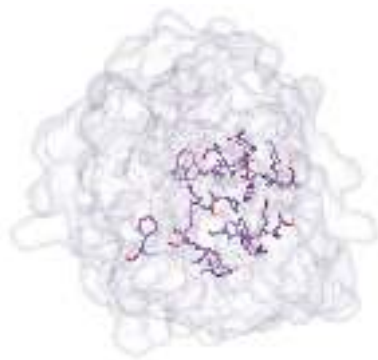
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Acne caused by *Cutibacterium acnes* (*C. acnes*) is a skin disease commonly affecting teenager worldwide. Lipase breaking sebum into free fatty acids is one of the key drug targets. Although there are various types of lipase-targeted drugs, new drugs are still needed due to drug resistance. Using herbal remedies can be an alternative. Recently, sappan wood (*Caesalpinia sappan* Linn.) was reported to exhibit anti-acne properties, containing bioactive compounds such as brazilin (BRA) and hematein (HEM). Many studies have investigated the biological activities of sappan wood and found that it can inhibit *C. acnes*, but no molecular detail is available. This study focuses on the inhibitory efficacy of BRA and HEM, bioactive compounds in sappan wood, which are studied in comparison to an existing drug lipase, using molecular docking to study the binding of ligands. Then, molecular dynamics (MD) simulations were employed to understand the structural and dynamic properties. BRA and HEM show better binding than drug lipase. The ligand-binding mechanisms and residues used for binding are revealed here. The results suggest the possibility of using BRA and HEM for acne treatment.

**Keywords:** *Cutibacterium acnes*; Lipase; *Caesalpinia sappan* Linn.; Molecular docking; Molecular dynamic simulation



## The binding mechanism of Atazanavir to drug-resistant HIV protease: A simulation study

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The problem of HIV drug resistance is caused by mutations of drug targets. One of major drug targets is HIV protease. This protein plays a crucial role in the life cycle of HIV. Atazanavir (ATV) is a commonly used drug for protease inhibition. However, the long-term use of ATV results in drug resistance. To date, there is no data on how ATV causes drug resistance. Thus, in this work, Molecular Dynamics (MD) simulations were conducted for 500 ns with a repeat to investigate the binding mechanism of ATV to mutated protease (I50L) in a drug resistance condition in comparison to wild-type protease. The mutation significantly alters the dynamics of protease. The mutation also causes the loose binding of ATV to protease. The key interactions for ATV binding are revealed. The mechanism by which protease rejects ATV is also revealed here. The obtained data can potentially be used to design and develop new potential drugs that are more effective and can inhibit drug-resistant HIV proteases.

**Keywords:** HIV protease; Atazanavir (ATV); MD simulation



Figure 1. A. HIV protease structure (PDB code : 2AQU ) with bound ATV in the active site. B. Structures of ATV

## The computational studies of Rilpivirine – resistant HIV Reverse Transcriptase for drug design and development

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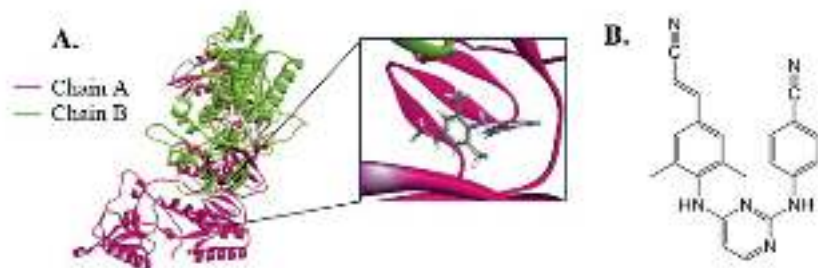
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Millions of individuals worldwide are impacted by HIV infection, which is one of serious global health concerns. The use of antiretroviral therapy (ART) has significantly reduced disease morbidity and mortality. However, the emergence of HIV drug resistance can lead to the treatment failure. Reverse transcriptase (RT) is one of targets causing drug resistance. Non-nucleoside reverse transcriptase inhibitor (NNRTI) is commonly used in HIV-infected patients, but it causes fast drug resistance. NNRTIs act by binding directly to RT and inhibiting its enzymatic function. Rilpivirine (RPV) is a second-generation NNRTI that is potent and widely prescribed to treat HIV. Even in a drug-resistant condition, RPV fails in some drug-resistant situations where no molecular detail is available. In this work, molecular dynamics (MD) simulations were employed to understand the binding of RPV to RT where prevalent mutated RT was studied in comparison to wild-type RT. MD simulations revealed the K101P mutation leads to a loss of hydrogen bonds. This loss of hydrogen bonds results in weaker binding affinity in mutated RT. The insights here can guide the future development of novel NNRTIs against drug-resistant strains.

**Keywords:** HIV; Reverse transcriptase; NNRTIs; Molecular dynamics



**Figure 1.** Structure (A.) HIV-1 NNRT structure (PDB code: 3MEE) with ligand (RPV) in the active site (B.) RPV structure

## Metabolite profiling of *Spirodela* by LC-QTOF

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Duckweed is a type of aquatic plant that has high nutritional value and medicinal benefits. It also grows widely in freshwater. Divided into five genera (i.e., *Spirodela*, *Landoltia*, *Lemna*, *Wolffiella* and *Wolffia*) and 36 species, *Spirodela* is morphologically composed of multiple roots and leaves with a slightly purplish-red ventral surface. This purple pigment was proposed to originate from anthocyanin. Unlike in the natural environment, this purplish-red color found in *Spirodela* gradually disappears when raised in the laboratory. In this work, we investigated the MS-based metabolic profiling of *Spirodela* extract, aiming to qualitatively identify anthocyanin-based compounds. In the present study, *Spirodela* collected from a natural water pond in Angthong province was cleaned with distilled water, dried, and extracted by ethanol. The crude extracts were analyzed by using liquid chromatography coupled with high-resolution mass spectrometry (LC-QTOF) in both-positive and negative modes. Their chemical composition was identified by matching their MS and MS/MS spectra with the SciEx database including Natural Product and NIST. The results showed the presence of various classes of compounds including terpenoids, alkaloids, phenolics and flavonoids but no matching of anthocyanin. It is possible that the anthocyanin concentration was well below the detection limit or the ionization was suppressed from matrix effects. Nevertheless, our findings support the idea that *Spirodela* has a potential to be a new animal feed rich with bioactive compounds.

**Keywords:** Duckweed; *Spirodela*; Metabolites; LC-QTOF



## Chemical profile of hexane fraction of hydrosol from fresh *Wolffia globosa*

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*Wolffia globosa*, called in Thai as Khai Nam, Kai-Pum, or Kai Nhae, belongs to Lemnaceae or duckweed family. This plant is a tiny water plant, fast growing, and can be grown in small areas. It is commonly used as an ingredient in local foods. The investigation of the chemical profile, antioxidant, and antibacterial activities of hexane fraction (HF) of hydrosol from *Wolffia globosa* were focused herein. We are interested in the hexane fraction because hexane can effectively extract non-polar compounds in a hydrosol. In addition, the applications of the extract for food and cosmetic aspects were also investigated. In this work, we report the chemical profile of *W. globosa* hydrosol by using GC-MS. The HF was obtained from hydrosol by liquid-liquid extraction. The compounds in HF were annotated by using NIST14 library. The results revealed the presence of phytol, squalene, and cymene, all of which are bioactive compounds and have been used as cosmetic ingredients. This finding could potentially promote duckweed as a new natural ingredient for cosmetic products.

**Keywords:** Duckweed; *Wolffia globosa*; Hydrosol; GC-MS

## Bioactive substances in the Peel of immature *Dictyophora indusiata* mushrooms expressed antioxidant and anti-tyrosinase properties

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Bioactive agents in natural resources have been developed for foods, functional foods, pharmaceuticals, and traditional medicine. This study aims to extract the biomolecules from the peel of immature *D. indusiata* mushrooms to determine antioxidant, anti-tyrosinase activity, and analyze types of biomolecules. Raw materials were collected, and the extracts were used at different temperatures and solvents. All extracts were determined for antioxidant and anti-tyrosinase activities, including a comparison of total phenolics, total flavonoids, and total terpenoids contents. The results showed that the hot air oven machine (O) with ID number (01) was performed at 80 °C (80) using water solvent (W) of the peel mushrooms (A1) by ID series of O-A1-01-80W represented the potential of antioxidant activity at the IC<sub>50</sub> value of 0.230 mg/mL and FRAP value of 212.46 ± 0.20 mM Fe<sup>2+</sup>/g extract. The total phenolics, total flavonoids, and total terpenoids contents expressed 26.98 ± 0.34 mg GAE/g, 14.49 ± 0.25 mg QE/g, 98.93 ± 1.02 mg MT/g O-A1-01-80W extract, respectively. The result expressed that the lyophilizing machine (L) with ID number (02) was performed at 80 °C (80) using water solvent (W) of the peel mushrooms (A1) by ID series of L-A1-02-80W extract high efficacy of anti-tyrosinase activity and the IC<sub>50</sub> value of 0.430 mg/mL. Therefore, the biological potential represented in the extracts could develop as a functional food ingredient to prevent the risk of non-communicable diseases (NCDs).

**Keywords:** Antioxidant; Anti-tyrosinase; Biomolecules; Non-communicable diseases; *Dictyophora indusiata*



## Extraction, preliminary phytochemical screening and antioxidant properties of ethanolic crude extract of Madan (*Garcinia schomburgkiana* Pierre)

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Madan (*Garcinia schomburgkiana* Pierre) is an edible perennial fruit belonging to the Guttiferae family. Local people consumed it fresh and fermented. Madan leaves, root and fruit are also traditionally used as an expectorant, improvement of menstrual blood quality, treatment of coughs, treatment of diabetes and as a laxative. The aim of the present study was to explore the phytochemical constituents, to evaluate the total phenolic and total flavonoid contents and antioxidant activity of the crude extracts fruits and leaves of *G. schomburgkiana* Pierre. The extraction process was performed using 50 g each of the dried powder of *G. schomburgkiana* fruit and leaves soaked in 250 ml of ethanol and macerated for 7 days at room temperature. The crude extract yields obtained were  $23.13 \pm 3.17$  g and  $6.46 \pm 2.64$  g for fruit and leaf extracts, respectively. The phytochemical screening of the Madan fruit extracts revealed the presence of flavonoids, tannins and saponins, while the Madan leaf extracts were found to contain flavonoid, steroids, tannins, glycosides, sterols, and saponins. The total phenolic contents in Madan fruit and leaf extracts using Folin–Ciocalteu method were estimated to be  $22.0 \pm 1.47$  and  $10 \pm 5.28$  mg gallic acid equivalent per 1 g of extract, respectively. Total flavonoid contents of Madan fruit and leaf extracts using aluminum chloride colorimetric method were found to be  $0.4083 \pm 0.034$  and  $92.1486 \pm 0.614$  mg quercetin equivalent per 1 g of extract, respectively. The antioxidant activity of fruit and leaf extracts and standard gallic acid using 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay showed the  $IC_{50}$  values of  $1694.42 \pm 39.50$ ,  $275.55 \pm 2.78$  and  $140.68 \pm 14.70$  mg/ml, respectively.

**Keywords:** *Garcinia schomburgkiana* Pierre; Phytochemical screening; Antioxidant activity; Total phenolic content; Total flavonoid content

## OM : Organic Synthesis and Medicinal Chemistry

## Stannylation as the key strategy for the synthesis of C2-substituted cordycepin derivatives for antiviral drug development

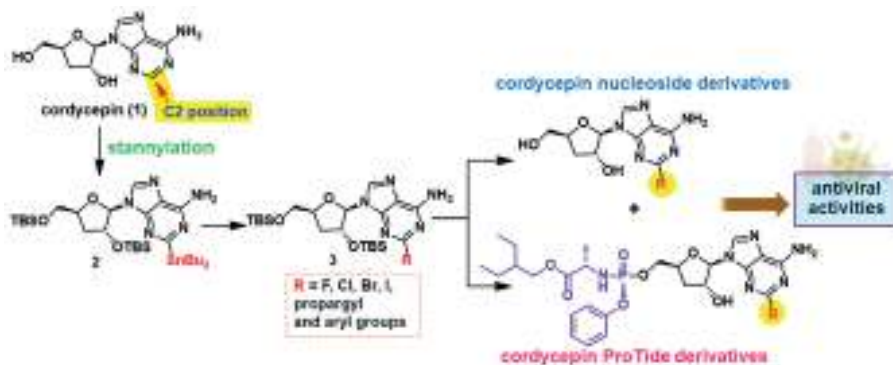
A. Thiraporn, P. Mee-udorn, R. Thiabma, N. Sooksai, S. Onnome, A. Suphatrakul, T. Uengwetwanit, B. Siridechadilok, and N. Srimongkolpithak\*

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Cordycepin (**1**) or 3'-deoxyadenosine is a derivative of the natural nucleoside. It has been found to exhibit a wide range of biological activities, including anti-inflammatory and antiviral activities. While adenosine analogs substituted at the 2-position demonstrate interesting activity in several biological systems, the current synthesis and biological evaluation of C2-substituted cordycepin (**1**) has been underexplored. Our research group develop the synthetic route towards C2-modified cordycepin library, following by further evaluation of their antiviral activities. The synthesis started with the preparation of 2-stannylated adenosine **2** from cordycepin (**1**) in 4 steps by using stannylation as the key strategy. Stannyl group at 2-position of **2** could be converted to various groups, such as F, Cl, Br, I, propargyl and aryl groups, resulting into silylated key intermediate **3**. These intermediates were subsequently converted to be either C2 modified nucleoside through desilylation or nucleotide though Prodrug nucleotide (ProTide) approach. To exemplify, 2-fluorocordycepin nucleoside and 2-fluorocordycepin phosphoramidate were synthesized and found to exhibit potent inhibitory activity against dengue virus without being cytotoxic to Vero cells. These studies could lead to the establishment of BIOTEC's nucleoside library for further drug discovery endeavors.

**Keywords:** Cordycepin; Nucleoside; Prodrug nucleotide; Stannylation; Dengue virus



# Synthetic study of natural antimalarial, (+)-febrifugine, from D-glucose and D-serine: Development of new pathways via azide and azide free approaches

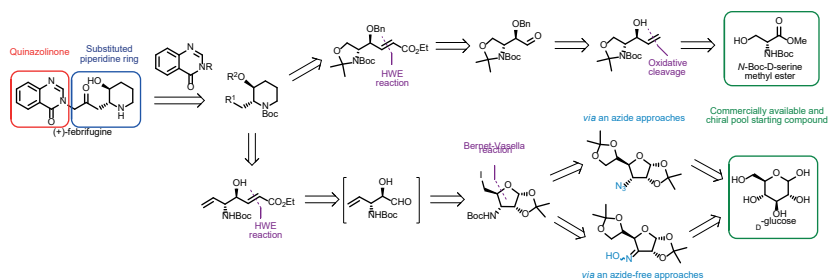
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(+)-Febrifugine, a quinazolinone-containing alkaloid was isolated from the roots and leaves of Chang shan (*Dichroa febrifuga*) and hydrangea families, has exhibited a significant antimalarial activity by inhibiting prolyl-transfer RNA synthetase (ProRS) in *Plasmodium falciparum*. The structure of (+)-febrifugine consists of two crucial parts, which are a quinazolinone and a substituted chiral piperidine ring. The substituted piperidine ring could be synthesized from both chiral pool compounds, D-glucose and D-serine. The stereochemistry of these two precursors can be easily handled and controlled to produce (+)-febrifugine with the desired chiral centers. The synthetic plans were designed through azide and azide-free methods. In this research, Bernet-Vasella reaction, and Horner-Wadsworth-Emmons reaction could be utilized as key reactions. The piperidine structure was successfully synthesized in 19 steps from D-glucose and 10 steps from N-Boc-D-serine methyl ester.

**Keywords:** Febrifugine; Natural antimalarial; D-glucose; D-serine; Natural products synthesis



**Scheme 1** Retrosynthetic analysis of (+)-febrifugine from D-glucose and D-serine via an azide and azide-free approaches.

## Amination of 1,2,4-oxadiazol-5(4H)-ones with tertiary amines

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5-Amino-1,2,4-oxadiazoles are essential building blocks extensively employed in drug discovery due to their diverse pharmacological and biological properties. Although various methods have been devised for their synthesis, access to the 5-*N,N*-dialkylamino derivatives remains somewhat limited. Traditional methods often involve restricted reagent availability, multi-step preparation, and harsh conditions, resulting in inefficient and costly processes. Therefore, in this work, a facile and direct synthetic method toward 5-amino-1,2,4-oxadiazoles via the deoxygenative amination of 1,2,4-oxadiazol-5(4H)-ones using tertiary amines as nitrogen sources was developed under a sonochemical process. A combination of inexpensive and commercially available triphenylphosphine ( $\text{Ph}_3\text{P}$ ) and iodine ( $\text{I}_2$ ) was applied as key activating reagents. Several types of tertiary amines comprising both cyclic and acyclic structures were compatible with the reaction conditions with the preferential selectivity toward the cleavage of benzyl moiety over the methyl group. Various functional groups on the oxadiazolones were also well tolerated. Moreover, piperazine-linked 1,2,4-oxadiazole analogs can be readily accessed through a direct one-pot amination using *N*-methylpiperazine as a key building block enabling *in-situ* *N*-functionalization and coupling without protecting group strategy. Real-time reaction monitoring by  $^{31}\text{P}$ - and  $^1\text{H}$  NMR spectroscopy provided mechanistic insights into the reaction pathway.

**Keywords:** 5-Amino-1,2,4-oxadiazoles; Tertiary amines; Deoxygenative amination



## Comparison synthesis of picric acid from phenol and salicylic acid for crystallization of mitragynine as picrate salt at difference percent purity

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Kratom, or *Mitragyna Speciosa* Korth, contains several alkaloids, one of which is mitragynine. However, a significant number of impurities, including wax and other undesirable alkaloid-derived substances, were included in the mitragynine that was obtained via the extraction method. For this reason, picric acid was used to crystallize mitragynine from a crude extraction. Picric acid is a highly explosive material that can't be bought without authority, so we have to synthesize it on our own and must be extremely cautious when using it due to its properties to form complexes with other compounds like creatinine and metals. These properties were applied to the crystallization of mitragynine. Upon crystallization, the mitragynine became a mitragynine picrate. We are eager to compare the formation of mitragynine picrate from picric acid, which was produced using phenol and salicylic acid as substrates, to study whether different substrates will affect the formation of a mitragynine complex. In this study, we employ a 36.90% (Figure 1) crude mitragynine extract for crystallization with picric acid. Numerous contaminants are visible on the peak of the 36.90% <sup>1</sup>H-NMR analysis (Figure 2). In order to produce a mitragynine crystal, mitragynine picrate from both substrates was depicrated. <sup>1</sup>H-NMR analysis revealed that the outcome was satisfactory (Figures 3 & 4) compare to the mitragynine standard (Figure 5). Although the two depicrated products displayed a crisp peak, they weren't the same. We hypothesize that the characteristics of picric acid, which is derived from salicylic acid and phenol, differ slightly, causing the difference in peak.

**Keywords:** kratom; mitragynine; phenol; salicylic acid; picric acid; mitragynine picrate



Figure 1



Figure 2



Figure 3



Figure 4



Figure 5

\*\*\*Please hold ctrl + left click on the hyperlink to see the full picture.

## Synthesis and evaluation of chrysin derivatives as histone deacetylase inhibitors

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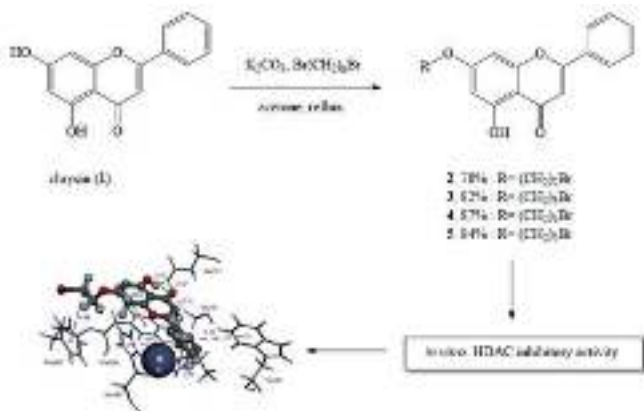
<sup>2</sup>Department of Biochemistry, Faculty of Science, Khon Kaen University, Khon Kaen 40002, Thailand

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Four bromo derivatives of chrysin (**1**) were synthesized by dissolving chrysin and potassium carbonate in acetone followed with dibromoalkyl halides including 1,2-dibromoethane, 1,3-dibromopropane, 1,4-dibromobutane and 1,5-dibromopentane to give compounds **2–5**, respectively. All synthesized derivatives were gained in 78–84% yield and were characterized by spectroscopy techniques (IR, <sup>1</sup>H NMR, and <sup>13</sup>C NMR). Biological activity of the obtained compounds against histone deacetylases (HDACs) was tested *in vitro* using trichostatin A (TSA) as a positive control (91 % inhibition at 25  $\mu$ M). The preliminary findings showed that bromo compounds had the moderate inhibitory effect against HDACs with 33–43 % inhibition at 100  $\mu$ M. HDAC inhibitory activity of the investigated compounds demonstrated that 7-(2-bromoethoxy)-5-hydroxy-2-phenyl-4H-chromen-4-one (**2**) (78% yield) possessed the highest inhibitory activity, with a value of 43 % inhibition when compared to the lead compound (chrysin, (**1**) 51 % inhibition). Moreover, molecular docking of the synthesized compounds with class I HDACs was studied. The results showed that compound **2** had the most selectivity against HDAC8 with the  $\Delta G$  value as -8.76 kcal/mol compared to chrysin (**1**,  $\Delta G$  = -8.08 kcal/mol). The side-chain alkyl bromo of compound **2** strongly interacted with Phe207 and aromatic region chelated the HDAC cofactor, zinc ion.

**Keywords:** Chrysin; Structural modification; HDACs; Docking



## Structural simplification of maytansine and synthesis efficiency for antitumor activity

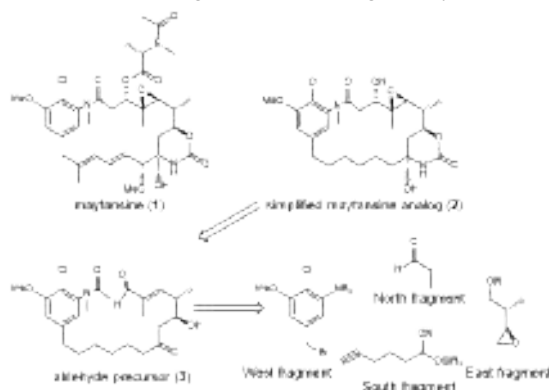
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Maytansine, an antitumor agent, binds to tubulin and exhibits antitumor activity. Its complex structures have attracted many organic chemists, and total synthesis was achieved in the 1980s. Despite concerns about high toxicity in clinical use, recent interest has been revitalized due to advancements in drug delivery systems, including those utilizing antibodies. This study aims to simplify the structure of maytansine while preserving its antitumor activity, allowing for practical total synthesis. Based on the reported X-ray crystal structure of the maytansine-tubulin complex, some moieties that would not affect its antitumor activity were selected. Significantly, the dienyl structure and methoxy group, located away from the critical binding site, offer the potential for simplification. In addition, they are unconjugated to the aromatic ring, which can destabilize the overall structure of maytansine and pose challenges in stereoselective synthesis. Consequently, a novel simplified maytansine analog was designed, replacing these synthetically challenging and unnecessary components for antitumor activity with the unfunctionalized methylene chain. DFT calculations indicated that the structural simplifications would not influence the overall steric structure since the stable conformation of the analog resembled natural maytansine. With aldol condensation and cyanohydrin chemistry as the key steps, the retrosynthetic analysis of this analog yielded four fragments—East, West, North, and South—along established total synthesis routes. The East and the West fragments have been synthesized, and the current focus involves considering the linkage of each fragment to the South fragment.

**Keywords:** Maytansine; Anti-tumor agent; Tubulin; Fragment synthesis; Simplification



**Figure 1.** Structures of maytansine (1) and the simplified maytansine analog (2). Open arrows indicate the retrosynthetic analysis of 2 through the aldehyde precursor (3), which would be obtained from the four fragments.

## Syntheses and mechanistic investigations of formamides, formamidines, and formimides

Chhorvy Kong<sup>1\*</sup>, Piyabutr Wanichpongpan<sup>2</sup>, and Kittichai Chaiseeda<sup>1</sup>

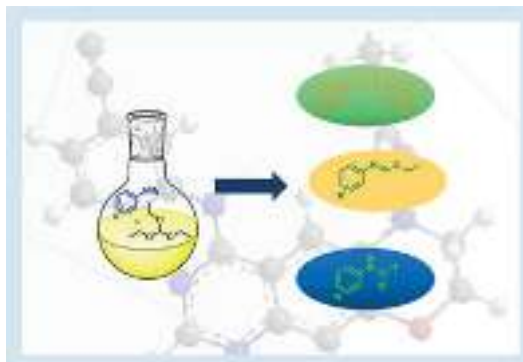
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Formamide, formidine, and formimide compounds are the organic compounds that have been used in the synthesis of pharmaceutically active compounds, and industries. This work presents convenient and efficient methods for preparing 3 kinds of products: formidine, formimide, and formamide from amines and triethyl orthoformate (TEOF) under varied reaction conditions. Aniline was chosen as a model compound. Various experimental parameters were varied including type of solvent, mole ratio, reaction time, and reaction temperature. It was found that to obtain formidine, using ethanol as a solvent and 1 equivalent of TEOF at 60 °C in 2 h produced the desired product at 91% yield. The highly efficient protocol for formimide was carried out under solvent-free condition using 5 equivalents of TEOF at 60 °C and the formimide product was obtained at 98% yield within 24 h. To produce formamide, 12 equivalents of TEOF in deionized water at 70 °C were used to achieve 86% yield in 24 h. Mechanistic investigations were also carried out to learn about the behavior and properties of these compounds and propose a reaction mechanism to produce these three types of compounds. The optimized reaction conditions were later applied for other amines as well. Due to its catalyst-free, low-cost, easy reaction, fast reaction time, and excellent yields, the current method is favorable.

**Keywords:** Formidine; Formimide; Formamide; Triethyl orthoformate; Catalyst-free



## Synthetic and chiroptical studies on novel fluorophores based on chiral bipyrenyl platform

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Axially chiral compounds based on polycyclic aromatic hydrocarbons are expected to show enhanced chiroptical properties such as optical rotation, circular dichroism (CD), and circularly polarized luminescence (CPL). Focusing on the rich optical properties of pyrene, we have previously reported axially chiral bipyrenes. With an aim at obtaining a photo-induced energy/electron transfer chiral-material mimicking photosynthesis, we designed and synthesized the bipyrene **1** having quaterphenyl chromophores (Figure 1a). The optical resolution of the resulting *rac*-**1** was carried out using a HPLC with ChiralPak IA<sup>®</sup>. The values of anisotropy factors ( $g_{CD}$ ,  $g_{CPL}$ ) of CD and CPL were  $2.5 \times 10^{-3}$  and  $1.5 \times 10^{-3}$ , respectively (Figure 1(b)). The fluorescence quantum yield of *rac*-**1** was 0.54, leading to the CPL brightness ( $B_{CPL}$ ) of 34.0. In the presentation, the details of the synthesis and the spectroscopic studies will be discussed.

**Keywords :** Circularly polarized luminescence; Axially chiral molecule; Pyrene;  $\pi$ -conjugated molecules

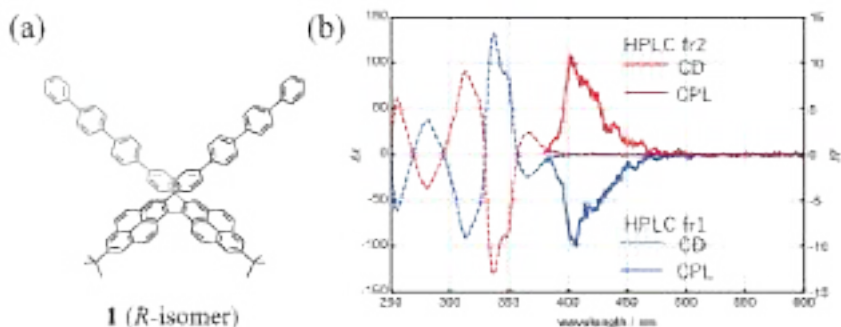


Figure 1. (a) Molecular structure of **1**. (b) CD and CPL spectra of **1** in  $CH_2Cl_2$  ( $1 \times 10^{-5}$  M).



## Gallic acid encapsulated Pamam dendrimers: A promising antioxidant delivery system for controlled release and reduced toxicity

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Poly(amidoamine) (PAMAM) dendrimers have generated significant interest in various research areas, particularly in the field of medicinal compound delivery. Their versatility stems from their capability to conjugate with functional molecules on their surface and encapsulate small molecules, rendering them suitable for a wide range of applications. Gallic acid, a potent antioxidant that has gained recent attention, is the focal point of our research. The gallic acid content in the PAMAM dendrimers were evaluated using NMR spectroscopy and UV-vis techniques. We aim to investigate whether gallic acid-encapsulated PAMAM dendrimers of generations 4 and 5 (G4(OH)-Ga, G5(OH)-Ga) can enhance radical scavenging, potentially delaying the progression of age-related macular degeneration (AMD). The encapsulation of gallic acid in PAMAM dendrimers serves as a viable method for preserving its stability and reduce toxicity. *In vitro* antioxidant activity was assessed using the DPPH and ABTS, as well as the FRAP assay, to determine IC<sub>50</sub> values for antioxidant potential. These results indicate that the order of antioxidant potency in scavenging the DPPH, ABTS and FRAP assay are as follows: Gallic acid > G4(OH)-Ga > G5(OH)-Ga. Additionally, the cytotoxic effect of gallic acid and gallic acid encapsulated-PAMAM dendrimers on ARPE-19 cells was determined via the MTT assay, it was observed that both gallic acid and G5(OH)-Ga demonstrated cytotoxic effects on ARPE-19 cells.

**Keywords:** Poly(amidoamine) dendrimers; PAMAM; Gallic acid; Age-related macular degeneration (AMD); Antioxidant; Encapsulation

## Synthesis of azanorbornadienes as building blocks to complex aryl products

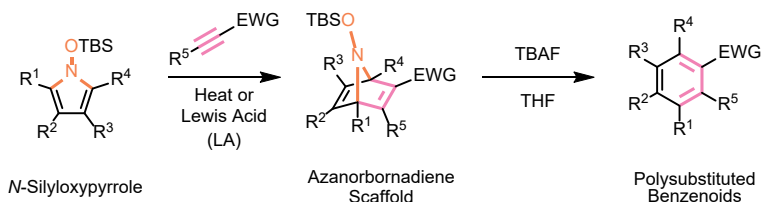
Thomas Whatton<sup>1</sup>, Dr Ben Emery<sup>1</sup>, Dr James Taylor<sup>1</sup>, and Prof. Steven Bull<sup>2\*</sup>

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Complex, highly substituted aryl products are highly prevalent in pharmaceuticals, with most small molecule drugs containing at least one aromatic motif. However, these aromatic compounds are often limited in variety of substitution patterns with more easily accessible patterns dominating the active pharmaceutical ingredient (API) space. We describe a novel synthetic route to access these extremely underrepresented 1,2,3,4-; 1,2,3; 1,2,4 and 1,2,4,5 substituted benzenoids. This was achieved through the modular synthesis of azanorbornadienes (Aznobs) via the Diels-Alder [4+2] cycloaddition between *N*-silyloxypyrroles and electron deficient alkynes. Twenty-seven examples of these Aznobs have been synthesised, with yields ranging from 22-93% yields. The synthesised Aznobs were then diversified, using cross-coupling methodology such as the Suzuki-Miyaura coupling, the Sonogashira coupling and the Buchwald-Hartwig amination. Twelve examples of compounds ranging from 23-84% yields were made in this way. The Aznobs were then subjected to tetrabutylammonium fluoride, which triggered the cheletropic elimination of Aznobs to produce 26 substituted benzenoids in 12-87% yields. The *de-novo* synthesis of *N*-silyloxypyrroles was also explored, using the Paal-Knorr synthesis and *aza*-conjugate addition to produce 8 examples in 10-58% yields. This powerful synthetic pathway allows for synthesis within relatively unexplored chemical space, which provides new ways to produce previously difficult to access benzenoid scaffolds.

**Keywords:** Diels-Alder; Synthesis; Pyrrole; Paal-Knorr; Benzenoid



## Synthesis and properties of helical oligothiophenes anchored to binaphthyl

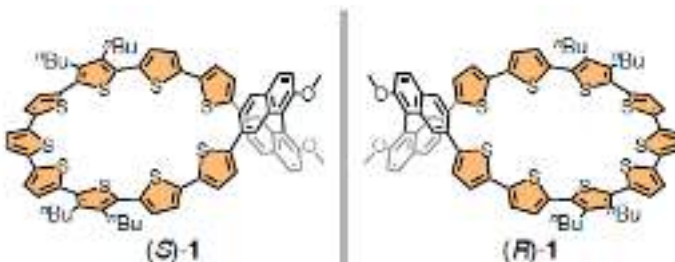
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Recently, shape-persistent  $\pi$ -conjugated chiral macrocycles have been attracted attention due to their intensive chiroptical properties such as circularly dichroism (CD) and circularly polarized luminescence (CPL). To gain insight into the correlation between chiroptical properties and molecular structure, we newly designed macrocyclic oligothiophene (*R*)/(*S*)-**1** embedded into a chiral binaphthyl moiety. Target compounds were prepared from racemic 7,7'-dibromo-2,2'-methoxy-1,1'-binaphthyl via several steps. Then, the optical resolution by a chiral HPLC method gave two-enantiomers of (*R*)/(*S*)-**1**. The molecular structure was confirmed by  $^1\text{H}$  and  $^{13}\text{C}$  NMR, and HRMS spectra. The absolute configuration of these enantiomers was validated by the comparison of CD spectra and TD-DFT calculations. Compound **1** exhibited absorption and fluorescence maximum at 475 nm and 561 nm, respectively, in  $\text{CH}_2\text{Cl}_2$  solution. The quantum yield of *rac*-**1** was found to be 15%. Both enantiomers exhibited clear CPL spectra, and their dissymmetry factor ( $|g_{\text{lum}}|$ ) was  $3.5 \times 10^{-3}$ . Furthermore, cyclic voltammetry of *rac*-**1** showed four pairs of reversible waves at  $E_{\text{ox}} = 0.26, 0.41, 0.69$  and  $0.85$  V, suggesting successive formation of radical cations. In the future, we plan to investigate host-guest chemistry using the chiral cavity of **1**.

**Keywords:** Macrocycle; Chiroptical properties; Oligothiophene; Circular dichroism; Circularly polarized luminescence



# Organic Synthesis and Medicinal Chemistry (OM)

## Poster Presentation

# Development of visible-light-induced hydrogen atom transfer (HAT) process as a tool for C–H functionalization of indole derivatives

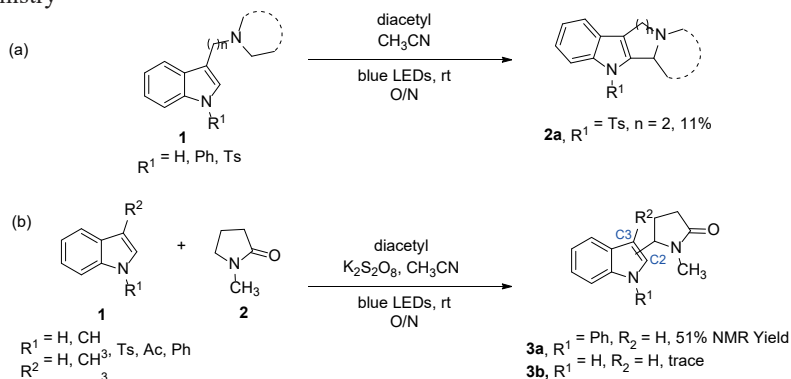
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Indole is a core structure commonly found in alkaloids and is also present as a pharmacophore in numerous medicinal drugs. These indole-containing biologically active compounds exhibit various activities, including anticancer, antifungal, anti-HIV, antitubercular, anti-inflammatory, and antimicrobial activities. To extensively study these bioactivities, a fast and practical methodology, used for generating a library of the compounds, is needed to be investigated. Herein, we are interested in developing a new synthetic route to access indole derivatives using the photoinduced hydrogen atom transfer (HAT) process, which is a simple way to generate radical intermediates from C–H bonds and has a unique potential for green and sustainable synthesis. We have been investigated the intramolecular C–H functionalization of the indole derivative *via* HAT process (Scheme 1a) and it was found that Ts-derivative can provide the desired  $\alpha$ -amidoalkylated product in 11% yield. To study the improvement of the reaction efficiency, the intramolecular reaction and model substrates (indoles and *N*-methyl-2-pyrrolidinone) were subjected to optimization by the treatment of HAT reagent, *e.g.* diacetyl, under blue LEDs irradiation (Scheme 1b). By the treatment of diacetyl and  $K_2S_2O_8$ , the reaction of 1-phenylindole and *N*-methyl-2-pyrrolidinone provided the C3-alkylated product in 51% NMR yield with a high regioselectivity. However, we expected that this strategy could be used to prepare pyrrolo- or piperidoindole derivatives in an intramolecular manner, which are similar to the core structures of natural products, such as harmacine, cuscutamine, *etc.*

**Keywords:** Indole; C–H functionalization; Hydrogen atom transfer; Photoredox Chemistry



**Scheme 1.**  $\alpha$ -Amidoalkylation of indole derivatives via (a) intra- and (b) intermolecular HAT.

## Synthetic and theoretical study on the homodimerization mechanism of coumarin derivatives

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Nevena I. Petkova-Yankova, Hristiyan A. Aleksandrov, Petko St. Petkov, and  
Rositca D. Nikolova\*

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Study on the reaction conditions for homodimerization process of 3-substituted coumarins were achieved under sonication. The mechanism of the reaction was investigated on the basis of first principal calculations and experimental results for 3-acetylcoumarin. Relative stability of the possible intermediates has been compared. Two reaction pathways were considered: ionic and radical. The comparison between the experimental data and the relative stability of the intermediates suggest that the most plausible reaction pathway proceeds via formation of radical species. The important role for the dimerization process of the implied metal and metal salts in the reaction mixture was emphasized. Quantum-chemical calculations also demonstrated the necessity of both Zn and Zn-salt in the reaction mixture and not Cu/Cu-salt. The activation role of the solvent on the reactivity of the Zn-salt was also clarified. The coordination of the solvent molecules to the Zn-atom of the  $\text{ZnCl}_2$  reduces the energy barrier for the Zn-Cl bond dissociation, thus facilitating the formation of I-B-Zn to the final biscoumarin structure.

The authors acknowledges the support by the EXTREME project, funded by the Bulgarian Ministry of Education and Science, D01-76/30.03.2021 through the programme "European Scientific Networks".

**Keywords:** Coumarins; Homodimerization; Sonochemistry; Mechanism; Quantum-chemical investigation

# Synthesis of ceramide IIIB, a natural skin protective lipid barrier, from commercially available protected L-serine

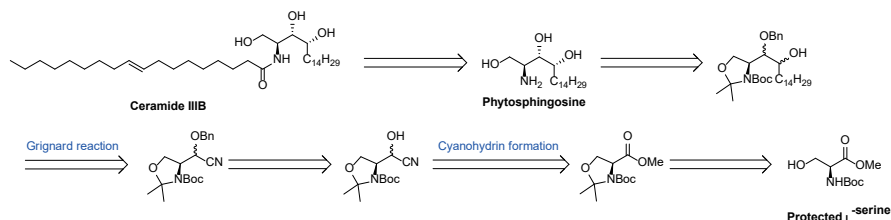
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Ceramides, the major lipid components of the stratum corneum, help keep the skin hydrated and reduce dehydration, which are two causes of skin weakness. Ceramides are typically found in various forms, but ceramide IIIB is an essential lipid in the skin and the most popular compound in the cosmetics industry. Imported ceramide IIIB is very expensive, and there is no synthetic approach in Thailand. This research will focus on the synthesis of ceramide IIIB using protected L-serine as a precursor. The synthesis was designed in nine steps, with cyanohydrin formation and Grignard reactions being utilized as key reactions.

**Keywords:** Ceramide; L-serine; Stratum corneum; Sphingolipids; Keratin



**Scheme 1.** Retrosynthesis of ceramide IIIB.

## Investigation of the aqueous-mediated green synthesis of squarate esters and squarate thioesters

Siraporn Soonthonhut and Peera Acharasatian\*

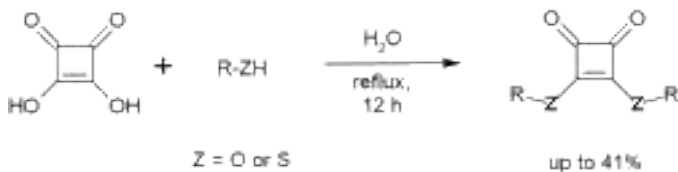
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Squaric acid and squaramides are well studied and found applications in various fields. On the other hand, the exploration of squarate esters and squarate thioesters is rather limited. The aqueous mediated green synthesis of squarate esters and squarate thioesters was investigated. The mixture of squaric acid and the corresponding alcohol (or thiol) was refluxed in water without addition of a catalyst or any other reagent. Although water molecules could facilitate proton transfer process in the reaction, it also triggered hydrolysis (the reverse reaction). The syntheses of squarate esters and squarate thioesters are therefore quite challenging since the desired reaction must compete with the hydrolysis. This competition will certainly affect the product yields. Five examples of alcohols/thiols were examined in this study. Ethane-1,2-dithiol provided the highest yield since the dithiol could undergo cyclization. The cyclized product, 2,5-dithia-bicyclo[4.2.0]oct-1(6)-ene-7,8-dione which is a bicyclic squarate thioester was afforded in 41%.

**Keywords:** Squarate thioester; Squarate ester; Aqueous mediated reaction; Green synthesis; Cyclization



## Synthesis, structural modification and biological activity evaluation of triazole derivatives derived from *S*-benzylhomocysteines

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1,2,3-Triazole derivatives are well-known compounds showing various biological activities such as antitumor, antimicrobial, antiviral, antituberculosis, antidiabetic, anticancer, and so on. The structure of 1,2,3-triazole is composed of a pentagonal three nitrogen atoms containing aromatic ring which plays a significant role in biological activities. The 1,2,3-triazole ring can be synthesized easily in one step via 1,3-dipolar cycloaddition or Click reaction. In this research, the preparation of 1,2,3-triazole derivatives would be planned by using Click reaction and starting from *N*-propargyl quinazolinone and modified azido derivatives derived from *S*-benzyl homocysteine. These synthetic compounds will be submitted for bioactivity screening such as anticancer, antidiabetic, antimelanogenesis, and antialzheimer. We expected that three main parts, quinazolinone, 1,2,3-triazole and *S*-substituted homocysteine, will show some engaging biological activities. The strategy can be applied and developed into medical scale and also a drug used in Thailand, resulting in the reduction in the cost of treatment. Including the prototype substance that may be developed to be a drug sent abroad.

**Keywords:** 1,2,3-Triazole; Click reaction; Quinazolinone; Homocysteine; 1,3-Dipolar cycloaddition

**Scheme 1.** Retrosynthesis analysis of 1,2,3-Triazole derivatives.

## An *In Silico* study of phloretin as a potential of class I glucose transporters inhibitor for targeted hepatocellular carcinoma treatment

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Hepatocellular carcinoma (HCC) is the most common liver cancer and a primary cause of cancer deaths worldwide. Within cancer cells, there is an increased demand for glucose compared to normal cells, resulting from metabolic alterations known as the Warburg effect, leading to an excessive expression of class I glucose transporter proteins (GLUTs). Therefore, most therapeutic strategies for HCC focus on inhibiting the function of class I GLUTs to effectively regulate glucose uptake in cancer cells. Phloretin, a polyphenol derived from apples, which has been proven to be class I GLUTs inhibitor, was selected as a ligand to investigate the reaction and binding positions to the class I GLUTs; including GLUT-1, GLUT-3, and GLUT-4, except for GLUT-2, whose crystal structure has yet to be determined. Phloretin and glucose, the two ligands of interest, were compared in this study. The results revealed the competitive mechanism between phloretin and glucose when interacting with class I GLUTs with calculated docking scores for complex formation of phloretin in GLUT-1, GLUT-3, and GLUT-4 (-192.44, -171.23, and -141.76, respectively). While the docking scores for glucose with GLUT-1, GLUT-3, and GLUT-4 were -131.52, -138.50, and -112.94, respectively, confirming the effectiveness of the phloretin in interacting with these transporter proteins since the binding occurred around the same position as glucose, suggesting a possible pathway for inhibiting glucose uptake by blocking glucose in cancer cells through the transporters. Finally, this study may contribute to the advancement of potential inhibitors targeting class I GLUTs through the further design of phloretin.

**Keywords:** Phloretin; Glucose transporter proteins; GLUTs inhibitor; Hepatocellular carcinoma (HCC); Molecular docking

## Applications of Methyl Itaconate-Anthracene Adducts as Chiral Resolving Agents for Binaphthol Derivatives

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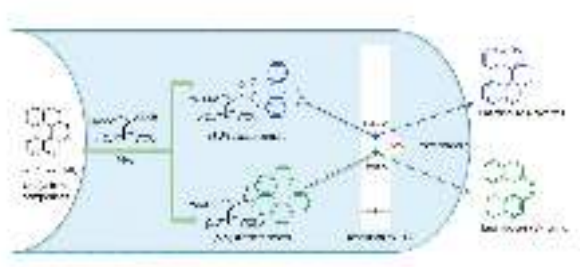
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Chiral BINOL derivatives have several applications such as asymmetric synthesis, circularly polarized luminescence (CPL) dyes and charge transfer host system. There are several methods for enantiopure BINOLs preparation which are asymmetric synthesis from 2-naphthol, enzymatic resolution, and chiral resolution by crystallization or chromatography. Herein, we applied the latter method with methyl itaconate-anthracene adducts (MIAs) as chiral auxiliaries. Diastereomeric pairs of MIAs and BINOLs were prepared through esterification reaction and obtained with moderate yield. Spectroscopic analysis was applied for the structural characterization and confirmation. Chiral resolution was further investigated using thin layer chromatographic (TLC) technique. The difference of retention factor ( $\Delta R_f$ ) values between (*S*)-MIA-(*S*)-BINOL and (*S*)-MIA-(*R*)-BINOL was determined to be 0.11. For other BINOL derivatives, H<sub>8</sub>-BINOL and BINAM were selected to validate the efficiency of MIA. The results demonstrated the effectiveness of MIA in chiral resolution process of BINOL and its derivatives, as indicated by significant differences in  $\Delta R_f$  values. Interestingly, both diastereomers of BINOL and BINAM derivatives with (*S*,*R*)-configuration displayed a distinct characteristic on TLC, appearing at a higher position compared to the (*S*,*S*)-configuration. Diastereomers of BINOL were investigated to study methanolysis for deriving enantiopure forms of BINOL with high optical purity.

**Keywords:** Chiral BINOL derivatives; Chiral auxiliary, Chiral resolving agent; Thin layer chromatography.



## Cyclodextrin conjugated fluorescein dye for drug delivery

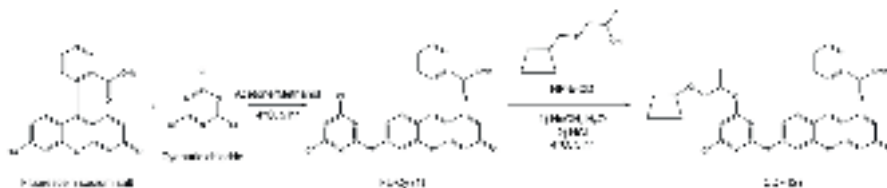
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Cyclodextrins (CD) are cyclic glucose units that are extensively used in the food, pharmaceutical, and cosmetic industries. It is a vehicle for delivering odors, flavors, bioactive substances, and medicines. However, it is difficult to follow the delivery since CD has no UV absorption or fluorescence emission. In this research, cyclodextrins conjugated fluorescein (CDF) dye was synthesized in two steps. In the first step, fluorescein sodium salt was reacted with cyanuric chloride resulting in yellow precipitate of FL-Cy (1). Then FL-Cy (1) was reacted with HP-b-CD to obtain CDF (2). The chemical structures were characterized by using  $^1\text{H-NMR}$ ,  $^{13}\text{C-NMR}$ , IR and MS. The UV-Vis absorption and fluorescence emission of CDF have been studied in PBS buffer pH 4, 7.4 and 9. The results showed that the UV-Vis absorption and fluorescence emission of CDF depended on pH. In addition, CDF will be used for further study of drug or active compounds delivery.

**Keywords:** Cyclodextrin; Fluorescein; CDF



**Figure 1.** Synthesis scheme of CDF.

## Synthesis and characterization of gallic acid derivatives for investigating antioxidant properties

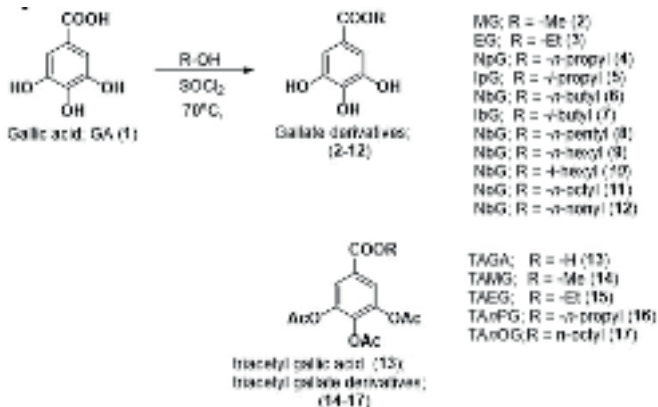
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Gallic acid (**1**) exhibits anti-bacterial, anti-fungal, anti-viral, anti-inflammatory, anti-cancer, and anti-oxidative properties. One of the main factors contributing to changes in food processing is oxidation. This process causes changes in the nutritional quality of the food, such as the safety, color, smell, and texture, leading to deterioration and safety. The researchers successfully synthesized all 13 gallic acid derivatives (**2-12**) through an esterification reaction with a high %yield. The structural characterization of each synthesized derivative was accomplished using Fourier transform infrared (FTIR) and nuclear magnetic resonance (NMR) spectroscopy. Subsequently, the antioxidant properties were evaluated using 2, 2-diphenyl-1-picrylhydrazyl (DPPH) radicals or DPPH radical scavenging methods. Compounds (**1-12**) exhibited excellent antioxidant capacity. Additionally, the five *tri*-acetyl gallate derivatives (**13-17**), which lack any residual hydroxyl groups, demonstrated noteworthy antioxidant capacity compared to the positive control, gallic acid. A compound must contain at least two adjacent hydroxyl groups (-OH) to be a good antioxidant. This sentence needs to be consistent with the experimental results. The researchers recommend cutting it out. Therefore, this information could be used as scientific information in the anti-oxidation group and lead to further development for industrial use.

**Keywords:** Gallic acid; Gallic acid derivatives; Gallate derivatives; Antioxidant activity



## The synthesis of benzazepine analogs via intramolecular ritter reaction

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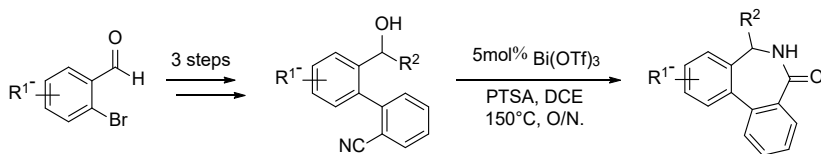
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The seven-membered ring benzazepine belongs to a significant class of heterocyclic compounds and this core structure is an important scaffold found in synthetic and natural compounds. Benzazepine moiety has received a great attention from researchers around the world due to its biological and pharmacological activities. For example, fenoldopam is used as an anti-hypertensive agent, lorazepam is used to treat severe anxiety and panic attacks, and galantamine is a cholinesterase inhibitor which is used to treat Alzheimer's disease. For these reasons, our research group intends to develop a new method for synthesizing benzazepine analogs via intramolecular Ritter reaction employing bismuth(III) trifluoromethanesulfonate ( $\text{Bi}(\text{OTf})_3$ ) and *p*-toluenesulfonic acid. The key substrate of this conversion is 1,1'-biphenyl]-2-carbonitrile alcohol which can be prepared from Suzuki cross coupling between 2-bromobenzaldehydes and *ortho*-cyanophenyl boronic acid, followed by Grignard addition. Based on prior research,  $\text{Bi}(\text{OTf})_3$  is considered to be one of the most effective catalysts for converting benzylic alcohol into benzylic cations. Consequently, we used this catalyst in our procedure. We anticipate that the outcome of the synthesis of benzazepine libraries may result in the identification of novel bioactive compounds.

**Keywords:** Benzazepine; Intramolecular cyclization; Ritter reaction; Bismuth(III) trifluoromethanesulfonate; Suzuki coupling



# Phospha-1,4-addition promoted highly regioselective cyclization of *N*-propargyl azlactone: Unprecedented synthesis of benzopyrroloazepine

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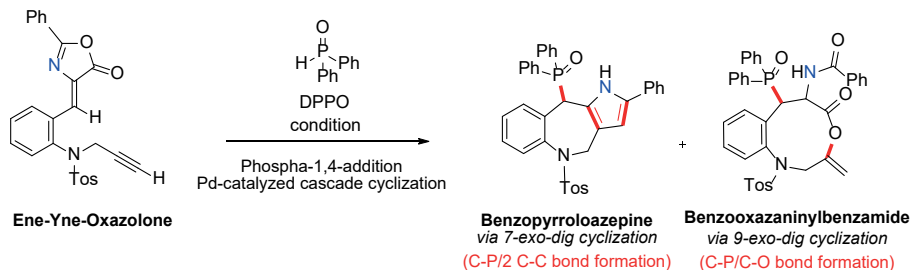
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Phosphorylated heterocycles have significant value in both chemical and biological properties. Despite their importance, there are relatively few reports on these compounds. Therefore, the development of efficient methods for synthesizing heterocyclic compounds bearing a phosphonate group on the ring is of great interest. In this study, we successfully employed a highly regioselective approach to synthesize benzopyrroloazepine characterized by 6/7/5 ring systems containing a phosphorus atom, resulting in moderate yield. Our approach involves *N*-propargyl azlactone and diphenylphosphine oxide (DPPO) as precursors in a Pd-catalyzed cascade cyclization. The reaction encompasses phospha-1,4-addition, 7-exo-dig cyclization, ring-opening of the oxazolone, and the construction of a 5-membered pyrrole ring, respectively. This sequence leads to the formation of both C-P and two C-C bonds of benzopyrroloazepine. Additionally, a minor product, benzooxazaninylbenzamide, was also obtained through 9-exo-dig cyclization.

**Keywords:** Phosphorylated heterocycle; Cascade cyclization; Pd-catalyst; Ene-yne-oxazolone; Benzopyrroloazepine; Benzooxazaninylbenzamide



## Synthesis and anticancer evaluation of indolo[1,2-*a*]quinoline derivatives

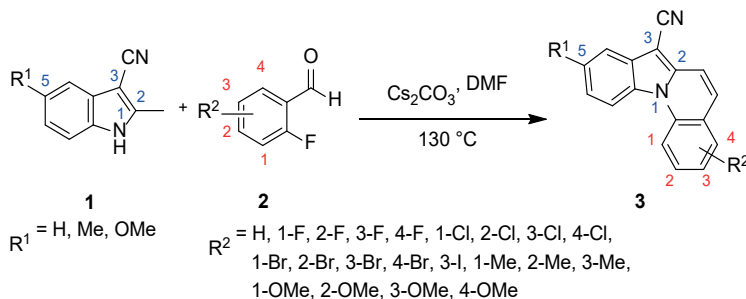
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Indolo[1,2-*a*]quinoline is a nitrogen-containing tetracyclic compound, and some of its derivatives exhibit biological activities such as anticancer and antibacterial activities, making them potential drug candidates. Additionally, indolo[1,2-*a*]quinoline and its derivatives possess luminescent properties, which could be used as organic semiconductors and organic sensitizers for solar cells. Previously, the synthesis of indolo[1,2-*a*]quinolines typically used transition metals such as Pd, Cu, Au, and Rh for coupling reactions. In this work, indolo[1,2-*a*]quinolines **3** were prepared in one pot under transition-metal-free conditions via nucleophilic aromatic substitution and Knoevenagel condensation of indole-3-carbonitriles **1** and 2-fluorobenzaldehydes **2** in the presence of  $\text{Cs}_2\text{CO}_3$ . This method was simple and efficient, and most of the desired products were obtained in moderate to good yields. All synthesized compounds were evaluated against colorectal cancer (HT-29 and HCT-116) and breast cancer (MCF-7) cell lines, and some exhibited significant activity against these cell lines.

**Keywords:** indolo[1,2-*a*]quinoline; nucleophilic aromatic substitution; Knoevenagel condensation





## Potential of flavonoids from Thai natural products as SARS-CoV-2 3CL<sup>Pro</sup> inhibitor: *In silico* and experimental perspectives

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The emergence of the COVID-19 situation has become a global issue due to the lack of effective antiviral drugs for treatment. Flavonoids are a class of plant secondary metabolites that have antiviral activity against SARS-CoV-2 through inhibition of the main protease (3CL<sup>Pro</sup>), a crucial enzyme in the viral replication cycle. In this study, 22 flavonoids obtained from natural and semi-synthetic approaches were investigated for their inhibitory activity against SARS-CoV-2 3CL<sup>Pro</sup>, along with cytotoxicity on Vero cells. The protein-ligand interactions were examined using molecular dynamics simulation and binding free energy calculation using molecular mechanics Poisson-Boltzmann surface area (MM-PBSA) and molecular mechanics with generalized Born and surface area (MM-GBSA) calculations. Moreover, 3D-QSAR analysis was conducted to clarify the structural effects on their antiviral activity. Accordingly, the *in vitro* investigation demonstrated that four flavonoids, namely tectochrysin, 6'',6''-dimethylchromeno-[2'',3'':7,8]-flavone, panduratin A, and genistein, showed higher protease inhibitory activity compared to the standard flavonoid baicalein, with IC<sub>50</sub> in the range of 13.25 to 24.00  $\mu$ M. Finally, our finding suggests that genistein, an isoflavone discovered in *Millettia brandisiana* Kurz. or Kra Pee Jun, has potential for further development as a SARS-CoV-2 3CL<sup>Pro</sup> inhibitor.

**Keywords:** SARS-CoV-2; COVID; Antiviral; Molecular Dynamics; QSAR

## A novel synthetic approach to 2,3-diaryl-1,3-thiazolidin-4-ones and their anticancer activity

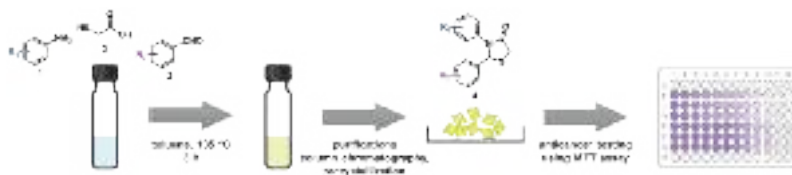
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Nowadays, health issues remain a significant global concern such as diabetes, hyperlipidemia, hypertension, cardiovascular disease, cancer and others. Although effective drugs and treatment guidelines are now available for many illnesses, the improvements in drug efficacy, specificity and safety are still needed. Thiazolidinone is a class of the heterocyclic compounds that exhibit a wide range of pharmacological activities, i.e. anticancer, anti-tuberculosis, antimicrobial and anti-inflammatory activity. There are many reported methodologies to prepare 1,3-thiazolidin-4-one analogues, for example, acid-catalyzed, coupling reagent-catalyzed, ionic liquid-assisted and microwave-assisted synthesis. In this research work, 2,3-diaryl-1,3-thiazolidin-4-ones (**4**) were synthesized via acid-catalyzed three-component one-pot reaction in seal tube which was used aniline (**1**), benzaldehyde (**2**) and thioglycolic acid (**3**) as starting material. The reaction condition required only three hours, which was faster than previous reports and resulted the clean reaction mixture, yielding moderated to high product yield. This developed condition can be applied to electron donating, electron withdrawing and hetero aromatic compounds. Anticancer activities were tested against ten cell lines including SW1088, U87-MG, A549, H460, MCF-7, MDA-MB-231, HepG2, HCT116 and HT-29 cell line via MTT assay. A series of synthetic 2,3-diaryl-1,3-thiazolidin-4-ones (**4**) shows low ( $IC_{50} = 50-100 \mu M$ ) to no activity ( $IC_{50} > 100 \mu M$ ) against all tested strains. However, the other analogues will be synthesized and evaluated their activity to study the relationship between the structures and activity.

**Keywords:** Heterocyclic compound; 1,3-Thiazolidin-4-one; Anticancer; Drug discovery; Structure-activity relationships



## Synthesis and molecular docking studies on SAR-CoV-2, AChE and MPO inhibitors of chalcone-caffeine hybrids

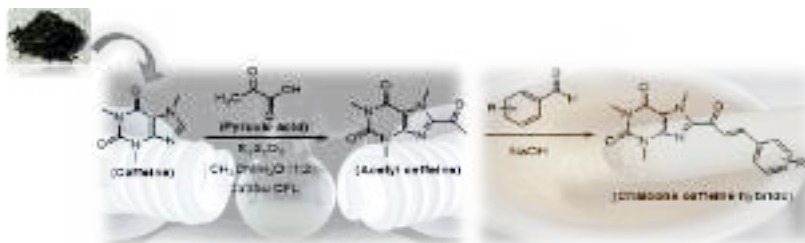
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Chalcone-caffeine hybrids were synthesized through 2 steps starting from caffeine separated from tea leaf extracts. Photocatalysis reaction employing pyruvic acid as acyl precursor was performed to synthesize acetyl caffeine. Thereafter, Claisen-Smidth condensation of acetyl caffeine with benzaldehyde and its derivatives was investigated to provide 12 chalcone-caffeine hybrids containing various e-withdrawing and e-donating groups on the phenyl ligand (H, 2Cl, 3Cl, 4Cl, 2Me, 3Me, 4Me, 2MeO, 3MeO, 4MeO, 2NO<sub>2</sub> and 3NO<sub>2</sub>). The results provided moderate to high yields of the desired adducts that *para*-substituted derivatives gave higher yield than *ortho* and *meta* substituents. Additionally, their bioactivities to inhibit SARS-CoV-2, human acetylcholinesterase (AChE) and human myeloperoxidase (MPO) were evaluated by using molecular docking calculation. The excellent results indicated that all derivatives afforded high efficiency against SARS-CoV-2, AChE and MPO in comparison to caffeine with lower binding energy values. Interesting results displayed that 3Cl and 3Me derivatives of chalcone-caffeine hybrid exhibiting as SARS-CoV-2 inhibitor more than other substituents. Likewise, 4Me derivatives showed the highest efficiency to inhibit AchE, and 3NO<sub>2</sub> substituted adduct gave higher efficacy for MPO inhibitors than other derivatives. Consequently, all substituted chalcone-caffeine adducts might be further developed in pharmaceutical industries.

**Keywords:** Caffeine; Chalcone-caffeine hybrid; SARS-CoV-2; Acetylcholinesterase; Myeloperoxidase



## The synthesis of phenanthrene-9-ols *via* palladium-catalyzed annulation

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Jumreang Tummatorn<sup>1,2</sup>, and Somsak Ruchirawat<sup>1,2</sup>

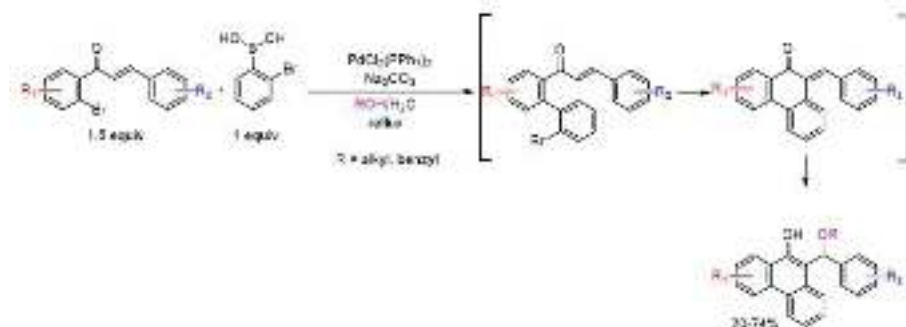
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Phenanthrene is a crucial component of many chemical compounds that exhibit intriguing biological properties like antimalarial, anticancer, and antibacterial properties. The synthetic phenanthrene is also used in many organic photoelectronic materials such as carbon nanotubes, superconducting materials, and chelating ligands. Furthermore, these core structures have been employed as substrates for a variety of applications which includes the creation of numerous libraries of compounds which are useful for drug discovery and development. As this core structure shows several biological activities which draws our attention to develop a novel method for the synthesis of phenanthrene-9-ols using palladium-catalyzed cascade annulation, *via* Suzuki cross-coupling reaction, followed by intramolecular Heck reaction to produce the desired products in low to good yields along with trace amount of indenone side products. The chemoselectivity of sequential reaction is controlled by concentration and temperature of the reactions. The scope of substrate is studied as shown in Scheme below.

**Keywords:** Phenanthrene; 9-phenanthrol; Suzuki cross-coupling; Intramolecular Heck reaction; 2-bromochalcone





## Development of the cobra antivenom production efficiency by using radioactive tracer techniques

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An envenomation from Thai cobra (*Naja kaouthia*) has been one of the most occurred incidents in Thailand along with other terrestrial inland snakebites. Even a number of antivenoms produced inland covers seven most encountered snakes, the antivenom production of Thai cobra is especially cumbersome as shown by a low antibody titer after an immunization on horses with cobratoxin. In order to comprehend the circulation of the cobratoxin within hosts and enhance the antivenom production capability, a radioactive tracer technique, together with the use of adjuvants, *i.e.* Freund's incomplete adjuvant (FIA) and Alum, are of interest. Radiolabeled cobratoxin can be visualized by means of gamma camera to reveal a pharmacodynamic through biodistribution, organ accumulation profiles, and a dynamic whole-body scan. The radioisotope used in this study was I-131 due to its high energy gamma rays, low cost, and easy to radiolabel *via* electrophilic substitution (ES) reaction on phenolic group of tyrosine in cobratoxin molecules. At first, the <sup>131</sup>I-cobratoxin has been produced *via* ES with a high radiochemical yield (85-95%). To maintain a specific activity, the product has been used without further purification and subjected into three parts; without addition of adjuvant, mixing with FIA, and using Alum as additives, respectively. Each solution was injected separately into three groups of rats, and the biodistribution and organ accumulation profiles has been acquired. FIA has proved to be the additive effectively extended the duration of cobratoxin in rats, while the effect of Alum or without adjuvant could not be notably observed.

**Keywords:** Antivenom; Radioactive tracer technique; Cobratoxin; Adjuvant

## Studies toward the synthesis of dibenzo[*b,f*]azepine derivatives

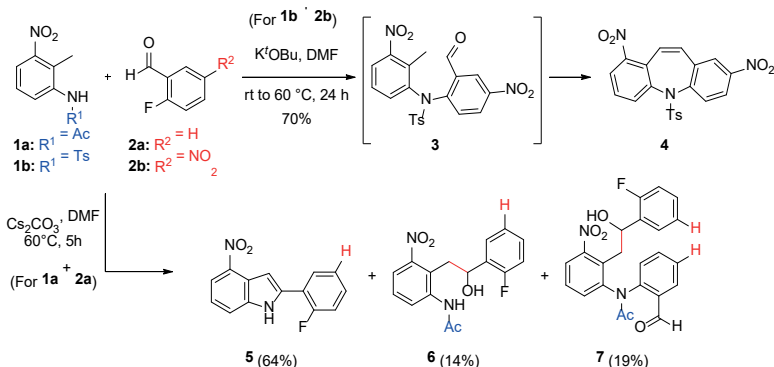
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Dibenzo[*b,f*]azepine, a heterocyclic compound composed of two benzene rings fused to an azepine ring, serves as the focus of this study. Dibenzo[*b,f*]azepine derivatives are vital in the pharmaceutical industry, serving not only in established antidepressants, anxiolytics, and anticonvulsants but also offering the potential for reengineering in various applications. Moreover, most reported methods use multi-step synthesis and transition metals such as Cu, Pd, or Rh. In this work, we have developed a novel method to synthesize 1-nitro-5*H*-dibenzo[*b,f*]azepine derivatives **4**. With the presence of a nitro group in the target structures, we envisioned that these compounds could be synthesized in one pot without using transition metals from anilines **1** and 2-fluorobenzaldehydes **2**. Under basic conditions, we anticipated that compounds **1** and **2** would participate in a nucleophilic aromatic substitution ( $S_NAr$ ) reaction to generate intermediates **3**, which would subsequently undergo an intramolecular Knoevenagel condensation reaction to provide the desired products. When **1a** and **2a** were employed in the presence of  $Cs_2CO_3$ , the reaction sequence did not proceed as expected since the  $S_NAr$  reaction seemed to occur in the second step to give compound **7**. Fortunately, the reaction of **1b** and **2b**, which contains an additional electron-withdrawing group ( $-NO_2$ ) required for the  $S_NAr$  reaction, successfully provided the product **4** in 70% yield when it was performed with  $tBuOK$  in DMF at room temperature to 60 °C.

**Keywords:** carbocyclization reaction; cascade reaction; dibenzo[*b,f*]azepine



## Design, synthesis, and biological activity evaluation of novel colchicine derivative as anticancer agent

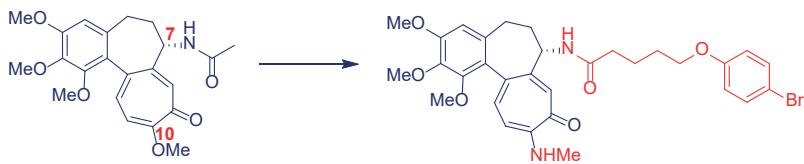
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Colchicine has been identified as a potential anticancer agent due to its ability to inhibit the formation of microtubules by interacting with  $\beta$ -tubulin at the 'colchicine binding site'. However, it exhibits high systemic toxicity and lacks selectivity, leading to various side effects. Several structural modifications of the colchicine scaffold, specifically at the C7, and C10 positions have been reported with significant improvement to its potential in cancer treatment. Notably, the replacement of the C7-acetamide with long-chain amides was shown to significantly increase the activity due to the interaction of alkyl moieties with the hydrophobic groove of  $\alpha$ -tubulin. In this work, we designed a novel structure of colchicine derivative with a 4-bromophenyl ring linked to the C7 via an aliphatic linker, together with the replacement of C10-OMe with NHMe. The synthesis was performed by the substitution of the C10-OMe of an ester-protected colchicine with methylamine. A newly optimized hydrolysis of the C7-acetamide gave the amino-colchicine, which was then coupled with our pre-synthesized linker via amide coupling to give the 4-bromophenyl-linked colchicine derivative in good yield over six steps. Next, this newly synthesized colchicine derivative underwent *in vitro* testing and demonstrated potent anticancer activity against Miapaca and HCT human cancer cell lines, with  $IC_{50}$  values of  $6.77 \pm 0.40$  nM and  $0.71 \pm 0.14$  nM respectively.

**Keywords:** Colchicine; Microtubules; Tubulin; Synthesis; Cancer



**Figure 1.** Graphical Representation of Novel Colchicine Derivative.

## Acid-catalyzed formylation reaction of indole derivatives with trialkyl orthoformate

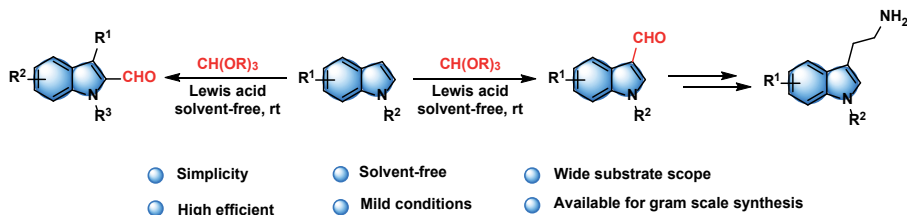
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2- and 3-Formyl indoles are highly versatile compounds with various applications in the pharmaceutical and chemical industries. Furthermore, these formyl indoles are versatile key intermediates involved in various functional group transformations to provide valuable simple to complex indole scaffolds. Although several convenient methods for synthesizing 3-formyl indoles have been reported in the past decade, most of them had the limitations of having harsh reaction conditions and typical requirements of electron-rich indoles with the use of costly heavy transition metals. Moreover, some methods involve reactions under volatile organic solvents and dry conditions. In this work, efficient synthesis of 3- and 2-formyl indole has been achieved through an acid-catalyzed formylation reaction of indoles with trialkyl orthoformate. The present approach offers the advantages of simplicity, high efficiency, solvent-free, mild reaction conditions, wide substrate scope, and excellent regioselectivity. The strategy could be performed on a gram scale to allow access to structurally versatile 3-formyl indoles, of which a key intermediate of tryptamine and its analogs, could be synthesized efficiently.

**Keywords:** Formylation; 2-Formyl indole; 3-Formyl indole; Trialkyl orthoformate; Tryptamine



## Development of a PSMA-11 lyophilized kit for convenient radiolabeling with $^{68}\text{Ga}$

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Prostate specific membrane antigen (PSMA) targeting ligands labeled with various types of radionuclides have been developed and used for diagnosis of prostate cancer. The positron-emitting radionuclide gallium-68 ( $^{68}\text{Ga}$ ) produced from a  $^{68}\text{Ge}/^{68}\text{Ga}$  generator has an excellent advantage in terms of on-site synthesis. It is similar in principle to  $^{99}\text{Mo}/^{99\text{m}}\text{Tc}$  generator which makes the cold kits for  $^{99\text{m}}\text{Tc}$  radiolabeling become widely used in medical imaging.  $^{68}\text{Ga}$ -PSMA-11 has been increasingly used in Thailand since 2017. This radiopharmaceutical is often produced by commercial synthesis modules which have high consumable costs and require hot cell facilities. While the kit-based production has advantages of lower cost, shorter preparation time and easier to operate. The aim of this work was to develop the PSMA-11 kit in a form of lyophilized powder to be ready for radiolabel with  $^{68}\text{Ga}$ . The lyophilization process was performed under sterile conditions. The kit could be radiolabeled with 5 – 20 mCi of  $^{68}\text{Ga}$  at room temperature in 15 min. The radiopharmaceutical  $^{68}\text{Ga}$ -PSMA-11 produced from the kit had high radiochemical purity without purification and was stable for at least 4 h. The biological quality control showed that the lyophilized product was a sterile, nonpyrogenic kit. It could be said that, by using the PSMA-11 kit, the production of  $^{68}\text{Ga}$ -PSMA-11 was relatively easy, cost effective and radiologically safe.

**Keywords:** Kit formulation; Prostate cancer; PSMA-11; Radiopharmaceutical

## Toward the synthesis of dauphinol B, a novel antimalarial natural product

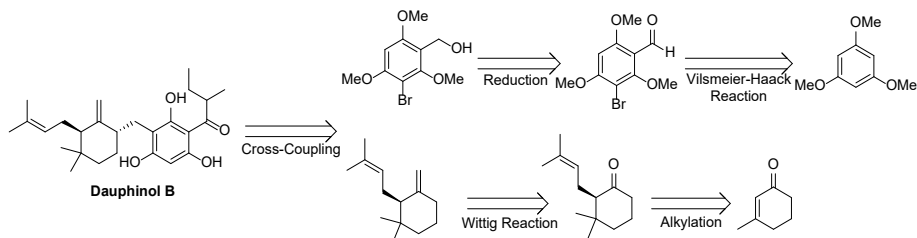
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Dauphinol B, a sesquiterpene linked to a phloroglucinol derivative, was isolated from the Madagascan plant *Garcinia dauphinensis* by Kingston and colleagues in 2018. Dauphinol B was found to possess potent antiplasmodial activities with an  $IC_{50}$  value of  $0.8 \pm 0.1 \mu M$  against the drug-resistant Dd2 strain of *P. falciparum*. In this research, the synthesis of dauphinol B will commence from commercially available 1,3,5-trimethoxybenzene and 3-methyl-2-cyclohexen-1-one. Vilsmeier–Haack reaction, alkylation and cross coupling reactions were planned as key steps.

**Keywords:** Antiplasmodial; Dauphinol B; Natural product synthesis



**Scheme 1.** Retrosynthetic analysis of dauphinol B.

## Chemical synthesis research of sea urchin feeding inhibitory substances

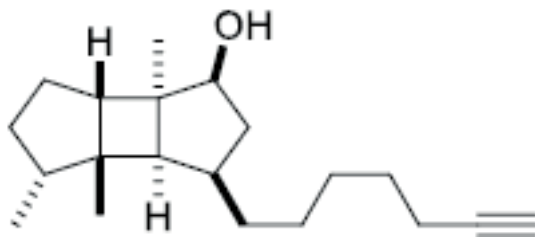
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In recent years, coastal regions of Japan have been facing an environmental issue known as “rocky shore denudation” which has led to the depletion of fisheries resources and the loss of marine biodiversity. rocky shore denudation refers to a phenomenon where coastal seaweed beds decline significantly or disappear beyond the scope of seasonal fluctuations or minor long-term changes. This is often described as “sea desertification”. The primary cause of this is the overconsumption of seaweed by sea urchins. In light of these circumstances, this study focused on spatane-type diterpene compounds with feeding inhibitory properties as a measure to prevent rocky shore degradation caused by sea urchins. Spatane-type diterpene compounds are produced from brown algae (*Dilophus okamurae*) and are characterized by a tricyclic structure with consecutive 5-4-5-membered rings. The objective of this study is to establish a method for immobilizing the chemical structure of spatane-type diterpenoid compounds within a polymer, and provide a technique to prevent “rocky shore denudation by sea urchins” in the coastal areas of Japan. Our research began the synthesis of spatane-type diterpene compounds using commercially available 5-norbornene-2-yl acetate as the starting material. First, we constructed the spatane framework by [2+2] photocyclization reaction between cyclopentanone and bicycloheptene. Subsequently, we successfully synthesized the lactone through a Baeyer-Villiger oxidation reaction, followed by hydrolysis to induce the hydroxyester. In the future, we will synthesize the desired non-natural molecule by modifying the ester moiety and converting it to a methylene chain with a terminal alkyne.

**Keywords:** Rocky shore denudation; *Dilophus okamurae*; Spatane-type diterpene; [2+2] Photocyclization reaction



## The modified formula of aggregated human albumin in lyophilization form (MAA-Cold kit) by adding human albumin solution.

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Macro aggregated human albumin (MAA) are labelled with Tc-99m for lung perfusion imaging. However, the MAA kit in-house formula was adsorbed on plastic syringe after labelled by Tc-99m. To solve this problem, a modified formula of the MAA-cold kit was studied by adding surfactant. The human albumin solution (HSA) was used as surfactant of aggregated particles by themselves. The preparation of MAA-cold kit was modified by varying the amount of HSA surfactant added [0.75 mg/vial (0.75AS) and 1.50 mg/vial (1.5AS)]. Radiochemical purity (%RCP), percent of MAA adsorbed on plastic syringe (%adsorb), particles size distribution, and water content were determined for both preparation. The radiochemical purity (%RCP) of 0.75AS and 1.50AS formula were 96.54 and 96.43 respectively. The both formula had similarly the particles size distribution. Moreover, the water determination of 0.75AS and 1.50AS formula were 3.22% and 4.28% respectively. Percent of MAA adsorbed on plastic syringe of original formula, 0.75AS and 1.50AS formula were 38.45, 11.90 and 9.56 respectively. The results reveal that MAA adsorbed 0.75AS and 1.50AS formula decrease form original formula, therefore the both formula can solve this problem.

**Keywords:** Human albumin; Aggregated human albumin; MAA-Cold kit; Surfactant; 99mTc-MAA



## Design, synthesis, and evaluation of *N*<sup>2</sup>-phenylurea-*N*<sup>4</sup>-aminoquinazolines targeting *Plasmodium falciparum* histone lysine methyltransferase

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Histone lysine methyltransferase (HKMT) is an important epigenetic enzyme that regulates the gene expression by histone methylation. HKMT protein represents a high potential target in *Plasmodium falciparum* parasite bound with the quinazoline scaffold as a peptide substrate competitive inhibitor, BIX-01294. Forty-six *N*<sup>2</sup>-anilinophenylurea-*N*<sup>4</sup>-aminoquinazoline derivatives were synthesized to gain a better understanding of the antimalarial SARs. The antimalarial activity against *P. falciparum* strain 3D7 (*Pf*.3D7) was evaluated ranging from 0.012 to 4.20  $\mu$ M which is consistent with the previous work. The cytotoxicity was measured to represent the cytotoxicity in range from 1.1 to >100  $\mu$ M. Ten compounds that exhibit inhibitory activity against the *Pf*.3D7 less than 0.050  $\mu$ M with a selectivity index (SI) over cytotoxicity more than 75-fold were selected for undertaken the solubility and logD at pH 7.4 to profile the ADME properties show the values ranging from 0.001 to 1.2 mg/mL. Compound **36** exhibited the most potent antimalarial activity with an IC<sub>50</sub> value of 0.012  $\mu$ M and 423-fold selectivity index (SI) over HepG2 cytotoxicity. Moreover, this compound possesses solubility and logD at pH 7.4 values of 0.061 mg/mL (0.12 mM) and 4.45, respectively. The molecular docking and molecular dynamics were used to predict the binding mode of our series consistent with the EHMT crystal structure for further *Pf*HKMT inhibitor validation.

**Keywords:** *N*<sup>2</sup>-anilinophenylurea-*N*<sup>4</sup>-aminoquinazoline; *P. falciparum* 3D7 strain; *P. falciparum* Histone Lysine Methyltransferase (*Pf*HKMT); HKMT MD

## Synthesis and structural modification of thymidine derivatives via multicomponent Pd-catalyzed coupling reaction

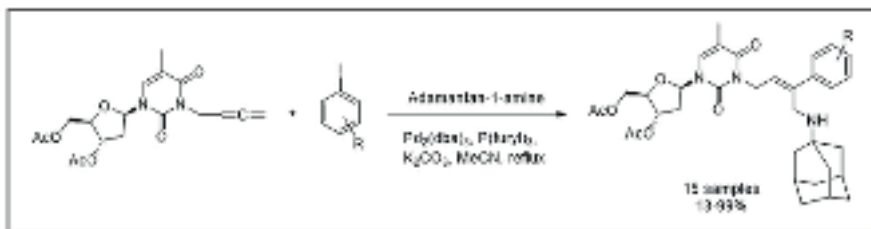
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Thymidine, a naturally occurring nucleoside, can be structurally modified to yield derivatives with promising biological activities and potential medicinal applications. This research investigates the synthesis and structural modification of thymidine derivatives through a multicomponent Pd-catalyzed coupling reaction involving *N*-allenylthymidine, aryl halides with varying substituents, and adamantan-1-amine, the nitrogen nucleophile. This one-pot reaction facilitates the straightforward synthesis of diverse thymidine derivatives. The thymidine synthesized samples will be evaluated for their biological activities, including antidiabetic, anticancer, and anti-Alzheimer properties.

**Keywords:** Thymidine; multicomponent Pd-catalyzed coupling; synthesis; one - pot reaction



**Scheme 1.** The synthesis of Thymidine derivatives.

## Production and quality control of $^{177}\text{Lu}$ -PSMA for prostate cancer treatment

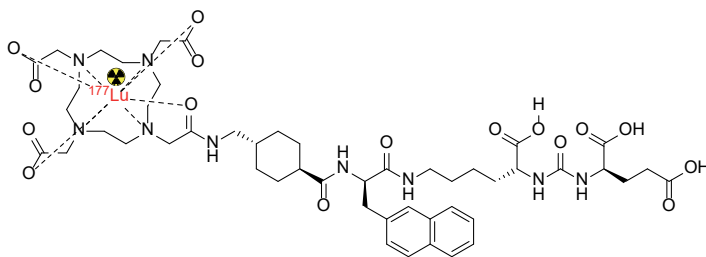
Suppamat Makjan\*, Kanyapat Lumyong, Chotiwid Wiriyachailerd, Sudkanung Phumkem,  
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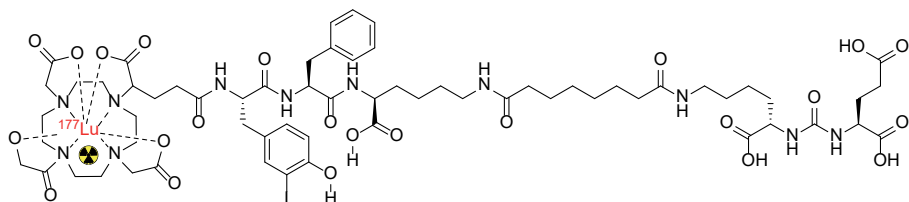
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Prostate Specific Membrane Antigen (PSMA) is an important target in nuclear medicine owing to its overexpression in metastatic castration-resistant prostate cancer.  $^{177}\text{Lu}$ -PSMA is a targeted radionuclide therapy that is currently an alternative for prostate cancer treatment. The aim of this research was to study the preparation and quality control of  $^{177}\text{Lu}$ -PSMA-617 and  $^{177}\text{Lu}$ -PSMA-I&T. The radiochemical purity (RCP) was carried out by high-performance liquid chromatography (HPLC) and thin-layer chromatography (TLC). The results of  $^{177}\text{Lu}$ -PSMA-617 and  $^{177}\text{Lu}$ -PSMA-I&T prepared in this study revealed that the RCP was >95.0% at room temperature, pH 5. The two radiopharmaceuticals remained stable in saline up to 48 h after radiolabeling and bacterial endotoxins complied with the endotoxin limit for parenteral drugs. In conclusion, both  $^{177}\text{Lu}$ -PSMA-617 and  $^{177}\text{Lu}$ -PSMA-I&T are highly stable radiolabeled compounds. The combination of HPLC and TLC provides a reliable quality control method for  $^{177}\text{Lu}$ -PSMA-617 and  $^{177}\text{Lu}$ -PSMA-I&T.

**Keywords:** Prostate specific membrane antigen; Metastatic castration-resistant prostate cancer;  $^{177}\text{Lu}$ -PSMA-617;  $^{177}\text{Lu}$ -PSMA-I&T; Targeted radionuclide therapy



Structure of  $^{177}\text{Lu}$ -PSMA-617



Structure of  $^{177}\text{Lu}$ -PSMA-I&T

## Radiolabeling of DFO-NCS and DFO\*-NCS siderophore chelator with zirconium-89 radiometal

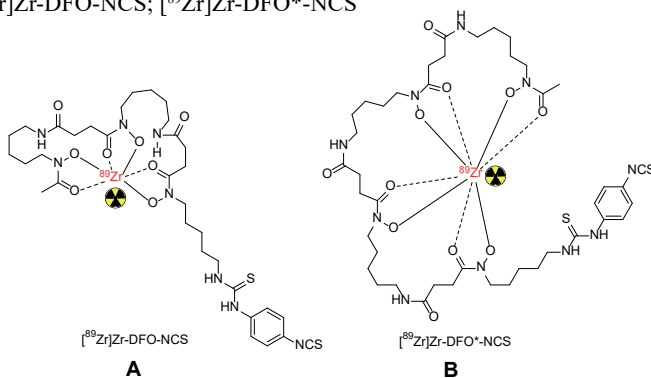
Kanyapat Lumyong<sup>1\*</sup>, Thidarat Kohud<sup>1</sup>, Suppamat Makjan<sup>1</sup>, Thanete Duangta<sup>1</sup>, Boon-Uma Jowanaridhi<sup>1</sup>, Chotiwid Wiriyachailerd<sup>1</sup>, Sudkanung Phumkem<sup>1</sup>, Siriwat Thida<sup>1</sup>, Wiranee Sriwiang<sup>2</sup>, and Piriya Kaepookum<sup>2</sup>

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Over the past few years, zirconium-89 (<sup>89</sup>Zr) labeled with monoclonal antibodies (mAbs) has emerged as a crucial diagnostic tool for a wide range of cancer types, for example, [<sup>89</sup>Zr]Zr-J591 is used to identify PSMA-expressing tumors in patients with prostate cancer, and [<sup>89</sup>Zr]Zr-trastuzumab is used to detect breast cancer. Chelation agents play the important roles for the radiometal <sup>89</sup>Zr to compound and attach to the mAbs. Although desferrioxamine (DFO) is now widely employed in clinical purposes, it has been demonstrated that in many of these cases, the [<sup>89</sup>Zr]Zr-DFO complex has low stability and can release the radiometal <sup>89</sup>Zr, resulting in unnecessary bone uptake. In order to increase the stability of the [<sup>89</sup>Zr]Zr-DFO complex, DFO derivatives have been developed. The aim of this research was to compare the radiolabeling yield of DFO\*-NCS octadentate chelator and DFO-NCS hexadentate chelator labeled with <sup>89</sup>Zr. The results have shown that the [<sup>89</sup>Zr]Zr-DFO-NCS had a high radiochemical yield of up to >99% in 30 minutes at room temperature and pH 7.5. On the contrary, [<sup>89</sup>Zr]Zr-DFO\*-NCS had a high radiochemical yield of up to >99% in 1 hour at the same conditions. But after 90 minutes, the radiochemical purity of [<sup>89</sup>Zr]Zr-DFO-NCS slightly declined to 98%, whereas [<sup>89</sup>Zr]Zr-DFO\*-NCS continued to have a high radiochemical yield of up to >99% throughout the same period. In conclusion, as a comparison, DFO\*-NCS was more stable than DFO-NCS throughout the same duration, although the DFO-NCS chelator connected to the <sup>89</sup>Zr more rapidly. This investigation is intended to be preliminary exploration for the development of Zr-89 radiopharmaceuticals.

**Keywords:** Zirconium-89; Hexadentate-desferrioxamine complex; Octadentate-desferrioxamine complex; [<sup>89</sup>Zr]Zr-DFO-NCS; [<sup>89</sup>Zr]Zr-DFO\*-NCS



**Figure 1.** Structures of [<sup>89</sup>Zr]Zr-DFO-NCS (A) and [<sup>89</sup>Zr]Zr-DFO\*-NCS (B).

## The development of new azobenzene derivatives within three-colors range absorption for biological applications.

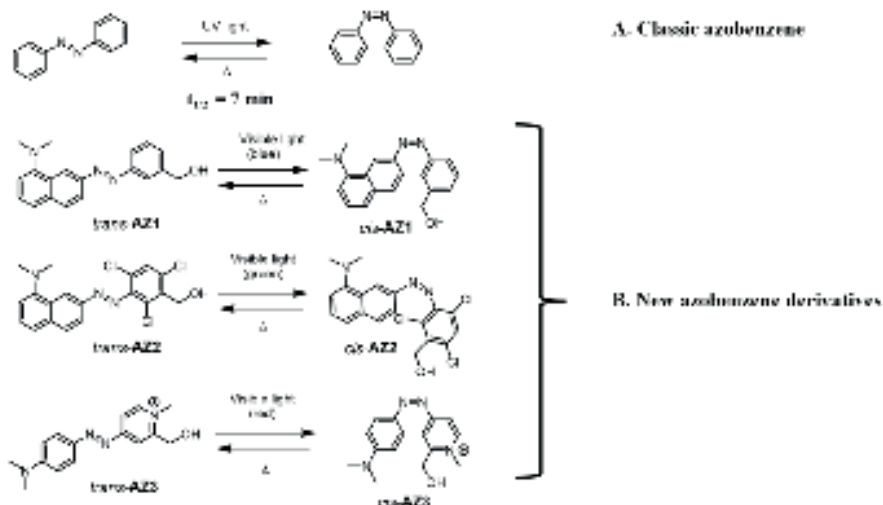
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Azobenzene is one of the molecular photoswitches that can undergo reversible isomerization between cis- and trans-isomers when exposed to light (normally UV-light). In the present, azobenzene that can be activated via visible light is more focusing. With good rational design, we can synthesize azobenzene derivatives (AZ1, AZ2) by using a push-pull substituent on the phenyl group of azobenzene, which includes attaching the donor and acceptor group to the azobenzene moiety. As a result, the energy gap between the ground state and the excited state is small, resulting in more red shift adsorption. These two molecules can be light-activated by blue and green light (visible light) to switch between cis-trans isomers. In this study, we include a new azobenzene (AZ3) that can absorb light in a longer wavelength (550–650 nm) than previous molecules (AZ1 and AZ2). Furthermore, all compounds showed faster thermal relaxation (cis- back to trans-) than classic azobenzene, which will be further useful for biological and medical applications such as 11-cis-retinal in rhodopsin with a half- life of 80 milliseconds (thermal isomerization).

**Keywords:** Azobenzene; Molecular switches; Cis-trans isomerization; Push-pull azobenzene



## Diastereoselective synthesis of spiro[indolizidine-oxindole]-isoxazolidine via tandem Cope oxidation/[3+2]-nitronc cycloaddition

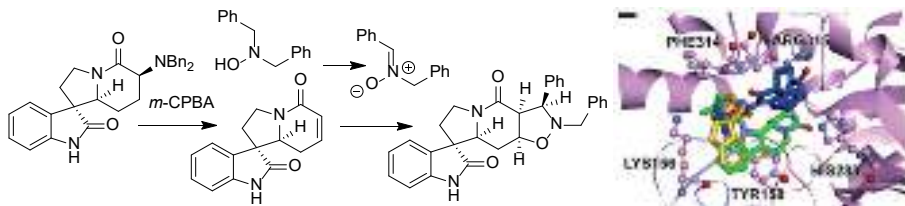
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Indoloquinolizidine and spiro[indolizidine-oxindole] are common core structures of alkaloids found in oriental medicinal plants such as Kratom (*Mitragyna speciosa*) and 'fish hook vine' (*Uncaria rhynchophylla*). In our diastereoselective synthesis of indoloquinolizidine and related alkaloids from L-glutamic acid, the dibenzylamino group on the heterocyclic systems was used for stereocontrol during the reaction sequences. Its subsequent removal generated unsaturated lactam moiety which provided the point for further derivatization. In particular, during Cope elimination of the dibenzylamino group on the spiro[indolizidine-1,3'-oxindole], the by-product dibenzylhydroxylamine was oxidized to give the corresponding nitronc. This reactive intermediate underwent tandem [3+2]-cycloaddition with the resulted unsaturated lactam to give spiro[indolizidine-oxindole]-isoxazolidine as a single diastereomer. In addition, hetero-Michael addition of the unsaturated lactam with methanol and dibenzylhydroxylamine gave additional derivatives. All synthetic indoloquinolizidine and spiro[indolizidine-oxindole] and isoxazolidine compounds were tested for their anti- $\alpha$ -glucosidase activity where an indoloquinolizidine and a spiro[indolizidine-oxindole] were found to be active against  $\alpha$ -glucosidase with  $IC_{50}$  of 18 mM and 13 mM, respectively. Molecular docking experiments of selected compounds were conducted to gain insight into their mode of action and showed that our most active compounds bind to the same site as the positive control, acarbose.

**Keywords:** Indoloquinolizidine; Spiro[indolizidine-oxindole]; Isoxazolidine; Synthesis; Anti- $\alpha$ -glucosidase; Molecular docking



## Synthesis of Dibenzylamino Derivative of (+)-and (-)-Chabamide

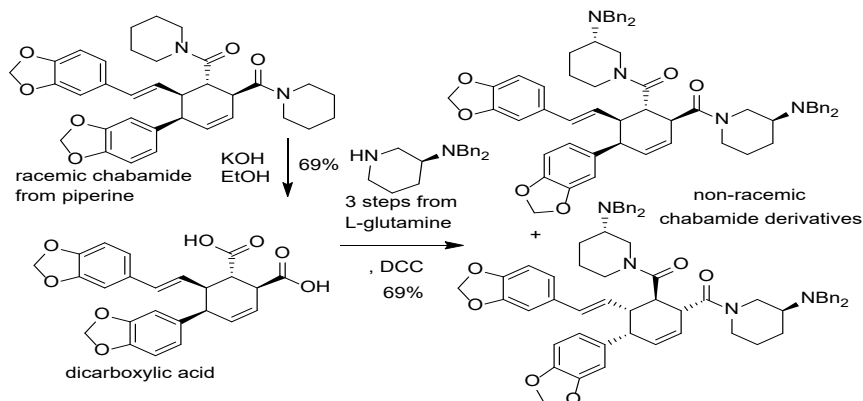
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Chabamide is a cytotoxic dimeric bis-amide alkaloid found in long pepper [Dee-plee, Piper chaba (Thai), Piper longum (Indian, hindi), and Piper retrofractum (Indonesian)] which is used as spice and medicinal herb in Thailand and other countries in South and South East Asia. It is a dimer from a [4+2]-cycloaddition of piperine, the main chemical constituent found in many plants in Piperaceae family. Both chabamide and piperine were reported to display a wide spectrum of biological activities such as anti-oxidant, anti-inflammatory and anti-cancer. In this work we synthesized chabamide from piperine via Diels-Alder reaction using reported procedure. Hydrolysis of chabamide obtained from Diels-Alder reaction of piperine gave the corresponding dicarboxylic acid in racemic form with 69% yield. To obtain enantiomerically active compounds, we applied a resolution method using chiral (S)-3-dibenzylaminopiperidine synthesized in 3-steps from L-glutamine. N-Benzoylation was followed by cyclization in the presence of CDI in basic condition to give (S)-2-dibenzylaminoglutarimide. Reduction of the glutarimide carbonyls with lithium aluminum hydride gave (S)-3-dibenzylaminopiperidine. Coupling of this chiral piperidine with the racemic dicarboxylic acid intermediate in the presence of DCC then gave two diastereomeric products which were separated chromatographically to give dibenzylamino derivatives of both (+)-chabamide and (-)-chabamide as non-racemates with 69 % yield. We also envision that the dibenzylamino group will provide a variation point for further synthesis of other derivatives of piperine dimer.

**Keywords:** Chabamide; Piperine; Synthesis; Diels-Alder; Chiral Resolution



## Asymmetric heptamethine cyanine photosensitizer for near-infrared photodynamic cancer therapy

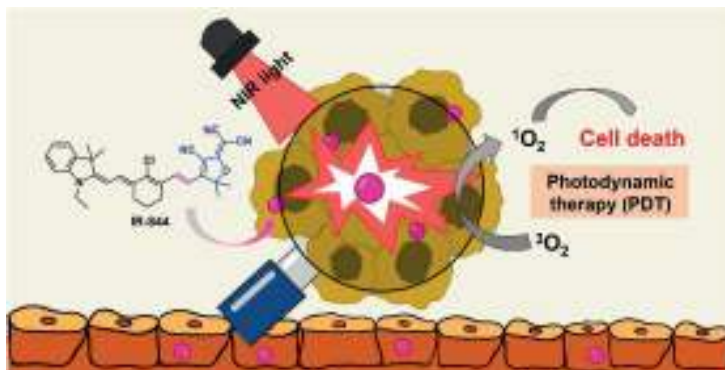
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Photodynamic therapy (PDT) is an attractive cancer therapeutic method, involving a light activation of a photosensitizer at a specific wavelength and subsequent reactive oxygen species (ROS) generation, which leads to cancer cell death. PDT's therapeutic efficacy is determined by both photosensitizers and light. Photosensitizers with near-infrared (NIR) absorption (680–900 nm) are in demand due to their greater penetrating capabilities. A well-known class of NIR fluorophores utilized as PDT photosensitizers are heptamethine cyanine dyes. Herein we described an asymmetric heptamethine cyanine probe (**IR-844**), containing a 2-dicyanomethylene-3-cyano-4,5,5-trimethyl-2,5-dihydrofuran (TCF) acceptor and an indole donor, for NIR fluorescent imaging and NIR photosensitizer that aimed to target cancer cells. A NIR light (850 nm) can activate **IR-844**, which generated a notably high singlet oxygen quantum yield ( $\Phi_{\Delta}=0.71$ ). In addition, **IR-844** exhibited cancer-targeting capacity as specific visualization in hepatocellular carcinoma (HepG2) cells relative to normal liver cells, alpha mouse liver 12 (AML12) cells. Remarkably, at a concentration of 30  $\mu\text{M}$ , **IR-844** showed negligible dark cytotoxicity with a cell survival rate above 80% and significant photocytotoxicity with a cell survival rate below 5%. As a result, **IR-844** could be a great candidate for cancer cell targeting agents for photodynamic treatment.

**Keywords:** photodynamic therapy (PDT); photosensitizers; asymmetric heptamethine cyanine



## Synthesis and $\alpha$ -glucosidase inhibitory activity of bis-coumarin derivatives

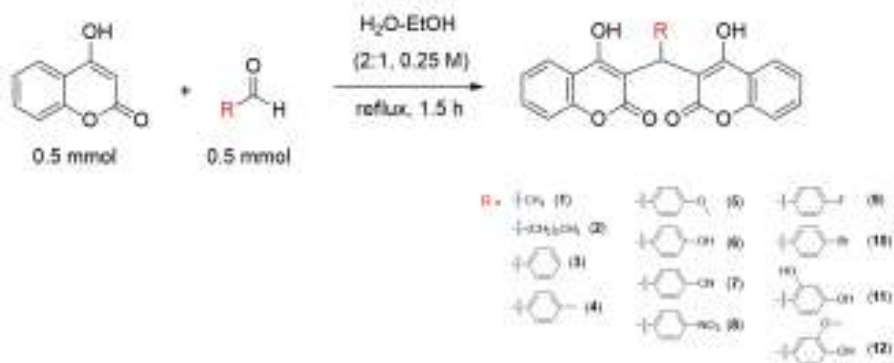
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Diabetes is the most common type of chronic metabolic disease that affects a large number of elderly people.  $\alpha$ -Glucosidase inhibitors, such as acarbose, nojirimycin, voglibose, and miglitol, display an essential role in the treatment of diabetes by inhibiting the digesting  $\alpha$ -glucosidase. However, new and more efficient compounds are still necessary as an alternative approach for treating this enzyme. In the present study, bis-coumarin derivatives were synthesized from the condensation of 4-hydroxycoumarin with various aldehydes under environmentally friendly conditions. Under optimized conditions, aromatic aldehydes could be transformed into the corresponding products in high to excellent yields, whereas the products produced from aliphatic aldehydes were obtained in moderate yields. All synthesized bis-coumarin derivatives were further evaluated for their  $\alpha$ -glucosidase inhibitory activity. The results found that compound **8** was the most potent inhibitor, with an  $IC_{50}$  value of  $7.03 \pm 0.57 \mu M$ . This compound could be developed into a new potential antidiabetic drug.

**Keywords:** 4-Hydroxycoumarin; Bis-coumarin derivatives;  $\alpha$ -Glucosidase inhibitory activity; Diabetes



# Polymer Chemistry and Bio-based materials (PC)

## Oral Presentation

## A study of pre-vulcanization time affected on the nano-porous structure preservation in Silica aerogel/Natural rubber composite

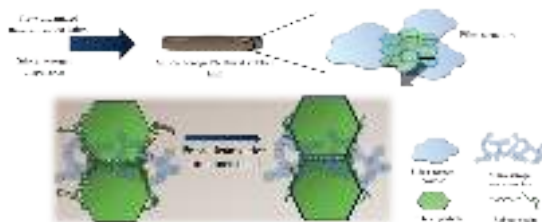
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Silica aerogel (SA)/polymer is the mechanical property enhancement from a fragile issue as a result of the characteristic extremely high porosity, surface areas, and low density of the SA porous structure to utilize properly in super thermal insulation, and hydrophobic surface materials. However, the pores of SA filled by the moving chains freely of the mixing polymer in solution and melting stage reduce porosity and increase density leading to malfunction of SA in the composite. To overcome this problem, the limitation of the free-moving polymer chains becomes the key. The pre-vulcanized natural rubber latex (PVNRL) is the promising solution, since the chain motion is confined in a naturally dense chain pack as particles, and the pre-vulcanization generates crosslink rubber chains inside rubber particles (RPs), in the liquid stage. This study aims to preserve the nano-porous structure of SA by carrying out PVNRL at different times at room temperature prior to the mixing with SA dispersion and then post-vulcanization. The crosslink density of the casted film with and without SA depended on the pre-vulcanization periods, relating to the remaining nano-porous structure of SA in the composite. The film formation study revealed that the withstanding deformation of RPs by the vulcanization process hindered the diffusion of rubber chains between particles in the film formation process involved in the reduction of the free-moving rubber chains, resulting in the existence of nano-porous structure of SA in the composite.

**Keywords:** Silica aerogel; Natural rubber latex; Pre-vulcanization; composites; preserved pores



## Production and characterization of cellulose powders from brewery' spent grain

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Brewery Spent Grain (BSG) is a byproduct of the brewing industry, primarily consisting of cellulose, hemicellulose, lignin, and protein, sourced from malted barley. Although often discarded as waste, BSG holds untapped potential as animal feed and contains valuable cellulose, applicable across various industries like food, pharmaceuticals and cosmetics. This study aims to optimize extraction process to produce cellulose from BSG. The Box-Behnken Design was applied to optimize the cellulose yield with three critical variables as alkaline concentration (1-2% w/v NaOH), temperature (90-100 °C) and extracting time (1-3 h). The extracted cellulose samples were then bleached with H<sub>2</sub>O<sub>2</sub> g at 70 °C for 40 minutes, followed by washing and drying to obtain pure cellulose powders. Result found that the cellulose yield was 10.89 with 60.32 % crystallinity under 1.69 %w/v alkaline concentration, at 100 °C and 1h extracting time. The assessment of the structural features and bonds, with a particular emphasis on eliminating undesirable components of lignin and hemicellulose via Fourier Transform Infrared (FT-IR) analysis. Revealed that a strong sharp lignin stretching vibration positioned at 1633 cm<sup>-1</sup> (C=stretching) of lignin was reduced by 34.70 % compared with the untreated BSG. 11% reduction of lignin (Aromatic skeletal vibration) and hemicellulose (COO<sup>-</sup>stretching) were also observed. These purified cellulose powders was further analyzed using X-ray Diffraction (XRD) to determine crystallinity and obtained 58.59% cellulose purity while the cellulose powder standard gained 65.85% of crystallinity. This research contributes to the value-added of BSG and its potential integration into the wider food industry, opening new possibilities for its use beyond traditional waste disposal.

**Keywords:** Brewer's spent grain; Cellulose powders; Alkaline treatment; Crystallinity; Box-Behnken design

## Development and characterization of amidated pectin-PVA hydrogels for enhanced drug delivery and antimicrobial properties

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Hydrogel-based drug delivery systems have gained significant attention due to their unique properties and applications. In this study, hydrogels were prepared from polyvinyl alcohol (PVA), pectin-PVA, and amidated pectin (AMDP)-PVA for potential drug delivery and antimicrobial applications. Pectin was extracted from pomelo peel through acid extraction, and amidation was carried out using ethanolamine. The hydrogels were created using a freeze-thaw (FT) cycle, with varying freezing times of 24, 48, and 72 hours. The FT cycle duration had a significant impact on the hydrogels' properties. The swelling behavior of the hydrogel at different FT cycles and types was thoroughly investigated. Furthermore, loading and release studies were conducted by using Chlorhexidine as a model drug, revealing that AMDP-PVA hydrogels exhibited superior loading and release profiles compared to PVA and pectin-PVA hydrogels. These findings emphasize the potential of amidated pectin as a valuable component for controlled drug delivery systems. To assess their suitability for biomedical applications, the antimicrobial properties of these hydrogels were evaluated against *E. coli*, *S. aureus*, and *C. albicans*. The results indicated that the hydrogels, especially those prepared with amidated pectin, possess remarkable antimicrobial activity. This study emphasized the importance of modifying hydrogel characteristics by selecting appropriate constituents and processing conditions for drug delivery applications and the potential of amidated pectin-PVA hydrogels in the field of pharmaceutical and medical research.

**Keywords:** Hydrogel-based drug delivery; Pectin; Controlled drug delivery systems; Antibacterial hydrogel properties; Amidated pectin

## Comparison properties of hybrid carbon-based nanocomposites between engineering-thermoplastic Acrylonitrile-Butadiene-Styrene and commodity-thermoplastic polypropylene for electrical and thermal application

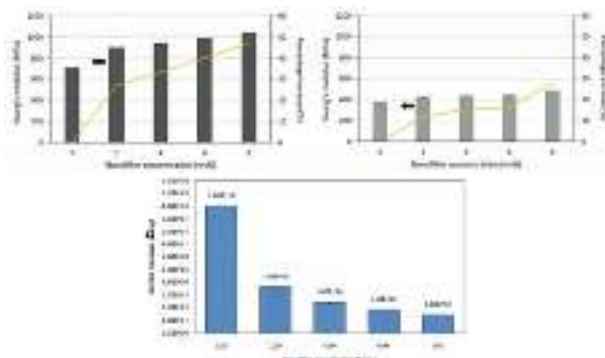
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Electronic based industry has become one of the highest growth industries in the world, which electrostatic discharge (ESD) could be a serious problem associated for a specific application. Due to the low price and availability of pristine graphite in large quantities, graphene nanoplatelets (GNPs) is considered an ideal choice as conductive fillers to replace carbon nanotube (CNTs) or mix them to produce hybrid conductive fillers. Accordingly, this report was focused on using suitable surface oxygen gas modified nanofiller hybrid as a filler in Acrylonitrile-Butadiene-Styrene (ABS) and polypropylene (PP) was used to represent an amorphous and a semi-crystalline polymer respectively, which these composites could be used mainly for electronic packaging. Nanocomposites were successfully prepared using a twin-screw extruder, which ABS/Nanofiller or PP/Nanofiller masterbatch was mixed with neat polymer to the desired concentrations of Nanofillers (2, 4, 6, and 8 wt%). Based on the static dissipative range of surface electrical resistivity, the suitable ratio of nanofiller was found to be 80:20 of  $O_2$ -CNTs: $O_2$ -GNPs, and the critical amount of nanofiller loading on mechanical properties was found to be 2.0 wt%. ABS reinforced with 2.0 wt% of Nanofiller resulted in an increase of Young's modulus 27% and of tensile strength 24%, with a reduction of elongation at break 75%. PP reinforced with 2.0 wt% of Nanofiller resulted in an increase of Young's modulus 12% and of tensile strength 6%, with a reduction of elongation at break 71%. The surface resistivity and Thermal conductivity of nanocomposites was sharply decreased from  $10^{16}$  to  $10^6$  ohm/square and increased from 0.208 to 0.349 W/m.K respectively which could be designated as a static dissipative material.

**Keywords:** Graphene nanoplatelet (GNP); Carbon nanotube (CNTs); Acrylonitrile-Butadiene-Styrene (ABS); Polypropylene (PP); Electronic packaging



**Figure1.** Young's modulus and the percentage increase of ABS (A) and PP (B) reinforced with  $O_2$ -modified nanofiller and Surface resistance (C) in various filler concentrations.

## Apatite growth of bioactive glass containing elephant dung cellulose

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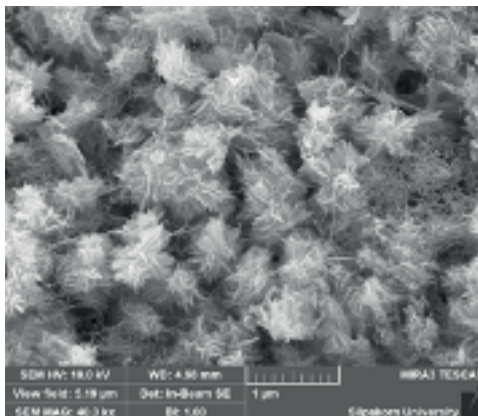
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Bioactive glass (BG) is an effective scaffold for the growth of hydroxyapatite when in contact with body fluid. To increase its mechanical strength, various biopolymers like gelatin, cellulose and cellulose derivatives, were added into the glass matrix. In this research, cellulose, extracted from elephant dung, was being used to prepare hydrogel via DMAc/LiCl solvent system. Cellulose gel (CH\_ED) mixed with bioactive glass solution (BG sol) using the volume ratio of 3.75:1, was subsequently poured into a petri dish and left still for 1 week to obtain BG/CH\_ED scaffold. The bio-mineralization was performed by keeping BG/CH\_ED scaffolds in simulated body fluids (SBF) for 8, 16 and 24 days at 37 °C. The SBF solution was then collected and replaced with the freshly prepared SBF solution every 2 days. The collected solutions were analyzed for  $\text{Ca}^{2+}$  and  $\text{PO}_4^{3-}$  concentrations using atomic absorption spectroscopy (AAS) and UV-VIS spectroscopy. BG/CH after bio-mineralization was characterized by FTIR, SEM-EDX and XRD. The results confirmed the existence of the formed hydroxyapatite on the surface of the cellulose-bioactive glass surface as the SEM image shown in Figure 1.

**Keywords:** Bioactive glass; Cellulose hydrogel; Elephant dung



**Figure 1.** SEM image of apatite growth (flower-like crystals) on the surface of BG/CH\_ED scaffold after being mineralized in SBF for 24 days

# Polymer Chemistry and Bio-Based Materials (PC)

## Poster Presentation

# Tumor microenvironment modulation using nano-formulated drug for cancer immunotherapy

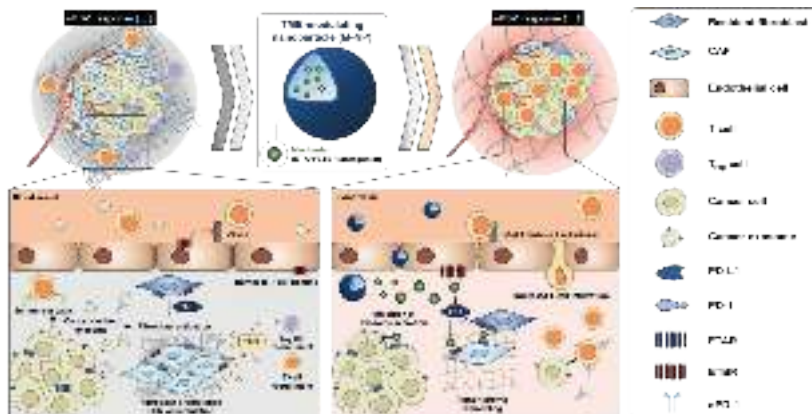
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Immune checkpoint therapy (ICT), which primes cytotoxic T cells, provides clinical benefits as a promising option to conventional cancer therapies. However, its clinical outcome is poor for treating an immune-excluded tumor, owing to stiff tumor tissue impeding the penetration of immune cells. Here, we report that macitentan, a dual endothelin receptor antagonist approved by the FDA to treat pulmonary arterial hypertension, can be repurposed to modulate the desmoplastic tumor microenvironment (TME). In the 4T1 orthotopic tumor model, the polymeric nanoparticles bearing macitentan (M-NPs) prevent fibrotic progression by regulating the function of cancer-associated fibroblasts, attenuating the biogenesis of cancer cell-derived exosomes, and modulating the T cell subsets and distribution in TME. These results demonstrate that the M-NPs effectively reorganize the immunosuppressive TME by targeting the endothelin-1 axis and consequently exhibit synergistic antitumor effects in combination with ICT.

**Keywords:** Nanomedicine; Cancer immunotherapy; Tumor microenvironment



**Figure1.** Schematic illustration of macitentan-loaded nanoparticle for cancer immunotherapy.

# Exploring electrohydrodynamically printed organic semiconductors for high-performance solution-processed organic field-effect transistors and integrated logic devices

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Solution-processable organic semiconductors (OSCs) have emerged as captivating contenders for advancing printed electronics manufacturing. In this study, we present an exploration into the electrohydrodynamic (EHD) jet printing of p- and n-type OSCs: 6,13-bis((triisopropylsilyl)ethynyl)pentacene (TIPS-PEN) and 6,13-bis((triisopropylsilyl)ethynyl)-5,7,12,14-tetraazapentacene (TIPS-TAP). We prepared three types of such solutions: one with TIPS-PEN, another with mixed OSCs of TIPS-PEN and TIPS-TAP in a 1:1 ratio, and the third with TIPS-TAP. These OSCs are employed both individually and in mixed p-n layers to craft solution-processed p-, n-, and ambipolar-type organic field-effect transistors (OFETs). The devices based on the printed single p- and n-type OSC channel layers showed average charge mobility values of 0.16 and 0.28  $\text{cm}^2\text{V}^{-1}\text{s}^{-1}$ . This approach capitalizes on the akin molecular structures of TIPS-PEN and TIPS-TAP, resulting in a homogeneous solid solution that exhibits ambipolar transport characteristics in OFETs. The amalgamation of single- and mixed-OSC layers facilitates the creation of diverse charge-transport devices, spanning from basic units to integrated systems encompassing NOT, NAND, NOR, and multivalued logic circuits.

**Keywords:** organic field-effect transistors; electrohydrodynamic jet printing; organic semiconductors; integrated devices; printed electronics

## Release characteristic of Curcumin (Zingiberaceae) from sodium alginate and polyvinyl alcohol-based hydrogel composite: Antioxidant properties

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Pongpat Sukhavattanukul <sup>2</sup>, and Sarute Ummartyotin <sup>2\*</sup>

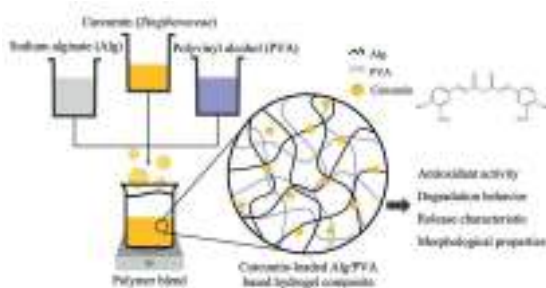
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The local herbal in Thailand such as Curcumin (Zingiberaceae) was considered as one of the most naturally occurring resources. It was investigated the phytochemical and antioxidant activity of curcumin. In this work, Sodium alginate and polyvinyl alcohol-based hydrogel composite was loaded with Curcumin at different concentration and was investigated the functional group by FTIR. the thermal behavior and the crystallinity of composite were observed using DSC and XRD, respectively. (figure 1) The results confirm that no significant change of functional group, crystallinity and thermal behavior of sodium alginate and polyvinyl alcohol-based hydrogel composite were observed because of less amount of curcumin powder. The porous network was created due to freeze thaw technique. At the initial stage, the swelling characteristic was occurred. Water molecule was penetrated into porous network. The role of curcumin particle significantly offered antioxidant activity as reported by DPPH assay, ABTS assay and FRAP assay. The release characteristic curves of hydrogel composite presented the burst release at the initial stage. It was rapidly released within 500 min. After that, the trend of release behavior was stable. Therefore, as prepared curcumin loaded into sodium alginate and poly vinyl alcohol-based hydrogel composite has the potential for applications such as drug delivery system, nutraceutical food as well as horticulture.

**Keywords:** Antioxidant activities; Curcumin; Hydrogel; Phytochemical



**Figure 1.** Graphical abstract of Sodium Alginate and Polyvinyl Alcohol-Based Hydrogel Composite loaded Curcumin (Zingiberaceae)

## Preparation of hyaluronic acid-PVA-cyclodextrin biocompatible film

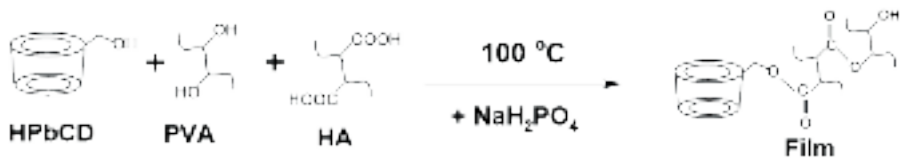
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In this research, the biocompatible films contained hyaluronic acid (HA), polyvinyl alcohol (PVA) and 2-hydroxypropyl- $\beta$ -cyclodextrin (HPbCD) were prepared. The  $\text{NaH}_2\text{PO}_4$  at different concentrations of 10%, 20%, 30% mol were used as catalyst for cross-linking process. The solution of HA-PVA-HPbCD was more continuous heated at 100 °C with different times of 10, 20 and 30 min before film forming. The water solubility of the films was then studied. It was found that increasing the concentration of  $\text{NaH}_2\text{PO}_4$  and the reaction time caused the decreasing of water solubility of the films due to the cross-linking was occurred. The FT-IR showed the signal at 1732  $\text{cm}^{-1}$  corresponding to the C=O bond of the ester group from cross-linking process. TGA at 245-280°C found films with 30% catalyst had the least decomposition of HA and DSC found endothermic properties of HA at 155°C but it was not found in films. It can be confirmed that  $\text{NaH}_2\text{PO}_4$  has an effect on the interaction of the components in the film. The SEM technique shows the porous nature of all types of films. It can prepare HA-PVA-HPbCD film containing vitamin E and reduce the water solubility of the film. These results can be applied as a carrier for active ingredients in cosmetics or drugs.

**Keywords:** hydrogel film, hyaluronic acid, poly (vinyl alcohol), 2-hydroxypropyl-beta-cyclodextrin, vitamin E



## Hyaluronic acid conjugated amino-beta-cyclodextrin schiff base hydrogels for drug control releasing

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Hydrogel with schiff base linkages or imine bonds are potential candidates to improve accuracy and efficiency of drug delivery due to rapidly proceeding under mild conditions without catalysts. In this research, Schiff base hydrogel based on hyaluronic acid dialdehyde (HAD) conjugated amino-beta-cyclodextrin (EDA-CD) was prepared by various component ratios. HAD was synthesized through periodate oxidation of hyaluronic acid (HA, 80-100 kDa). EDA-CD was prepared by two following steps. The first step, hydroxyl group of CD was activated by tosyl group (OTs), then ethylenediamine was used to substitute the OTs groups. Schiff base linkage occurs the reaction between aldehyde group of HAD and amino group of EDA-CD or CS. HAD and EDA-CD could form Schiff base linkages *in situ* at room temperature. Chitosan (CS, 70 kDa, 90 %DD) was used to stabilize hydrogel system by forming the schiff base linkages with the remaining aldehyde groups. These schiff base linkages can be hydrolyzed in acid condition. All chemical structures were characterized by  $^1\text{H}$  NMR and FTIR. The hydrogel network was observed by SEM.

**Keywords:** Schiff base; Hyaluronic acid; Cyclodextrin; Chitosan

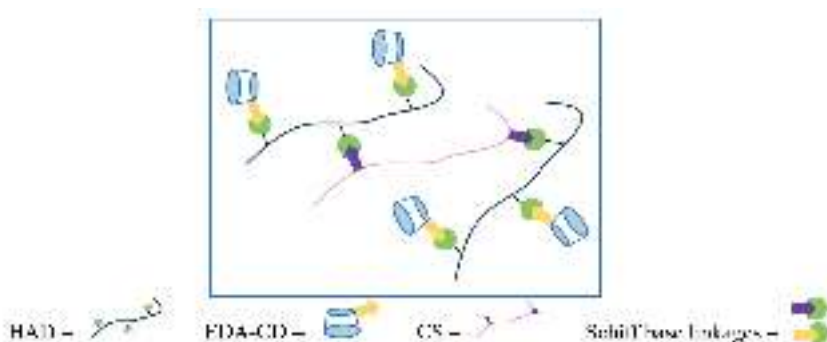


Figure 1. HAD-EDACD-CS hydrogels.

# Preparation and properties of poly(vinyl chloride) composites recycled from used peritoneal dialysis solution containers and reinforced with silane-treated pineapple leaf fibers

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In addressing environmental concerns about plastic waste accumulation, recycling is acknowledged as a valuable approach. This research study aimed to develop PVC composites from used peritoneal dialysis solution containers (PDCs), made of medical-grade PVC plastic, by incorporating them into PVC composites reinforced with the silane treated pineapple leaf fibers (APS-PALF). The research sought to investigate the impact of varying the amount of APS-PALF (10-40 phr) on the mechanical and thermal properties of the resulting composites. The PALF treatment consisted of alkaline treatment with NaOH solution, followed by silane treatment with (3-aminopropyl) triethoxysilane (APS). The investigation the amounts of neat PVC and PDCs were fixed at 50 and 50 phr, respectively. The composite sheets were fabricated by an internal mixer and two-roll mill into thin sheets before subjected to compression molding. The untreated and treated PALFs and the composite sheets were characterized by ATR-FTIR and SEM techniques. The mechanical properties of the composite sheets including tensile, flexural and impact properties were investigated. The thermal property of the composite sheets was assessed by a TGA technique. In terms of mechanical strength, the composite sheet with 40 phr APS-PALF excelled in both tensile and flexural strengths while the composite sheet with 10 phr APS-PALF showed the highest impact strength. FTIR confirm the success of all fiber treatments and the interfacial interaction between phases. SEM reveals favorable compatibility in APS composites, phase separation in UT and Na composites, and TGA highlights component degradation in all variations.

**Keywords:** Peritoneal dialysis solution containers; Plastic recycling; Pineapple leaf fibers; Fiber-reinforced composites; Silane treatment



## Dyeing silk fabric with natural dyes from *Garcinia Dulcis* (Roxb.) Kurz bark

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Natural dyes extracted from *Garcinia Dulcis* Kurz bark were applied to a silk fabric by an exhaustion dyeing process. Silk fabrics were conducted with and without metallic salt mordants, using three types of mordants: aluminum potassium sulfate, copper sulfate and ferrous sulfate. - Three different mordanting methods were employed: pre-mordanting, meta-mordanting and post-mordanting. The dyed fabric was investigated in terms of the CIELAB (L\*, a\* and b\*) and K/S values. The colorfastness to washing and colorfastness to light of the *Garcinia Dulcis* Kurz bark dyes were investigated. It was found that the mordants had a significant effect on the color of silk fabrics. Silk fabrics dyed with *Garcinia Dulcis* Kurz bark extraction showed a pale-yellow shade. Silk fabric mordanted with aluminum potassium sulfate and copper sulfate appeared more yellow, while that mordanted with ferrous sulfate turned darker brown. The results showed that meta-mordanting was the optimal dyeing conditions to yield dark yellow on dyed fabric with K/S change from 4.32 to 15.95., the colorfastness to washing was better; from level of (1-2) to (4-5). However, the colorfastness to light was lower; from level of (4-5) to (3-4). It can be concluded that *Garcinia Dulcis* Kurz bark extraction can be used for silk dyeing to obtain high color intensity as well as good colorfastness properties for special event cloth.

**Keywords:** Dyeing; Silk fabric; Natural dye; *Garcinia Dulcis* (Roxb.) Kurz; Colorastness

## Natural and synthetic fibers on mechanical properties and degradation of fiber cements

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Nowadays fiber cement (FC) is drawn much attention for construction applications such as ceiling, wall, roof, and floor due to its functionalized and modernized designs. Their manufacturing processes are also improved for better mechanical properties and lifetime. Fiber cement is composed of portland cement, fine sand, and water in a majority with adding of filler including minerals (asbestos), natural fibers and synthetic fibers, etc. Due to the hazard of asbestos in fiber cement to respiration system during prolong period of usage, several alternative fibers have been replaced. Therefore, the objective of this study was to compare the properties of fiber cement from natural waste plant fibers (banana; B and water hyacinth; WHC) and synthetic fiber (glass reinforced concrete; GRC) fabricated by mimic hatschek process. The type of fiber, method of fiber treatment and degradation of fiber cement were studied in terms of microstructure, flexural strength, flexural strain, and degradation, respectively. The results demonstrated that all fiber cement samples showed flexural strength in a range of 8-10 MPa in which pass the requirement of the Thai standard (TIS no. 1472-2561). FCs (B-NaOH, WHC-NaOH, GRC) possess deformation behavior observed by non-linear S-E curve. The degradation of FC-WHC-NaOH and GRC was found to be 10 and 12 percent, respectively. It could be concluded that the fiber cements with NaOH treated-natural waste plant fibers demonstrated comparable properties to those of synthetic glass fiber. Thus, such natural waste plant fibers have a potential to act as the filler in fiber cement application.

**Keywords:** Fiber cement; Water hyacinth fiber; Banana fiber



## Bacterial cellulose from kombucha for oil adsorption

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Kombucha is well-known as a beverage consumed worldwide. The fermentation process of Kombucha produces symbiotic culture of bacteria and yeast (SCOBY) as a byproduct, which is currently considered of little value. The SCOBY possesses highly porous structure consist of bacterial cellulose fiber, which is a non-toxic and biodegradable biopolymer. High porosity of SCOBY have potentials as adsorbent materials. In this work, initially hydrophilic SCOBY was modified with trimethylchlorosilane (TMCS) to increase hydrophobicity for oil absorption application. The SCOBY aerogel was obtained from freeze-drying of SCOBY hydrogel and was treated with TMSC via chemical vapor deposition (CVD) to yield oleophilic aerogel in high yield. Hence, this research focuses on characterizing the properties of SCOBY that have been modified by TMCS. The resulting bacterial cellulose aerogels exhibit hydrophobicity, making it highly suitable for oil adsorption applications. This work presents a method to prepare green aerogels and provides a feasible strategy for solving oil spill problem.

**Keywords:** Kombucha; SCOBY; Bacterial cellulose; Aerogel; Oil adsorption

## Simulated gastrointestinal digestion of microencapsulated *Lactobacillus salivarius* culture in biopolymer

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*Lactobacillus salivarius* assumes a crucial role as a probiotic organism, significantly contributing to bacteriocin production and both innate and acquired immunity. This study evaluated the survival of encapsulated *L. salivarius* TISTR 1112 under simulated gastrointestinal conditions using a 5-L batch fermentation in de Man-Rogosa-Sharpe broth over 7 days of cultivation time. The microencapsulation technique was applied to entrap the freeze-dried cell with the single biopolymer alginate (A) and alginate mixed octenyl succinic anhydride modified starch (A+O) and the dual biopolymer alginate coated with chitosan (A+C) and alginate mixed octenyl succinic anhydride modified starch coated with chitosan (A+O+C). The results showed that in all treatments, encapsulation efficiency reached 95%. To simulate the replete and fasting states of humans, only the pH was altered in each section of the intestinal tract. The pH of the simulated gastrointestinal fluid (SGIF) was regulated throughout the procedure. The results found that both the release and viability of probiotics in the SGIF were pH-dependent; at the end, the pH of the caecum showed that a biopolymer coated with chitosan provided superior protection for probiotics when exposed to gastrointestinal fluid, A+O+C, A+C, A+O, and A, respectively. The findings indicate that all heteropolysaccharides have the potential to serve as a promising material for microencapsulation in functional foods.

**Keywords:** Encapsulation; Probiotics; *Lactobacillus salivarius*; Biopolymer; Simulated gastrointestinal fluid

## Chitosan coated on magnetic nanoparticles for a simple *Escherichia coli* detection

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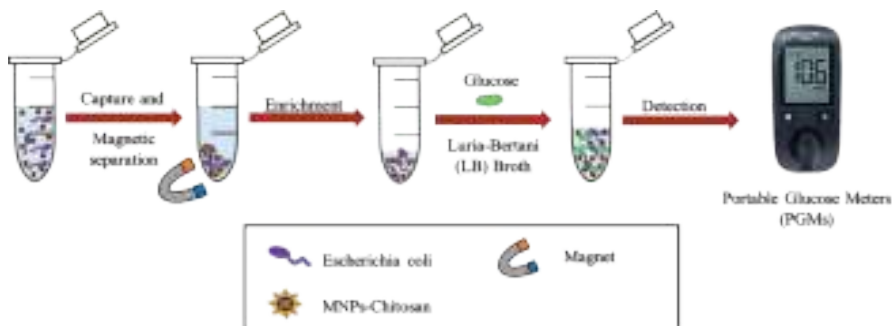
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The rapid and high-efficiency measurement of *Escherichia coli* can help prevent diseases caused by food. In this research, a simple method for *Escherichia coli* detection was designed using an integrated approach under chitosan coated magnetic nanoparticles and portable glucose meter (PGMs). Magnetic nanoparticles (MNPs) were synthesized using the co-precipitation of  $\text{Fe}^{2+}$  and  $\text{Fe}^{3+}$  in the presence of  $\text{NH}_3\text{OH}$ . To increase particle stability, citric acid was added after MNPs formation. The MNPs are subsequently coated with chitosan polymer. ATR-FTIR spectrum confirmed the effectiveness of chitosan-coated MNPs. Zeta-potential analysis also confirmed this success in which the surface charge of MNPs changes from a negative to a positive upon chitosan coating. Chitosan coated magnetic nanoparticles (MNPs-CH) demonstrated strong capture capability for *Escherichia coli* (*E. coli*) through electrostatic adsorption between the positively charged MNPs-CH and the negatively charged bacteria. MNPs-CH demonstrated a 98.22% efficiency in capturing *E. coli*. Subsequently, the captured *E. coli* was detected using PGMs in the presence of LB broth and glucose. A decrease in glucose concentration was observed upon the introduction of *E. coli*. By measuring the glucose consumption by *E. coli*, this method can achieve simple and cost-effective detection of *E. coli* in food samples, water, and other samples.

**Keywords:** Magnetic nanoparticles; Chitosan; *Escherichia coli* detection; Portable glucose meter (PGMs)



## Preparation of carboxymethylcellulose (CMC)-polyethylene glycol (PEG) hydrogel for the growth of plants

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Hydrogels are three-dimensional polymeric networks prepared from chemical crosslinks. Their outstanding properties are the capability of swelling and retaining water within their structure without dissolving in water. These properties are interesting therefore the hydrogel was applied to mix within cultivated soil for moisture control and plant growth. This research was to study the preparation of hydrogel film from carboxymethylcellulose (CMC)-polyethylene glycol (PEG) using citric acid as a non-toxic crosslinking agent. The hydrogel films were measured by solid-state using an FTIR spectrophotometer to confirm the formation of ester crosslinks between CMC and PEG. The intensity of the carbonyl peak of the ester crosslink was found to increase, as the amount of PEG was increased. Corresponding with determining the carboxyl content of hydrogel film using acid-base titration and evaluating of swelling behavior were augmented. Accordingly, the maximum content of PEG (20% w/w in total polymer) was chosen to mix within cultivated soil. The results showed the weight ratio of 1:1 of hydrogel film and cultivated soil was suitable for growing plants because of the highest stem and root for 40 days.

**Keywords:** Hydrogel; Carboxymethylcellulose (CMC); Polyethylene glycol (PEG); Plant grown

## Preparation of HPMC/chitosan blend films incorporated with chrysin and wintergreen essential oil for strawberry preservation

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In Bangkok, the total generation of food waste each day has doubled from 2,860 metric tons in 2003 to 5,669 metric tons in 2018. In addition, approximately one-third of agricultural products, including vegetables and fruits, are perishable before consumption because their shelf lives are limited. To address these issues, traditional techniques such as freeze-drying, irradiation, refrigeration, controlled atmosphere storage, and coating protection surfaces are commonly utilized for reducing food waste and prolonging the freshness of food spoilage. Herein, to enhance the freshness of strawberries, different weight ratios of hydroxypropyl methylcellulose (HPMC)/chitosan-based edible films were prepared at 4:1, 3:2, 2.5:2.5, 2:3, and 1:4. Firstly, chitosan was dissolved in an aqueous solution of citric acid (4% w/v) at 50°C for 3 hours. HPMC was blended into a chitosan solution at 80°C. Afterwards, chrysin (0.1% w/w) and wintergreen essential oil (1% v/v) as antioxidant and antimicrobial agents and glycerol (20% w/w) as a plasticizer were incorporated into HPMC/chitosan solutions at room temperature. Edible blending films were characterized by their mechanical and structural properties, and barrier performance. Moisture absorption of 4HM-1CS, 3HM-2CS, 2.5HM-2.5CS, 2HM-3CS, and 1HM-4CS were 13.7%, 16.9%, 17.8%, 19.5%, and 22.8% respectively. Furthermore, the edible films were wrapped with strawberries and stored at ambient temperature and their physicochemical properties (appearance changes, and weight loss) were evaluated. Overall, chrysin and wintergreen essential oil incorporated into HPMC/chitosan composite films could be used to extend the shelf life of strawberries for 7 days at room temperature.

**Keywords:** HPMC; Chitosan; Chrysin; Edible films; Wintergreen essential oil

## Mechanical properties of hybrid fibers paper sheet from pineapple leaf fiber and banana fiber for packaging

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Agricultural waste of pineapple leaves and leaf sheaves of banana trees, which are eco-friendly, are abundantly found in Thailand. The natural fibers also have good mechanical properties. The pineapple leaf fibers (PLF) have high stiffness while the elongation of banana fibers (BF) is good. This study aimed to investigate the mechanical properties of hybrid fibers paper sheet from PLF and BF for packaging. The PLF and BF were treated with 5 wt% KOH alkali solutions at 80 °C for 5 h and subsequently 2 wt% H<sub>2</sub>O<sub>2</sub> solutions at 80 °C for 3 h to remove lignin and the other contaminants. The PLF and BF were then beaten to mix in the following PLF:BF ratios of 80:20, 60:40, 40:60, and 20:80, respectively. The findings indicated that increasing BF contents exhibited the continuous increase in tensile, tear, and burst indices in the hybrid fibers sheet. The SEM analysis revealed that PLF and BF occurred a partial adhesion. As a result, the optimal condition produced for the hybrid fibers paper sheet for packing comprising PLF:BF with a 20:80 ratio is the highest of all mechanical properties.

**Keywords:** Pineapple leaf fibers; Banana fibers; Mechanical properties; Hybrid fibers paper sheet; Eco-friendly packaging

## Preparation of microcrystalline cellulose from corn cob and synthesis of microcrystalline cellulose-derived polyol for polyurethane foam

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Corn cob is agricultural waste that is available in large quantities and can be used as renewable materials. In this study, corn cob was converted into microcrystalline cellulose (MCC) by chemical treatments. The corn cob was treated with an alkaline solution, followed by sodium chlorite ( $\text{NaClO}_2$ ) solution as a bleaching agent, and then treated with hydrogen peroxide to obtain MCC. The morphology, crystallinity, and thermal stability of the prepared MCC were analyzed. The results revealed that the MCC showed a porous fibrous structure with an average diameter size and porous size of 13.73 and 1.08  $\mu\text{m}$ , respectively. The crystallinity of the corn cob-derived MCC investigated by X-ray diffraction was 34.39 %. Moreover, it was found that the thermal stability of the MCC was higher than the untreated corn cob. Furthermore, the polyol was synthesized from the corn cob-derived MCC by reacting with glycidol in water. The obtained polyol was characterized by FT-IR,  $^1\text{H}$ -NMR, and gel permeation chromatography (GPC). The FT-IR and  $^1\text{H}$ -NMR results confirmed the presence of ether bond formed in the synthesized polyol due to reaction between hydroxy groups of MCC and epoxide rings of glycidol. The number average and weight average molecular weight of polyol were 213 and 304, respectively with a polydispersity index (PDI,  $M_w/M_n$ ) of 1.4. The synthesized polyol is expected that be used as a component for the preparation of polyurethane foam in our further research.

**Keywords:** Corn cob; Microcrystalline cellulose; Chemical treatments; polyol

## Study and Development Process for Reed Dyeing with *Garcinia Mangostana* Linn. Leaves dyes extraction

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This research aimed to study dyeing on Chantaburi Reed with dyes extracted from *Garcinia Mangostana* Linn. leaves, using the same technique employed for cotton fabric dyed with direct dyes. The study examined various dyeing factors, including dyeing method, the type and concentration of mordants. The effect of mordanting method during dyeing; pre-mordant, meta-mordant and post mordant; along with four concentrations of three different mordants: were studied. The color measurements were done with spectrophotometer to obtain CIE  $L^*a^*b^*$  values, and color strength (K/S), as along with the study on color fastness to light and color fastness to crocking. It was found that the type of mordant affected on the shades of the dyed reed. When calcium hydroxide ( $\text{Ca}(\text{OH})_2$ ) and aluminium potassium sulfate ( $\text{AlK}(\text{SO})_4$ ) was used as a mordant, those dyed reed with dyes extracted from *Garcinia Mangostana* Linn. leaves turned red. When  $\text{Fe}(\text{SO})_4$  was used as a mordant, those dyed reed turned black. Furthermore, the red dyed reed had the highest color strength when meta-mordant method was used, with 4 g/l of  $\text{Ca}(\text{OH})_2$ . On the other hand, the black dyed reed had the highest color strength when post-mordant method was used, with 4 g/l of  $\text{Fe}(\text{SO})_4$ . The results showed that the colorfastness to light of every condition dyed reed were good; they showed value of 4 out of 8. But their colorfastness to crocking for wet condition decreased with mordant dyeing. However, their colorfastness to crocking for dry condition mostly increased with mordant dyeing.

**Keywords:** Reed Dyeing; *Garcinia Mangostana* Linn.; Mordant; Coorfastness to light; Colorfastness to crocking.



## Hybrid interpenetrating polymer networks of $\kappa$ -carrageenan/poly(vinyl alcohol) films

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In this work, interpenetrating polymer networks (IPNs) of  $\kappa$ -carrageenan/poly(vinyl alcohol) films were developed. In order to improve physical properties of the films, the crosslinking contents and the compositions between both homopolymers were optimized with  $\kappa$ -carrageenan/poly(vinyl alcohol) ratios of 40:60, 50:50 and 60:40. The sol-gel process involving hydrolysis and polycondensation reactions and the solution casting were used to fabricate the hybrid films. The results obtained from ATR-FTIR, SEM-EDX, swelling test and thermal analysis confirmed that the crosslinked films containing covalent coupling between organic and inorganic hybrid networks were successfully formed. The hybridization resulted in enhancement of mechanical properties and dimensional stability in aqueous swollen state. The films were colorless and transparent. Their homogeneous microstructure morphology was confirmed by SEM micrographs indicating compatibility between both homopolymers. The combination of their physical properties, mechanical strength as well as simplicity of fabrication process made these IPNs films promising for packaging application.

**Keywords:**  $\kappa$ -Carrageenan; Poly(vinyl alcohol); Sol-gel reaction; Polymer blend; IPNs

## Investigation of mechanical properties on TPS/PLA bio-plastic composite with oil palm fiber

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Environmental pollution problems from burning of agricultural waste and plastic waste from petroleum-based plastic which cannot be degraded in nature are recently considered on global problem. The utilization of agricultural residue from oil palm fiber and bio-plastic composite might solve this global issue and lead to Bio-Circular-Green Economy (BCG) model. In this research, thermoplastic starch (TPS) and polylactic acid (PLA) blend were chosen for biodegradable plastic composite with and without oil palm fiber. The amount of palm oil fibers was added from 0 wt% to 5 wt% of TPS. The ratios of TPS/PLA as 40 : 60 and 70 : 30 with and without oil palm fiber were compared to pure PLA. Then, pellets of TPS/PLA mixing with oil palm fiber were prepared by using a twin-screw extruder. After that, the melt-flowable characteristic of TPS/PLA composite pellets was investigated. Mechanical properties of TPS/PLA with and without oil palm fiber compared to pure PLA were also investigated. The results revealed that the addition of oil palm fiber decreased the melt flow rate of TPS/PLA composite. In addition, the strength of TPS/PLA composite increased with increasing the amount of oil palm fibers, however, increasing oil palm fibers up to 5 wt% caused a reducing in tensile strength. Thus, the results indicated that the optimum tensile strength of TPS/PLA composite with 1 wt% oil palm fiber could reinforce the bio-plastic composite.

**Keywords:** Oil palm fiber; Agricultural waste; Plastic waste; Biodegradable; Bio-plastic composite



## Enhancing the mechanical properties of pineapple leaf fiber paper sheets with a dispersing agent

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Pineapple leaf fiber (PALF) is an agricultural waste material valued for its abundant cellulose content and eco-friendly characteristics. This research aimed to investigate the mechanical properties of PALF paper. To enhance its quality, PALF paper underwent a process that involved the removal of lignin and other components through treatment with a NaOH alkali solution, followed by bleaching with an  $\text{H}_2\text{O}_2$  solution. Additionally, varying concentrations of a dispersing agent (0, 1, 3, 5, and 7 g/l) were incorporated into the PALF paper preparation to aid in the paper formation process. The outcomes demonstrated that the inclusion of a dispersing agent led to significant improvements in the properties of PALF papers, particularly in terms of enhanced bursting and tearing strengths. To gain a deeper insight into the structural transformations, scanning electron microscopy (SEM) was employed to examine the surface morphology of the PALF papers. The SEM images revealed a dense and closely packed arrangement of fibers within the PALF papers.

**Keywords:** Pineapple leaf fiber; Dispersing agent; Bursting strength; Tearing strength; PLAF paper

## Developing hydrophobic cellulose fibers from pineapple leaves for oil absorption

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The process of developing hydrophobic cellulose fibers from pineapple leaves for oil absorption involves several key steps. Initially, raw pineapple leaf fibers are treated with a sodium hydroxide solution to remove hemicellulose, a component that attracts water. Subsequently, these fibers are coated with a gel solution and a surfactant to make them hydrophobic. This transformation is achieved through a gelation process and surface modification, resulting in cellulose fibers with hydrophobic properties. The experimental results reveal that these treated fibers exhibit outstanding water repellency and oil absorption capabilities. The combination of surface coating with a surfactant and the fiber preparation process directly affects the interaction between the surfactant and the hydroxyl groups on cellulose molecules, leading to improved fiber strength. This is evident from the increased contact angle of water droplets on the fiber surface, which falls within the range of  $145.3^\circ$  to  $144.6^\circ$ , signifying enhanced water resistance. Regarding their performance in oil absorption, the treated fibers prove to be highly effective. They demonstrate oil absorption efficiencies ranging from 93.42% to 91.40% after the first use and 87.44% to 85.65% after five uses, highlighting their sustained effectiveness over multiple applications.

**Keywords:** Hydrophobic cellulose fibers; Pineapple leaf fibers; Oil absorption fibers; Water resistance fibers





## Synthesis of conjugated network polymers from thieno[3,4-b]pyrazine derivatives

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Conjugated polymers have been widely used in many applications such as organic field effect transistors, organic light-emitting diodes (OLEDs), sensors, and organic photovoltaic (OPV) cells. They consist of  $\pi$ -conjugated system with alternating single and double bonds along the main chain. The naturally rotating linking single bonds can decrease the efficiency of  $\pi$ -delocalization on the main chain and limit the conjugated properties of the polymer. Conjugated network polymers (CNPs), derived from monomers joined together in more than 2 directions, could block such rotations, and flatten the polymer plane, hence improving the efficiency of electron delocalization. Derivatives of thienopyrazine have been reported to be excellent precursors for delivering visible-NIR absorbed low bandgap conjugated polymer. In this research, we use 2,3-di-(bromomethyl)thieno[3,4-b]pyrazine as a monomer with 4 connection sites to form novel CNPs through solid-state polymerizations (SSPs), oxidative polymerizations and substitutions. Poly(2,3-di-(bromomethyl)thieno[3,4-b]pyrazine) had been prepared, characterized by solid UV and IR, exhibited broad absorption in the visible regions extending into the near-infrared. The facile synthesis of these materials could expand the scope of their applications in organic devices.

**Keywords:** Conjugated polymer; Network polymer; Thienopyrazine; Solid-state polymerization

## Volatile organic compound absorption and photocatalytic degradation of natural rubber foam with modified $\text{TiO}_2$ composites

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The present work aims to study the effects of modified titanium dioxide ( $\text{TiO}_2$ ) with zinc oxide on mechanical properties and volatile organic compounds (VOC) absorption of the natural rubber (NR) foam composites filled with  $\text{ZnO-TiO}_2$  at different concentration. It was found that the values of 100% modulus, tensile strength, hardness and density increased with varying the  $\text{ZnO-TiO}_2$  concentration. Absorption and photodegradation of methylene blue (MB) solution were the composition determination indicator increased significantly with increasing the irradiation time under lighting conditions compared to dark conditions especially NR with the addition of modified  $\text{ZnO-TiO}_2$  at 5 phr. In terms of the relationship between absorption and volume change under benzene gas condition (BZ-95), it was found that natural rubber (NR) composite foam filled with  $\text{ZnO-TiO}_2$  can absorb benzene gas higher and longer than natural rubber composite foam without added  $\text{ZnO-TiO}_2$ .

**Keywords:** Benzene; Filtration; Natural rubber; Photocatalytic degradation; Titanium dioxide



## Effects of plasticizers on light transmission of silk fibroin films

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It is widely acknowledged that sugar alcohols, identified as environmentally friendly plasticizers, can be employed to tailor the properties of polymer films. In this study, silk fibroin was extracted from white silk cocoons using  $\text{Na}_2\text{CO}_3$  solution. The recovery percentages for silk fibroin and silk sericin were determined to be  $64.81 \pm 0.01$  % w/w and  $35.19 \pm 0.01$  % w/w, respectively. Subsequently, a silk fibroin solution was formulated through the dissolution of degummed silk fibroin in a mixture of  $\text{CaCl}_2/\text{C}_2\text{H}_5\text{OH}/\text{H}_2\text{O}$ , with a molar ratio of 1:2:8. This solution was further refined through dialysis against distilled water. The concentration of the silk fibroin solution after dialysis was  $4.56 \pm 0.01$  %w/v. Following this, a silk fibroin film was fabricated using a solution casting method. The resulting silk fibroin film exhibited notable transparency within the visible spectrum and demonstrated distinctive UV absorption properties. The impact of various plasticizers, with different numbers of C atom and OH group, specifically glycerol (Gly), sorbitol (Sor), and maltitol (Mal), on the light transmission of silk fibroin films was examined through UV-VIS spectroscopy. All three plasticizers were employed at an identical concentration of 30% w/w relative to the dry weight of silk fibroin. The experimental findings indicated that the light transmission percentage of the films varied based on the type of plasticizers used. The UV transmission at a wavelength of 250 nm increased in correlation with the number of carbon atoms in the plasticizers. Conversely, the light transmittance at 600 nm in the films decreased with an increasing number of carbon atoms. Nonetheless, the values fell within the range of 86-90%, signifying the films' exceptional transparency. Conclusively, through the utilization of different plasticizers, it becomes feasible to produce transparent silk films endowed with UV shielding properties. These films hold significant potential for applications in high-optical-transparency coatings.

**Keywords:** Silk cocoons; Silk fibroin; Light absorption; Plasticizer

## Preparation of levan from *B. subtilis* under different cultivation conditions

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Levan is a fructan biopolymer consisting of fructose molecules linked via beta-2, 6 glycosidic bond. It is typically synthesized through the catalysis levansucrase, secreted from certain microorganisms. Interestingly, variations in the molecular weight (MW) of levan have been associated with different levels of biological activities, including anti-bacterial and antitumor effects. However, the preparation of different MW of microbial levan is still challenging. Herein, we investigated the MW of levan produced from *Bacillus subtilis* under different cultivation conditions. Our findings revealed that the MW of levan from *B. subtilis* cultured in a minimal medium was  $1.8 \times 10^4$  Da. It was higher than the MW of levan from bacteria in a complete medium, which was  $9 \times 10^3$  Da. Additionally, shaking speed (Round Per Minute, RPM) also impacted the levan MW. Specifically, the levan MW of  $1.7 \times 10^4$  Da and  $9.8 \times 10^3$  Da were detected at the shaking speed of 100 and 180 RPM, respectively. The results of this study thus provided cultivation conditions for preparing levan with different MWs from *B. subtilis*. Also, it will facilitate further investigation of biological activities associated with levan of varying MW.

**Keywords:** Levan; Fructan; *B. subtilis*; Molecular weight



## Production of nanocellulose from green algae

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Green algae are the most common algae found in freshwater sources in Thailand. In this research, nanocellulose was prepared from green algae. Cellulose was extracted with sodium hydroxide solution and nanocellulose was produced via acid hydrolysis. The optimum conditions for cellulose extraction and nanocellulose production were studied. The chemical structure of cellulose was determined with Fourier transform infrared spectroscopy. The morphology and size of produced nanocellulose were obtained using transmission electron microscope. The results show that concentrations of sodium hydroxide solutions (0.5, 1.0 and 1.5 M) and temperatures (30 and 60 °C) did not affect the percentage yield of extracted cellulose fibers. Nanocellulose was hydrolyzed with sulfuric acid at 50, 60 and 80 °C, respectively, for 3 h. The results from Transmission electron microscope analysis displayed that the average diameter of nanocellulose fibers was 18.54, 18.37 and 18.30 nm, respectively, which has no significant difference. The shortest length of nanocellulose fibers was observed with an average length of 675.52 nm when hydrolysis at 80 °C.

**Keywords:** Nanocellulose; Freshwater; Chlorophyta; Biopolymer; Green algae

## Silk yarn dyeing with extracted dye from spent coffee grounds using a moka pot

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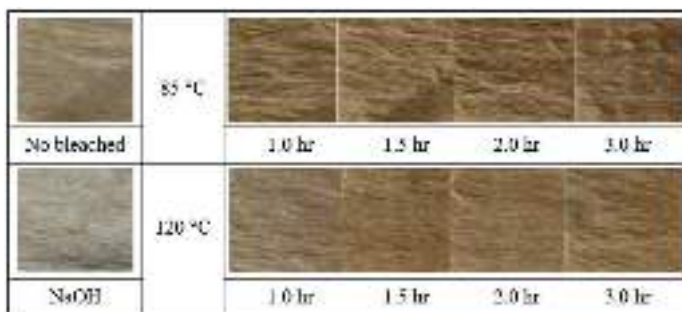
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Coffee, the second most globally traded commodity after petroleum, has seen a surge in popularity, especially in out-of-home settings, driving market growth. Concerns about the environmental impact of leftover coffee grounds have prompted exploration into their conversion into a valuable dye for natural silk yarn. Employing an eco-friendly approach, we utilized a Moka pot for straightforward extraction, eliminating the need for toxic solvents. Unlike previous studies on fabrics and wool, our focus was on dyeing silk yarn using the derived coffee dye. Varying dyeing time (1.0, 1.5, 2.0, and 3.0 h) and temperature (85 °C and 120 °C), we used a pressure cooker for dyeing at 120 °C. UV-vis spectrometry quantified the absorptivity of the coffee-extracted dye and the dyeing medium under diverse conditions. The absorptivity slightly decreased with a pressure cooker for 3.0 h compared to extraction at 85 °C. Various conditions were assessed for color properties in all types of dyed silk yarn using CIELAB parameters (L\*, a\*, and b\*). Dyed silk yarn exhibited a natural brown shade and alkali bleaching enhanced elongation without affecting strength. Prolonged dyeing significantly reduced tensile properties. FT-IR analysis distinguished coffee-extracted dye, dyed silk yarn under various conditions, and untreated yarn. This innovative approach highlights the potential of utilizing coffee remnants as an environmentally sustainable dye for silk yarn, offering conscientious alternatives in the textile sector. The research emphasizes efficient coffee ground utilization and eco-conscious dyeing practices for sustainable textile production.

**Keywords:** Coffee extract dye; Dyeing process; Moka pot; Silk yarn; Spent coffee grounds



**Figure 1.** Silk yarn before dyeing (no bleached and bleached with NaOH) and after dyeing at various conditions.



## Utilization of silk sericin as an ingredient in acne hydrogels: effects of tea tree oil on the inhibitory effect against *Staphylococcus aureus*

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Silk sericin, a naturally occurring polymer, is synthesized by the silkworm *Bombyx mori*. The cosmetic industry can benefit from the extended application of sericin due to its antioxidant activity. In this study, silk sericin was extracted from white silk cocoons using distilled water at 100 °C. The resulting silk sericin solution with the concentration of 0.52 %w/v was obtained. Acne hydrogel was prepared from carbomer with the addition of the sericin solution, glycerol and tea tree oil at different concentrations. The chemical structure of the acne hydrogel was analyzed using Fourier transform infrared spectroscopy (FT-IR). The inhibitory effect of the acne hydrogel was also tested against *Staphylococcus aureus* (*S. aureus*). The results showed that tea tree oil was effective in inhibiting the infection, and the effectiveness increased with increasing tea tree oil concentration. Acne hydrogels containing 10, 12.5 and 15%w/v of tea tree oil inhibited the growth of *Staphylococcus aureus*, with the mean inhibition zone diameters of  $7.33 \pm 0.57$ ,  $8.66 \pm 0.28$  and  $10.66 \pm 1.60$  mm, respectively. In the absence of tea tree oil supplementation, the hydrogel exhibited no inhibitory effects on the growth of *Staphylococcus aureus*, with recorded mean inhibition zone diameters of 0 mm. Additionally, the skin irritation test showed that the acne hydrogel did not irritate human skin.

**Keywords:** White silk cocoons; Sericin; Acne hydrogel; Tea tree oil

## Influence of functionalized graphene on properties of short glass fiber reinforced polyamide12 composites

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Polyamide12 (PA12) composites reinforced with short glass fibers (GF) of 12.6-13.0  $\mu\text{m}$  diameter and 6 mm length in the weight ratio of 2, 4, and 6 wt% were compounded using a twin-screw extruder. The influence of functionalized graphene (Gr-O2) was investigated by incorporating Gr-O2 of 0.3 and 0.5 wt% into the composites. As characterized by the supplier, these Gr-O2 were plasma functionalized by oxygen to obtain the carbonyl and the hydroxyl groups onto the surface. Mechanical, thermal and morphological properties of the injection molded composites were evaluated. It was found that Young's modulus and the ultimate tensile strength of the PA12-based composites increased linearly with respect to the GF concentration. Incorporating Gr-O2 of 0.3 wt% further increased both modulus and ultimate tensile strength of the PA12-based composites, which the highest ultimate tensile strength was achieved when adding GF of 6 wt% and Gr-O2 of 0.3 wt%. Due to plasticizing effect by the Gr-O2, the energy at break of the GF-reinforced PA12 composites was higher when incorporating Gr-O2 of 0.3-0.5 wt%. However, these Gr-O2 did not dissipate the shock loading well enough to improve the impact resistance. Two crystal melting temperatures of the PA12 were observed after annealing, and the merging of them occurred with the presence of Gr-O2 implying the physical interaction between the PA12 molecules and the nanoplatelets. SEM micrographs indicated the interfacial adhesion between the PA12 matrix and the GFs was improved due to the inclusion of Gr-O2 nanoplatelets that provided chemical compatibility via the functionalized groups.

**Keywords:** Polyamide 12; Functionalized graphene; Short glass fibers; Polymer composite



Figure 1. Ultimate tensile strength of PA12 and PA12-based composites.

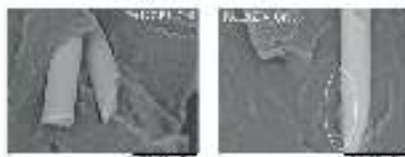


Figure 2. SEM micrographs (magnification of 2000X) of PA12-based composites with and without Gr-O2.

## Investigation of physicochemical properties of pomegranate extract loaded nanoliposome for cosmetic application

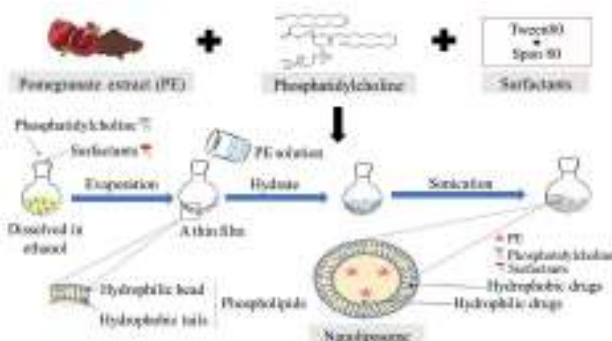
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Pomegranate extract (PE) contains phenolic compounds which are very sensitive to light and heat. In order to improve the stability of PE, nanoliposomes (NLPs) are an efficient way to encapsulate the compounds and controlled release. Therefore, the aim of this study was to produce pomegranate extract loaded nanoliposomes (PE-NLPs) by thin-film hydration method, using phosphatidylcholine as phospholipids and tween 80 and span 80 as surfactants. (Figure 1). The studied variables were different concentrations of PE (0.25, 0.50, 1.00 mg/mL). Then, the morphology, physicochemical properties, encapsulation efficiency, antioxidant activity, and *in vitro* release study of PE-NLPs were investigated. The prepared PE-NLPs were spherical with an average size of 277 to 424 nm. The zeta potential and polydispersity index of PE-NLPs were in the range of -8 to -10 mV and 0.3 to 0.5, respectively. The encapsulation efficiency of PE-NLPs was 14 to 49% which showed the capability for retention of active ingredients in the bilayer membrane or the central core of nanocarrier. The antioxidant activities of PE-NLPs were determined by 2,2-diphenyl-1-picrylhydrazyl (DPPH) assay and 2,2'-azino-bis (3-ethylbenzothiazoline-6-sulfonic acid) (ABTS) assay. The antioxidant activities ranged from 43 to 74% and 44 to 79% for DPPH and ABTS assay, respectively. In addition, *in vitro* release study of PE-NLPs showed 28 to 40% release of the extract in 24 hours. Consequently, result showed potential of PE-NLPs would be an option in innovative development of natural products for cosmetic application.

**Keywords:** Nanoliposome; Pomegranate extract; Thin-film hydration method; Phosphatidylcholine



**Figure 1.** Pomegranate extract loaded nanoliposomes (PE-NLPs)

## Effect of kappa-carrageenan concentration on encapsulating and releasing vitamin C

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Benefits of Vitamin C (VC) include boosting the body's immune system, strengthening collagen, and making the skin smoother and more radiant. However, VC can be broken down by heat, air, or acids, so there needs to be a proper way to release VC into the body. At present, the mask has been developed in the form of a hydrogel sheet to deliver the active ingredients through the skin because it can retain more moisture and does not cause irritation to the skin. Thus, this study aims to fabricate the hydrogel for loading and releasing VC from kappa-carrageenan (k-CAR). The k-CAR hydrogel was prepared by the solvent casting method based on the effect of k-CAR concentrations of 2-5% wt before VC was encapsulated into the k-CAR hydrogel by soaking the hydrogel in the VC solution. The amount of VC loaded in the k-CAR hydrogel was 2.1 mg. The amount of VC release decreased with increasing k-CAR concentration, which was consistent with decreasing swelling behavior. The amount of VC release from k-CAR hydrogel was more than 50% of the amount of VC loading within 1.5 h.

**Keywords:** Carrageenan; Vitamin C; Hydrogel; Release

# Physical and Theoretical Chemistry (PT)

## Oral Presentation

## The development of a new hypothetical MOF database for high-efficiency MOFs targeted for CO<sub>2</sub> utilization

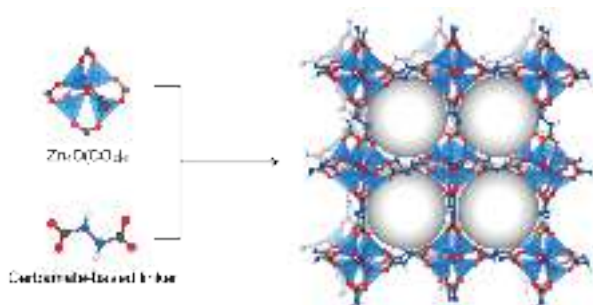
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Due to the fascinating properties of metal-organic frameworks (MOFs) such as porosity, large surface area, and active site, it has been getting attention as potential absorbents for CO<sub>2</sub> uptake. The large diversity of MOFs is ascribed to the enormous possible combinations of the metal nodes and the crossable organic linkers. Recently, the concept of turning CO<sub>2</sub> into MOF's linker has been proposed, and CO<sub>2</sub> content is defined as the amount of CO<sub>2</sub> in the MOF's structures. Despite the simplicity of the concept, the limitation of the experiment leaves large possibilities unexplored. In this study, we theoretically proposed new carbamate-type organic linkers using CO<sub>2</sub> as a raw material. The assembly of MOFs from those 14 designed CO<sub>2</sub>-based linkers, in combination with 15 types of metal nodes across over 40 topologies, results in nearly 2,000 possible MOFs generated as candidates for CO<sub>2</sub> uptake. All generated MOFs and their total CO<sub>2</sub> utilization (content + uptake) are collected as a database and to be published online, including key information such as physical properties and CO<sub>2</sub> adsorption isotherms from grand canonical Monte Carlo simulation. We hope that our designed database will contribute as a guideline for the upcoming experiments.

**Keywords:** Metal organic frameworks; Database; CO<sub>2</sub> utilization; CO<sub>2</sub> adsorption; CO<sub>2</sub> storage



# Computational investigation of double-atoms catalysts decorated on defective boron nitride for catalyzing CO oxidation: A DFT study

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Carbon monoxide (CO) is an environmental pollutant and poses a threat to human health. Therefore, the conversion of CO plays a crucial role in addressing environmental concerns. CO oxidation is the most effective method for converting CO to carbon dioxide (CO<sub>2</sub>) through heterogeneous catalysis. In this study, we conducted a systematic investigation using density functional theory calculations to examine the decoration of defective boron nitride with dual-metal atoms (TM<sub>2</sub> = Mn, Fe, Co, Ni, Cu, Pd, Ag, Pt, and Au). We modeled three distinct configurations of defective BN by introducing boron-boron vacancies (V<sub>BB</sub>), nitrogen-nitrogen vacancies (V<sub>NN</sub>), and boron-nitrogen vacancies (V<sub>BN</sub>). We explored the stability and structural properties of dual-metal atoms on defective BN. The calculation results demonstrate that anchoring dual-TM atoms onto defective BN stabilizes the system and prevents the aggregation of metal clusters on the substrate. Interestingly, all dual-TM atoms decorated on BNV<sub>BB</sub> exhibit greater durability than the others. As a result, we assessed the adsorption abilities of CO, O<sub>2</sub>, and CO<sub>2</sub> on TM<sub>2</sub>@BNV<sub>BB</sub> to identify a suitable catalyst for CO oxidation. Our findings indicate that Ag and Pd atoms show superior performance for this task, primarily because the difference in adsorption energy between O<sub>2</sub> and CO on Ag<sub>2</sub>@BNV<sub>BB</sub> and Pd<sub>2</sub>@BNV<sub>BB</sub> is smaller compared to the other catalysts. We anticipate that Ag<sub>2</sub>@BNV<sub>BB</sub> and Pd<sub>2</sub>@BNV<sub>BB</sub> exhibit the highest catalytic performance for CO oxidation. Our calculations provide insights into the stability of transition metals on defective boron nitride and offer guidance for selecting an appropriate catalyst for the CO oxidation reaction.

**Keywords:** Dual atom catalysts; CO oxidation; Density functional theory; Boron nitride; Transition metal



## Enhanced formic acid production through catalytic CO<sub>2</sub> hydrogenation on frustrated Lewis pair functionalized UiO-67

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The promising approach of capturing and transforming CO<sub>2</sub> into formic acid using a sustainable supply of H<sub>2</sub> offers a way to reduce overall CO<sub>2</sub> emissions while generating valuable fuels. In this study, we used computational methods to design eight functional groups containing both Lewis acid and Lewis base properties for incorporation into metal-organic frameworks (MOFs). We then assessed their effectiveness as catalysts for CO<sub>2</sub> hydrogenation, focusing on the reaction pathways, particularly the role of Frustrated Lewis Pairs (FLPs) in efficiently breaking down H<sub>2</sub> through heterolytic dissociation. This was followed by the simultaneous addition of a hydride and a proton to CO<sub>2</sub> in a single step to produce an HCOOH product. Notably, we discovered a linear relationship between the reaction energies of H<sub>2</sub> dissociation and the FLP acidity, highlighting the critical role of FLP acidity in determining their catalytic activity. Further calculations revealed that FLP acidity influences the reaction barriers in CO<sub>2</sub> hydrogenation, which also correlates linearly with the energy of H<sub>2</sub> dissociation. Furthermore, our microkinetic modeling demonstrated that at the lowest temperature of 400 K and a pressure of 1 bar, UiO-67-B(CH<sub>3</sub>)<sub>2</sub> exhibited higher reactivity (0.70 eV), resulting in a greater reaction rate and production rate of HCOOH compared to other catalysts. In summary, this study illustrates the process of constructing metal-free heterogeneous FLPs on MOFs and uncovers a direct link between the N-BX<sub>2</sub> composition, FLP acidity, and the catalytic capabilities of these FLPs.

**Keywords:** Lewis acid; Lewis base; Density functional theory; CO<sub>2</sub> hydrogenation; CO<sub>2</sub> utilization; formic acid

## A DFT study on a single transition metal doped C<sub>3</sub>N for oxidation reaction

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Carbon monoxide (CO) is one of the major common toxic gases in the atmosphere, originating from car exhausts, industrial processes and incomplete burning of fuels or petroleum products. The catalytic oxidation of carbon monoxide (CO) by oxygen (O<sub>2</sub>) molecule is one of the most popular methods for conversion of CO to the less toxic molecules, i.e., CO<sub>2</sub>. The C<sub>3</sub>N monolayer is an interesting catalyst for CO oxidation reactions due to its unique electronic and structural properties as well as high surface area. In this work, we investigated the catalytic oxidation of CO by O<sub>2</sub> over the transition metals (TM = Cu, Ni, Pt and Pd) decorated on the single (Cv and Nv) and double vacancy (CCv and CNv) of C<sub>3</sub>N monolayer using density functional theory (DFT) calculation. The results show that both CO and O<sub>2</sub> favorably adsorb on the TM deposited on the N-vacancy C<sub>3</sub>N (TM@Nv-C<sub>3</sub>N), with O<sub>2</sub> adhering more strongly than CO molecule. Among the metals studied, Pt@Nv-C<sub>3</sub>N exhibits the strongest binding affinity with O<sub>2</sub> molecule with E<sub>ads</sub> of -3.07 eV. According to the activation energies, the oxidation of CO by O<sub>2</sub> on Pt@Nv-C<sub>3</sub>N preferentially proceeds through Eley-Rideal (ER) mechanism rather than Langmuir-Hinshelwood (LH) mechanism with the rate-limiting step of 0.41 eV as illustrated in Figure 1. By comparison, Pt@Nv-C<sub>3</sub>N is predicted to have the highest catalytic performance for the CO oxidation reaction.

**Keywords:** Density functional theory (DFT); ER mechanism; LH mechanism; CO oxidation

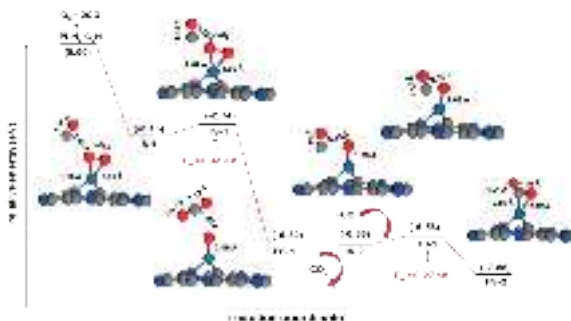


Figure 1. The potential energy profile for the oxidation of CO via the ER mechanism.



## The effect of non-metal doped graphitic carbon nitride for carbon dioxide reduction reaction: A DFT study

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The carbon dioxide reduction reaction (CO<sub>2</sub>RR) is one of the most promising processes for converting CO<sub>2</sub> into clean fuel. In this study, we applied the CO<sub>2</sub>RR method to produce C1 products (CO, HCOOH, CH<sub>2</sub>O, CH<sub>3</sub>OH, and CH<sub>4</sub>) on pristine g-C<sub>3</sub>N<sub>4</sub> incorporating non-metal dopants (B, P, O, and S). We examined this process through the density functional theory (DFT) calculations. Pristine g-C<sub>3</sub>N<sub>4</sub> offers six potential substitution sites: the top site on two carbon atoms (C1 and C2), three nitrogen atoms (N1, N2, and N3), and one interstitial site (int.). The results found that substituting B and P atoms at the C1 site yielded the most stable configuration while replacing O and S atoms at the N2 site was consistent with the formation energy calculation. In comparison to pristine g-C<sub>3</sub>N<sub>4</sub> and non-metal doped g-C<sub>3</sub>N<sub>4</sub>, the analysis of non-metal doped g-C<sub>3</sub>N<sub>4</sub> indicates a reduction in the first protonation step. Furthermore, when investigating the CO<sub>2</sub>RR pathways and limiting potentials on S-C<sub>3</sub>N<sub>4</sub>, we observed low limiting potentials of -0.17, -0.58, -0.58, and -0.58 V for HCOOH, CH<sub>2</sub>O, CH<sub>3</sub>OH, and CH<sub>4</sub>, respectively, along with a high limiting potential of -0.77 V for CO. This work highlights non-metal doped g-C<sub>3</sub>N<sub>4</sub> as a promising electrocatalyst for CO<sub>2</sub>RR due to its elevated CO<sub>2</sub>RR activity and enhanced selectivity.

**Keywords:** Non-metal atoms; g-C<sub>3</sub>N<sub>4</sub>; CO<sub>2</sub> reduction reaction; C1 product; DFT

## Enhancing carbon dioxide reduction through single and dual heteroatoms doped diamond: A DFT study

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In the field of catalyst development for electrochemistry, diamond doping has attracted more attention worldwide because diamond surface structure and its electronic states can be improved by the process. In this study, we employed Density Functional Theory (DFT) approaches to explore the catalytic potential of single and dual heteroatoms; boron (B), nitrogen (N), and phosphorous (P), integrated into a diamond structure for the Carbon Dioxide Reduction Reaction (CO<sub>2</sub>RR). Our computational results revealed that the existence of dual dopants on the diamond can enhance more catalytic activity of CO<sub>2</sub>RR as compared to the single-doped ones especially in the cases of BB and NN. The primary product in both pathways is HCOOH, which requires overpotentials of 0.40 V and 0.09 V, respectively. Note, the single P doped diamond supports a competing pathway Hydrogen Evolution Reaction (HER). Notably, the B and N co-doped diamond (BN) demonstrated its capability to produce HCOOH with no need for applied overpotentials. Also, the BN was found to emerge as the top of a 2D volcano plot, showing the lowest limiting potential (), an exceptional thermal stability, and an ability to suppress the HER pathway. The more effective catalytic potential of BN surface for CO<sub>2</sub>RR was confirmed by the analysis of density of states (DOS) and crystal orbital Hamilton population (COHP). This research offers valuable insights for both experimental and theoretical investigations into the electroreduction of carbon dioxide.

**Keywords:** Dopants-doped diamond; CO<sub>2</sub>RR; Density functional theory; Electrochemical properties





## How many water molecules react with simplest Criegee intermediates at atmospheric conditions?

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Due to its importance in atmospheric chemistry, the reactions involving Criegee intermediates and trace gases have attracted significant attention. This has led to a great number of experimental and computational studies on this topic in the past decade. For most computational studies, conventional transition state theory (CTST) has been utilized to predict rate coefficients. In this most basic form, CTST assumes a barrier geometry and calculates free energies based on harmonic approximation with rigid rotor approximations. For the reaction between the simplest Criegee intermediate and water vapor, this approach has given room temperature rate coefficients that are consistent with experimental ones for the  $\text{CH}_2\text{OO}+\text{H}_2\text{O}$  (calc: 5.00 exp:  $4.2 \times 10^{-16} \text{ cm}^3 \text{ s}^{-1}$ ) and  $\text{CH}_2\text{OO}+2\text{H}_2\text{O}$  (calc: 9.02 exp:  $10.7 \times 10^{-33} \text{ cm}^6 \text{ s}^{-1}$ ) reactions. However, TST calculation for the  $\text{CH}_2\text{OO}+3\text{H}_2\text{O}$  reaction ( $0.29 \times 10^{-50} \text{ cm}^9 \text{ s}^{-1}$ ) underestimates the rate coefficient compared to a very recent experimental study ( $1.48 \times 10^{-50} \text{ cm}^9 \text{ s}^{-1}$ ).

To remedy this difference, we utilized QCISD(T)/CBS//B3LYP/6-311+G(2d,2p) method and simulated the barrierless approach of  $\text{CH}_2\text{OO} \dots \text{H}_2\text{O}$  and  $(\text{H}_2\text{O})_2$ . Performing the variational TST calculation on this effective potential, we were able to obtain an effective reaction rate of  $1.47 \times 10^{-50} \text{ cm}^9 \text{ s}^{-1}$ , consistent with experimental results. Detailed discussion concerning the reaction path for this barrierless reaction will be given in more detail at the talk.

**Keywords:** Criegee mediate; Water cluster; Barrierless reaction; Rate coefficient; Variational transition state theory

## Enhancing $V_2O_5$ cathodes in magnesium-ion batteries through aqueous electrolyte-induced hydrogen insertion: A first-principles approach

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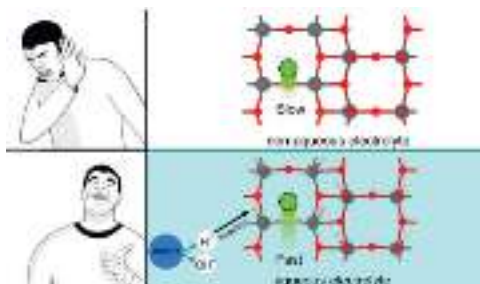
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Magnesium-ion batteries (MIBs) have emerged as a promising alternative to conventional Li-ion batteries, but the quest for a suitable electrode material remains a significant challenge. Among various cathode materials,  $V_2O_5$  stands out as a potential candidate due to its high theoretical capacity and cost-effectiveness. However, it still faces issues of high capacity fading and slow charge/discharge kinetics. In this talk, I will explain how we can use first-principles tools to suggest strategies to improve performance of  $V_2O_5$  cathodes. In particular, I will demonstrate the effect of H insertion – originated from using aqueous electrolyte – on the structural stability and Mg diffusion kinetics of the cathode. In brief, H insertion enhances ion transport kinetics and suppresses phase transformation of Mg-intercalated  $V_2O_5$ , which stems from the weakened electrostatic interaction between Mg-ion and the lattice oxygen upon the H insertion. The findings provide insights for the design of high-performance  $V_2O_5$ -based cathode materials in MIBs, highlighting advantages of employing aqueous electrolytes.

**Keywords:** Aqueous electrolyte;  $V_2O_5$ ; First-principles calculations; Mg-ion batteries; H insertion





## Roles of reactants for Suzuki C-C cross-coupling reaction using molecular volcano plots

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Suzuki-Miyaura C-C cross-coupling reaction is well-known reaction used for constructing C-C bond; however, this reaction does not always provide excellent efficiency especially when changing reactants, and the reasons behind are still unclear. To understand more complete picture, we have investigated the effects of both electrophile ( $R_1$ -Br) and nucleophile ( $R_2$ -B(OH)<sub>2</sub>) reactants catalyzed by Pd(PMe<sub>3</sub>)<sub>2</sub> using DFT calculations and further analyzed using molecular volcano plots to demonstrate relationship between intermediate energetic descriptor and reaction free energy. Among five selected substituent groups on  $R_1$  and  $R_2$  (furan, pyridine, phenyl, styrene, ethylene), we found that when using 2-bromofuran as an electrophile substrate, the reaction can easily proceed with any of boronic acid choices as the reactions with 2-bromofuran always have the lowest energy barrier in the rate-determining step compared to others. Molecular volcano plots also illustrate that the feasible reaction with 2-bromofuran reactant is resulting from the balance of interaction between reactants and Pd(PMe<sub>3</sub>)<sub>2</sub> catalyst, i.e., not too strong nor too weak which lead to the effortless oxidative addition and reductive elimination processes. The order of the interaction between each reactant and catalyst is furan, pyridine, styrene, phenyl and ethylene where furan has the most balanced interaction and reactant with ethylene has weakest interaction.

**Keywords:** Suzuki-Miyaura reaction; Reactants effects; Molecular volcano plot; Reactant-catalyst interaction

## Molecular docking and dynamic simulations of anti-apoptotic Bcl-2 proteins as targets for bioactive compounds in *Durio Zibethinus* for anti-cancer activity

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Different extracts of *Durio Zibethinus* showcase multiple cancer activities, from antioxidant and anti-inflammatory to cytotoxic in different cancer models. Many cancers are occurred due to the overexpression of antiapoptotic protein B-Cell Lymphoma 2 (Bcl-2), which impedes programmed cell death and contributes to uncontrolled cell differentiation. The BH3 domain in Bcl-2 is crucial for suppressing its expression, making BH3 mimetics essential in promoting apoptosis in malignant cells. However, mutations in the BH3 domain can confer resistance to existing BH3 mimetics, prompting ongoing efforts to develop more effective Bcl-2 inhibitors. This study explores the binding interactions between five bioactive compounds from *Durio Zibethinus* with both wild-type (WT) Bcl-2 and mutant Bcl-2G101V protein, with a focus on their BH3 mimetic potential. Flexible receptor docking revealed procyanidin B2 as a standout candidate, demonstrating good binding with docking scores of -8.30 and -8.80 kcal/mol for Bcl-2WT and Bcl-2G101V, respectively. The stability and structural parameters of the Bcl-2/Procyanidin B2 complexes were further analyzed using molecular dynamic simulations. Procyanidin B2 exhibits significant potential as a Bcl-2 inhibitor, displaying a good affinity for binding within the hydrophobic groove of Bcl-2.

**Keywords:** Apoptosis; Bcl-2 inhibitors; BH3-mimetics; Binding affinity; Flexible binding pocket; Structure-based drug design

# Physical and Theoretical Chemistry (PT)

## Poster Presentation

## Transient luminescence studies for excited-state kinetics of organic sensitizer dyes in solar cells

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Dye sensitized solar cells (DSSCs) are typical photovoltaics made of mesoscopic titanium dioxide  $\text{TiO}_2$ , sensitizer dye, and liquid electrolyte containing  $\text{I}_3^-/\text{I}^-$  redox couple. The primary photovoltaic process is electron injection from photoexcited dye to the conduction band (CB) of  $\text{TiO}_2$ . Regeneration of dye proceeds through recapturing of the excess electron of  $\text{I}^-$  by the oxidized dye species. Several authors have argued that introducing 4-tert-butyl pyridine (TBP) to the electrolyte raises the CB edge and suppresses unwanted electron-hole recombination between the CB electrons and  $\text{I}_3^-$ . Such a negative displacement of the CB edge may affect the rate of electron injection  $k_{\text{inj}}$  because the conditions of interfacing area should be significantly changed. In this study, we have conducted time-resolved fluorescence spectroscopy of the DSSC containing indoline dyes D149 and D205, and determined  $k_{\text{inj}}$  by following the analyses described in our preceding abstract. Figure 1 shows the results of time-correlated single photon counting for a D205/ $\text{TiO}_2$  film in DSSC at 470 nm excitation. The red and blue curves show the fluorescence decays with and without TBP, yielding  $k_{\text{inj}}$  of  $2.6 \times 10^9$  and  $1.1 \times 10^{10} \text{ s}^{-1}$ , respectively. The former value is smaller than  $k_{\text{inj}} = 1.3 \times 10^{10} \text{ s}^{-1}$  obtained for a D205/ $\text{TiO}_2$  film on an isolated anode apart from the electrolyte. Hence, TBP is considered to have a role of retarding electron injection the rate of which is just high enough to compete with the rate of the internal conversion of  $\text{S}_1^*(\nu)$  to  $\text{S}_0$  ( $k_{\text{nr}} = 8.9 \times 10^8 \text{ s}^{-1}$ ).

**Keywords:** Dye-sensitized solar cells; Indoline dyes; Electrolyte; Fluorescence; Electron injection

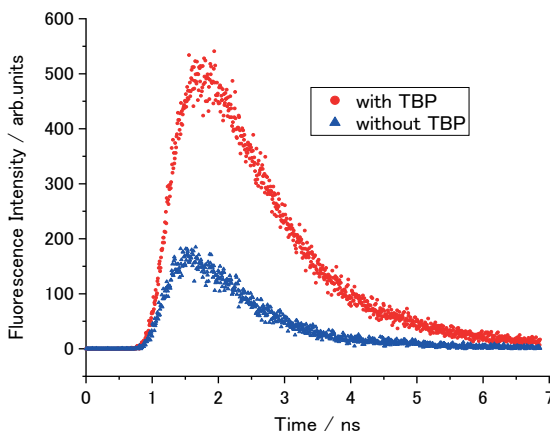


Figure1. Time correlated fluorescence signal from  $\text{TiO}_2/\text{D205}$  in DSSC at 470 nm photoexcitation.

## Modeling metal-atom-based hydrogen storage materials in the presence of non-inert gaseous species

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Studies on H<sub>2</sub> storage predominantly concentrate on interactions between hydrogen and H<sub>2</sub> storage materials, neglecting the influence of non-inert gases like oxygen and water. This study focuses on the interaction between H<sub>2</sub> storage materials and these gases. We utilized a simple model featuring a single lithium or scandium atom adsorbed on graphene, representing H<sub>2</sub> storage materials. We used periodic DFT calculations based on the PBE functional and the D3-type van der Waals corrections to determine the adsorption energies for hydrogen, oxygen, and water on these metal centers. Oxygen exhibited significantly more exothermic adsorption energies than water and hydrogen on both Li and Sc. In the case of Sc, the difference in adsorption energy between oxygen and hydrogen was 5.0 eV, while for Li, it was 1.6 eV, indicating Sc's heightened sensitivity to oxygen during hydrogen adsorption. Analyzing adsorption energies alone does not provide a comprehensive understanding of how hydrogen storage performance varies under different operating conditions. Therefore, we employed the kinetic Monte Carlo (kMC) method to get more insights. For this, we have estimated the rate constants from the adsorption energies within the framework of collision theory and used them to simulate the coverage rates of different adsorbates. Within the kMC method, the rate constants serve as weighting factors for the likelihood of specific molecular processes occurring. By randomly executing adsorption and desorption processes based on their respective probabilities, we have shown that O<sub>2</sub> is the biggest problem for H<sub>2</sub> storage, while H<sub>2</sub>O does not significantly interfere with H<sub>2</sub> adsorption.

**Keywords:** DFT calculation; Hydrogen storage; kMC method

## Structural investigation on chiral recognition of dapoxetine enantiomers with methylated cyclodextrins

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Dapoxetine (Dpx), a premature ejaculation drug, as the eutomer (*S*)-Dpx is 3.5 times more potent than (*R*)-Dpx. Enantiomeric purity of pharmaceutical preparation is necessary to be controlled. Chiral selection of cyclodextrin (CyD) is one of the most commonly used methods. Permethylated- $\beta$ -CyD and methylated- $\gamma$ -CyD as chiral selector for racemic Dpx were achieved with high enantioresolution. Unfortunately, there is no information related to the conformation of inclusion complexes and the molecular interaction between Dpx and CyD, which are important for assessment of the inclusion mechanism of Dpx encapsulated with CyD to develop pharmaceutical production. Molecular docking and semi-empirical PM6 calculations were performed to predict the conformations and interaction of the inclusion complexes between Dpx enantiomers with  $\beta$ -CyD,  $\gamma$ -CyD, permethylated- $\beta$ -CyD, and methylated- $\gamma$ -CyD. The results indicate the formation processes of the 1:1 host-guest ratio complexes are possible with three orientations, as depicted in **Figure 1**. The complexation energies of each molecular structure as well as the interaction between host and guest components in the inclusion complex are further determined by M062X/6-31G(d,p) calculations.

**Keywords:** Inclusion complex; Host-guest interaction; Molecular docking; Semi-empirical method, Density functional theory



Conformation 1



Conformation 2



Conformation 3

**Figure 1:** PM6 energy-optimized structure of 1:1 inclusion complex between (*S*)-Dpx with  $\beta$ -CyD.

## Chiral recognition of terbutaline enantiomers with $\beta$ -cyclodextrin and its three methylated derivatives: molecular modeling approaches

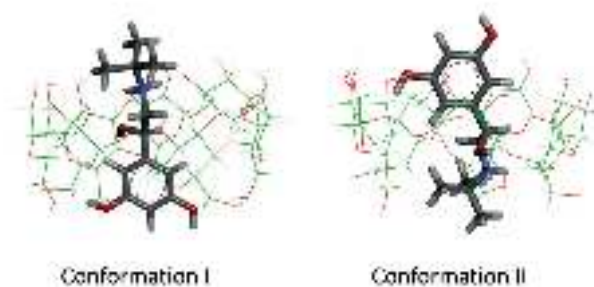
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Terbutaline (TBT) is a  $\beta$ 2-adrenoceptor agonist, the mainstay to relax airway smooth muscle then increasing the airflow in asthma and chronic obstructive pulmonary disease patients. TBT has two enantiomers. (*R*)-TBT was found to be the potent substance in generating therapeutic effects, while (*S*)-TBT has been reported to show side effects. Attempts at the resolution of enantiomeric forms of TBT have been done previously, either by absolute asymmetric synthesis, or using chiral selectors such as  $\beta$ -cyclodextrin or its derivatives. The molecular interaction and the mechanism of chiral recognition of the molecules are necessary for further pharmaceutical development. Molecular docking and AM1 calculations for the enantiomeric recognition of (*R*)-TBT and (*S*)-TBT were developed by means of native  $\beta$ -cyclodextrin (BCD) as well as three of its derivatives namely heptakis(2-O-methyl)- $\beta$ -cyclodextrin (2-MEB), heptakis(6-O-methyl)- $\beta$ -cyclodextrin (6-MEB) and heptakis(2,6-di-O-methyl)- $\beta$ -cyclodextrin (2,6-DIMEB). Results suggest two different orientations of TBT inside cyclodextrin's cavity with 1:1 molecular ratio as shown in Figure 1. The complexation energy results for the (*R*)-TBT/BCD system at the M062X/6-31G(d,p) level suggest that Conformation I is more stable (-49.24 kcal/mol) than Conformation II (-33.15 kcal/mol).

**Keywords:** Inclusion complex; Host-guest interaction, Molecular docking, Semi-empirical method, Density functional theory



**Figure 1:** The minimized M062X/6-31G(d,p) structure of (*R*)TBT/BCD inclusion complexes.

## Cross-docking, ONIOM and molecular dynamic studies of potent antiviral HIV-1 nonnucleoside reverse transcriptase inhibitors

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This study goals to develop HIV-1 RT inhibitors using quinoline as the foundational structure. Employing a molecular hybridization approach, quinoline derivatives yielded two key compounds: (1) 4-(2',6'-dimethyl-4'-cyanophenoxy)-6-(4''-cyanophenyl)-aminoquinoline and (2) 4-(2',6'-dimethyl-4'-cyanophenoxy)-2-(4''-cyanophenyl)-aminoquinoline. The study explored binding interactions between nonnucleoside reverse transcriptase inhibitors (NNRTIs), quinoline derivatives, and HIV-1 RT using cross-docking, molecular docking, ONIOM, and molecular dynamic (MD) approaches. Cross-docking analysis highlighted the superiority of the WT RT conformation (PDB ID: 4G1Q) due to its favorable binding energy compared to other HIV-1 RT conformations. Molecular docking and ONIOM analyses revealed that compound **(2)** notably interacts with LYS101 residues via H-bonding and exhibits pi-pi stacking interactions involving TYR181 and TRP229 residues within the HIV-1 RT binding pocket, akin to those observed with rilpivirine. The interaction energy between **(2)** and rilpivirine showed the lowest total among all ligands. MD simulations emphasized the robust stability of the binding between HIV-1 RT and both **(1)** and **(2)**. This stability was further confirmed by binding free energy calculations using MMPBSA and MMGBSA methods, indicating the enhanced binding affinity of HIV-1RT-**(2)** over HIV-1RT-**(1)**. The development of 2-amino-4-phenoxy-substituted quinoline as an HIV-1 RT inhibitor holds promise for future research, marking a pivotal step in advancing anti-HIV-1 drug discovery.

**Keywords:** Cross-docking; Quinoline; ONIOM; Anti-HIV-1 activity; Molecular Dynamic



Figure 1. The docking conformation of the ligands in HIV-1 RT using molecular docking

## A DFT study on cracking and dehydrogenation of propane on H-ZSM-5

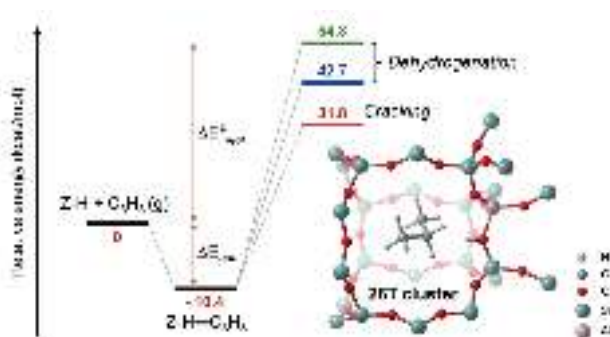
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Propane conversion is one of the hydrocarbon transformations that has been widely examined for determining the selectivity and activity of the catalysts. In this work, theoretical calculations based on density functional theory (DFT) were performed to shed light on the molecular reaction mechanisms involved in the protolytic cracking and dehydrogenation of propane on H-ZSM-5. By using the H-ZSM-5 cluster model containing 26 tetrahedral (26T) atoms to calculate the activation energies of the reactions at the M062X/6-311G(d,p) level theory, the activity and selectivity of this catalyst were ascertained. While the cracking reaction is slightly exothermic, overall, the dehydrogenation processes are endothermic. It is clear that the cracking reaction takes place more favorably than the dehydrogenation processes. The apparent activation energies were calculated to be 31.8, 54.8, and 42.7 kcal mol<sup>-1</sup> for cracking and dehydrogenation at the primary and secondary carbon atom, respectively, in good agreement with the experimental data published previously. These results are explained by the stability of the transition states, which are associated with the ionic structures resembling carbonium ions. The intrinsic reaction coordinate (IRC) calculation and the natural bond orbital (NBO) analysis were used to highlight the mechanistic details of the reactions.

**Keywords:** Propane; Cracking; Dehydrogenation; Zeolite; DFT



**Figure 1** Energy profiles for the protolytic cracking and dehydrogenation of propane of H-ZSM-5.



## Investigating electronic and phosphorescent characteristics in cycloplatinated complexes through DFT/TD-DFT analysis: Insights for OLED applications

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Density functional and time-dependent density functional (DFT, TD-DFT) theoretical methodologies were employed for the investigation of the photophysical characteristics of five inorganic compounds derived from Pt(II) and ppy (2-phenyl-pyridine) ligands. The primary objective of this study is to gain insights into the potential suitability of the selected systems for use in OLED devices. In addition to examining their ground and excited state geometries and electronic structures, an in-depth analysis of the electronic transitions responsible for absorption and spectra, along with other photophysical properties, was conducted. This encompassed the study of charge transfer parameters, triplet exciton generation, phosphorescence quantum yield, and radiative decay rates. The comprehensive results affirm that the chosen systems exhibit promising attributes for application in OLED devices. Furthermore, the findings contribute to a better understanding of the photophysical properties inherent in Pt(II) complexes with ppy ligands.

**Keywords:** Density functional theory; Time-dependent density functional; Photophysical properties; Cyclometalated Pt(II) complexes

## Density functional theory study on the antioxidant mechanism and electronic properties of hydroxybenzoic acid derivatives

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Density functional theory (DFT) has been performed to analyze the antioxidant mechanism of four hydroxybenzoic acid derivatives: 3-hydroxybenzoic acid, 4-hydroxybenzoic acid, protocatechuic acid, and gentisic acid. Gallic acid has been selected as an antioxidant reference molecule. Geometry optimization and frequency calculation of all natural compounds and their corresponding ionic and radical species have been calculated at the B3LYP/6-311++G(2d,2p) level of theory. The solvent effect at the single point level on the optimized geometries of the gas phase has been explored in water and ethanol by the integral-equation-formalism polarizable continuum model (IEF-PCM). Three main mechanisms; hydrogen atom transfer (HAT), single-electron transfer followed by proton transfer (SET-PT), and sequential proton loss electron transfer (SPLET) have been investigated to explain the radical scavenging ability of phenolic antioxidants. As the results, the calculated O-H bond dissociation enthalpies (BDEs) suggest that protocatechuic acid at the 3OH position is the most potent compound, with BDEs of 77.46, 78.24, and 78.20 kcal/mol in the gas phase, water, and ethanol, respectively. The results of protocatechuic acid are comparable to those of gallic acid, suggesting their similar activity. The results suggested that HAT would be the most favorable mechanism for explaining the radical-scavenging activity of phenolic compounds in the gas phase, whereas the SPLET mechanism is the thermodynamically favorable pathway in polar solvents.

**Keywords:** Density functional theory (DFT); Radical scavenging ability; Phenolic antioxidant; Hydroxybenzoic acid



## Binding investigation of 7,8-dimethoxy-4-isochromanone derivatives as Acetylcholinesterase inhibitors by computational study

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Alzheimer's Disease (AD) is a neurological disorder that affects the nerves found throughout the human body and the spinal cord. The FDA approved therapeutic drugs such as donepezil, rivastigmine, and memantine hydrochloride, revealed limitations in terms of side effects and an inability to stop the progression of AD. Recently, the 7,8-dimethoxy-4-isochromanone derivatives have been identified as potent AChE inhibitors demonstrating efficient experimental  $IC_{50}$  values in low nanomolar units. Therefore, this work has studied the binding investigation to describe how these derivatives exhibit excellent inhibition against acetylcholinesterase (AChE) activity through computational studies, which are molecular docking and molecular dynamics (MD) simulations, including MM/PBSA analysis. As a result, the key amino acid residues of these derivatives identified in the AChE are Trp286, and Tyr341. The binding interactions between the AChE and these derivatives include Van der Waals forces, Pi-Pi interactions, alkyl interactions, and hydrogen bonds. Notably, Pi-Pi and alkyl-Pi interactions with Trp286 are observed exclusively between an aromatic ring and the methoxy group of 4-isochromanone structure in the derivatives. In addition, pi-pi interaction is found to Tyr341 via an aromatic part of 4-isochromanone structure. Consequently, the 7,8-dimethoxy-4-isochromanone derivatives have been confirmed through computational methods as a promising scaffold for future AChE drug development.

**Keywords:** Alzheimer's Disease; Acetylcholinesterase; MD simulations; MM/PBSA

## ***In Silico* screening for repurposing anticancer drugs against *Plasmodium falciparum* dihydrofolate reductase-thymidylate synthase (*Pf*DHFR-TS)**

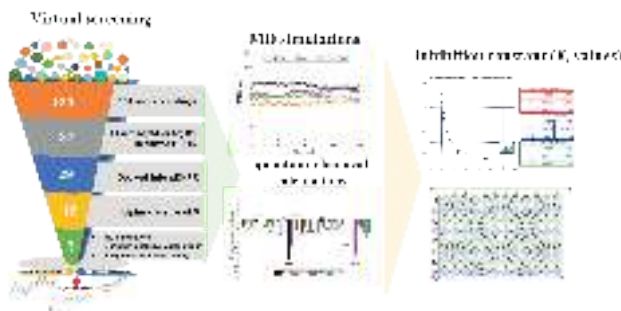
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*Plasmodium falciparum* dihydrofolate reductase-thymidylate synthase (*Pf*DHFR-TS) is an important antimalarial target of antifolate drugs such as Pyrimethamine (PYR). However, the parasite resistance to antifolate drugs causes a serious problem on unsuccessful malaria treatment. The anticancer drugs have already been shown to possess different levels of antimalarial inhibitions. In this work, we employed repurposing drug strategies, performing a stepwise-virtual screening by molecular docking to quickly identify promising drug candidates from 120 anticancer drugs. Three anticancer drugs namely pralatrexate: PRA, pemetrexed: PME, and dasatinib: DAS were identified. Additionally, MD simulations were performed to investigate the stability, fluctuation, and conformational changes during protein–ligand interaction of these anticancer. We found that the systems reached the equilibrium state of the binding site after 20 ns. The RMSF, Rg, SASA, PCA analysis revealed that these systems showed stability and compactness of protein–ligand complexes. Further investigation by quantum chemical calculations to identify key interactive residues of *Pf*DHFR with these anticancer showed that PRA, PME, and DAS bound in *Pf*DHFR active site through H-bond interactions with Asp54 and Ile164, and  $\pi$ - $\pi$  interaction with Phe58. Interestingly, PRA and PME also formed H-bonds interaction with Arg122. There is no H-bond interaction with Ile14 in PME and DAS systems. Finally, the strong inhibitory effect of PRA against wildtype *Pf*DHFR was confirmed by enzyme inhibition assay with inhibition constant of  $0.31 \pm 0.01$  nM, as compared to PYR ( $0.60 \pm 0.02$  nM). The others were with poorer inhibition constant. Based on these results, PRA could be a promising antifolate candidate against *P. falciparum*.

**Keywords:** DHFR; *Plasmodium falciparum*, drug repurposing; virtual screening; anticancer drugs; quantum chemical calculations



**Figure 1.** Discovery of new antimalarials from anticancer drugs through virtual screening and confirmed by enzymatic inhibitory against of *Pf*DHFR.



## Evaluating the binding modes of hepatitis B e-antigen inhibitor by in silico method

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Hepatitis B is a disease caused by the hepatitis virus, which is found in patients' livers and can lead to other harmful diseases. Many studies have shown that drug resistance and chronic hepatitis B infection are associated with the presence of hepatitis B core antigen (HBcAg) and hepatitis B e antigen (HBeAg). In addition, HBeAg could impair patients' innate immunity, leading to a lack of stimulated immunity to disease, and large amounts of HBeAg could weaken patients' immune systems, leading to slow disease diagnosis and treatment. However, knowledge of the structure and interactions between the inhibitor and HBeAg at the molecular level is still elusive, and this molecular detail is the essential key for the study and development of treatments. This work focused on exploring the potential basis of the molecular details between the core protein allosteric modulator (HAP\_R01) and the protein, including the simulation structures and interactions, by performing molecular dynamic simulations. The simulation results were analyzed to discover molecular properties of interactions, along with the simulation of the protein-ligand system. These properties of interactions helped us understand HBeAg inhibition abilities. Due to the similarity of the two antigens, they share similar interaction sites with HAP\_R01. Ultimately, this work will hopefully provide supportive information in molecular detail for acquiring new potential treatments for hepatitis B.

**Keywords:** Hepatitis B virus; Capsid assembly modulator; Core protein allosteric modulator; Molecular dynamic simulation

## Charaterization of volatile compound adsorbed on metal oxide

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Volatile compounds such as acetone ( $C_3H_6O$ ), formaldehyde ( $CH_2O$ ), etc. have been known as hazardous substance. They were utilized in various applications as well as a biomarker. Recently, many materials have been developed for volatile compounds detection because of their advantages in physical and chemical properties. Nevertheless, metal oxide has been recently a renowned material because of its excellent properties compared with the other, such as electrical property, optical property, etc. However, the investigation of volatile compounds sensing response has been still a limitation. In the present research, iron plate was treated by using alkaline solution. Then metal oxide was formed based on hydrothermal method. The previous FTIR results revealed spectral changes in the range of  $1800 - 1000\text{ cm}^{-1}$  when acetone adsorbed on the surface of iron oxide. By reason of cost and simple sample preparation, volatile compounds detection on metal oxide has been monitored. Volatile compounds adsorbed on metal oxide surface caused change of conductivity of the metal oxide.

**Keywords:** Volatile compounds; Metal oxide; Electrical property; Acetone; Formaldehyde



## Binding study of acetylcholinesterase inhibitors from *Centella Asiatica* using molecular dynamics simulations

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Currently, Alzheimer's disease (AD) has been found in over 55 million people around the world, especially elderly people. The dementia is caused by the low neurotransmitter, such as acetylcholine, in the brain leading to the slow communication between brain cells. Currently used drugs such as donepezil can inhibit the activity of acetylcholinesterase (AChE), however most drugs showed various side effects. Search for the new AChE inhibitors from natural products is still challenging. Compounds extracted from *Centella Asiatica* which are asiatic acid, madecassic acid, asiaticoside, and madecassoside, exhibited the AChE activity as compared to eserine, an AChE inhibitor. Therefore, in this work, we investigate how these compounds bind to AChE using molecular docking, molecular dynamics simulations, and the Molecular Mechanics Poisson-Boltzmann Surface Area (MM-PBSA) method. The results showed that the equilibrated MD structures bind deeper in the catalytic site similar to the donepezil, except eserine and a form of madecassic acid which slightly shift from the catalytic site and mainly bind in the peripheral site. The binding energy and residual interaction energies from MM-PBSA are also obtained and confirmed that the key interactions for all compounds are interaction with Trp86, Trp286, and Tyr341. The pharmacokinetics and drug-likeness are also predicted by using ADMET. The results of this work will be helpful to the development of AChE drugs.

**Keywords:** *Centella Asiatica*; MD simulations; Alzheimer's disease; Acetylcholinesterase; MM-PBSA

## A theoretical investigation on depsidones as potential candidates for small cell lung cancer targeting PARP-1 enzyme

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According to the latest Global Cancer Observatory (GLOBOCAN) estimates 2,094,000 new cases of lung cancer were diagnosed globally in 2018, making lung cancer the leading cancer incidence worldwide. Small cell lung cancer (SCLC) is an aggressive form of lung cancer and accounts for approximately 15% of all lung cancers. It is a violent neuroendocrine tumor, with rapid growth and early development of multiple organ metastases. Depsidones are compounds containing two aromatic rings joined by one ester bond and one ether bond. They are found as secondary metabolites in lichens. Each depsidone exists in two major forms, “up” conformation and “down” conformation. Therefore, 14 depsidones, isolated from the fungus *Chaetomium brasiliense*, have been theoretically studied for their potency to be small cell lung cancer drug candidates in terms of their binding affinity to poly(ADP-ribose)polymerase-1 (PARP-1), a DNA-repairing protein, as a protein target of SCLC. In this study, density functional theory (M062X/6-31G(d) method) was used to optimize the geometry of depsidone in both forms. Then, the binding of each compound was investigated using the molecular docking technique. From the molecular docking results, all 14 depsidones in both forms are bound to the active site of PARP-1; however, the depsidone mollicellin E in “up” form gave distinct Goldscore. The obtained findings reveal the most suitable candidate for inhibiting the PARP-1 enzyme and gaining insights into the properties and behavior of depsidones, with the ultimate goal of identifying promising candidates for future drug development.

**Keywords:** Small cell lung cancer (SCLC); Depsidone; Poly(ADP-ribose)polymerase-1 (PARP-1); Molecular modelling; Quantum chemical calculations

## Transient luminescence studies for excited-state kinetics of organic indoline dyes adsorbed on nanocrystalline TiO<sub>2</sub> films

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Dye sensitized solar cells (DSSCs) are typical photovoltaics made of sensitizer dye and mesoporous oxides such as nanoparticles of titanium dioxide TiO<sub>2</sub>. The primary photovoltaic process is electron injection from photoexcited dye molecules to a film of TiO<sub>2</sub>. This process may compete with other intramolecular decay pathways involving radiative and nonradiative transitions. In the present study, we have conducted time-resolved fluorescence spectroscopy of the DSSC anodes containing indoline dyes D149 and D205. These dyes were made to adsorb on thin films of TiO<sub>2</sub> and ZrO<sub>2</sub>, which allowed us to make a comparison between the fluorescence lifetimes, respectively, with and without electron injection. Figure 1 shows the results of time-correlated single photon counting (TCSPC) measured at 470 nm photoexcitation, that is, fluorescence decay curves of D149 on the TiO<sub>2</sub> film (red) and on the ZrO<sub>2</sub> film (blue), as well as the curve of D149 dissolved in chloroform (black). We assumed that the fluorescence lifetime for D149 in chloroform agrees with its radiative lifetime from the S<sub>1</sub> state. Thereby we could determine the rate constants for the following deexcitation processes of high-vibrational levels of the S<sub>1</sub> state (hereafter denoted as S<sub>1</sub><sup>\*</sup>(v)): (a) relaxation to the vibrational ground state of S<sub>1</sub>, (b) non-radiative internal conversion to the S<sub>0</sub> state, and (c) electron injection from S<sub>1</sub><sup>\*</sup>(v) to the conduction band of TiO<sub>2</sub> film. Evaluating the rate constant for the electron injection required the ratio of fluorescence intensity on the ZrO<sub>2</sub> electrode to that on TiO<sub>2</sub>.

**Keywords:** Indoline dyes; Fluorescence; TCSPC; Electron injection; Solar cells

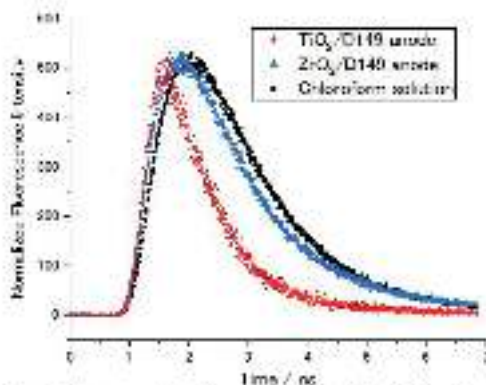


Figure 1. Time-correlated fluorescence signal from D149 on the TiO<sub>2</sub> and ZrO<sub>2</sub> films, as well as from D149 in chloroform

## Theoretical study on butylone inclusion complexes with $\beta$ -cyclodextrin and its three methylated derivatives

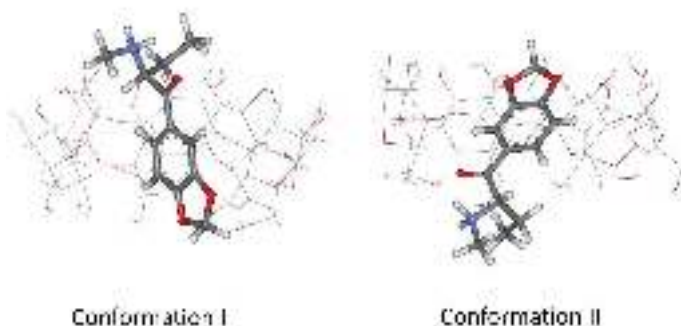
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Butylone, or  $\beta$ -keto-N-methylbenzodioxolylbutanamine, is a class of psychoactive substances with a chiral center, so it may exist as two stereoisomers with different biological activities. However, the process of enantiomeric separation can be quite complex as enantiomers are difficult to separate from one another. Cyclodextrins (CDs) are cyclic oligosaccharides with a central hydrophobic cavity. CDs are the most commonly used as chiral selectors because they possess a wide variety of cavity sizes, side chains, degrees of substitution, and charges. The hydrophobic cavity of the CDs is responsible for the formation of inclusion complexes with enantiomers, where one enantiomer shows higher binding affinity than the other. In this study, molecular docking and PM6 calculations for the enantiomeric recognition of (*R*)- and (*S*)-butylone were developed by means of native  $\beta$ -cyclodextrin (BCD) as well as three of its derivatives, namely heptakis(2-*O*-methyl)- $\beta$ -cyclodextrin (2-MEB), heptakis(2,6-di-*O*-methyl)- $\beta$ -cyclodextrin (2,6-DIMEB), and heptakis(2,3,6-tri-*O*-methyl)- $\beta$ -cyclodextrin (TRIMEB). The findings indicate two distinct orientations of butylone within cyclodextrin's cavity, depicted in Figure 1, with a 1:1 molecular ratio. According to the complexation energy results for the (*S*)-butylone/BCD system at the M062X/6-31G(d,p) level, Conformation II exhibits a lower complexation energy (-16.52 kcal/mol) compared to Conformation I. This suggests that Conformation II is more favorable.

**Keywords:** Inclusion complex; Host-guest interaction; Molecular docking; Semi-empirical method; Density functional theory



**Figure 1.** The M062X/6-31G(d,p) structure of (*S*)butylone/BCD inclusion complexes.



## Virtual screening of “Prab-Chompoo-Taweep” remedy targeting acetylcholinesterase for Alzheimer disease

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At present, thirty percent of people worldwide suffer from Alzheimer's disease (AD) especially for older adults with 60 years of age or older. The primary factor is a reduction in neurotransmitters, specifically acetylcholine, which prevents communication between brain cells. Medication like donepezil and possible natural therapies are among the current treatments for AD. However, current approved drugs exhibit some side effects and cannot successfully cure the AD. Therefore, the searching for new AD drugs is challenging. In this work, we looked for the natural compounds from herbs in one of the Thai traditional medicines, “Prab-Chompoo-Taweep” remedy, which can inhibit Acetylcholinesterase (AChE) using virtual screening techniques. Molecular docking methods using GOLD program and ADMET prediction were applied in this study. From the literatures, about 1,102 compounds were found from herbs which are ingredient of “Prab-Chompoo-Taweep” remedy. From molecular docking, Dahuribirin A was identified as a candidate to inhibit AChE with the goldscore of 108.35. As compared to the donepezil which is the approved drug, Dahuribirin A also revealed the similar interaction to AChE which are Trp86, Trp286, Tyr337, and Tyr341. ADMET profiles of Dahuribirin A were also predicted to confirm the drug-likeness property. Therefore, this study suggested that Dahuribirin A might be the potent AChE inhibitor and was selected for further study for the development of AD drug.

**Keywords:** Alzheimer's disease; Acetylcholinesterase; Donepezil; Molecular docking; ADMET

## Improving hydrophobicity in 3D printing of resin inks with porogen additives and micro-pillar structures

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The study of hydrophobicity is significant for applications such as self-cleaning, anti-fouling, and water-repellency in materials. It has recently gained particular interest for enhancing 3D printed surfaces. Common methods to achieve hydrophobicity include coatings, the use of inherently water-repellent additives, or surface texture modifications. However, coatings often suffer from mechanical instability and limited durability. This study aimed to enhance the resin inks used in stereolithographic LCD 3D printing by introducing specific additives that could interfere with polymerization. Porous agents, or porogens, containing different long-chain alcohols (PP, BT, PT, PH, CH, and DD), were blended into commercial resin inks (AA, AB, AH, and JS) and solidified using a 405-nm curing machine. The results showed that the AB:CH mixture with a ratio of 60:40 significantly increased the water contact angle from 61.5 to 122.2 degrees. The hydrophobic properties were attributed to the nanoscale roughness of inherent pores observed via scanning electron microscopy. This modification likely affected material hardness, reducing the shore D hardness from 85.9 to 65.0. Additionally, an array of micro conical pillars, each 300  $\mu\text{m}$  in height and 240  $\mu\text{m}$  in width, was designed and printed using the developed resin ink with a commercial LCD 3D printer. The capillary pressure from the pillars further improved the material superhydrophobicity, achieving a water contact angle higher than 140.0 degrees. These results present a promising strategy for enhancing hydrophobicity in 3D printed materials, potentially benefiting fields such as medicine, automotive, and electronics.

**Keywords:** LCD 3D printing; Hydrophobicity; Contact angle; Nanopore

## Elucidation of the specific interactions between benzimidazole derivatives and InhA based on *ab initio* fragment molecular orbital calculation

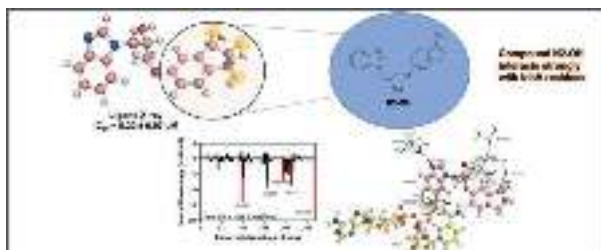
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2-trans enoyl-acyl carrier protein reductase (InhA) has been identified as a potential drug target in the field of anti-tuberculosis drug development. In the present study, we first designed novel compounds based on ligand X-ray structure that obtained from our previous study (PDB code: 6R9W) as well as benzimidazole derivatives. To elucidate the binding energies and the specific interactions between InhA and our designed derivatives using *ab initio* fragment molecular orbital calculation. Only hydrogen atoms were optimized using the B3LYP/6-31G (d, p) method. We fitted the structure of our designed derivatives to the ligand X-ray structure of its complex with InhA, using GROMACS version 2016.5. The structures were fully optimized using MM optimizations. We designed novel compounds by replacing H atom at the R1, R2, or R3 site of the 2,3-dihydro-1H-indene ring of ligand X-ray structure. The results evaluated by FMO highlight some key interactions between InhA and the derivatives, indicating that the most potent derivative has strong interaction with a water molecule, Gln100, Ala157, Ile215, and NAD<sup>+</sup>. In addition, as compared with the conformation of ligand obtained from the X-ray crystallographic data, the enhancement of the size of R2 substitution results in the changes in total IFIE from -103.1 to -118.2 kcal/mol. Finally, the results obtained from this study enhances our understanding of the structural basis for benzimidazole derivatives, enabling the rational design of more potent InhA inhibitors as potential tuberculosis agents.

**Keywords** benzimidazole derivatives; InhA inhibitors; anti-tuberculosis drug; *ab initio* fragment molecular orbital calculation; binding energies



## Development of catalytic performance of heterogeneous catalysts based on Cu embedded in graphitic carbon nitride for CO<sub>2</sub> hydrogenation reaction to formic acid: A DFT study

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Carbon dioxide (CO<sub>2</sub>) is one of the greenhouse gases released from fossil fuel combustion. The enhancement of CO<sub>2</sub> concentration leads to the global warming effect. The hydrogenation of carbon dioxide into formic acid (CO<sub>2</sub> + H<sub>2</sub> → HCOOH) is a promising reaction that can both reduce greenhouse gases and produce useful value-added compounds. In this work, the mechanism of CO<sub>2</sub> hydrogenation over the Cu-based catalyst has been investigated by means of Density Functional Theory (DFT). The Cu atom embedded in the g-C<sub>3</sub>N<sub>4</sub> monolayer has been constructed for the conversion of CO<sub>2</sub> into formic acid. Firstly, the stability of CO<sub>2</sub>, H<sub>2</sub> molecule, and co-adsorption complex (Co-Ads) were examined. Our calculations found that the adsorption energies of CO<sub>2</sub>, H<sub>2</sub>, and co-Ads are calculated to be -0.23, -0.44, and -0.63 eV, respectively. Moreover, co-Ads can be formed on Cu-g-C<sub>3</sub>N<sub>4</sub> catalysts which implies that CO<sub>2</sub> hydrogenation can proceed *via* a co-adsorption pathway via two important intermediates, namely (i) formate (HCOO) and (ii) carboxylate (COOH). To gain insight into the HCOOH formation, the mechanistic study of CO<sub>2</sub> hydrogenation has been investigated by the DFT method. The future applicability of Cu-based catalysts was also evaluated in this work.

**Keywords:** DFT; CO<sub>2</sub> conversion; Cu-based catalysts; g-C<sub>3</sub>N<sub>4</sub>; Formic acid



## Density functional theory study on the radical scavenging activity of five hydroxycinnamic acid derivatives from wine

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Hydroxycinnamic acids are the abundant group of polyphenols in grapes and the predominant group in wine. In this study, density functional theory (DFT) has been employed to investigate the radical scavenging activity of five hydroxycinnamic acid derivatives: caffeic acid, ferulic acid, p-coumaric acid, o-coumaric acid, and sinapic acid. Geometry optimization and frequency analysis of all naturally occurring systems including neutrals, radicals, radical cations, and anions have been calculated at the B3LYP functional and 6-311++G(2d,2p) basis set. The solvent effect has been explored in water and ethanol by using the integral-equation-formalism polarizable continuum model (IEF-PCM). Their global reactivity descriptors have been calculated to reveal their reactivity as an antioxidant. As a result, sinapic acid is the most reactive antioxidant according to the lowest phenolic O-H bond dissociation enthalpy (BDE) at 50.43 kcal/mol. It has been found that hydrogen atom transfer (HAT) is more favored in the gas phase. Also, the effect of solvent polarity on antioxidant activity has been explored for sinapic acid. The results disclosed that the polarity of the solvent increases the contribution of single-electron transfer followed by proton transfer (SET-PT) and sequential proton loss electron transfer (SPLET).

**Keywords:** Density functional theory (DFT); Radical scavenging activity; Polyphenols; Hydroxycinnamic acids

# Mechanisms of nickel and palladium catalyzed ethylene and carbon monoxide copolymerization: a density functional study

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Nickel and palladium catalysts have been developed for the copolymerization of ethylene with carbon monoxide (CO). The copolymerization involves two main pathways: (i) the alternating copolymerization resulting in polyketone, and (ii) the non-alternating copolymerization resulting in the high ratio of ethylene to CO in the polymerization product. The cationic Ni(II) and Pd(II) complexes with the diphosphazane monoxide ligand (PNPO) have been reported to perform copolymerization of C<sub>2</sub>H<sub>4</sub> with CO resulting in polyketone. Herein, we performed density functional calculations using the cationic Ni(II) and Pd(II) complexes with the PNPO ligand to study their mechanisms that involve (i) the alternating pathway, in which the CO insertion is followed by the C<sub>2</sub>H<sub>4</sub> insertion, and (ii) the non-alternating pathway, in which the C<sub>2</sub>H<sub>4</sub> insertions occur consecutively at M06/LANL2DZ/6-311++G(d,p)(SMD,solvent=THF)//B3LYP/LANL2DZ/6-31G(d) level of theory. According to the calculated free-energy profiles, the alternating pathway is more favorable than the non-alternating pathway for both Ni and Pd catalysts. For the alternating pathway, the CO insertion into the M-R bond (M = Ni, Pd) is facile while the C<sub>2</sub>H<sub>4</sub> insertion into the M-(CO)R bond is the rate determining step. The overall energy barrier using the Ni(II) catalyst is lower than that using the Pd(II) catalyst. Especially, the energy barrier of the C<sub>2</sub>H<sub>4</sub> insertion in the alternating pathway using the Ni(II) catalyst is notably lower than using the Pd(II) catalyst. This is in agreement with the experiment in that the activity of the copolymerization catalyzed by the cationic Ni(II) was found higher than that catalyzed by the corresponding cationic Pd(II).

**Keywords:** Ni catalyst; Pd catalyst; Copolymerization; Polyketone; Density functional theory

## Incorporating organic pigments as photoblockers in commercial resin inks to improve micro-scale resolution in 3D printing

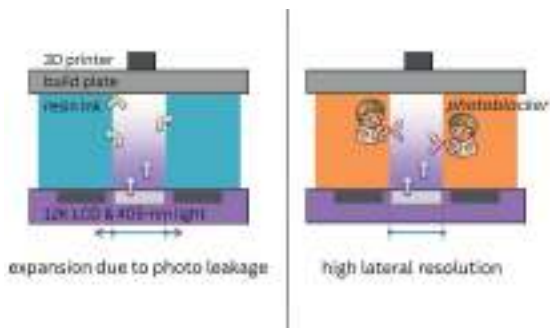
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In recent years, 3D printing has undergone rapid development, enabling the creation of objects ranging from microscale components to large-scale structures. LCD 3D printing, a popular and inexpensive method, employs an LCD screen to project an illumination pattern that solidifies liquid resin into 3D objects. However, this process often encounters challenges like shrinkage, warping, and limited resolution, potentially leading to defects in the final product. This study investigated the polymerization kinetics of five commercial colorless resin inks (JS, AB, AH, and AA). The polymerization reaction was initiated using a blueish 405-nm excitation wavelength with a gentle illumination intensity of  $6.2 \text{ mW/cm}^2$  generated by a curing machine. Among the tested resins, JS exhibited the highest polymerization depth rate at  $63.32 \text{ }\mu\text{m/s}$ . The research then explored the effect of five commercial organic pigments (Y12, O13, R112, G7, and B15) as photoblockers or excitation absorbers on polymerization depth rate and printing resolution. The addition of 0.05% w/v O13 coloring agent to JS significantly reduced the polymerization rate by a factor of five. This could improve lateral resolution to  $12.6 \text{ }\mu\text{m}$  in a 12K-LCD 3D printer, while maintaining a high-speed printing rate of under 3 seconds per layer. These findings suggest the feasibility of developing new resin inks tailored for LCD 3D printing, capable of achieving high-resolution results. Such advancements have the potential to drive the creation of innovative commercial products requiring exceptional precision.

**Keywords:** Photoblocker; 3D printing; Resin ink; Organic pigment; High resolution



## Utilization of *Dialium Cochinchinensis* Shell: Preparation and characterization of composite beads activated carbon

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*Dialium cochinchinense* shell (DS) as Pattani local agricultural waste were prepared two composite bead adsorbents: Gelatin/DS (GE-DAC) and Polylactic acid/DS (PLA- DAC) for adsorption process. Under characterization, it was found that the iodine number is highest in the ratio Char and KOH was 1:1.5 giving the highest iodine adsorption value of 603.61 mg g<sup>-1</sup>. The SEM image shows that GE-DAC has less porosity than PLA-DAC and has an average pore size in mesopore. The GE-DAC and PLA-DAC had the specific surface area of 80.96 and 154.65 m<sup>2</sup> g<sup>-1</sup>, respectively. The composite bead adsorbents could provide an alternative granular adsorbent for the adsorption process.

**Keywords;** Polylactic acid; Gelatin; *Dialium cochinchinensis* seed; Activated carbon; Composite Beads

## Computer predictions of hydrogen energy storage on boron nitrogen four-membered ring structure

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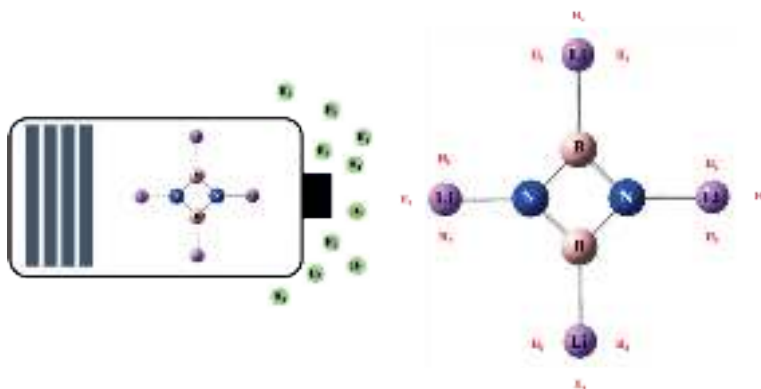
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Clean and sustainable energy is refining the role of decisive attraction based on renewable fuels. A new platform of boron nitrogen heterocyclic ring is in charge demonstration on Lithium-ion batteries (LIBs) and hydrogen ( $H_2$ ) storage systems. In this work, the possible boron nitrogen four-membered structure was particularly investigated regarding the capacity of lithium (Li) atom and  $H_2$  molecule via Density Function Theory (DFT) calculations by second-order Møller-Plesset perturbation theory (MP2) utilized in a def2-TZVP basis set with the Gaussian 16 package. The results showed the promising storage performance of the four Li-decorated  $B_2N_2$  structure ( $B_2N_2Li_4$ ), where the maximum adsorption energy of  $H_2$  is up to 12 molecules. This calculation has a potential to develop boron nitrogen materials for exploration in short- and long-term hydrogen technology.

**Keywords:** Sustainable energy; Hydrogen energy storage; Lithium



Lithium-ion batteries (LIBs) and hydrogen ( $H_2$ ) storage systems on boron nitrogen four-membered ring structure

## A theoretical study focusing on the design and development of efficient photocatalysts for water-splitting for hydrogen production

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Excessive consumption of fossil fuels leads to carbon dioxide ( $\text{CO}_2$ ) emissions and climate change. Hydrogen ( $\text{H}_2$ ) is an alternative energy source that can replace fossil fuels due to its clean and sustainable nature. This work aims to investigate the photocatalytic hydrogen evolution reaction (HER) on nitrogen-doped zigzag (7,0) and (8,0) carbon nanotubes (CNT) incorporating platinum metal (Pt) and hydroxyl additives ( $\text{C}_2\text{H}_6\text{O}_2$ ,  $\text{C}_6\text{H}_7\text{O}_6$  and  $\text{C}_6\text{H}_{15}\text{NO}_3$ ). The density functional theory (DFT) method with the M06-2X function enhances hydrogen production efficiency. The 6-311G\* basis set is used for C, N, O, and H atoms, while the LANL2DZ basis set is applied to the Pt atom. To assess the structural stability by considering the binding energy, the  $\text{PtN}_4$ -CNT (7,0) and  $\text{PtN}_4$ -CNT (8,0) exhibit a binding energy of -9.27 eV and -5.05 eV, respectively. These binding energy values confirm the presence of a strong interaction between Pt and the supporting substrates. Energy gaps (HOMO-LUMO gaps) were also calculated, as these gaps are crucial for the photocatalyst's water-splitting capability. The energy gaps are 1.80 eV and 1.43 eV for  $\text{PtN}_4$ -CNT (7,0) and  $\text{PtN}_4$ -CNT (8,0), respectively. The calculation results revealed that the energy gap between HOMO and LUMO was not within the optimum range for water splitting using photocatalysts. Consequently, it was improved by introducing hydroxyl groups. In the next step, we will investigate detailed information regarding hydrogen adsorption efficiency and the HER reaction mechanism on the catalysts.

**Keywords:** Hydrogen evolution reaction; Carbon nanotubes; Density functional theory; Hydroxyl additives; Photocatalysis



## Development of a new reaction for amide synthesis from Benzocyclobutenone and amines based on the reaction path network

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Amides are an important functional group found in many natural products and medicines. Synthesis of amides is one of the most frequent transformations and still has been intensively studied. To discover new chemical reactions, our group has developed a new quantum chemical calculation method of the retro-synthesis pathways. It enables us to predict the starting materials using only information about the target product molecules. One of the calculation results revealed the new transformation to affording amide from Benzocyclobutenone (BCB) and amine. In this work, chemical experiments will be conducted to confirm the calculation results, and the additional quantum chemical calculations of the BCB and several amines will be investigated. A protic solvent, high concentration, excess amount of an amine, and stoichiometric amount of acid as an additive under thermal condition were found to be important factors in achieving a high yield of amide products. The Gibbs energy of activation ( $\Delta G^\ddagger$ ) of the ring opening of BCB with different amine structures was calculated using GRRM20 program with Gaussian 16 rev. C.02. The calculation results showed that lower  $\Delta G^\ddagger$  of the amide productions were observed when BCB reacts with amines having aliphatic character, high basicity, and low steric hindrance.

**Keywords:** Amide; Amine; Benzocyclobutenone; DFT; GRRM

## Role of trace elements affecting coloration in blue, yellow, and green synthetic corundum

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Corundum ( $\text{Al}_2\text{O}_3$ ), commonly known as sapphire, is an allochromatic mineral that can produce a variety of colors depending on the transition metal inclusions present in its crystal structure such as  $\text{Fe}^{3+}$  in yellow corundum or Fe-Ti pair in blue corundum. Although we have a general knowledge of the factors that give corundum its color, the underlying mechanism for each color variety is still being debated and is a topic of controversy to this day. Green corundum is one color for which there has not been a dedicated study focused on its color mechanism. The leading theory suggests that it is a combination of blue and yellow corundum. To study the theory, we selected and analyzed blue, green, yellow, and colorless synthetic corundum using Colorimeter, Energy Dispersive X-ray Fluorescence (EDXRF), Ultraviolet-Visible-Near Infrared Spectroscopy (UV-Vis-NIR), and X-ray Absorption Spectroscopy (XAS). These analyses aim to determine the underlying color mechanism and construct an energy band model for the corundum samples. The energy band gap ( $E_g$ ) calculations for synthetic corundum resulted in values of 4.30 eV for blue, 4.01 eV for green, and 3.62 eV for yellow. While the colorless specimen has a narrow  $E_g$  of 4.10 eV due to high turbidity. The energy band model for synthetic blue corundum incorporates the  $\text{Fe}^{3+}\text{-Ti}^{4+}$  mixed acceptor state while the model for synthetic yellow corundum utilizes the  $\text{Fe}^{3+}$  neutral energy state. Synthetic green corundum, on the other hand, employs both  $\text{Fe}^{3+}\text{-Ti}^{4+}$  mixed acceptor state and  $\text{Fe}^{3+}$  neutral state to explain its energy band model.

**Keywords:** Synthetic corundum; Color mechanism; Energy band model; X-ray absorption spectroscopy; UV-Vis-NIR spectroscopy.

## Evaluation of the aromaticity of two star[3]calicene isomers

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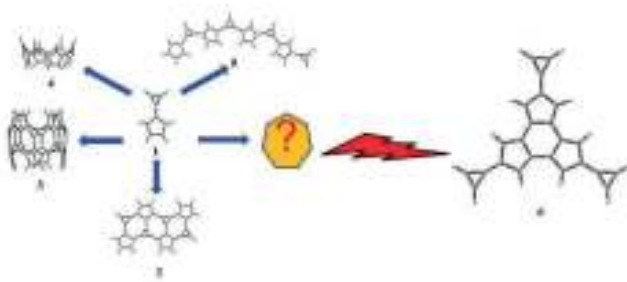
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Polycalicenes are an essentially unexplored region of chemical space. Polycalicenes are polymers of the monomer calicene **1**, also known as triapentafulvalene. One provocative feature of polycalicenes is that even though calicene has never been synthesized, a few polycalicenes have been synthesized and shown to be aromatic. Polycalicenes encompass a vast region of chemical space as it is easy to envision different polycalicene families by changing the bonding motif between the calicene monomers. In previous studies, we have investigated several polycalicene families (2-5) as illustrated in **Figure 1**. This study explores the aromaticity of two isomers of a new polycalicene family, star[3]calicene **6** (shown in **Figure 1**), using density functional theory (DFT). Star[3]calicenes have a star shape where [3] indicates the number of calicene monomers. The aromaticities of these two star[3]calicene isomers were evaluated using Schleyer's nucleus independent chemical shift (NICS). All geometries, vibrational frequencies, and properties (dipoles, NMR, etc.) of all molecules are reported at the B3LYP/6-31+G(d,p) level of theory. Calicene, benzene, cyclopentadienyl anion, and cyclopropenyl cation are reported as references.

**Keywords:** Calicene; Polycalicene; Aromaticity; NICS; DFT



**Figure 1** Star[3]calicene **6** representing a new family of polycalicenes

## Computational design of Ni catalysts for C-H activation and hydroarylation of alkenes

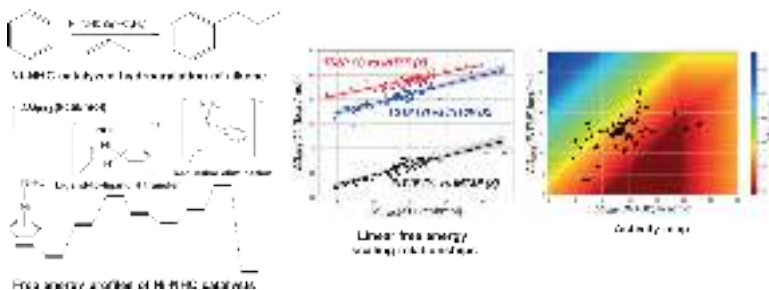
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Nickel N-heterocyclic carbene (Ni–NHC) complex-catalyzed hydroarylation of alkenes is a promising method for linear alkylbenzene synthesis. For unsubstituted arene, i.e., benzene, the reaction yields are still moderate. The structural modification of the ligand can potentially improve the catalytic activity. In this work, free energy profiles and linear free energy scaling relationships (LFESRs) for 70 Ni catalysts were explored by varying the NHC ligand structures. An activity map was plotted linking the energy span to two descriptors: (i) the relative free energy of an intermediate formed from ligand-to-ligand hydrogen transfer ( $\Delta G_{\text{RRS}}(\text{INT3P})$ ) and (ii) the relative free energy of an intermediate undergoing reductive elimination ( $\Delta G_{\text{RRS}}(\text{INT5P})$ ). Achieving a relatively low energy span requires minimizing  $\Delta G_{\text{RRS}}(\text{INT5P})$  while maintaining  $\Delta G_{\text{RRS}}(\text{INT3P})$  within a certain range. Additionally, linear relationships between buried volume and energy span were observed within groups of NHC ligands sharing common structural moieties. Overall, the favorable NHC characteristics for Ni catalysts were those with substantially large backbone, and with a diisopropylphenyl group or larger substituent group at the nitrogen on the backbone of the NHC. These insights pave the way for optimizing the catalytic activity of Ni catalysts in the hydroarylation of alkene with benzene facilitating the catalyst design process.

**Keywords:** Ni catalysts; Hydroarylation of alkene; Linear free energy scaling relationships; Activity map; Catalyst design





## A potential approach for modeling the time-evolution of the properties of defective MoS<sub>2</sub>

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Vacancies on MoS<sub>2</sub> are important for its catalytic activity, which in return depends on the size and shape of the vacancies. This study addresses whether the S-vacancies on MoS<sub>2</sub> tend to form specific patterns and how fast the surface patterns change. Using activation barriers at DFT-PBE level as input, we have constructed a kinetic Monte Carlo (kMC) model to simulate a 25×25 MoS<sub>2</sub> supercell with 6% vacancy coverage rate. It could be shown that the S-vacancies are highly dynamical, and tend to form an alternating pattern of S-atoms and vacancies. However, this provides only limited information about the chemical properties, which are related to the electronic structure as characterized by the electronic density of states (DOS). Unfortunately, evaluating the DOS at DFT level is only possible for a system of limited size. Thus, we propose an approach to estimate a large structure's DOS from a DFT-level database of projected DOS (PDOS) for atoms in varying environments. The DOS of the total system can be obtained by analyzing the environment of each atom in the system and adding up the corresponding PDOS. It has been found that, to get the DOS, the PDOS data from different calculations have to be normalized and aligned at the low lying electronic bands. So far, we have a proof-of-concept that this approach can be used to estimate the DOS of a system. In the future, this approach will be coupled with the kMC program to simulate the time evolution of the electronic structure.

**Keywords:** Kinetic Monte-Carlo; First-principles modeling; Electronic structure; DOS; PDOS