



اَللّٰهُمَّ صَلِّ وَسَلِّمْ عَلٰى نَبِيِّنَا  
UNIVERSITI  
TEKNOLOGI  
MARA

# The 5th International Conference on Chemistry and Material Sciences 2023



## **Book of Abstracts:**

Analytical / Bio / Inorganic / Organic / Physical  
Chemistry

Molecular Science

Functional Materials

Renewable Energy and Fuel Cell

Material: Synthesis and Characterization

Nanomaterials and Nanodevices

## Opening Speech Rector of Universitas Brawijaya

Assalamualaikum Warahmatullahi Wabarakatuh



On behalf of organizing committee of IC2MS 2023, I would like to extend my warmest welcome to all delegates of IC2MS 2023. Welcome to Malang, one of the educational cities in Indonesia. There are about 40 universities in Malang. The largest university in Malang is Universitas Brawijaya. Universitas Brawijaya is also included in the top ten best universities in Indonesia.

IC2MS is an international conference conducted every year, formerly organized by Chemistry Department, Faculty of Science, Universitas Brawijaya. And next IC2MS is co-organized by other universities, including Universitas Negeri Malang, Universitas Jember, and Universiti Teknologi Mara, Malaysia.

IC2MS 2023 aimed to promote mutual exchange between scientists and experts, to discuss of new research results in the fields of chemistry and materials science. The conference will facilitate researchers and academic members from universities, government institutions, private sectors, and non-government organization to share their knowledge through the discussion on plenary session, and parallel session of oral presentation.

This year the topic of IC2MS 2023 is "Post Pandemic Challenges: The Role of Chemistry and Material Sciences". This topic is suitable with the condition of our nation this year, where we are ready to achieve more prosperity and development post COVID-19 pandemic.

I believe that IC2MS 2023 should bring advantages for all participants. They will learn many new aspects of research in the related topics, either from keynote speakers, invited speakers, or general participants. In addition, collaborations between Universitas Brawijaya and other universities both from Indonesia and overseas can be initiated.

Finally, I would like to express my gratitude to keynote and invited speakers of IC2MS 2023, for their expertise and knowledge they will bring to the conference, and of course the warm discussion of their talks. Special thanks are also extended to the members of organizing committee for their hard work in bringing this conference together. And last but not least, I would like to thank all of the conference participants who will contribute to making the most memorable IC2MS 2023.

I will also officially open IC2MS 2023, Please enjoy IC2MS 2023 and have a delightful seminar.

Wassalamualaikum Warahmatullahi Wabarakatuh

Sincerely yours

**Rector of Universitas Brawijaya**

## Welcoming Remarks from the IC2MS 2023 Chairman



On behalf of the Organizing Committee, I would like to welcome all of you, keynote speakers, invited speakers, distinguished guests, presenters, and participants, to the 5<sup>th</sup> International Conference on Chemistry and Materials Science (IC2MS 2023). The IC2MS is an annual scientific meeting co-organized by Universitas Brawijaya, Universitas Negeri Malang, Universitas Jember, and this year together with Universiti Teknologi Mara, Malaysia. This meeting aimed to promote mutual exchange between scientists and experts, to discuss innovative ideas in scientific research, and to handle contemporary problems through the application of knowledge that rise from chemistry and materials science fields.

The IC2MS 2023 runs for 2 days, 11-12 October 2023. This year topic for IC2MS 2023 is "Post Pandemic Challenges: The Role of Chemistry and Material Sciences,"

and consists of several related topics, including:

- Analytical / Bio / Inorganic / Organic / Physical Chemistry
- Molecular Science
- Functional Materials
- Renewable Energy and Fuel Cell
- Material: Synthesis and Characterization
- Nanomaterials and Nanodevices

This year conference will be held as a full offline conference, no more online presentations.

Around 100 people are attending this conference. They consist of 70 presenting participants, 20 non-presenting participants, 5 keynote speakers, and 5 invited speakers. In terms of country of origin, the participants of the IC2MS 2023 are coming from 5 different countries, including Indonesia, Japan, Malaysia, Australia, and Thailand.

The IC2MS 2023 covers broad range of research in the fields of chemistry and materials science. This international forum also provides a platform where national and international academia or researchers, policy makers, and other stakeholders to translate technology, exchange ideas, and help stimulate multidisciplinary international collaborations for shaping a worldwide sustainable development. It is worth noting that, IC2MS 2023 event genuinely highlights the important of recent advances in chemistry and materials science to address community life in post pandemic era.

The IC2MS 2023 could not become a reality without the help and assistance of many parties. Thus, in this occasion I would like to sincerely thank to our keynote speakers:

- Prof. Nobuyuki Matubayasi from Osaka University
- Prof. Masato Tominaga from Saga University
- Prof. Justin M. Chalker from Flinders University
- Prof. Dr. Mohd Fazli Mohammat from Universiti Teknologi Mara
- And Assoc. Prof. Atitaya Siripinyanond from Mahidol University

I also thank to our invited speakers, Rector of Universitas Brawijaya, Dean of Faculty of Mathematics and Natural Sciences, Universitas Brawijaya, Head of Chemistry Department, Universitas Negeri Malang, Universitas Jember, Universitas Teknologi Mara, and all members of the Organizing Committee, who have provided meaningful help and assistance for the implementation of this conference.

Finally, we have tried to do our best to prepare IC2MS 2023. Nevertheless, there is nothing completely perfect in the world, including this conference. Therefore, please accept our deep apologizes for any inconveniences found in this conference.

Please enjoy the ICMS2 2023, and your stay in Malang.

Malang, 11 October 2023

Chairman of the Organizing Committee

**Dr. Elvina Dhiaul Iftitah**

## **KEYNOTE ADDRESSES**

# Innovative Material and Electrochemistry for Sensing Application Advancement and Microbial Energy Conversion

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**Keywords:** carbon nanotubes, cobalt nanoparticles, cellulose nanofiber, electrode, fuel cell

## Abstract

Electrochemistry has become increasingly important recent years in maintaining a sustainable environment and solving energy problems. Additionally, innovative materials have been developed for supporting electrochemical reaction. Nanomaterials such as nanocarbon and nanometallic nanoparticle are a typical innovative material. In the present study, I would like to introduce latest achievement by using nanocarbon, nanometallic particle and nanofiber in Tominaga laboratory group as follows.

### Phosphate ion detection at cobalt oxide nanoparticles supported MWCNTs electrodes

A new phosphate ion sensor based on cobalt oxide nanoparticles (CoONPs) hybridized with polybenzimidazole (PBI) and multi-walled carbon nanotubes (MWCNTs) was developed (Fig. 1) [1,2]. The synthesized CoONPs were shown to be well dispersed on the MWCNTs and exhibit a uniform size of 3.5–5.5 nm, mainly comprising hexagonal  $\text{Co}_3\text{O}_4$  with a fraction of CoO. The effects of morphology and microstructure on electrochemical performance were investigated to reveal that the CoONPs-containing electrode exhibited a considerably higher sensitivity than that of the bulk Co wire electrode. Specifically, the former electrode could sense phosphate at pH 4 and 7 and at concentrations (0.1–100 nM) lower than the eutrophication threshold. The CoONPs/PBI/MWCNT electrode was successfully used to detect phosphate in actual creek water samples.

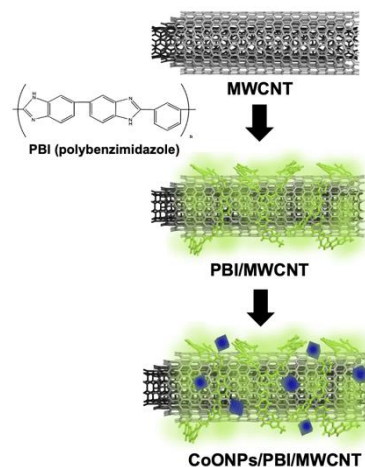


Fig. 1 CoONPs/PBI/MWCNT electrode.

### Amoxicillin detection at green cellulose nanofiber-based MWCNTs printed electrode

Single-use printed cellulose nanofiber (CNF)-based electrode modified with polybenzimidazole (PBI)-wrapped multi-walled carbon nanotubes (MWCNTs) has been developed for amoxicillin (AMX) detection [3]. The CNF-based printed electrode achieved a detection limit of 0.3  $\mu\text{M}$  and exhibited a wider detection range of 0.3–500  $\mu\text{M}$ . In addition, the electrode reactions of AMX were electrochemically investigated and found to primarily involve the adsorbed species at low AMX concentrations and be diffusion-controlled at high AMX concentrations. The developed CNF-based electrodes were used for the easy and practical determination of AMX in seawater and tap water via a soaking method.

## Skin alcohol gas detection at CNF-based MWCNTs electrode modified with enzyme

Gases of various components are released from skin and breath of the human body. Since the composition of the gas depends on health conditions and diseases, this sensing is useful for health science technology. Biogas sensing technology with specific, high-sensitivity, and low-cost measurements will greatly contribute to human health care. Our group has developed ultra-high sensitive alcohol gas sensor to detect alcohol gas on skin utilizing MWCNT electrode modified with PQQ-ADH (pyrroloquinoline quinone–alcohol dehydrogenase) on a CNF film platform. We have achieved alcohol gas detection at 25 ppb level (Fig. 2).

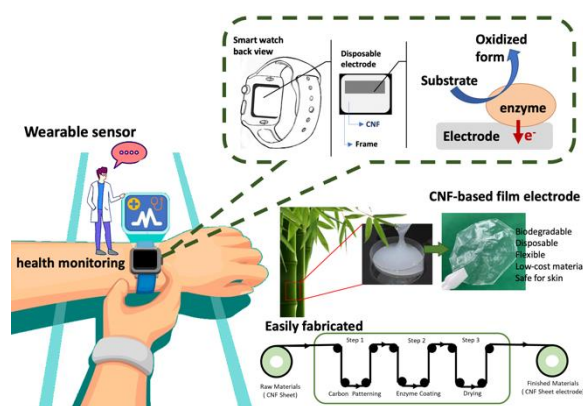


Fig. 2 Image of future use of a skin gas sensor.

## Microbial fuel cell for energy conversion

Microbial fuel cell (MFC) converts chemical energy to electrical energy with the aid of microorganisms as biocatalysts [4]. Recently, we have developed new type of MFC, which has cylinder shape and easily operating inside a sediment such as paddy field. The MFC was applied to operate a sensor for humidity and temperature measurement as well as a power source to transmit the data (Fig. 3). The MFC provided the maximum voltage of 400 mV and the maximum current of 2.5 mA. This sensor has been running for more than 18 months with only the MFC power supply.

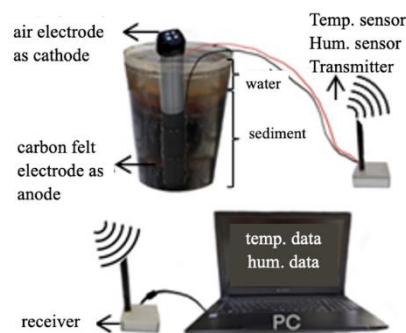


Fig. 3 Image of future use of a skin gas sensor.

## References

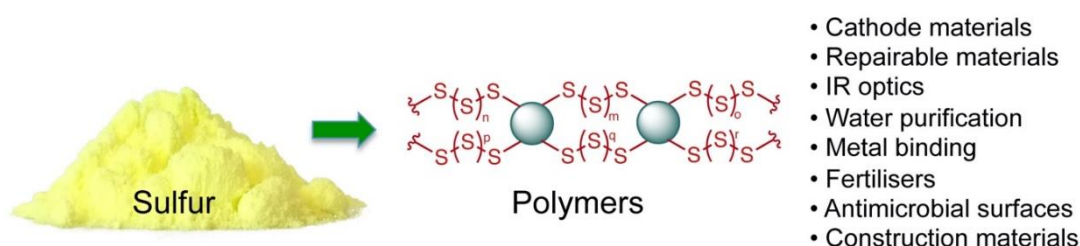
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# New Frontiers in Polymers Made from Sulfur

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Sulfur is an abundant feedstock generated in millions of tonnes each year in petroleum refining. Converting this sulfur into useful polymers is one way to repurpose this surplus industrial product (1). In our laboratory, the overarching goal is to use these polymers in applications that benefit the environment and human well-being (2,3). In this presentation, I will discuss design principles for making these sulfur polymers with tailored thermal, mechanical, and optical properties (4, 5). I will then present case studies in using these polymers as repairable and recyclable materials (6,7), smart coatings (8), next-generation lenses for thermal imaging (9), and versatile sorbents for pollution and precious metals (10).



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# All-Atom Analysis of Intermolecular Interactions in Polymeric Materials: Water Absorption and Mutual Miscibility

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The performance of a polymeric material as a medium for dissolution of small molecules is determined by atomic-level interactions. In the present work, we develop a free-energy method to assess the extent of dissolution into polymer by combining all-atom MD simulation and a statistical-mechanical theory of solvation. It is demonstrated that all-atom treatment is predictive for the free energy of water dissolution, and the structural units within copolymers that determine the dissolution free energy are identified. Polymer functions may be further tuned by preparing blends. An all-atom method is also presented to assess the mutual miscibility of polymers.

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# Exploring Gamma-Lactam as New Potential Lead Compound for Medicinally Active MRSA Antibiotics

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## ABSTRACT

Methicillin-resistant *Staphylococcus aureus* (MRSA) continues to be one of the main causes of hospital-acquired infections in all regions of the world, while linezolid is one of the only commercially available oral antibiotics available against this dangerous gram-positive pathogen. In this research project, the antibacterial activity from different analogues derived from gamma-lactam heterocycles against MRSA was determined. Different analogues were synthesized from hydrazonation reaction, intramolecular hydrazine-lactamization and diastereoselective fused-annulation to furnished gamma-lactam hydrazone, pyrazolidinone and oxazepanone gamma-lactam compounds, respectively. Amongst screened different analogues for the minimum inhibitory concentration (MIC) assay, compound **MF514** displayed good inhibitory activity with MIC values of 7.8–15.6 µg/mL against 30 MRSA and 12 methicillin-sensitive *S. aureus* (MSSA) clinical isolates, while cytotoxicity evaluations displayed a mean inhibitory concentration (IC<sub>50</sub>) value of > 625 µg/mL, displaying a potential to becoming as a lead compound. In subsequent animal studies for **MF514**, a single-dose oral acute toxicity test revealed an estimated mean lethal dose (LD<sub>50</sub>) value of <5000 mg/kg, while in the mice infection test, a mean effective dose (ED<sub>50</sub>) value of 29.39 mg/kg was obtained via oral administration. These results suggest that gamma-lactam class of compound, show its potential to be further explored as a new safe and efficacious orally delivered antibacterial agent against MRSA.

# Characterization of Nanoparticles Using Field-Flow Fractionation and Inductively Coupled Plasma Mass Spectrometry

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## ABSTRACT

The use of field-flow fractionation (FFF) and inductively coupled plasma mass spectrometry (ICP-MS) for characterization of nanoparticles will be presented. Field-flow fractionation is a separation-based method for hydrodynamic size determination of nanoparticles or colloidal particles. An ICP-MS is a trace element detection technique, which offers information on concentration when operated in conventional mode and information on nanoparticle size and number of particles when operated in single particle mode.

With FFF, various types of laboratory synthesized particles were characterized including selenium nanoparticles<sup>[1]</sup>, silver and gold nanoparticles<sup>[2]</sup>, bimetallic gold-silver nanoparticles<sup>[3]</sup>, and silver nanoplates<sup>[4,5]</sup>. Coupling FFF with ICP-MS provides element specific detection with high sensitivity. With single particle ICP-MS (SP-ICP-MS), various types of information were obtained as follow: core diameter for selenium nanoparticles<sup>[1]</sup>; core diameter and shell thickness for bimetallic gold-silver nanoparticles<sup>[2]</sup>; and equivalent spherical diameter and plate thickness for silver nanoplates<sup>[4]</sup>. The use of FFF and SP-ICP-MS was also demonstrated for tracking changes of triangular silver nanoplates during their synthesis and colorimetric sensing of mercury ions by anti-etching mechanism from bromide ions<sup>[5]</sup>. FFF-ICP-MS was employed to observe the association between silver and mercury ions to confirm the selectivity of silver nanoplates towards mercury ions.

Furthermore, application of SP-ICP-MS was demonstrated for study the release of ZnO nanoparticles from fabric face mask samples upon washing in deionized water and 4% detergent<sup>[6]</sup>. The released ZnO nanoparticles from fabric face mask were in the range of 100 – 200 nm with the release percentage of Zn from mask samples approximately 0.25 – 1.17% in the first washing cycle in deionized water, and around 1.97 – 3.12% in 4% detergent. This work illustrates the capability of SP-ICP-MS for providing the information which can also be applied to study the release of nanoparticles from other consumable products.

**Keywords:** hydrodynamic diameter; core diameter; field-flow fractionation; single particle ICP-MS; nanoparticles

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## **INVITED ADDRESSES**

# **Artificial Intelligence in Drug Discovery leveraging pChemBL.ID: Unlocking the Potential of Billions of Compounds**

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## **ABSTRACT**

Harnessing the power of AI in pChemBL.ID as a screening tool, this innovative application offers a transformative approach to drug discovery. By swiftly predicting the viability of new compounds as potential drug candidates for a wide array of diseases, it significantly streamlines the drug development process. These predictive insights serve as a valuable compass, guiding researchers in the design and development stages, enabling them to make informed decisions before embarking on costly and time-consuming laboratory trials, both in vitro and in vivo, as well as clinical trials. This application not only accelerates the pace of drug development but also enhances its efficiency by pinpointing the most promising candidates for further investigation.

# 3D-Connector Microfluidic Paper-based Analytical Devices for Rapid Detection of Nephropathy

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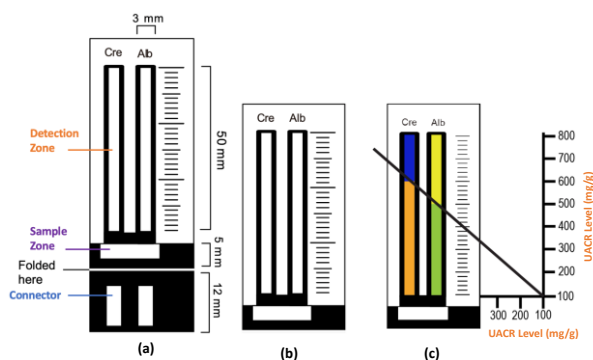
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## ABSTRACT

The detection resolution of the distance-based microfluidic paper-based analytical devices (mPADs) suffers from the mixing of reagents between the sampling and detection zones caused by capillary action. This problem has been solved by developing a three-dimensional connector (3DC) connecting the sampling and detection zones, as shown in Figure 1. The innovative design of the connector has effectively prevented the mixing of the reagents in these two zones, and it also offers another function as a masking zone to solve potential interferences. This 3DC- mPADs is applied to the semiquantitative analysis of the urinary albumin-to-creatinine ratio (UACR), allowing an instrumentation-free approach for rapid detection of nephropathy. The concept of this device is based on a dual color-change length found in the detection zones, followed by drawing a line/slope connecting the upper color-change of these two zones of the 3DC-mPADs, enabling the semiquantitative UACR detection by showing its level in the card reader. In this work, the picric acid-capped gold nanoparticles (AuNPs) and/or complex of palladium with Chrome Azurol S (Pd<sup>2+</sup>-CAS) are used as creatinine (Cre) reagents detection. Protein error of pH indicator and full corona protein formation mechanisms are applied for the detection of albumin (Alb) through its reaction with dyes in the presence of AuNPs. In comparison to the UACR gold standard, the proposed method resulted in good accuracy (>90%).



**Figure 1.** Desain of 3D-uPADs before (a) and after (b) folded, and illustration of UACR detection (c)

**Keywords:** Albumin; Creatinine; Kidney;  $\mu$ PADs; Urine

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# Heterogeneous Catalyst Potential of Modified Magnesium Fluoride to Enhance Both Sides of Lewis Acid and Brønsted Acid and Its Application in Some Organic Synthesis

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## ABSTRACT

Some organic compound synthesis reactions require acid catalysts, Lewis acids or Brønsted acids to take place. Fluoride-based catalysts such as  $\text{MgF}_2$  are catalysts that already contain these two acids, although they are still low.  $\text{MgF}_2$  is a potential solid as a Lewis or Brønsted acid catalyst for heterogeneous catalysis of various organic compound synthesis reactions. Synthesis and characterization of metal fluoride (Mg, Ca) alkaline earth fluoride have been carried out. Different compositions and synthesis methods have been tried for various purposes according to requirements.  $\text{MgF}_2$  synthesized by the sol gel method has a large surface area, thermal stability, chemical stability, high hardness and has a mesoporous structure. Modification of magnesium fluoride synthesized by the sol-gel method produces catalysts with different acidities, which can be effective heterogeneous catalysts. Modification has been carried out by impregnation of transition metals on  $\text{MgF}_2$ . The resulting catalyst can be applied in CFC hydrodechlorination, nitrate reduction, vitamin E synthesis, methyl ester (biodiesel) production, phenol acylation. In the hydrodechlorination of  $\text{CF}_3\text{-CCl}_3$  with the catalyst of impregnated Pd and Pt on the  $\text{MgF}_2$  were obtained conversions of 15 and 27%, respectively. The products  $\text{CF}_3\text{-CHCl}_2$ ,  $\text{CF}_3\text{-CH}_2\text{Cl}$ ,  $\text{CF}_3\text{-CH}_3$  are 4, 6, 5% for the Pd/ $\text{MgF}_2$  catalyst and 7, 8, 15% for the Pt/ $\text{MgF}_2$  catalyst. In nitrate reduction with Cu/ $\text{MgF}_2$ , Pd/ $\text{MgF}_2$  and Cu-Pd/ $\text{MgF}_2$  catalysts were obtained conversions of 60.35, 65.28 and 87.07%, respectively. Nitrogen gas products from these reaction are 15, 42, 50%, ammonium hydroxyde 2, 5, 10%, and nitrite acid 0, 0, 0.5%. In the synthesis of vitamin E from the reaction between trimethyl hydroquinone and isofitol with the FeEDTA/ $\text{MgF}_2$  catalyst, a conversion of 95.81% was obtained with a yield of vitamin E of 69.5% and benzofuran of 26.31%. In the production of biodiesel from palm oil with the  $\text{Fe}_2\text{O}_3/\text{MgF}_2$  catalyst, the total yield of methyl palmitate and methyl stearate was 93.2%. The same catalyst ( $\text{Fe}_2\text{O}_3/\text{MgF}_2$ ) in the phenol acylation reaction with acetic acid as the acyl source were obtained a conversion of 86% with yields of p-hydroxy aceto phenon and phenyl acetate of 55 and 28%, respectively.

# EXPLORING VERSATILE APPLICATIONS OF COORDINATION CHEMISTRY WITH N, S, AND O DONOR ATOMS

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## Abstract

Schiff bases, thiourea, and thiosemicarbazide are versatile ligands known for their ability to donate nitrogen (N), sulfur (S), and oxygen (O) atoms in coordination chemistry. This review explores the versatile applications of N,S, and O donor ligands and their metal complexes in various fields of chemistry, including medicinal chemistry, catalysis, materials science, and environmental chemistry. The ligands and their metal complexes are synthesized and characterized using various analytical techniques, such as FTIR, UV-Vis, and NMR spectroscopy. The synthesized compound was also studied theoretically using Density Functional Theory (DFT) method to compare the experimental and calculated results. In medicinal chemistry, N, S, and O donor ligands and their metal complexes have shown promising activities against a wide range of diseases, including cancer, bacterial and viral infections, and inflammation. Additionally, the metal complexes have been used as diagnostic and imaging agents in medical applications. Overall, this study highlights the diverse applications of N,S, and O donor ligands and their metal complexes in various fields of chemistry and underscores their potential for the development of new materials and therapeutic agents.

Keywords: Schiff Base, thiourea, thiosemicarbazide, corrosion inhibitor, anticancer agent



# Modification of Metal-Organic Frameworks: A Route to Enhance Its Catalytic Performance in Organic Transformation

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**Abstract.** Metal-Organic Frameworks, a material constructed by metal ions or metal cluster with organic linker, offer enormous potential in a wide variety of applications including catalysis. High surface area, tunable pore size, diverse structures, and easy geometric control are among benefits used to enhance its chemical properties. Herein, our group has utilized various approaches to transform catalytically inert MOFs into highly active MOFs in various organic transformations. Three novel Zirconium-based MOFs with phenoxy-imine-based organic linker have been successfully synthesized through an in-situ formation of imine organic linker by reacting a Zr salt with 4-aminobenzoic acid, and 4-formylbenzoic acid. These MOFs were employed as catalyst support for Ni(II) as active sites in the transformation of ethylene to oligomers of olefins with high catalytic activity. Functionalization of the phenoxy-imine-based organic linker with electron donating group and electron withdrawing group further tunes the catalytic performance of the MOFs. In addition, our group has also been successfully enhance the catalytic performance of ZIF-8, a Zinc-based MOF with 2-methylimidazolate linker, in the oxidation of alcohol by substituting Zn(II) ions with other late transition metals, i.e, Cu(II), Ni(II), and Co(II). These modified ZIF-8 show a higher catalytic performance compared to the pristine ZIF-8, even to their metal salts acting as homogenous catalysts. Since all the MOFs acting as heterogenous catalysts for both reactions, recyclability and reusability of the MOFs have been achieved.

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## CONFERENCE SCHEDULE

<b>Wednesday, 11 October 2023 (1<sup>st</sup> day)</b>		
07.30-08.30	<b>Registration</b>	Lobby
08.30-08.35	<b>Opening Ceremony</b>	Grand Ballroom
08.35-08.40	<b>Indonesia Raya Anthem</b>	Grand Ballroom
08.40-08.50	<b>Welcome Speech from IC2MS Chairman</b>	Grand Ballroom
08.50-09.00	<b>Opening Speech from Rector/Dean</b>	Grand Ballroom
09.00-09.45	<b>Moderator:</b> Anna Safitri, S.Si, M.Sc, PhD	Grand Ballroom
	<b>Keynote 1:</b> Innovative Material and Electrochemistry for Sensing Application Advancement and Microbial Energy Conversion <b>Prof. Masato Tominaga - Saga University, JPN</b>	
09.45-09.55	<b>Discussion</b>	Grand Ballroom
09.55-10.25	<b>Poster Session</b>	Ballroom #1
10.25-11.10	<b>Moderator:</b> Lukman Hakim, S.Si, M.Sc, Dr.Sc	Grand Ballroom
	<b>Keynote 2:</b> All-Atom Analysis of Intermolecular Interactions in Polymeric Materials: Water Absorption and Mutual Miscibility <b>Prof. Nobuyuki Matubayasi - Osaka University, JPN</b>	

11.10-11.20	<b>Discussion</b>			Grand Ballroom
11.20-12.05	<b>Moderator:</b> Lukman Hakim, S.Si, M.Sc, Dr.Sc			Grand Ballroom
	<b>Keynote 3:</b> New Frontiers in Polymers Made from Sulfur <b>Prof. Justin M. Chalker - Flinders University, AUS</b>			
12.05-12.15	<b>Discussion</b>			Grand Ballroom
12.15-13.00	<b>Lunch Break</b>			
	<b>Contributed Talks 1 (Parallel oral presentation)</b>			
	<b>Molecular Science (Room 1)</b> <i>Seoul</i>	<b>Nanomaterials and Nanodevices (Room 2)</b> <i>Osaka</i>	<b>Inorganic Chemistry (Room 3)</b> <i>Manila</i>	
13.00-13.20	<b>Moderator :</b> Dr. Noor Hidayat binti Punqot	<b>Moderator :</b> Dr. Ika Oktavia W, S.Si., M.Si	<b>Moderator :</b> Alif Alfariysi, S.Si	
	<b>Invited Speaker :</b> Artificial Intelligence in Drug Discovery leveraging pChemBL.ID: Unlocking the Potential of Billions of Compounds <b>Drs. Sudarko, PhD</b>	<b>Invited Speaker :</b> 3D-Connector Microfluidic Paper-based Analytical Devices for Rapid Detection of Nephropathy <b>Prof. A. Sabarudin, S.Si, M.Sc., Dr.Sc.</b>	<b>Invited Speaker :</b> Modification of Metal-Organic Framework: A Route to Enhance Its Catalytic Performance in Organic Transformation <b>Dr. rer. nat. Ubed Sonai Fahrudin Arrozi</b>	
13.20-13.30	<b>Discussion</b>			
13.30-13.40	<b><u>MS/O-001</u></b> Detection Performance of Thyroid Peroxidase and Thyroid Stimulating	<b><u>NN/O-001</u></b> Single-step green synthesis of gold-conjugated polyphenol nanoparticles using extracts of <i>Cajanus cajan</i> as	<b><u>MSC/O-010</u></b> The Behaviour Study Of Sumbermanjing's Pyrophyllite-Water Interaction	

	Hormone Receptor (TPO-TSHR) Rapid Test with Lateral Flow Immunoassay (LFIA) <b>Aulanni'am</b>	chemical probes for heavy metal detection and its biological applications <b>Dini Nur Fauzia</b>	<b>Siti Mutrofin</b>
13.40-13.50	<u><b>MS/O-006</b></u> Solvation free-energy of transthyretin in the mixture of water and urea as co-solvent from molecular dynamics simulation <b>Ellya Indahyanti, M.Eng</b>	<u><b>NN/O-002</b></u> Stability Test Of Nanogold Synthesized Using Ascorbic Acid At Room Temperature As Preparation For The Commercialization Nanogold Healthy Drink <b>Titik Taufikurohmah</b>	<u><b>REF/O-001</b></u> Fabrication of Activated Carbon-NiCo <sub>2</sub> O <sub>4</sub> with Hybrid Structure for Supercapacitor Electrode Materials <b>Silvi Rahmawati Wibowo</b>
13.50-14.00	<u><b>MS/O-004</b></u> Computational Characterization of Zr-Oxide MOFs for Post-Combustion CO <sub>2</sub> Capture <b>Rama Oktavian</b>	<u><b>MSC/O-006</b></u> Effects of Crosslinker Concentration on The Synthesis of Thermoresponsive P(SPE-co-NIPAM) Hydrogels for Drug Delivery <b>Kayla Aliya</b>	<u><b>MSC/O-007</b></u> Tracking Ag-Au Bimetallic Nanoparticles during Their Synthesis by Field Flow Fractionation and Inductively Coupled Plasma Mass Spectrometry: Implications for Colorimetric Sensing of Cobalt Ions <b>Luluil Maknun</b>
14.00-14.10	<b>Discussion</b>		
14.10-14.20	<u><b>CHE/O-005</b></u> Benzene Complexes Of Triruthenium Derived From Thermal Reaction Of Ru <sub>3</sub> (CO) <sub>9</sub> (M-Ph <sub>2</sub> P(CH <sub>2</sub> ) <sub>4</sub> PPh <sub>2</sub> )(L) Where [L = PPh <sub>3</sub> And AsPh <sub>3</sub> ] <b>Siti Syaida Sirat</b>	<u><b>MSC/O-011</b></u> Synthesis and Characterization of Keratin Nanoparticles from Chicken Feather by Sonification Method <b>Darjito</b>	<u><b>MSC/O-012</b></u> One-pot Synthesis of Chitosan-Reduced Gold Nanocomposites as Novel Functional Material <b>Elvira Nurraida</b>
14.20-14.30	<u><b>MSC/O-001</b></u>	<u><b>NN/O-003</b></u>	<u><b>FM/O-006</b></u>

	<p>Synthesis and Characterization of Hematite (<math>\alpha</math>-Fe<sub>2</sub>O<sub>3</sub>) from Iron Sand Using Coprecipitation Method</p> <p><b>Marzuki Naibaho</b></p>	<p>Synthesis of TiO<sub>2</sub> nanotubes using a two-stage hydrothermal process with variations in the TiO<sub>2</sub>/NaOH molar ratio.</p> <p><b>Tanti Haryati</b></p>	<p>Modification of Functional Porous Material Based on Ni(II)-terephthalate Metal-Organic Frameworks</p> <p><b>Yuniar Ponco Prananto</b></p>
14.30-14.40	<p><b><u>MSC/O-004</u></b></p> <p>Characterization of Na<sub>2</sub>/3[Fe<sub>1</sub>/2Mn<sub>1</sub>/2]O<sub>2</sub> as cathode material for sodium-ion batteries</p> <p><b>Diah Agustina Puspitasari</b></p>	<p><b><u>MSC/O-003</u></b></p> <p>Fabrication and Characterization of Cellulose Acetate/N-Methyl-2-Pyrrolidone Membranes for Separation of Microplastics in Water</p> <p><b>Annisa Alifia Rahmah</b></p>	<p><b><u>CHE/O-021</u></b></p> <p>Computational Insight For Electric Field-Driven Catalytic Activity in Reduced Graphene Oxide</p> <p><b>Fazira Ilyana Abdul Razak</b></p>
14.40-14.50	<p><b><u>MSC/O-005</u></b></p> <p>Facile Synthesis of Activated Carbon-PANi Composites as Electrode Material for Application in Supercapacitor</p> <p><b>Viona Lidya Haryati Putri</b></p>	<p><b><u>MSC/O-013</u></b></p> <p>Synthesis, Quality Control and Stability Test of [177Lu]Lu-PSMA I&amp;T Radiopharmaceutical as a Theranostic Agent for Prostate Cancer Treatment</p> <p><b>Titis Sekar Humani</b></p>	<p><b><u>CHE/O-010</u></b></p> <p>Phosphorescent Cyclometallated Iridium(III) Complex with (E)-N-cyano-N-(4-methylbenzyl)-N'-(pyridin-2-yl)formimidamide Ancillary Ligand : Synthesis, Spectroscopic and Theoretical Studies</p> <p><b>Nurul Husna As Saedah Bain</b></p>
14.50-15.00	<b>Discussion</b>		
15.00-15.15	<b>Coffee Break</b>		Ballroom #1

<b>Thursday, 12 October 2023 (2<sup>nd</sup> day)</b>		
07.30-08.00	<b>Registration</b>	Lobby
08.00-08.45	<p><b>Moderator:</b> Prof. A. Sabarudin, S.Si, M.Sc, Dr.Sc</p>	Grand Ballroom

	<b>Keynote 4:</b> Exploring gamma-lactam as new potential lead compound for medicinally active MRSA antibiotics <b>Prof. Dr. Mohd Fazli Mohammat - Universiti Teknologi MARA, MAS</b>		
08.45-08.55	<b>Discussion</b>		Grand Ballroom
08.55-09.40	<b>Moderator:</b> Prof. A. Sabarudin, S.Si, M.Sc, Dr.Sc		Grand Ballroom
	<b>Keynote 5:</b> Characterization of Nanoparticles Using Field-Flow Fractionation and Inductively Coupled Plasma Mass Spectrometry <b>Assoc. Prof. Atitaya Siripinyanond - Mahidol University, THA</b>		
09.40-10.50	<b>Discussion</b>		Grand Ballroom
11.15-11.55	<b>Poster Session</b>		Ballroom #1
	<b>Contributed Talks 1 (Parallel oral presentation)</b>		
	<b>Inorganic Material (Room 1)</b>  <i>Seoul</i>	<b>Material : Synthesis and Characterization (Room 2)</b>  <i>Osaka</i>	<b>Organic Chemistry (Room 3)</b>  <i>Manila</i>
10.15-10.25	<b>Moderator :</b> Layta Dinira, S.Si., M.Si	<b>Moderator :</b> Dr. Bambang Piluharto, S.Si., M.Si	<b>Moderator :</b> Anisa Ul Husna, S.Si., M.Sc
	<b>Invited Speaker :</b> EXPLORING VERSATILE APPLICATIONS OF COORDINATION CHEMISTRY WITH N, S, AND O DONOR ATOMS	<b>Invited Speaker :</b> Heterogeneous catalyst potential of modified magnesium fluoride to enhance both sides of Lewis acid and Brønsted acid	<b><u>CHE/O-001</u></b> Linked Hybridization Approach in the Development of Quinoline-Based Anticancer Compounds from Methyl Eugenol and Methyl Salicylate Essential Oils

	<b>Assoc. Prof. Dr. Karimah Kassim</b>	and its application in some organic synthesis	<b>Dwika Putri Pangesti</b>
10.25-10.35		<b>Prof. Dr.rer.nat. Irminda Kris M</b>	<b><u>CHE/O-002</u></b> The Impact of Ultrasound-Assisted Extraction Time on the Toxicity and Antioxidant Activity of Hydrilla verticillata Ethanol Extract <b>A. Ghanaim Fasya</b>
10.35-10.45	<b>Discussion</b>		
10.45-10.55	<b><u>MS/O-005</u></b> Expression and Characterization of Recombinant Endo- $\beta$ -1,4-D-xylanases XynBTN63D from Soil Termite Abdomen in Escherichia coli BL21 (DE3) <b>Anak Agung Istri Ratnadewi</b>	<b><u>CHE/O-014</u></b> Characteristic of lignin isolated from the wood of <i>Paraserianthes falcataria</i> (L) Nelson <b>Masruri</b>	<b><u>CHE/O-003</u></b> Screening Multitarget Anticancer Compounds from Salicylic Acid Derivatives: Without and with Amino Acid Linkage <b>Warsito</b>
10.55-11.05	<b><u>MS/O-002</u></b> In vitro and in silico Approaches to Evaluating The Cytotoxicity Activity of $^{177}\text{Lu}$ -EDTMP and Cisplatin Combination Against the MDA-MB-231 Human Breast Cancer Cell Line <b>Alfian M. Forentin</b>	<b><u>MSC/O-009</u></b> Preparation of High Specific Capacitance Material Based on Activated Carbon-Manganese Dioxide Composite Using Lemon Peel ( <i>Citrus limon</i> ) Extract for Supercapacitor Electrode <b>Muhammad Hafidz Ramadhan</b>	<b><u>CHE/O-004</u></b> Single-Step Hydrogenolysis of Furfural to 1,2-Pentanediol by Nickel Catalyst <b>Nova Pratiwi Indriyani</b>
11.05-11.15	<b><u>MS/O-003</u></b> Computational Molecular and Material Design Environment (CMMDE) <b>Aditya Wibawa Sakti</b>	<b><u>CHE/O-017</u></b> Optimization of pH and Solution Concentration in the Determination of Paracetamol and p-Aminophenol Using	<b><u>CHE/O-012</u></b> The Influence of Extraction Method and Solvent Type on Natural Pigment Profile Purple Sweet Potato Anthocyanins (PSPAs) in Purple Sweet Potatoes ( <i>Ipomoea batatas</i> L.)



		Carbon Electrode by Voltammetric Method <b>Hanandayu Widwastuti</b>	<b>Rurini Retnowati</b>
11.15-11.25	<b>Discussion</b>		
11.25-11.35	<b><u>FM/O-001</u></b> Modification Of Natural Rubber Via Sulphur Curing System As Basic Design On Seismic Bearing Compound Formulation <b>Adi Cifriadi</b>	<b><u>MSC/O-008</u></b> Effect of mole Ratio of Si/Al on the Acidity and Crystal Structure of Aluminosilicate <b>Suardiyanto</b>	<b><u>CHE/O-020</u></b> Isolation and Screening for The Potential of Polypropylene Degradation Bacteria Isolated from Bestari Landfill of Probolinggo City <b>Shinta Yuliana</b>
11.35-11.45	<b><u>CHE/O-018</u></b> EFFECT OF BASE TYPE AND CONCENTRATION ON CHITOSAN'S DEGREE OF DEACETYLATION FROM CHITIN ISOLATED BY ECO-FRIENDLY METHOD FOR SMART PACKAGING APPLICATIONS <b>Dyah Ayu Nastiti</b>	<b><u>NN/O-004</u></b> Biosynthesis of TiO <sub>2</sub> Nanoparticle using Aloe Vera for the photodegradation of of Linear Alkyl Benzene sulphonate (LAS) <b>Novita Andarini</b>	<b><u>CHE/O-022</u></b> NUTRITIVE VALUES AND POTENTIAL USES OF TWO VARIETY OF LEUCAENA LEUCOCEPHALA (TARAMBA AND WONDERGRAZE) AS ANIMAL FEED <b>Firstca Aulia Rachma</b>
11.55-12.05	<b>Discussion</b>		
12.05-13.00	<b>Lunch Break</b>		Grand Ballroom
	<b>Contributed Talks 2 (Parallel oral presentation)</b>		
	<b>Biochemistry / Organic (Room 1)</b>  <i>Seoul</i>	<b>Material : Synthesis and Characterization (Room 2)</b>  <i>Osaka</i>	<b>Functional Material (Room 3)</b>  <i>Manila</i>
	<b>Moderator</b> : Dr. Arie Srihardyastutie, S.Si.,M.Kes	<b>Moderator</b> : Siti Maryah Ulfa, S.Si., M.Sc., Dr.Sc	<b>Moderator</b> : Barlah Rumhayati, S.Si., M.Si., Ph.D

13.00-13.10	<p><b><u>CHE/O-006</u></b></p> <p>In-Silico Analysis of Hyptolide Compound and Its Derivatives in HDAC Class Ila Protein reveals their impact on Protein-ligand Binding Affinities</p> <p><b>Lulut Tutik Margi Rahayu</b></p>	<p><b><u>CHE/O-013</u></b></p> <p>The Effect of Concentration and pH on Phosphate Adsorption Efficiency in Fe<sub>3</sub>O<sub>4</sub>-Agarose-Oxalic Acid as Binding Gel for DGT</p> <p><b>Layta Dinira</b></p>	<p><b><u>FM/O-002</u></b></p> <p>Physical Modification Cellulose Nanofibril with Poly(vinyl alcohol) and Carboxymethyl cellulose as Coating on Paper for Food Packaging</p> <p><b>Noverra Mardhatillah Nizado</b></p>
13.10-13.20	<p><b><u>CHE/O-007</u></b></p> <p>Mechanical and Antibacterial Properties of Biocompatible Modified Mineral Trioxide Aggregate from Natural Waste</p> <p><b>Mariyam</b></p>	<p><b><u>CHE/O-015</u></b></p> <p>A New Diagnoses Approach for Iron Deficiency Anemia Based on Iron-silver Nanoparticles Interaction</p> <p><b>Hermin Sulistyarti</b></p>	<p><b><u>MSC/O-015</u></b></p> <p>The Effect of Poly(L-Lactic Acid) (PLLA) and Polyethylene Glycol 200 (PEG200) Addition in Cellulose-Based Biocomposite Beads on Adsorption of Methylene Blue in Batch Systems</p> <p><b>Ferdy Hermawan</b></p>
13.20-13.30	<p><b><u>CHE/O-009</u></b></p> <p>Unveiling the Synthetic Approach Towards Daibucarboline A and Its Derivatives via Tetrahydro-β-Carbolines Intermediates for Anti-Inflammatory Potential</p> <p><b>Noor Hidayah Pungot</b></p>	<p><b><u>CHE/O-016</u></b></p> <p>Green Analytical Approach for Gastric Acid Diagnosis Based On Salivary Ammonia Using Flow Injection-Spectrophotometry</p> <p><b>Hermin Sulistyarti</b></p>	<p><b><u>REF/O-004</u></b></p> <p>Crude Biodiesel Production from Palm Fatty Acid Distillate (PFAD) By Ultrasound-Assisted Esterification Method</p> <p><b>Muhammad Alif Aditya Febriyadi</b></p>
13.30-13.40	<p><b><u>REF/O-003</u></b></p> <p>In Situ Transesterification of Nannochloropsis sp Microalgae to Produce Biodiesel with CaO/Hydrotalcite Catalyst: Analysis of The Effect of CaO Loading</p> <p><b>Yustia Wulandari Mirzayanti</b></p>	<p><b><u>MSC/O-014</u></b></p> <p>Kappa Number Analysis in the Production of Abaca Fiber Pulp using Ultrasound-Assisted Organosolv Method with Alkaline Pretreatment</p> <p><b>Rania Sekar Kinasih</b></p>	<p><b><u>CHE/O-019</u></b></p> <p>SYNTHESIS OPTIMIZATION OF CHITOSAN FROM CHITIN ISOLATED BY ENVIRONMENTALLY FRIENDLY METHOD FOR SMART PACKAGING APPLICATIONS</p> <p><b>Jauhairiyah Gailani</b></p>

13.40-13.50	<b>Discussion</b>		
13.50-14.00	<p><b><u>CHE/O-011</u></b></p> <p>Potential of the Bacteria Consortium as A Domestic Liquid Waste Bioremediation Agent</p> <p><b>Dita Ayu Eka Saputri</b></p>	<p><b><u>FM/O-004</u></b></p> <p>Effect of Composition and Thickness of Polyaniline-Polypyrrole Composites as Gas Sensor Electrode Material on Responses to Robusta Coffee Aromas</p> <p><b>Yeni Maulidah Muflihah</b></p>	<p><b><u>REF/O-002</u></b></p> <p>Synthesis of MgO Nanoparticles Using Water Hyacinths Leaves Extract and Its Application on Biodiesel Production from Waste Cooking Oil</p> <p><b>Celine Audyta Berlian</b></p>
14.00-14.10	<p><b><u>MSC/O-002</u></b></p> <p>MODELING AND SIMULATION OF THE DISTRIBUTION OF UREA CONCENTRATIONS IN HEMODIALYSIS HOLLOW FIBER MEMBRANES WITH VARIATIONS OF BLOOD FLOW RATE</p> <p><b>Belinda Kezia Purwanto</b></p>	<p><b><u>FM/O-003</u></b></p> <p>Separation of Sunset Yellow based on Molecularly Imprinted Polymers using Acrylamide Functional Monomer</p> <p><b>Fazia Almas Nathifa</b></p>	<p><b><u>NN/O-006</u></b></p> <p>The stability of human serum albumin nanocolloid based on the type of sugar molecule and their radiochemical purity</p> <p><b>Ratna Dini Haryuni</b></p>
14.10-14.20	<p><b><u>FM/O-007</u></b></p> <p>Effect of molecular weight of chitosan in the coating solutions on the shelf life of Tuna fish fillets</p> <p><b>Bambang Piluharto</b></p>	<p><b><u>CHE/O-008</u></b></p> <p>pH Effect of Caesalpinia sappan L. Extract as Green Reducing Agents on Synthesis of Reduced Graphene Oxide</p> <p><b>Lia Destiarti</b></p>	<p><b><u>CHE/O-023</u></b></p> <p>Flow Injection Potentiometry using Cobalt-Carbon Electrodes for Determination of Phosphate in Soil</p> <p><b>Siswoyo</b></p>
14.20-14.30		<p><b><u>MSC/O-016</u></b></p> <p>Synthesis and Structure of <math>[\text{Ni}(\text{4-ampy})_4(\text{dca})_2] \cdot 4\text{-ampy}</math> (ampy = aminopyridine, dca = dicyanamide ion)</p> <p><b>Moch Robitul Choir</b></p>	<p><b><u>FM/O-005</u></b></p> <p>Evaluation of the functionality of pectin from cocoa pod husk to modify the characteristic and starch digestibility of bread</p> <p><b>Ariza Budi Tunjung Sari</b></p>

14.30-14.40	<b>Discussion</b>	
14.45-15.05	<b>Closing Ceremony</b>	Grand Ballroom
15.05-14.55	<b>Award Announcement</b>	Grand Ballroom
14.55-15.00	<b>Closing Speech from Dean</b>	Grand Ballroom

## Poster Session (1<sup>st</sup> day)

<p><b>Wednesday, 11 October 2023</b></p> <p><b>09.55-10.25</b></p>	<p><b>Poster Presenter 1 (CHE/P-001)</b> Isolation and Optimization of Incubation Time, pH, and Temperature for Amylase Enzyme Production from Indigenous Bacteria in Sugar Factory Waste <b>Silvia Febriana</b></p>
	<p><b>Poster Presenter 2 (CHE/P-002)</b> Biotransformation of Vanillin from Isoeugenol Using <i>Pseudomonas aeruginosa</i> as an Enzyme Biocatalyst Agent: Effect of Substrate Concentration and Incubation Time <b>Mochamad Hendy Fathur Rahman</b></p>
	<p><b>Poster Presenter 3 (CHE/P-003)</b> Comparative phytochemical analysis of the fresh and fermented leaves of two varieties of <i>Leucaena leucocephala</i> L. (Taramba and Wondergraze) using Gas chromatography–mass spectrometry (GC–MS) method <b>Agustono Wibowo</b></p>
	<p><b>Poster Presenter 4 (CHE/P-004)</b> Structure analysis of <math>Ru_3(CO)_9(\mu-Ph_2AsCH_2AsPh_2)(AsPh_3)</math>: Single crystal X-ray diffraction, thermal analysis, Density Functional Theory (DFT) and Hirshfeld surface analysis. <b>Husna Izzati Muhammad Nor Azharan</b></p>
	<p><b>Poster Presenter 5 (CHE/P-005)</b> Analysis Of The Sources And Impacts Of Mercury Concentrations In Sediments Of Belawan Harbor Waters, Medan <b>Lilik Sulistyowati</b></p>
	<p><b>Poster Presenter 6 (CHE/P-006)</b> Green Synthesis of p-Hydroxychalcones Using <math>FeCl_3 \cdot 6H_2O</math> as A Catalyst Under Solvent-Free Conditions <b>Muhammad Ainur Hasan</b></p>
	<p><b>Poster Presenter 7 (MSC/P-001)</b> Solvothermal Synthesis of Ni(II)-BDC-Pyrazine complex: Effect of solvent toward the yield, surface morphology, and crystallite size of the complex <b>Yenni Finisia</b></p>
	<p><b>Poster Presenter 8 (MSC/P-002)</b> Synthesis and Characterization of Thermoresponsive Hydrogels of P(SPE-ko-NIPAM) as a Carrier for a Model Drug of Metformin HCl <b>Fauziah Damayanti</b></p>
	<p><b>Poster Presenter 9 (REF/P-002)</b> PHOTOESTERIFICATION OF WASTE COOKING OIL USING ZNO DOPED EMPTY FRUIT BUNCHES ASH HETEROGENEOUS CATALYST <b>Norshahidatul Akmar Mohd Shohaimi</b></p>
	<p><b>Poster Presenter 10 (CHE/P-015)</b> Quantum Molecular Simulations for Lithium-Ion Transport in Solid Polymer Electrolyte of Layered Cellulose and Its Derivatives <b>Kensuke Ishida</b></p>
	<p><b>Poster Presenter 11 (MSC/P-003)</b> Magnetite Coated with Oxalic Acid Crosslinked Chitosan Hydrogel for <math>Zn^{2+}</math> and <math>Cd^{2+}</math> Removal from Aqueous Media <b>Danar Purwonugroho</b></p>
	<p><b>Poster Presenter 12 (CHE/P-013)</b> Passive Samplers for Inorganic Phosphate Measurement in Water System <b>Barlah Rumhayati</b></p>
	<p><b>Poster Presenter 13 (CHE/P-018)</b></p>

	Synthesis Cellulose Acetate From Corn Cobs With Varying Acetylation Times As A Material For Filtration Membranes <b>Sofiatul Hasanah</b>
	<b>Poster Presenter 14 (CHE/P-019)</b> Synthsis of Cellulose Acetate Based on Corn Cob As A Membrane Material With Variations In The Amount Of Acetic Acid <b>Ellyna Octaviana</b>

### Poster Session (2<sup>nd</sup> day)

<p style="text-align: center;"><b>Thursday</b> <b>12th October</b> <b>2023</b></p> <p style="text-align: center;"><b>11.15-11.55</b></p>	<b>Poster Presenter 1 (CHE/P-007)</b> Fractionation of Goat Liver Urikase Based on Carbonate Buffer with Variations in Ammonium Sulfate and Precipitation Time on Urikase Characteristics <b>Wuryanti Handayani</b>
	<b>Poster Presenter 2 (CHE/P-008)</b> Profile of flavonoid and phenolic compounds from ethyl acetate fraction of <i>Caesalpinia sappan</i> heartwood having antioxidant and anti-inflammatory properties <b>Siti Mariyah Ulfa</b>
	<b>Poster Presenter 3 (CHE/P-009)</b> The Effect of pH and Fe (VI) Concentration on the Coagulation Process of River Water Samples <b>Qonitah Fardiyah</b>
	<b>Poster Presenter 4 (CHE/P-010)</b> Biotransformation of Isoeugenol to Vanillin Using <i>Pseudomonas aeruginosa</i> in Various pH of Culture Medium <b>Elvina Dhiaul Iffitah</b>
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# **SYMPOSIUM**

**Analytics/Bio/Inorganic/Organic/Physical Chemistry (CHE)**



## **Linked Hybridization Approach in the Development of Quinoline-Based Anticancer Compounds from Methyl Eugenol and Methyl Salicylate Essential Oils**

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### **ABSTRACT**

Quinoline has demonstrated promising potential as an anticancer agent. In this study, we propose a hybridization approach, utilizing quinoline as a linked component or connector, to amalgamate compounds found in essential oils, namely methyl eugenol and methyl salicylate. The objective is to generate innovative compounds with the potential to be effective cancer therapeutics. The bioactivity of the synthesized compounds will undergo in-silico testing, targeting five breast cancer receptors: MMP9, MMP2, CDK2, TP53, and BAK. Docking results reveal that quinoline-derived compounds from hybridization exhibit promise against MMP9 and CDK2 receptors, with binding affinities of -8.5 and -7.1 kcal/mol, respectively. The synthesis of intermediate compounds to yield quinoline derivatives involves several stages, including the nitration and amination of methyl eugenol. Intermediate compounds are also derived through the oxidation of a derivative of methyl salicylate, specifically 2-hydroxybenzyl alcohol, into 2-hydroxybenzaldehyde. The use of sonication expedites the synthesis process, yielding compounds such as 1,2-dimethoxy-3-nitro-5-(prop-2-en-1-yl)benzene (58.71%), 2,3-dimethoxy-5-(prop-2-en-1-yl)aniline (56.9%), and 2-hydroxybenzaldehyde (28.91%). This research provides promising initial evidence regarding the potential of quinoline-based linked hybridization compounds as potential anticancer drugs. Subsequent steps involve experimental testing of compound bioactivity and further research endeavours in developing more effective cancer treatments.

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## **The Impact of Ultrasound-Assisted Extraction Time on the Toxicity and Antioxidant Activity of *Hydrilla verticillata* Ethanol Extract**

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### **ABSTRACT**

Ultrasound-assisted extraction (UAE) has emerged as a promising technique for extracting bioactive compounds from plant materials. In this study, we investigated the impact of varying extraction times on the toxicity and antioxidant activity of ethanol extracts obtained from *Hydrilla verticillata*. The extraction of *H. verticillata* biomass was conducted using ethanol solvent at a sonication frequency of 42 Hz, with extraction times ranging from 10 to 60 minutes. Toxicity assessment was carried out using the Brine Shrimp Lethality Test (BSLT), while antioxidant activity was evaluated using the DPPH (1,1-diphenyl-2-picrylhydrazyl) method. The results revealed that the yields of *H. verticillata* ethanol extracts at Ultrasound-Assisted Extraction Times of 10, 20, 30, 40, 50, and 60 minutes were 1.86%, 2.18%, 2.03%, 2.27%, 2.14%, and 2.23%, respectively. Toxicity testing using the BSLT method indicated that the ethanol extract of *H. verticillata* exhibited toxicity towards *Artemia salina* shrimp larvae with LC50 values of 4314 ppm, 1400 ppm, 1044 ppm, 572 ppm, 629 ppm, and 1995 ppm for extraction times of 10, 20, 30, 40, 50, and 60 minutes, respectively. Meanwhile, antioxidant activity testing yielded EC50 values of 2851 ppm, 1182 ppm, 1377 ppm, 1140 ppm, 1172 ppm, and 1863 ppm for the same extraction times. Based on these findings, it can be concluded that the optimal sonication time for extracting *H. verticillata* with ethanol solvent using the Ultrasound-assisted extraction method is 40 minutes.

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## Screening Multitarget Anticancer Compounds from Salicylic Acid Derivatives: Without and with Amino Acid Linkage

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### ABSTRACT

This research aims to design multitarget candidate anticancer molecules using salicylic acid derivatives that have combine with other natural molecules, both with and without amino acid linkages. The research primarily focuses on cancer, conducting screenings of the designed salicylic acid derivative molecules using an in-silico approach against receptors: MMP9 (Matrix Metalloproteinase 9), EGFR (Epidermal Growth Factor Receptor), and ADP Ribose Polymerase. The best docking results for multitarget cancer compounds were salicylic acid derivatives with amino acid linkages, namely salicylic acid-curcumin, salicylic acid-benzyl alcohol, salicylic acid-eugenol, and salicylic acid-citronellol, with binding affinities towards MMP9 of -9.6, -9.6, -8.9, and -8.1 kcal/mol, towards EGFR of -9.0, -7.6, -7.9, and -7.3 kcal/mol, and towards ADP Ribose Polymerase of -11.2, -9.0, -9.4, and -8.7 kcal/mol. The docking results indicate that the design of multitarget anticancer compounds from salicylic acid derivatives with amino acid linkages is significantly better than without. This docking result is attributed to the amino acid structure's wealthy functional groups that enhance ligand-receptor interactions. This research is expected to potential drug molecules as effective multitarget anticancer agents.

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## Single-Step Hydrogenolysis of Furfural to 1,2-Pentanediol by Nickel Catalyst

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### ABSTRACT

Biomass derivatives, especially furfural, are considered the most promising platform chemicals for producing value-added chemicals. Current methods for hydrogenolysis of furfural to furfuryl alcohol and 1,2-pentanediol are limited by their use of platinum metal catalysts (Ru, Pd, and Pt) in pressurized hydrogen (up to 100 bar). Here, hydrogenolysis of furfural to 1,2-pentanediol was investigated using a nickel-based catalyst in the absence of pressurized hydrogen. In this work, the air-stable and inexpensive Ni(II) phosphine complex,  $\text{NiCl}_2(\text{PPh}_3)_2$ , was observed to catalyze selective hydrogenation and hydrogenolysis to produce furfuryl alcohol and 1,2-pentanediol at 160-180 °C for 7 h. Experimental studies suggest the rule of Ni(0) phosphine complex as an active species in this catalytic reaction. Investigation of reaction mechanisms was conducted using Density Functional Theory (DFT) methods. The reaction mechanism for the hydrogenolysis of furfural to yield 1,2-Pentanediol with a source of alcohol hydrogen is proposed through the formation of furfuryl alcohol and tetrahydrofurfuryl alcohol. Based on the proposed reaction mechanism, the proton transfer steps from alcohol to furfural require a high electron density at the central metal site to enhance the nucleophilicity of the metal center, facilitating the attack on the electrophilic center of the C=O bond in furfural form a sigma bond between the metal center and the carbon in the C=O bond of furfural. Control of electron density on the catalyst can be achieved by varying ligands on the catalyst with electron-donating properties and variable electron-withdrawing abilities to manipulate the electron density at the metal center in the catalyst complex.

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**BENZYNE COMPLEXES OF TRIRUTHENIUM DERIVED FROM  
THERMAL REACTION OF  $\text{Ru}_3(\text{CO})_9(\mu\text{-Ph}_2\text{P}(\text{CH}_2)_4\text{PPh}_2)(\text{L})$   
WHERE  $[\text{L} = \text{PPh}_3 \text{ AND } \text{AsPh}_3]$**

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**ABSTRACT**

$\text{Ru}_3(\text{CO})_{12}$  is shown to readily undergo substitution of carbonyl groups by  $\text{Ph}_2\text{P}(\text{CH}_2)_4\text{PPh}_2$  ligand to give  $\text{Ru}_3(\text{CO})_{10}(\mu\text{-Ph}_2\text{P}(\text{CH}_2)_4\text{PPh}_2)$  which exhibit greater stability when compared with the parent compound. In continuation of our research interest in the reactivity of  $\text{Ru}_3(\text{CO})_{10}(\mu\text{-Ph}_2\text{P}(\text{CH}_2)_4\text{PPh}_2)$ , the synthesis and thermal reaction of  $\text{Ru}_3(\text{CO})_9(\mu\text{-Ph}_2\text{P}(\text{CH}_2)_4\text{PPh}_2)(\text{L})$  [where  $\text{L} = \text{PPh}_3$  (1) and  $\text{AsPh}_3$  (2)] were undertaken since previous studies of clusters bearing bidentate ligands have shown that they produce interesting new molecular structures via C-P/C-As bond cleavage and C-H bond activation. The thermal reaction of  $\text{Ru}_3(\text{CO})_9(\mu\text{-Ph}_2\text{P}(\text{CH}_2)_4\text{PPh}_2)(\text{L})$  [where  $\text{L} = \text{PPh}_3$  (1) and  $\text{AsPh}_3$  (2)] in toluene gives benzyne cluster complexes of  $\text{Ru}_3(\text{CO})_7(\mu\text{-C}_6\text{H}_4)(\mu\text{-PPh}_2)_2$  (1b) and  $\text{Ru}_3(\text{CO})_7(\mu\text{-C}_6\text{H}_4)(\mu\text{-AsPh}_2)(\mu\text{-PPh}_2)$  (2a) which might be considered to be suitable models of active species on a metal surface. Both structures have been established by Single Crystal X-ray diffraction, revealing that a benzyne is coordinated to two Ru atoms through two Ru-C  $\sigma$  bonds from ortho carbons, while the third Ru atom is also coordinated to these carbons in an  $\eta^2$ -mode. Herein discussion will be focused on the thermal reaction of 1 and 2 as well as the crystal structure of 1b and 1a.

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## **In-Silico Analysis of Hyptolide Compound and Its Derivatives in HDAC Class IIa Protein reveals their impact on Protein-ligand Binding Affinities**

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### **ABSTRACT**

HDAC proteins play a role in epigenetic changes in cancer-causing gene expression. In previous research reported that hyptolide and its derivatives inhibited several cancer cell growths in vitro. However, the potential of this anticancer compounds in preventing HDAC protein activity has not yet been evaluated. This study aims to determine the site-related inhibitory activity and binding affinity produced by hyptolide against HDAC class IIa protein compared to its derivative complexes. Hyptolida and its derivatives have previously been optimized using ORCA software with B3LYP/6-31G\*\* functional DFT theory. The optimization results on the hyptolide molecule show that the partial charge values of O4, O5, O6, and O7 atoms in the OAc group are -0.437; -0.444; -0.436, and -0.431 with a dipole moment 5.47363 Debye, while the partial charges of hyptolide derivatives on the same atom for epoxy-hyptolide are -0.465; -0.454; -0.448, and -0.415 with dipole moment value 8.57293 Debye and dimethylphenylamine-hyptolide molecules are -0.456; -0.442; -0.559 and -0.418 and dipole moment value 8.86020 Debye. The molecular docking process was conducted using AutoDock Vina software. The interaction of binding sites between hyptolide compounds with HDAC class IIa proteins occurs at zinc ion chelation Zn101A, Zn101B dan Zn101C. There are two hydrogen bonds in the hyptolide molecule, between atom O6 with Val708B (2.8 Å) and O4 with Trp7618B (2.83 Å) residue. In epoxy-hyptolide molecule between O7 with Leu729B (3.2 Å) residue. In addition, the dimethylphenylamine-hyptolide molecule, occurs at O5 with Arg731B (2.99 Å) and O7 with Val708B (3.00 Å) and Asp801B (3.11 Å) residues. In line with the partial charge value of the optimized hyptolide compound and its derivatives, binding affinity value will increase with the modification of the compound in the hyptolide molecule. These results confirm that prediction of hyptolide derivative with nitrogen group as alkylating agents will increase binding affinity between ligands and proteins. These results motivate researchers to conduct further studies on the activity of hyptolide derivative compounds in dimethylphenylamine-hyptolide against cancer cell growth in vitro.

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## **Mechanical and Antibacterial Properties of Biocompatible Modified Mineral Trioxide Aggregate from Natural Waste**

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### **ABSTRACT**

Mineral trioxide aggregate (MTA) is one of root canal filling materials used for pulpotomy. It is an imported material and has been marketed at high prices. Furthermore, MTA possessed low mechanical and antibacterial properties. In this study, MTA was synthesized using natural waste and modified with 4 wt% chitosan and 10 wt% ZnO to achieve ideal properties as a dental material. It was found that MTA synthesized using natural waste components experienced similar characteristics as a commercial MTA. Modified MTA using 4 wt% chitosan and 10 wt% ZnO resulted in higher mechanical properties and potential bioactivity. The MTA/Chitosan/ZnO was evaluated for its biocompatibility using an MTT assay. IC50 showed that MTA/Chitosan/ZnO was classified as a nontoxic material.

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## **pH Effect of *Caesalpinia sappan* L. Extract as Green Reducing Agents on Synthesis of Reduced Graphene Oxide**

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### **ABSTRACT**

Reduced graphene oxide (rGO) is a nanomaterial that can be applied for composite materials, energy storage, and field effect transistors. Reduction of graphene oxide (GO) to rGO is generally carried out using toxic hydrazine and sodium borohydride. Natural reducing agents are an alternative to these materials. The chemical compound in *Caesalpinia sappan* L. extract has a different structural form at acidic and alkaline pH. In this study, rGO was successfully produced using the green reducing agent. It was found that rGO-3 and rGO-7 show a significant decrease in the peak intensity of  $2\theta=10^\circ$  compared to GO, whereas in rGO-10, the peak almost disappears, and a peak of  $25^\circ$  is predominant than other rGOs. The C/O data derived from EDS is 3.8, 3.4, and 4.5 for rGO-3, rGO-7, and rGO-10, respectively. The Raman data shows a decrease in the ID/IG ratio value in all rGOs (compared to GO). The morphology of synthesized materials using SEM and TEM showed folded and clumpy areas, whereas lighter areas showed thinner parts than the dark zone. This research concludes that rGO obtained from synthesis using extracts in alkaline conditions (rGO-10) is the best rGO.

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## Unveiling the Synthetic Approach Towards Daibucarboline A and Its Derivatives via Tetrahydro- $\beta$ -Carbolines Intermediates for Anti-Inflammatory Potential

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### ABSTRACT

$\beta$ -Carbolines, belonging to the class of indole alkaloids, were isolated from wild Syrian rue (*Peganum harmala*), which is common in Iran. In recent years, there has been a growing fascination with the synthesis of  $\beta$ -carbolines, owing to their extensive utility in pharmaceutical and biological fields. Due to their unique rigid heterocyclic skeleton,  $\beta$ -carbolines demonstrate promising pharmacological diversity of neuroprotection, antioxidant, anticancer, antibacterial, antitumor, antiviral, anti-allergic, antimalarial, anti-leishmania, and anti-HIV. For instance, daibucarboline A, is proven to demonstrate interesting anti-inflammatory activity upon testing using iNOS assay with the IC<sub>50</sub> value of 18.41  $\mu$ M. However, a literature survey reveals there is no report found on the synthesis of daibucarboline A in addition to limited works on its isolated compound. Thus, the main objective of this work was to develop a novel synthetic approach towards daibucarboline A and its derivatives, which are anticipated to have similar biological potentials. Our synthetic strategy began with the synthesis of tetrahydro- $\beta$ -carboline intermediates as the key structural moiety using different starting materials (tryptamine and tryptophan derivatives) with different substituted aldehydes/phenylglyoxal via Pictet-Spengler condensation. Subsequent aromatization of the resulting intermediates by oxidative dehydrogenation reaction furnished the  $\beta$ -carboline frameworks. Subsequent aromatization of the resulting intermediates by oxidative dehydrogenation reaction furnished the  $\beta$ -carboline frameworks. The reaction proceeded with the reduction of carbonyl functionality on C-7 position of the precursor of daibucarboline A via Wolff-Kishner reduction using hydrazine hydrate and KOH to furnish a series of 1-substituted- $\beta$ -carboline derivatives in moderate yields. The synthesis was carried out without the use of expensive metal catalysts, prolonged reaction hours, and critical reaction conditions. Accordingly, Fischer esterification, carbonyl reduction, and Williamson ether synthesis were employed to obtain the desired natural compound, daibucarboline A. The essential derivative of daibucarboline A was successfully synthesized in four steps with an overall yield of 3.4 %. In the screening of anti-inflammatory activities of daibucarboline A and its derivatives using xanthine oxidase inhibitory assay at the concentration of 100  $\mu$ g/mL, six compounds showed anti-inflammatory activities against xanthine oxidase ranging from moderate to 63.17% inhibition. The structures of all synthesized intermediates and derivatives of  $\beta$ -carboline were confirmed by NMR, FTIR, and GC-MS spectroscopy.

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## Phosphorescent Cyclometallated Iridium(III) Complex with (E)-N-cyano-N-(4-methylbenzyl)-N'-(pyridin-2-yl)formimidamide Ancillary Ligand : Synthesis, Spectroscopic and Theoretical Studies

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### ABSTRACT

Phosphorescent Iridium(III) complexes have drawn tremendous research interest and are widely applied in organic light-emitting diodes (OLEDs) due to their excellent photophysical and chemical properties. Compared to most other transition metals, iridium exhibited a significant ligand-field splitting and a wide range of color changes. In this study, a complex of Ir(F<sub>2</sub>ppy)<sub>2</sub>(CNMBpyfo) utilizing 2-(2,4-difluorophenyl)pyridine (F<sub>2</sub>ppy) as the cyclometallating ligands and (E)-N-cyano-N-(4-methylbenzyl)-N'-(pyridine-2-yl)formimidamide (CNMBpyfo) as the ancillary ligand has successfully synthesized. Spectroscopic and crystallographic studies have shown that the starting cyclic (4-methylbenzyl)-1H-1,2,4-triazol-1-yl)pyridine ligand has converted into acyclic CNMBpyfo when cleavage to iridium atom. IR analysis demonstrated the presence of a prominent stretching of C=N at 2220 cm<sup>-1</sup>. Both pyridine and phenyl aromatic rings have C=N stretching bands at 1598 cm<sup>-1</sup> and C=C stretching bands at 1554 cm<sup>-1</sup> and 1400 cm<sup>-1</sup>, respectively. The <sup>1</sup>H NMR spectrum revealed phenylpyridine protons corresponding signals in the 5.00–9.00 ppm aromatic region, while the <sup>13</sup>C NMR spectrum indicated 37 carbon signals and was also consistent with the complex Ir(F<sub>2</sub>ppy)<sub>2</sub>(CNMBpyfo) structural formula. Steady-state emission spectroscopy determined that the Ir(III) complex emitted blue-green light in dichloromethane solution at room temperature with the vibronic structure at 462 nm and 487 nm. The simulated spectroscopic and photophysical properties of complex Ir(F<sub>2</sub>ppy)<sub>2</sub>(CNMBpyfo) were assessed at B3LYP/6-31G(d,p) and the LanL2DZ basis set and were in good agreement with the experimental results. The Frontier Molecular Orbital (FMO) study showed fluorine substituent at phenyl moiety has contributed to the 3.88 eV of HOMO-LUMO gap energy level. In addition, simulated gibbs free energy has supported the formation of acyclic pyridine-formimidamide ancillary ligand in the complex Ir(F<sub>2</sub>ppy)<sub>2</sub>(CNMBpyfo).

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## Potential of the Bacteria Consortium as A Domestic Liquid Waste Bioremediation Agent

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### ABSTRACT

Along with the increasing population in Indonesia, there has been an increase in domestic waste production. It is necessary to treat waste water before it goes to the environment to prevent pollution of the environment. This research was conducted with the aim of investigating the potential of isolates A, B and L from Biology Department Universitas Negeri Malang as a bacterial consortium in decomposing domestic waste with aerobic system to remove chemical oxygen demand using a batch system. Experimental trials were carried out using synthetic domestic waste with variations in bacterial formulation treatments and starter doses. The results show that a more stable COD removal performance was obtained in the batch test process. Sequentially, the COD reduction data efficiency includes B 20% (88.65%), L 20% (84.2%), A 10% (80%), A 20% (79.92%), ABL 10% (72.3%), B 10% (25.67%), ABL 20% (-10.87%), with the greatest efficiency occurring in the L10% treatment at 89.76%. The genotype analysis show that A, B and L isolates were indentified as *Alcaligenes ammonioxydans*.

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## **The Influence of Extraction Method and Solvent Type on Natural Pigment Profile Purple Sweet Potato Anthocyanins (PSPAs) in Purple Sweet Potatoes (*Ipomoea batatas* L.)**

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### **ABSTRACT**

Purple sweet potato (*Ipomoea batatas* L.) is a type of tuber plant that is often found in Indonesia and has a higher anthocyanin content than other sweet potato plants. Anthocyanin is a natural coloring pigment that has various types of colors. This study aims to analyze the influence of extraction method and solvent type on the color intensity profile, stability, and UV-vis spectrum profile of anthocyanins from purple sweet potato extract. Anthocyanin extraction was carried out using maceration and sonication and two solvents with different polarities, namely ethanol and butanol. The purple sweet potato extract was then tested for stability and analyzed for its UV-vis spectrum profile using a UV-vis spectrophotometer. The color resulting from anthocyanin extraction from purple sweet potatoes was analyzed using a color reader. The results showed that the ethanol extract of purple sweet potatoes was light red with a color intensity profile in the sonication results that was higher than the maceration, while the butanol extract of purple sweet potatoes was light yellow in color with a color intensity profile in the sonication results that was higher than the maceration results, as indicated by the difference in Commission values Internationale d'Eclairage (CIE) L\*, a\*, and b\*. The stability test of purple sweet potato extract showed that the extract was stable until the 20th day. Analysis of the UV-vis spectrum profile of purple sweet potato extract showed a typical anthocyanin spectrum characterized by absorption at 523, 327, 296, and 221 nm, with the absorbance value of the sonicated extract being higher than that of the maceration and the ethanol extract being higher than the butanol extract. In conclusion, the intensity profile of purple sweet potato extract resulting from sonication was higher than maceration and higher using ethanol as a solvent than butanol. Keyword: *Ipomoea batatas* L., maceration, sonication, color intensity profile, UV-vis spectrum

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## The Effect of Concentration and pH on Phosphate Adsorption Efficiency in Fe<sub>3</sub>O<sub>4</sub>-Agarose-Oxalic Acid as Binding Gel for DGT

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### ABSTRACT

Phosphate is a nutrient required by all organisms. However, its excessive abundance in waters negatively impacts water quality, causing the death of fish and invertebrates due to eutrophication. A passive sampling technique called diffusive gradient in thin films (DGT) can be applied to monitor the phosphate concentration in water. Iron oxide (Fe<sub>3</sub>O<sub>4</sub>) in agarose crosslinked with oxalic acid as a binding gel for DGT has been developed to adsorb phosphate. Fe<sub>3</sub>O<sub>4</sub>-agarose-oxalic acid gel was characterized by Scanning Electron Microscopy. Parameters affecting adsorption efficiency, such as concentration and pH, were examined. The adsorption efficiency was calculated based on the phosphate concentration in the solution before and after adsorption. Phosphate concentration was determined using the spectrophotometric method. The results showed that Fe<sub>3</sub>O<sub>4</sub> was immobilized in the agarose-oxalic acid gel network. The pores in the binding gel were non-uniform, ranging from 2.72 to 37.19 μm. Increasing the phosphate concentration increases adsorption efficiency. The adsorption efficiency of phosphate by the binding gel approached 100% at concentrations of 0.5 to 4 mg phosphate/L. The adsorption efficiency decreased to 51 ± 1%, especially when the phosphate concentration was 20 mg/L. The highest phosphate adsorption efficiency was obtained at pH 4 (89 ± 1%). However, phosphate adsorption efficiency tends to be constant at pH 4 - 8 (approximately 80%). This study demonstrates that oxalic acid crosslinked Fe<sub>3</sub>O<sub>4</sub>-agarose has good performance as a binding gel and can be applied to DGT passive samplers for measuring phosphate in the natural aquatic environment.

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## **Characteristic of lignin isolated from the wood of *Paraserianthes falcataria* (L) Nelson**

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### **ABSTRACT**

The indigenous fast-growing plant of *Paraserianthes falcataria* (L) Nelson has been our concerning research since the biomass wasted by local and small industry. The branch and sawdust are disposed of or burnt. Previously, the cellulose and its nano cellulose have been reported. The paper discloses our recent investigation of their prospective evaluation of lignin isolated from its sawdust wood. Characterization of the isolated lignin using spectroscopy for FTIR, UV-Vis, and DTA/TGA. The isolated lignin shows important properties for future application in adhesives, thermoplastic polymers, etc.

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## **A New Diagnoses Approach for Iron Deficiency Anemia Based on Iron-silver Nanoparticles Interaction**

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### **ABSTRACT**

A new spectrophotometric method based on green chemistry concept was developed using a natural reagent derived from pineapple peel extract (*Ananas comosus* L. Merr) as a metal ion detector. This research method is based on the principle of increased color intensity of silver nanoparticles (AgNPs) after the addition of Iron(II) ions which possibly due to aggregation. To achieve linearity, sensitivity, and method validity, optimization was performed on the parameters of AgNPs volume, reaction time, and pH solution. The results showed optimal under the conditions of 2.5 mL of AgNPs solution, 3 mins reaction time, and pH solution of 4. The method exhibited linearity in the measurement of Iron(II) ions in the range of 0-8 mg/L, with respective limits of detection (LOD) and quantification (LOQ) values of 0.41 mg/L and 1.37 mg/L. The method has been applied to synthetic urinary samples with satisfied results supported by recovery test ranging from 92-100%, indicating a reasonably good level of accuracy. Keywords: Iron, silver nanoparticles, pineapple peel, spectrophotometry, anemia

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## **Green analytical approach for gastric acid diagnosis based on salivary ammonia using flow injection-spectrophotometry**

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### **ABSTRACT**

Saliva is a collection of biological markers that have great potential as specimens for health surveillance and disease diagnosis. Salivary ammonia as the product of *Helicobacter pylori* bacteria metabolism in the stomach was proposed as an early detection for gastric acid using Gas Diffusion-Flow Injection (GD-FI) Spectrophotometry with natural reagent of purple sweet potato extract. The principle of determining ammonia is based on the total ammonia in saliva which is transformed to gas ammonia in NaOH donor stream which diffuses through the GD-membrane to the acceptor stream containing purple sweet potato extract. The presence of ammonia changed the extract color detected at a wavelength of 604 nm giving absorbance proportionally to the concentration of ammonia. Optimization to common parameters were done and produced optimal results under 1.5 M NaOH, 10 % extract, 50 cm mixing coil with 300  $\mu$ L sample. The method results was selective against sulfate, nitrite, phosphate, magnesium, and calcium with % error of less than 10% and give satisfactory validity when it was applied to salivary ammonia supported by recovery test in the range of 95-105%. Keywords: Ammonia, saliva, purple sweet potato extract, gastric acid, gas-diffusion flow injection (GD-FI), spectrophotometry

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## **Optimization of pH and Solution Concentration in the Determination of Paracetamol and p-Aminophenol Using Carbon Electrode by Voltammetric Method**

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### **ABSTRACT**

Paracetamol is one of the drugs that functions as an analgesic due to its anti-pyretic content. This drug is commonly used to relieve fever and pain and has no side effects if used according to dosage. However, if consumed continuously, it can cause kidney damage, liver disorders, and pancreatic inflammation. p-aminophenol is an important component in the synthesis of paracetamol so it is possible that this compound is present with paracetamol during degradation. p-aminophenol has aniline and phenol toxicity, when exposed to the skin it will cause dermatitis, eczema, and also significantly affects the occurrence of nephrotoxicity and teratogenic effects. The European Union and the US government set the maximum level of p-aminophenol allowed in paracetamol at 50 mg/L. Therefore, a sensitive detection method needs to be developed for the detection of paracetamol and p-aminophenol. In this study, carbon electrode was used for the determination of paracetamol and p-aminophenol by voltammetry method. The parameters analyzed were the effect of both the pH and the concentration of the solution. The result shown that the optimum measurement of paracetamol was obtained at pH 7 (260.88  $\mu$ A) and the optimum pH of p-aminophenol was pH 5 (60.34  $\mu$ A). The linearity of paracetamol measurement is  $r^2$  0.9862 while the linearity of p-aminophenol measurement is  $r^2$  0.9886. Based on these results, it can be concluded that the carbon electrode is sufficient to provide good results in measurement but the detection ability of p-aminophenol is quite low so it is necessary to optimize and develop the electrode so that the detection ability of p-aminophenol increases.

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## **EFFECT OF BASE TYPE AND CONCENTRATION ON CHITOSAN'S DEGREE OF DEACETYLATION FROM CHITIN ISOLATED BY ECO-FRIENDLY METHOD FOR SMART PACKAGING APPLICATIONS**

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### **ABSTRACT**

Frozen shrimp is one of the major export commodities of Indonesia. The desired part of shrimp is the meat while other parts, such as shells, tails, and entrails are thrown away. Besides, shrimp waste contains a high content of chitin which is potential to be used as a chitosan's precursor. Synthesis of chitosan is usually done by deproteination, demineralization, and deacetylation process. Deacetylation of chitin from shrimp waste isolated by eco-friendly method, i.e., autolysis, has never been reported before. Hence, this paper investigates the effect of base type and concentration on the degree of deacetylation of chitosan from chitin isolated by autolysis. Autolysis was carried out by an incubation at pH 2 using sulfuric acid for 10 d. Demineralization was performed by immersion in hydrochloric acid pH 1 for 24 h. The deacetylation of chitin was carried out at 120 °C for 120 min using two different bases, which are NaOH and KOH, respectively. The determination of chitosan's degree of deacetylation (DD) was carried out using a semi-quantitative method from IR spectra. The use of KOH resulted in the obtained DD of around 95%, while the NaOH usage produced around 50% of DD. Then, the NaOH was chosen and studied further to obtain a suitable DD for film applications, which is 60 - 90%. The deacetylation of chitosan was carried out by varying NaOH concentration from 60 to 70% (w/v). High concentration of NaOH tends to increase chitosan's DD and slightly decrease the yield. The optimum concentration of NaOH was obtained at 70% (w/v) producing DD of 65.57% and yield of 47.66%. Chitosan synthesized using 70% concentration of NaOH produced a relatively homogeneous thin film. Polyaniline was then introduced to the film to obtain a prototype of smart packaging. This smart packaging was able to detect the pH changes proven by the change of its color. **Keywords:** shrimp waste, chitin, chitosan, autolysis, degree of deacetylation

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## **SYNTHESIS OPTIMIZATION OF CHITOSAN FROM CHITIN ISOLATED BY ENVIRONMENTALLY FRIENDLY METHOD FOR SMART PACKAGING APPLICATIONS**

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### **ABSTRACT**

Shrimp is an Indonesian's export commodity with high economic value increasing every year. Usually, shrimp are exported in the form of frozen shrimp without shells, heads, tails, and entrails. It resulted in the accumulation of shrimp waste leading to the increasing environmental pollution. Shrimp waste contains high contents of chitin which can be processed to a chitosan owing several benefits. Synthesis of chitosan was done by several stages, such as deproteination, demineralization, and deacetylation. The deproteination using the autolysis method is environmentally friendly because it uses enzymes from the shrimp. The synthesis of chitosan from chitin isolated by autolysis method has never been reported before. Therefore, the purpose of this study is to determine the optimum condition of the synthesis of chitosan from chitin isolated by autolysis method. The deproteination was done by soaking the shrimp waste in a sulfuric acid solution at pH 2 - 3 for 10 d. The demineralization process was done by soaking the deproteinated solids in hydrochloric acid solution at pH 0 - 1 for 24 h. Parameters varied in this study were time (1 - 3 h), chitin to NaOH ratio (w/v) (1:10 - 1:30), and temperature (60 - 120 °C). The longer the time, the higher obtained degree of deacetylation (DD) which is in the range of 45.14±2.62 to 55.14±1.54%. On the other hand, the yield decreased from 48.45±2.69 to 47.78±0.81%. Similar trend was observed when the ratio of chitin to NaOH (w/v) was increased. The optimum condition was obtained at synthesis time of 2 h, chitin to NaOH ratio of 1:20 (w/v), and temperature of 90 °C producing chitosan with DD of 85.68±6.09% and yield of 49.27±3.70%. Chitosan synthesized using optimum conditions produced a relatively homogeneous thin film. Polyaniline was then introduced to the film to obtain a prototype of smart packaging. This smart packaging was able to detect the pH changes proven by the change of its color. **Keyword:** chitin, chitosan, autolysis, degree of deacetylation, smart packaging.

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## **Isolation and Screening for The Potential of Polypropylene Degradation Bacteria Isolated from Bestari Landfill of Probolinggo City**

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### **ABSTRACT**

The Bestari Final Processing Site (TPA) in Probolinggo City collects various kinds of plastic waste, and most of it has been degraded, so it is thought to contain isolates of polypropylene degrading bacteria adaptable to the Indonesian environment. This research aims to carry out isolation and selection to obtain bacterial isolates that have the potential to degrade polypropylene. The research stages included sampling, isolation of polypropylene-degrading bacteria using the Enrichment method, selection based on the ability of bacterial isolates to degrade polypropylene, and identification of selected isolates. Based on the research results, six isolates of polypropylene degrading bacteria were obtained from the Bestari landfill of Probolinggo City using enrichment techniques, namely B1UM1, B1UM2, B1UM3, B2UM1, B2UM2, and B2UM3. The selection results showed that the three selected potential isolates, namely B2UM1, B1UM1, and B1UM2, could degrade polypropylene after 15 days of incubation, respectively 8.25%, 7.15%, and 6.35%. Isolate B1UM1 has a similarity of 99.93% to *Staphylococcus hemolyticus*, and two other isolates are currently in the 16s rRNA determination stage. Key words: Biodegradation, landfill, polypropylene, screening.

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## Computational Insight For Electric Field-Driven Catalytic Activity in Reduced Graphene Oxide

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### ABSTRACT

The field of catalyst research has advanced significantly with a focus on enhancing catalyst performance through non-electric and electric field methods. The latter, especially the application of electric fields, holds promise in boosting catalytic activity. Both approaches have been investigated to improve catalyst performance, with non-electric methods concentrating on surface modification and support material selection, while applied electric fields modify catalysts' electronic properties, charge distribution, and surface interactions. These strategies offer insights into more efficient and sustainable catalytic systems. However, a challenge in electric field-driven catalysis lies in understanding the mechanisms underlying enhanced activity. While electric fields show potential in catalysis, the specific ways they influence reaction kinetics and selectivity remain unclear. This gap obstructs the optimization and design of such catalytic systems. This study delves into the theoretical basis of simulating heterogeneous catalysis under external electric fields, focusing on reduced graphene oxide (RGO) as a catalyst and exploring its behaviour under electric influence. The study employs density functional theory (DFT) calculations to investigate alkene hydrogenation using cotton textile-based reduced graphene oxide (CT-RGO) as a catalyst. Results reveal that when an external electric field is applied along the bond axis, the adsorption energy of H<sub>2</sub> on CT-RGO's surface increases significantly. This suggests that the alkene hydrogenation can be initiated by CT-RGO catalysts under external electric fields. The study elucidates the impact of external electric fields on the graphene-hydrogen complex, activation energy of graphene radicals, and hydrogen atom adsorption on the graphene surface. This research addresses the lack of comprehensive mechanism studies in electric field-driven catalysis, opening a promising path for further exploration. Bridging this knowledge gap could unlock the potential of electric field manipulation in catalysis, paving the way for more effective and sustainable catalytic systems with widespread applications across industries.

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## **NUTRITIVE VALUES AND POTENTIAL USES OF TWO VARIETY OF LEUCAENA LEUCOCEPHALA (TARAMBA AND WONDERGRAZE) AS ANIMAL FEED**

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### **ABSTRACT**

Leucaena leucocephala belongs to the family Leguminosae and is one of the fastest-growing leguminous trees. Leucaena leucocephala leaves have a great potential as an alternative protein, mineral and fiber source. Leucaena leucocephala varieties wondergraze leaves contain 22% of crude protein, 7.56% of ash, 1.50% of fat, 253.25 kcal/kg of metabolizable energy, 33.19% of acid detergent fiber (ADF), and 38% of neutral detergent fiber (NDF). Leucaena leucocephala varieties taramba leaves contain 19.66% of crude protein, 8.39% of ash, 1.99% of fat, 281.70 kcal/kg of metabolizable energy, 32.67% of acid detergent fiber (ADF), and 42.67% of neutral detergent fiber (NDF). Taramba can grow in infertile soil and Wondergraze produce many high proportion of leaf. Leucaena leucocephala also contains anti-nutritional substances, namely nonprotein amino acids called mimosine.

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## Flow Injection Potentiometry using Cobalt-Carbon Electrodes for Determination of Phosphate in Soil

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### ABSTRACT

Implementation of precision agriculture needs to involve an evaluation stage of the condition of nutrients in the soil, one of which is phosphate. Measuring phosphate content in soil generally uses spectrometric analysis methods. An analytical method that is not widely used for soil analysis is the potentiometric method. This research aims to develop a potentiometric method that uses cobalt carbon electrodes in continuous flow. Cobalt-carbon electrodes were made by electrodeposition using the linear sweep voltammetry (LSV) technique from cobalt sulfate and cobalt chloride materials. The electrode immersion time and the concentration of the immersion solution (potassium hydrogen phthalate/PHP) were observed for their effect on electrode performance. The electrodes with the best performance were then characterized and used in batch and flow potentiometric methods. Immersing the electrode in a PHP solution with a concentration of 0.025 M for 5 minutes showed optimal electrode performance results, which provided the best electrode sensitivity and linearity values. Electrodes made from cobalt chloride have better characteristics than those made from cobalt sulfate in terms of sensitivity, linearity, and working area parameters. Electrode application in the flow injection potentiometric (FIP) system with a flow rate of 2 mL/minute and an injection volume of 100  $\mu$ L shows a sensitivity value of -26.326 mV/decade, linearity of 0.9947 in the linear region of  $10^{-3}$  to  $10^2$  ppm, with a detection limit  $10^{-3}$  ppm and 3.415% reproducibility. Even though the sensitivity of the FIP system is lower than the batch system, the results of the analysis of plantation soil samples provide relatively similar results between the two analysis methods.

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# **SYMPOSIUM**

## **Molecular Science (MS)**





## **Detection Performance of Thyroid Peroxidase and Thyroid Stimulating Hormone Receptor (TPO-TSHR) Rapid Test with Lateral Flow Immunoassay (LFIA)**

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### **ABSTRACT**

Autoimmune Thyroid Diseases (AITD) are generally asymptomatic (showing symptoms like normal conditions). The large number of births of unhealthy babies due to worsening manifestations of symptoms in pregnant women suffering from hypothyroidism cannot be separated from a doctor's delay in determining early detection and prompt and appropriate treatment. In addition, this delay in detection causes delays in thyroid hormone therapy, causing these children to experience hampered intellectual development, as indicated by low intelligence quotient (IQ) scores. Thyroid Peroxidase (TPO) and Thyroid Stimulating Hormone Receptor (TSHR) antibody titters can be detected early before changes in T3 and T4 hormone levels occur. They can be used to monitor the success of treatment. Measuring TPO and TSHR antibodies is not yet a routine examination for evaluating thyroid disorders. Apart from limited costs, not all regions in Indonesia have sophisticated laboratory equipment for measuring the titter of these two antibodies. This condition moved the research team's form of creativity among the country's children to continue to innovate in designing an economical, rapid diagnostic test tool based on TPO and TSHR using the lateral flow immunoassay method. This work resulted in an excellent promise to apply this rapid test due to the high sensitivity (92-95%) and specificity of 91-100%. This detection also performs a negative predictive value (NPV) of 80+96% and a positive predictive value of 82-100 with an accuracy test of 91-96 %.

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## **In vitro and in silico Approaches to Evaluating The Cytotoxicity Activity of <sup>177</sup>Lu-EDTMP and Cisplatin Combination Against the MDA-MB-231 Human Breast Cancer Cell Line**

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### **ABSTRACT**

Metastasis is a complex process by which malignant cells can leave the primary tumor site and spread to other parts of the body, making cancer a leading cause of mortality worldwide. Bone is the most common site of metastasis for numerous malignancies, particularly breast cancers. PRTRRB-BRIN developed a new freeze-dried EDTMP kit composition. It was recently registered as a registered patent at the Ministry of Law and Human Rights of the Republic of Indonesia, register number P00202301920. Due to variations in the formulations of commercially available products, in vitro testing was conducted against cancer cell models. This study highlighted the influence of varying amounts of EDTMP on the quality of <sup>177</sup>Lu-EDTMP and its biology activity, both in vitro and in silico. The process involved the labeling of EDTMP with Luthetium-177 (<sup>177</sup>Lu) at room temperature for 10 minutes, resulting in a molecule known as <sup>177</sup>Lu-EDTMP. MDA-MB-231 cell lines were treated for 24 hours with <sup>177</sup>Lu-EDTMP (0.023-0.37 MBq) in the presence or absence of cisplatin. In addition, a computational simulation was performed to examine the influence of <sup>177</sup>Lu-labelling on the binding capacity of EDTMP to several receptors, including HER2, estrogen, and progesterone receptors. The freeze-dried EDTMP kit has been successfully labeled with <sup>177</sup>Lu, resulting in the formation of <sup>177</sup>Lu-EDTMP with a radiochemical purity over 99%. In the highest radioactivity, cellular viability was observed to be greater than 50%. Nevertheless, the combination of cisplatin has been observed to dramatically enhance the process of cell death in MDA-MB-231 (p<0.01). The findings of this study indicate that the reduction in the amount of EDTMP does not have a negative impact on both the radiochemical purity and the ability to kill cancer cells. According in silico studies, it has been observed that the binding affinity of <sup>177</sup>Lu-EDTMP for receptors is approximately two to three times greater than EDTMP. In summary, it can be concluded that both <sup>177</sup>Lu-EDTMP (half formula) and <sup>177</sup>Lu-EDTMP (full formula) demonstrated similar amounts of radiochemical purity and demonstrated equivalent efficacy in inhibiting cell growth. However, further biological activity testing, such as experimentation on bones cancer cells and in vivo assays, is necessary.

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## Computational Molecular and Material Design Environment (CMMDE)

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### ABSTRACT

Computational molecular and material design environment (CMMDE) is a set of Python codes for computing and simulating molecular and material objects. Using the CMMDE, experimental and computational chemists can easily perform their routine simulations, geometry optimizations, frequency calculations, molecular docking, and many more. The code supports input file preparation, geometry conversion, job submission in the supercomputer environment, and output analysis. Currently, the CMMDE code supports the calculations and simulations by using Orca, XTB, Dcdftbmd, Gromacs, DOCK6, and Quantum Espresso. The codes have been implemented in the command line interface in Linux or Mac OS. The graphical user interface has also been created with limited features, such as molecular and surface structure preparations, geometry optimization, frequency calculation, and thermochemical analysis. The presentation will introduce features implemented in the current version of CMMDE, particularly for molecular science research related to molecular design for homogeneous catalysis reactions. As a test case, a computational study on Diels-Alder reactions in various solvents will be presented. The thermodynamic properties of the chemical reactions can be obtained easily by using the CMMDE code. The IR spectra of the resulting reactant, transition states, and products can also be obtained easily. Finally, the CMMDE code is promising for an efficient computational study of molecular science and material design.

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## Computational Characterization of Zr-Oxide MOFs for Post-Combustion CO<sub>2</sub> Capture

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### ABSTRACT

Metal-organic frameworks (MOFs), one of the most exciting developments in recent active porous materials science, are now, more than ever, in the center of attention as they make their way successfully into industrial applications for gas storage and separation applications. In 2021, Svante reported successful scale up of an outstanding MOF material, CALF-20 with remarkable properties to capture CO<sub>2</sub> from flue gas while maintaining stability and resisting water[1]. Here, we demonstrate the power of molecular-level simulations to shed light on the excellent gas adsorption properties of Zr-oxide MOFs. Moreover, we show how CCDC's structural search tool, ConQuest can be used to develop search queries to extract 102 structures containing Zr-oxide secondary building units (SBUs). Importantly, we performed systematic periodic density functional theory (DFT) calculations comparing 25 different combinations of basis sets and functionals to calculate framework partial atomic charges. We used this subset to perform high-throughput adsorption simulations and identify top candidates for post-combustion CO<sub>2</sub> capture. Finally, we introduced augmented reality (AR) visualizations as a means to bring adsorption phenomena alive in porous adsorbents and to dynamically explore gas adsorption sites in MOFs[2]. This study highlights the power of using big data in combination with molecular-level simulations to discover new uses for a wide range of promising synthesized materials available in CSD MOFs subset[3,4].

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## **Expression and Characterization of Recombinant Endo- $\beta$ -1,4-D-xylanases XynBTN63D from Soil Termite Abdomen in *Escherichia coli* BL21 (DE3)**

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### **ABSTRACT**

The xynBTN63D gene subcloned on the plasmid shuttle vector pESC and pYHM1 in the host *Escherichia coli* BL21 (DE3) was successfully expressed and characterized. The xynBTN63D gene in the soluble fraction of each plasmid is expressed at induction temperatures of 25, 30, 35, 37, and 40°C with a molecular weight of  $\pm 30$  kDa. The insoluble fraction in the pESC expressed with inductions of 37 °C and 40 °C, and in the pYHM1 has a molecular weight of  $\pm 30$  kDa, in the induction temperature of 30, 35, 37, and 40°C. The recombinant XynBTN63D, purified using the fast protein liquid chromatography (FPLC) method also has a molecular weight of  $\pm 30$  kDa, observed using the sodium dodecyl polyacrylamide sodium electrophoresis (SDS-PAGE) method. The recombinant XynBTN63D shows the optimal temperature at 40 with an optimal pH of 5.5. It shows stability from 4 to 40 oC after preincubation for 1 hour with relative activity on the pCES and pMH1 plasmid of more than 50%. Recombinant XynBT63D also showed pH stability after being preincubated for 24 hours by showing relative activity of 86-100% at pH 5.0 to 6.0 for each plasmid. Key word: pESC, pYHM1, induction temperature, stability, FPLC

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## **Solvation free-energy of transthyretin in the mixture of water and urea as co-solvent from molecular dynamics simulation**

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### **ABSTRACT**

Transthyretin (TTR) is a transport protein whose aggregates play important roles in pathophysiological diseases. The aggregate stability depends on the interaction of between peptides and between the peptide with the surrounding solvent molecules. The thermodynamics potential that arises from the latter can be manipulated with the presence of co-solvent. Therefore, it is important to understand the influence of a particular co-solvent in altering the solvation free-energy that can either prevent the formation of aggregates or dissociate the formed aggregates. Here we perform molecular dynamics simulations at constant temperature and pressure to investigate the solvation free-energy of TTR under different solvent environments. Several n-mer structures of TTR are solvated and subject to investigation. In the absence of urea, TTR is shown to favor aggregation due to the increase of the solvent-accessible surface area.

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# **SYMPOSIUM**

## **Functional Materials (FM)**





# MODIFICATION OF NATURAL RUBBER VIA SULPHUR CURING SYSTEM AS BASIC DESIGN ON SEISMIC BEARING COMPOUND FORMULATION

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## ABSTRACT

Indonesia is highly prone to earthquakes. The southern and western coasts of Java, as well as Sumatra, have the most exposed locations. Because of this, it's critical to establish a culture of disaster mitigation in the most fertile and heavily populated islands to reduce the number of fatalities and economic losses caused by earthquakes. The rubber seismic bearing, which is constructed of rubber layers, is a promising real-world seismic base isolation technique. The aimed of the research was to examine the typical behaviour of natural rubber compounds that had undergone various sulfur-curing processes. Sulfur curing systems were arranged consisted of a conventional which applied N-cyclohexyl-2-benzothiazole sulfonamide (CBS)/Sulfur (S) ratio as 1.4/0.25 and 1.4/0.35; semi-efficient for CBS/S ratio as 1.4/1.4 and 1.4/1.7; and efficient for CBS/S ratio as 1.4/3.0 and 1.4/3.5. The experiment's findings demonstrated that the most ideal modification condition for the natural rubber macromolecule chain found in the seismic-bearing rubber compound was a semi-efficient sulfur curing system with a CBS/S ratio of 1.4/1.4. Therefore, it was appropriate to be implemented in the development of seismic rubber bearing especially low-damping rubber bearing types.

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## **Physical Modification Cellulose Nanofibril with Poly(vinyl alcohol) and Carboxymethyl cellulose as Coating on Paper for Food Packaging**

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### **ABSTRACT**

In these past few years, research have been carried out to find an alternative coating materials for food packaging paper that are environmentally friendly. One candidate for such plastic coatings for food packaging is biopolymers such as cellulose. Modified cellulose nanofibril (CNF) can be used on coating food packaging paper. Previous studies revealed that PVA/CNF composites had a poor viscosity; as a result, a thickening agent, such as carboxymethyl cellulose (CMC), is required. Therefore, this study investigated the effect of CMC addition on the composites. Characterization techniques of viscosity, zeta potential, and FTIR were used. According to the findings, PVA/CMC/CNF composites showed high viscosities and zeta potential, which lead to outstanding dispersion and stability. The performance of the composites as a coating was studied using various parameters, i.e., tearing resistance strength and water absorption. Suprisingly, PVA/CMC-1/CNF had an excellent performance in water absorption test. Meanwhile, increase of the CMC concentration leads to a better tearing resistance. Moreover, PVA/CMC-1/CNF exhibits lower water vapor transmission rate (WVTR) than the blank sample, thus, is promising as a coating for food packaging paper.

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## Separation of Sunset Yellow based on Molecularly Imprinted Polymers using Acrylamide Functional Monomer

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### ABSTRACT

The synthesis of Molecularly Imprinted Polymers (MIPs) with acrylamide functional monomer for separation of Sunset Yellow has been carried out using acrylamide and ethylene glycol dimethacrylate as the monomer and crosslinker, respectively, through free radical polymerization technique. This research aims to synthesize MIPs using acrylamide monomer to separate Sunset Yellow. The MIPs preparation involved several steps, starting with the pre-polymerization of the template and monomer, followed by the polymerization of MIPs Sunset Yellow (MIP-SY) in acetonitrile porogen. As a control, Non-Imprinted Polymers (NIPs) was also synthesized following the same procedure as MIPs, without template molecules. MIPs Sunset Yellow was characterized using Fourier Transform Infrared (FTIR) spectroscopy, and rebinding studies were examined. The MIPs was characterized using FTIR at 644 cm<sup>-1</sup>, confirming the presence of naphthalene functional groups from sunset yellow bending vibrations. This characteristic peak was observed in the MIPs before leaching, highlighting its specific molecular recognition capabilities in the synthesized polymer. The synthesized MIP-SY showed rebinding potential to sunset yellow samples. Performance evaluation with adsorption capacity parameters and imprinting factor (IF) was obtained at 1.172 mg.g<sup>-1</sup> and 4.903, respectively. Mass variation optimization revealed the optimal adsorption capacity at 25 mg mass with an adsorption capacity of 1.247 mg.g<sup>-1</sup>. These findings point to the potential of MIP-SY for water purification, notably in the remediation of water tainted with sunset yellow dyes, as well as applications in food samples containing the dye. Keywords: molecularly imprinted polymers, sunset yellow, acrylamide, dyes

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## **Effect of Composition and Thickness of Polyaniline-Polypyrrole Composites as Gas Sensor Electrode Material on Responses to Robusta Coffee Aromas**

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### **ABSTRACT**

This experiment aimed to study the effect of composition and thickness of polyaniline/polypyrrole (PANi/PPy) composites as alternative electrode materials in gas sensors. The early step was synthesizing PANi and PPy from their monomers, followed by results confirmation using FTIR and UV-visible spectrophotometer. Various compositions of PANi/PPy were layered on the surface of the Print Circuit Board (PCB) using a drop-casting technique and were tested on the gas sensor to assess Robusta coffee aroma, resulting in the optimum composition of PANi/PPy was 20:80. This exhibited that, the highest PANi/PPy ratio, the lower the conductivity. The optimum PANi/PPy composite was then tested with a thickness variation of 160, 200, 311, 362, and 576  $\mu\text{m}$ . The effect of PANi/PPy composite thickness was determined based on the highest conductivity and response time. The results showed that the conductivity increases with increasing the thickness. However, at a certain thickness, the conductivity decreased. The highest conductivity value was obtained from a 311  $\mu\text{m}$  thickness sensor with a conductivity value of  $7,5 \times 10^{-9}$  S/cm with a response time of 44 seconds. Electrode with optimum composition and thickness was applied to characterize Robusta coffee aroma from three locations. PANi/PPy gas sensor electrodes with optimum composition and thickness perform acceptable in sensitivity, repeatability, and reproducibility.

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## **Evaluation of the functionality of pectin from cocoa pod husk to modify the characteristic and starch digestibility of bread**

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### **ABSTRACT**

Pectin is a soluble fiber beneficial for digestive health. Its potential functionality in lowering blood glucose levels has been reported. In this study, pectin was extracted from cocoa pod husk and fortified to a loaf of bread at concentrations of 5% w/w. The physical and chemical properties of bread were evaluated comprising of color and hardness level, as well as the moisture, crude fiber, and total digestible starch contents. The characteristics of bread were significantly changed with the presence of pectin concentration. The crust color showed a decrease in the a\* (red/green) and b\* (blue/yellow) values from the control bread, while the lightness (L\*) values were relatively constant. The hardness levels, moisture content, and crude fiber content were dramatically increased from initially 16.43 g/mm, 17.53%, and 7.39% to 49.46 g/mm, 20.57%, and 19.69%, respectively. Despite its expected effects on blood glucose levels, in our experiment, the addition of pectin resulted in an increase in the total digestible starch content from 33.39 g/100g to 36.97 g/100g. In conclusion, the addition of pectin from cocoa pod husks could alter the properties of bread in addition to the starch digestibility of the bread. Further study is needed to explore the suitable applications of pectin-fortified bread. Keywords: pectin, cocoa pod husk, bread, digestible starch, texture.

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## Modification of Functional Porous Material Based on Ni(II)-terephthalate Metal-Organic Frameworks

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### ABSTRACT

Previously, the crystal structure of Ni(II)-terephthalate complex was reported to display a 2D polymeric structure. The 2D polymeric structure of Ni(II)-terephthalate complex can be improved into 3D networks to modify its structure and functionality by introducing bridging ligands, such as pyrazine, as pillars. This study aims to incorporate pyrazine as a pillar into the Ni(II)-terephthalate complex, not only to increase the complex's dimensionality from 2D to 3D but also to enhance its thermal stability and porosity. The targeted Ni(II)-terephthalate-pyrazine was synthesized by solvothermal reaction using dimethylformamide as a solvent in several different conditions, namely at 130 and 150 C and in Ni(II): terephthalic-acid:pyrazine mol ratios of 1:1:2 and 1:1:4. The solid product was characterized by infrared spectroscopy, SEM-EDX, and powder-XRD in order to confirm the presence of pyrazine in the synthesized compound. Meanwhile, the thermal stability and porosity of the synthesized compound were investigated by DTA-TGA and surface area analyzer, respectively. Experimental data shows that green pale powder was obtained from all reactions in considerably good yield, which is different from the dark green crystalline solid of Ni(II)-terephthalate complex. SEM imaging reveals that the product has a wave-like surface morphology. Infrared spectra of the product show characteristic functional groups, namely the C=O, C-O, C=N, and C-N groups, which confirm the presence of both ligands. Powder XRD analysis suggests that the crystal system of the synthesized compound is different from that of the Ni(II)-terephthalate complex. Based on these analyses, the targeted Ni(II)-terephthalate-pyrazine is successfully obtained. However, analyses for thermal stability and porosity of the synthesized compound are not fully finished yet and are being investigated.

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## **Effect of molecular weight of chitosan in the coating solutions on the shelf life of Tuna fish fillets**

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### **ABSTRACT**

Tuna fish is one of the greatest Indonesia marine commodities. Besides delicious in taste, tuna fish have high nutrients content. However, high protein content is susceptible to deterioration during storage. Therefore, it require strategies to inhibit deterioration of tuna fish during storage. The aim of research is to prepare the coating solution and utilize it for extended the shelf life of tuna fish. The coating solution is composed of chitosan and liquid smoke. In here, chitosan in different molecular weight were used as variable to study physical and chemical properties. As the result, physically, there were not significant change in tuna fillet after apply coating. Based on pH and TVB-N, shelf life of tuna fish was extended by the chitosan-based coating solutions. In this study showed that chitosan with high molecular weight in the coating solution is more efficient to delay deterioration of tuna fish than medium and low molecular weight.

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# **SYMPOSIUM**

## **Renewable Energy and Fuel Cell (REF)**



## Fabrication of Activated Carbon-NiCo<sub>2</sub>O<sub>4</sub> with Hybrid Structure for Supercapacitor Electrode Materials

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### ABSTRACT

State-of-the-art supercapacitors generally use various types of activated carbon (AC) as electrode materials. However, the use of AC is poor in conductivity performance and low energy density. Herein, we demonstrated the fabrication of AC-nickel cobaltite (NiCo<sub>2</sub>O<sub>4</sub>) used as an asymmetric material for supercapacitor electrodes. The purpose of this study was to determine the performance of modified AC-based electrodes as the anode and AC-NiCo<sub>2</sub>O<sub>4</sub> as the cathode. NiCo<sub>2</sub>O<sub>4</sub> has been successfully synthesized using the hydrothermal method. Then the sample results obtained are composited with AC as the cathode electrode. Furthermore, AC and AC-NiCo<sub>2</sub>O<sub>4</sub> are characterized using Fourier Transform Infrared Spectroscopy (FTIR), X-Ray Diffraction (XRD), and Scanning Electron Microscope-Energy Dispersive X-Ray (SEM-EDX) respectively. The FTIR AC-NiCo<sub>2</sub>O<sub>4</sub> reveal absorption band for AC shows peak at 1554 cm<sup>-1</sup>, which can be attributed to C=C are typical vibrations present in carbonaceous material, and the spectrum of NiCo<sub>2</sub>O<sub>4</sub> spinel exhibits two separate sharp bands in the stretching vibrations of Ni-O bond were assigned to the band at 567 cm<sup>-1</sup>, while the stretching vibrations of Co-O bond were attributed to the band at 648 cm<sup>-1</sup>. The XRD pattern confirm the crystalline structure be assigned of cubic spinel. Afterwards electrochemical measurements were carried out by assembling the electrodes into a prototype coin cell. Finally, the resulting prototype was tested for performance using Cyclic Voltammetry (CV), Electrochemical Impedance Spectroscopy (EIS), and Galvanostatic Charge-Discharge (GCD).

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## **Synthesis of MgO Nanoparticles Using Water Hyacinths Leaves Extract and Its Application on Biodiesel Production from Waste Cooking Oil**

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### **ABSTRACT**

This research is driven by the diminishing reserves of fossil fuels, which are in contrast to the increasing consumption of fuel oil. Hence, there is a growing demand for alternative fuels, particularly biodiesel. Waste cooking oil serves as a viable source for biodiesel production due to its abundance, affordability, and lack of reuse. In this study biodiesel was produced from waste cooking oil through two-step processes, namely esterification reactions using homogeneous  $H_2SO_4$  catalyst and transesterification using the heterogeneous base Magnesium oxide nanoparticles (MgO-NPs) catalyst. MgO-NPs have shown significant interest due to their broad applications in fields like pharmaceuticals, manufacturing, and dermatology. In our current study, we employed an environmentally friendly method to produce MgO-NPs. These nanoparticles were successfully synthesized using an aqueous leaf extract of water hyacinths. Subsequently, the MgO-NPs produced through this eco-friendly process underwent characterization after being subjected to calcination at 400°C. UV-Vis spectroscopy was used to confirm the formation of the nanoparticles. The MgO-NPs was also characterized by X-Ray Fluorescence (XRF), X-Ray Diffraction (XRD), Thermal Gravimetric Analysis (TGA) and Scanning Electron Microscope (SEM).

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## **In Situ Transesterification of *Nannochloropsis* sp Microalgae to Produce Biodiesel with CaO/Hydrotalcite Catalyst: Analysis of The Effect of CaO Loading**

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### **ABSTRACT**

The present study aims to determine the effect of CaO to hydrotalcite loading ratio in the catalyst and stirring speed in the reactor on biodiesel yield and FFA content produced from microalgae *Nannochloropsis* sp. by In-Situ transesterification. The microalgae was chosen because it does not compete with human food needs and is only used as animal feed for fish and shrimp. The optimal operating conditions and components of biodiesel purified by distillation were also determined in this study. The variables used were CaO/hydrotalcite load ratios of 1:1, 3:1 and 5:1 wt/wt and stirring speeds of 50, 100, 150, 200 and 250 rpm. The results showed that a catalyst ratio of 1:1 and a stirring speed of 250 rpm gave the highest yield of 38.36% with the lowest FFA content of 1.39%. The results of the GC/MS test showed that the biodiesel contained olefins and aliphatic alkanols that are classified as petrol.

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## **Crude Biodiesel Production from Palm Fatty Acid Distillate (PFAD) By Ultrasound-Assisted Esterification Method**

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### **ABSTRACT**

Indonesia is the largest crude palm oil (CPO) producing country in the world with a total area of oil palm plantations recorded in 2022 was 15.4 million hectares and total CPO production in the same year was 48.2 million tonnes. In overall, the palm oil refining process can produce 73% olein, 21% stearin, 5% PFAD, and 0.5% waste. Therefore, to overcome this problem, an alternative approach used in this study was utilization of CPO waste, palm fatty acid distillate (PFAD), because it does not interfere with consumption materials. The purpose of this study was to evaluate the effectiveness in term of % yield in the production of crude biodiesel from PFAD using intensified process, which is ultrasound-assisted esterification method. The intensified biodiesel production with assisting of ultrasound irradiation was conducted under various operational conditions of esterification reaction temperature (55°C, 60°C, 65°C), oxalic acid catalyst loading (4%, 6%, 8% (w/w)), and ultrasonic power (12%, 14%, 16% (maximum 900 Watts)). Characteristics of biodiesel were also evaluated. Experimental results showed that in general, the % yield of biodiesel increases with the increasing of time at various operational process conditions. The characteristics of the obtained biodiesel were in accordance with the crude biodiesel quality standard range of SNI 7182: 2015. The optimum yield of biodiesel was obtained at operational condition of temperature of 65°C, catalyst loading of 4%, and ultrasonic power of 16% with an optimum yield of 98.22%.

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# **SYMPOSIUM**

## **Material : Synthesis and Characterization (MSC)**





## **Synthesis and Characterization of Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) from Iron Sand Using Coprecipitation Method**

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### **ABSTRACT**

Hematite ( $\alpha$ -Fe<sub>2</sub>O<sub>3</sub>) has been synthesized from iron sand using the coprecipitation method. This study aims to determine the morphology and mineral content using SEM-EDX, crystal structure and phases formed using XRD, and magnetic properties using VSM on iron sand before and after synthesis. SEM-EDX results show that the average particle size of iron sand before and after synthesizing is 356.23nm and 12.40  $\mu$ m, respectively. XRD results show that iron sand before synthesizing has multiphase including Hematite, magnetic, and ilmenite and after synthesizing produces Single Phase hematite. VSM results show that iron sand before synthesizing has saturation, remanence, and coercivity of 47.56 emu/g, 5.97emu/g, and 121.03 Oe respectively, and after synthesizing has saturation, remanence, and coercivity of 9.47 emu/g, 1.53 emu/g and 102.97 Oe respectively.

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## **MODELING AND SIMULATION OF THE DISTRIBUTION OF UREA CONCENTRATIONS IN HEMODIALYSIS HOLLOW FIBER MEMBRANES WITH VARIATIONS OF BLOOD FLOWRATE**

Yeni Rahmawati<sup>1</sup>, Belinda Kezia Purwanto<sup>2</sup>, Fabio Emiguel Simanjuntak<sup>3</sup>, Siti Nurkhamidah<sup>4</sup>

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### **ABSTRACT**

The kidney is one of the important organs in the body that can filter around 120-150 liters of blood every day and excrete metabolic wastes, namely urea, creatinine, and foreign chemicals through urine. Kidney failure in carrying out these important functions can result in high levels of urea in the body so it can become toxic to the body. If the condition of the kidneys is not functioning above 75%, dialysis or hemodialysis is very helpful for sufferers. Hemodialysis is a process of taking blood through the extracorporeal circuit, through a device called a dialyzer. In this study, a hollow fiber type dialyzer was used which consisted of three parts, namely the shell (dialysate flow area), porous membrane, and tube (blood flow area). This research will be carried out theoretically by developing a mathematical model of mass transfer in hollow fiber membranes in the hemodialysis process to study the effect of blood flow rate on urea concentration in the axial and radial sections of the tube, membrane, and shell, the effect of length on urea clearance, and influence of dialysate flowrate on urea clearance using MATLAB R2022b. It was found that the greater the blood flow rate, the greater the concentration of urea coming out of the tube, because a small amount diffuses into the shell. In addition, the longer the membrane, the greater the clearance obtained. For dialysate flow rate, it does not affect the clearance of urea. With a dialysate flow rate of 500 mL/min and a membrane length of 27 cm, urea clearance was obtained successively at blood flow rates of 200, 300, 400, and 500 mL/min, including 21.95%; 17.06%; 14.31%; 12.52%.

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## **Fabrication and Characterization of Cellulose Acetate/N-Methyl-2-Pyrrolidone Membranes for Separation of Microplastics in Water**

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### **ABSTRACT**

Indonesia is the fifth ranked country with plastic waste that is not managed properly. Over time, plastic decomposes into microplastics (MPs) less than 5 mm in diameter, which in water can cause some harm. One method of removing MPs that is considered efficient is MPs microfiltration using membrane technology. To obtain an adequate membrane in removing MPs particles, it is necessary to modify the membrane both in the material and the membrane manufacturing process itself. So this study aims to study the effect of evaporation time and temperature on the characteristics and performance of microfiltration membranes to remove MPs in water. In this study, the membrane will be made using the phase inversion method with a flat sheet membrane finish. The membrane is made using Cellulose Acetate (CA) polymer with n-Methyl Pyrrolidone (NMP) solvent and aquadest as its non-solvent. The analysis of the results to be carried out is a characteristic analysis including SEM, water content, porosity, and contact angle. Also, membrane performance tests are carried out to determine the ability of membranes when separating microplastics in water. Fabrication of CA/NMP flat sheet membranes produces white membranes. All types of membranes that have been made have a thickness in the range of 68-75  $\mu\text{m}$ . These results are in accordance with the thickness range for microfiltration membranes. The results of measuring the contact angle on the CA/NMP membrane (15:85) show that the contact angle increases with the length of observation time. In addition, the contact angle also increases with increasing membrane immersion time. The contact angle formed is still in the range of 56°-79°, this indicates that the membrane formed is not yet hydrophobic. For membrane test performance, FTIR analysis was first carried out which showed that the synthetic water samples contained PET.

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## Characterization of $\text{Na}_{2/3}[\text{Fe}_{1/2}\text{Mn}_{1/2}]\text{O}_2$ as cathode material for sodium-ion batteries

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### ABSTRACT

Sodium-ion batteries have received significant attention recently due to element abundance, low price, and similar electrochemistry mechanism to lithium-ion batteries. However, the ionic radii of sodium larger than Lithium would trigger low ionic conductivity, leading to low electrochemical performance. Therefore, it needs a material design to accommodate sodium ion diffusion. Using a solid-state reaction, we developed the  $\text{Na}_{2/3}[\text{Fe}_{1/2}\text{Mn}_{1/2}]\text{O}_2$  cathode materials with various temperatures. X-ray diffraction (XRD) analysis confirms that  $\text{Na}_{2/3}[\text{Fe}_{1/2}\text{Mn}_{1/2}]\text{O}_2$  was a hexagonal structure that indexed to space group P63/mm. The various calcination temperatures result in various crystal sizes. Meanwhile, the existing carbon coating will improve the electrochemical performance. The  $\text{Na}_{2/3}[\text{Fe}_{1/2}\text{Mn}_{1/2}]\text{O}_2$  shows promising material properties for SIB application. Keyword: solid-state reaction, SIB,  $\text{Na}_{2/3}[\text{Fe}_{1/2}\text{Mn}_{1/2}]\text{O}_2$  Reference: [1] Yabuuchi, N., Kubota, K., Dahbi, M., Komaba, S. Research Development on Sodium-Ion Batteries. Chem. Rev. 2014, 114:p. 11636–11682. [2] Kalluri, S., Seng, K. H., Pang, W. K., Guo, Z., Chen, Z., Liu, H. -K., Dou, S. X. Electrospun P2-type  $\text{Na}_{2/3}(\text{Fe}_{1/2}\text{Mn}_{1/2})\text{O}_2$  Hierarchical Nanofibers as Cathode Material for Sodium-Ion Batteries. ACS Appl. Mater. Interfaces 2014, 6: p. 8953–8958. [3] Zhao, W., KiKirie, H., Tanaka, A., Unno, M., Yamamoto, S., Noguchi, H. Materials Letters 135 (2014) 131-134. [4] Wang, X., Gao, L., Yang, X. Materials Letters 341 (2023) 134262.

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## **Facile Synthesis of Activated Carbon-PANi Composites as Electrode Material for Application in Supercapacitor**

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### **ABSTRACT**

The development of energy storage systems has become the main focus in supporting the advancement of renewable energy technology and electric vehicles. One important device in this effort is the supercapacitor, which is known to have high capacity and low internal resistance. Although activated carbon-based supercapacitors have been widely used, they have weaknesses in energy density. Therefore, this study aims to modify the supercapacitor electrode with a composite between activated carbon and polyaniline (PANi) to improve its performance. This research uses a more efficient and flexible form of coin cell supercapacitor. Variations in the concentration of AC/PANi solutions are used as an approach to increase the capacity and energy density of supercapacitors. PANi has been successfully synthesized using the oxidation polymerization method and the results of the FTIR test show that one of the absorption peaks of stretching N=Q=N is at the wave number of  $1190\text{ cm}^{-1}$ , it indicates the delocalization of electron in the form of conductive properties of PANi. In the PANi X-ray diffraction pattern, 3 diffraction peaks appear at an angle of  $2\theta$ , at a peak of  $25.1^\circ(200)$  is a typical peak of PANi due to the characteristic level of conjugation- $\pi$  in PANi. The XRD pattern of PANi shows amorphous characteristics because PANi is a type of polymer. AC/PANi composite synthesis using the insitu polymerization method has been successfully carried out with AC as a commercial material. The results of FTIR characterization show that there are 8 absorption peaks, 2 of which show the peak of AC, namely at the values of  $1591\text{ cm}^{-1}$  and  $1527\text{ cm}^{-1}$ , while the other 6 peaks are the absorption peak of PANi. The results of this research are expected to prove that the use of PANi as an electrode material can improve the performance of supercapacitors with higher efficiency, supporting the development of renewable energy technology and electric vehicles. Keywords: AC, Electrode, Energy Density, PANi, Supercapacitor.

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## Effects of Crosslinker Concentration on The Synthesis of Thermoresponsive P(SPE-co-NIPAM) Hydrogels for Drug Delivery

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### ABSTRACT

Hydrogels have been widely applied in the biomedical field, especially smart hydrogels that can respond to stimulation such as temperature, light, electricity, etc. Among all stimulants, thermoresponsive hydrogels have emerged as appealing materials to be used in stimuli-controlled drug delivery systems, due to their ability to show reversible phase transition changes with stimulants in the form of human body temperature. This study focused on the synthesis of thermoresponsive hydrogels, specifically poly(sulfobetaine methacrylate-co-N-isopropylacrylamide) (P[SPE-co-NIPAM]), via free radical polymerization and investigating the impact of different concentrations of N,N'-methylenebisacrylamide (MBA) crosslinker on the properties of hydrogels and their potential application as drug carriers. It was found that the increasing MBA concentration led to increasing gel content of the hydrogels, and decreasing the equilibrium swelling ratio (ESR). According to the temperature-dependent swelling test, the ESR of the hydrogels decreased as temperature increased. The phase transition temperature ( $T_c$ ) of the hydrogels also exhibited a decrease with an increase in MBA concentration. Moreover, when the concentration of the initiator was doubled, the ESR was slightly increasing. The deswelling test revealed that the hydrogel with the highest concentration of MBA demonstrated an ability to retain more water. The hydrogel with the highest ESR was chosen for the drug carrier application studies. The ability of these hydrogels as a carrier was investigated using metformin-HCl as a model drug. The P(SPE-co-NIPAM) hydrogel was found to have entrapment efficiency of 4.8% and cumulative release of 19.34% for 15 hours in a simulated environment that mimicked physiological pH and temperature. Keywords : thermoresponsive hydrogels, poly(sulfobetaine methacrylate), poly(N-isopropylacrylamide), drug delivery, metformin-HCl

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# Tracking Ag-Au Bimetallic Nanoparticles during Their Synthesis by Field Flow Fractionation and Inductively Coupled Plasma Mass Spectrometry: Implications for Colorimetric Sensing of Cobalt Ions

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## ABSTRACT

A method using inductively coupled plasma mass spectrometry (ICP-MS) in the single particle mode and the conventional mode coupled to a flow field flow fractionation (Fl-FFF) was developed to select suitable conditions for the synthesis of Ag-Au bimetallic nanoparticles (Ag-Au BNPs) and to monitor the colorimetric changes due to aggregations. Ag-Au BNPs, synthesized by using citrate reduction of Ag and Au ions, were used as sensors for the detection of Co<sup>2+</sup>. To better understand the colorimetric sensing of Co<sup>2+</sup> using the Ag-Au BNPs, various mixtures were studied, viz. (i) only Ag-Au BNPs; (ii) Ag-Au BNPs with thiosulfate; (iii) Ag-Au BNPs with thiosulfate and ethylenediamine; and (iv) Ag-Au BNPs with thiosulfate, Co<sup>2+</sup> and ethylenediamine. Single particle ICP-MS (SP-ICP-MS) was used to determine the core size, size distribution, and number concentration, as well as the heterogeneity of the particles synthesized by using various citrate concentrations and metal ratios. Fl-FFF-ICP-MS was also used to observe the hydrodynamic size and the Ag: Au signal intensity ratio of the BNPs to support information obtained from the SP-ICP-MS. The combination of the proposed techniques has been applied to monitor the reaction during colorimetric sensing. Additional information from fractograms provided by Fl-FFF-ICP-MS was also useful for the understanding of the aggregation of BNPs arising from the [Co(II)(en)<sub>3</sub>]<sup>2+</sup> complex surrounding the surface of the BNPs. Furthermore, when compared to colorimetric sensing, the limit of detection for Co<sup>2+</sup> ion, using the BNPs and SP-ICP-MS, were 20-fold lower, decreasing from ppb to ppt levels. Keywords: Single particle inductively coupled plasma mass spectrometry (SP-ICP-MS), flow-field flow fractionation (Fl-FFF), bimetallic nanoparticles, size distribution, particle number concentration.

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## **Effect of mole Ratio of Si/Al on the Acidity and Crystal Structure of Aluminosilicate**

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### **ABSTRACT**

Aluminosilicate is a solid acid material that can be applied as a material catalyst for many purposes such as cracking, acetylation, and esterification reactions. The acidity can be controlled by the ratio of a combination of aluminium trivalent atoms on the tetrahedral silica frameworks. This study aimed to evaluate the effect of the mol ratio of Si/Al on its crystal structure and acidity prepared by hydrothermal and sol-gel methods. Both reaction methods were carried out in the mole ratios of Si/Al 30, 50, and 70. Besides, hydrothermal reactions were prepared at temperatures 110, 125, and 140 °C, while the sol-gel reactions were conducted at pH 2, 4, and 6. All of the materials were characterized by x-ray diffraction to evaluate the crystal structures, FTIR spectrophotometer to understand the functional groups, and FTIR-Pyridine to observe the acidity. The results exhibited all the aluminosilicate materials have an amorphous structure that can be seen by the hump diffractogram pattern in  $2\theta = 22^\circ$ . Moreover, increasing the mole ratio of Si/Al declined the total acidity of aluminosilicate. The rising hydrothermal temperature increased total acidity and Bronsted acid site and decreased the Lewis acid site. Meanwhile, the pH in sol-gel remained an insignificant effect on the total acidity of aluminosilicates.

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## **Preparation of High Specific Capacitance Material Based on Activated Carbon-Manganese Dioxide Composite Using Lemon Peel (*Citrus limon*) Extract for Supercapacitor Electrode**

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### **ABSTRACT**

This study, we prepare a high specific capacitance material based on activated carbon-manganese dioxide (AC/MnO<sub>2</sub>) composite. The MnO<sub>2</sub> particle was synthesized via redox reaction between KMnO<sub>4</sub> and lemon peel extract as a bioreductor. The steps taken in this research was first preparation of lemon peel extract, then synthesis of MnO<sub>2</sub> using lemon peel extract, synthesis of AC/MnO<sub>2</sub> composites, and finally electrodes characterization using XRD, SEM, and CV. Our findings reveal that the AC/MnO<sub>2</sub> composite electrode had a higher specific capacitance than that of the synthesized MnO<sub>2</sub>. This is because MnO<sub>2</sub> particles can be dispersed to the surface and pores of activated carbon, thus increasing the contact area of MnO<sub>2</sub> and electrolytes, which refers to the increase in specific capacitance. The XRD test results show that the formed MnO<sub>2</sub> consisted of  $\alpha$ ,  $\gamma$ , and  $\delta$  polymorphs. SEM data show that the average MnO<sub>2</sub> particle size is 482.80 nm. The CV test results show that the highest AC/MnO<sub>2</sub> capacitance is 188.17 F g<sup>-1</sup> when the AC/MnO<sub>2</sub> ratio is 1:1. This suggested that the AC/MnO<sub>2</sub> composite material has immense potential to be used as supercapacitor electrode material.

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## THE BEHAVIOUR STUDY OF SUMBERMANJING'S PYROPHYLLITE-WATER INTERACTION

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### ABSTRACT

Sumbermanjing pyrophyllite classified as 2:1 clay mineral carrying plasticity property and its hardness is 1-2 mohs scale. It is reported having no both hydrated cations and unhydrated cations between its interlayer structure. Pyrophyllite in general is classified has no charge and hydrophobic clay mineral. However, its fundamental structure consisting of two polymeric tetrahedral silicate and polymeric octahedral alumina sandwiched among the two tetrahedral silicate showing some reactive sites which is possible to react with other reactive compounds. There is no report elsewhere about the reactivity of Sumbermanjing's pyrophyllite toward water. This research reported the resulting study of Sumbermanjing's pyrophyllite reactivity to water using modified foster method. The measurement glass apparatus was used instead of biuret and beaker glass. Sumbermanjing's pyrophyllite was sized to fit 100-200 mesh, heated at 300oC for 5 hrs, washed at 1:2 ratio using water and re-heated for another 1 hrs at the same temperature. The sample (1 g) was immersed with water in the measurement glass up to 10.0 mL and was left to contact with water for 24 hrs, 48 hrs and 72 hrs. This time contact variation was applied to the different size of pyrophyllite, 100-200 mesh and 200-300 mesh. The dispersing pyrophyllite was treated with stirring and non-stirring. The data was taken based on the change of the height level of pyrophyllite in the measuring glass. After one -way ANOVA analysis, there were no significant differences among the shrinkage values of the applied parameter, except for the 200-300 mesh pyrophyllite under stirring. The highest value of shrinkage (31.75%) was obtained for 200-300 mesh pyrophyllite under stirring and the contact time for 48 hours.

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## **Synthesis and Characterization of Keratin Nanoparticles from Chicken Feather by Sonification Method**

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### **ABSTRACT**

Keratin is a protein biopolymer that can be isolated from chicken feathers by hydrolysis method. To increase the capability, keratin can be made in the form of nanoparticles. In this research, the synthesis of keratin nanoparticles was carried out from chicken feathers by sonication method. Addition of surfactant (span 80) and cross-linking reagent (NaTPP) was also carried out to increase the stability of the keratin nanoparticles. Keratin nanoparticles synthesis was started by determining the concentration of the dispersing medium in the form of acetic acid (1.0, 1.5, and 2.5%). Next is determining the optimum sonication conditions which was carried out by varying the amplitude (10, 50, and 100%) and the sonication time (8, 10, 12, and 30 minutes). The results were analyzed toward the yield of keratin nanoparticles. The stability level of nanoparticles keratin was observed by comparing the addition of span 80 or NaTPP with the absence of these two reagents. The synthesized keratin was then characterized using (1) FTIR to examine the changes in functional groups, and (2) using an electron microscope to observe the particle morphology. Meanwhile, the particle size was obtained through calculations using the ImageJ program. The research results showed that the IR spectrum of keratin nano particles does not have a significant difference when compared to the IR spectrum of non-nanoparticle keratin, in which there is a typical absorption of protein biopolymers in the form of amide and III (absorption). Furthermore, the morphology of keratin nanoparticles made with the addition of NaTPP has an irregular shape and various particle size with a size of around 300 nm, while the morphology of keratin nanoparticles obtained from the addition of span 80 has smaller and uniform round particles that are evenly distributed with the particle size of around 200 nm. Keratin nanoparticles obtained without the addition of NaTPP or span 80 have a non-uniform shape and tend to be stacked with each other with a particle size of around 275 nm. Keywords: Keratin, nanoparticles, sonication.

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## One-pot Synthesis of Chitosan-Reduced Gold Nanocomposites as Novel Functional Material

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### ABSTRACT

Chitosan-gold nanocomposites (Ch-AuNCs) have unique biocompatible properties that can be used for various biomedical applications, including drug delivery, sensing, and catalysis. However, the current method of Ch-AuNC synthesis is not efficient enough because it requires a lot of time and monitoring. In this study, we present a facile one-pot synthesis method to synthesize Ch-AuNCs from strach. The synthesis process involves the reduction of gold ions as well as the stabilization of nanoparticles within the chitosan matrix. The structural characteristics of the Ch-AuNCs were investigated using various analytical techniques, including UV-Vis spectroscopy, FTIR, and DLS. These analyses confirmed the successful formation of spherical gold nanoparticles with an average size of 173.5 nm embedded within the chitosan matrix. The concentration of HAuCl<sub>4</sub> used was varied from 0.1, 0.25, 0.5, 0.6, 0.8, and 1 mM to study the correlation between the concentration used and the nanoparticle size produced. The UV-Vis spectroscopy results showed that there is a maximum absorbance shift between each of the concentrations. Our research concluded that Ch-AuNCs can be synthesized using simple one-pot synthesis methods that are more efficient than conventional synthesis methods.

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## **Synthesis, Quality Control and Stability Test of [177Lu]Lu-PSMA I&T Radiopharmaceutical as a Theranostic Agent for Prostate Cancer Treatment**

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### **ABSTRACT**

The theranostic application of radiopharmaceutical [177Lu]Lu-PSMA I&T for Prostate Cancer (PCa) treatment is widely used worldwide and turned into clinical trials in many countries. However, in Indonesia, the application of [177Lu]Lu-PSMA I&T has not been reported. Therefore, we developed the production of [177Lu]Lu-PSMA I&T using carrier-added Luthesium-177 produced by an Indonesia nuclear research reactor. We optimized the production methods such as the TLC system for quality control, the amount of ligand, pH, temperature and incubation time. The stability and lipophilicity were also investigated. The radiochemical purity of [177Lu]Lu-PSMA I&T was checked using Instant Thin Layer Chromatography Silica Gel (ITLC-SG) with saline as a mobile phase, which clearly separates the free 177Lu (Rf=0) and the complex (Rf=1). High labelling yield was achieved by labelling the ligand with carrier-added 177LuCl<sub>3</sub> solution in the fourth molar excess of the ligand, and pH ±5 (adjusted with buffer acetate 1 M). The radiopharmaceutical, [177Lu]Lu-PSMA I&T was successfully produced with a high radiochemical yield and a high radiochemical purity of > 98% (both radio-TLC and radio-HPLC) after less than 10 min at a temperature of 90 °C, resulting in specific activity of 17-20 GBq/μmol. The complex of [177Lu]Lu-PSMA I&T showed high stability at both room temperature (22.5 °C) and refrigerator temperature (4-8 °C) for up to 96 hours. The complex exhibited high stability in saline and human serum in vitro for 96 hours and 48 hours, respectively. The radiopharmaceutical [177Lu]Lu-PSMA I&T showed higher hydrophilicity with a log-P value of -3,37 ± 0,03. Keywords: [177Lu]Lu-PSMA I&T, Luthesium-177, theranostic, prostate cancer

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## **Kappa Number Analysis in the Production of Abaca Fiber Pulp using Ultrasound-Assisted Organosolv Method with Alkaline Pretreatment**

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### **ABSTRACT**

An alternative raw material, which has great potential to replace wood source, is needed to continue the development of pulp and paper manufacturing industries. One of the choices of alternative raw materials is banana abaca fiber (*Musa Textilis*) as a source of non-wood fiber in the manufacture of pulp, because it contains about 68.32% cellulose, 19% hemicellulose, and 12-13% lignin. The use of abaca fiber is also promising in replacing wood source, because its plantation period is much shorter compared to that of wood source. The purpose of this study was to analyze the effect of time, temperature, NaOH concentration, and ultrasonic power on Kappa number of abaca fiber pulp obtained from organosolv method with ultrasound irradiation assistance followed by alkaline pre-treatment process. In addition, the best operational condition in organosolv method was evaluated. The COD and BOD<sub>5</sub> of the waste process for best variable condition were also observed. The ultrasound-assisted organosolv process was conducted under various operational conditions of temperatures (30, 50, 70, 90 °C), ultrasonic powers [117 W (13%), 162 W (18%), 210 W (23%), 256 W (28%)], process times (30, 45, 60, 90 minutes), and NaOH concentrations (5%, 10%, 15%, 20 wt.%). The experiment results showed that the best conditions were obtained at pulping reaction time of 30 min, ultrasonic power of 162 W (18%), NaOH catalyst concentration of 20 wt.%, and temperature of 50 °C with lowest kappa number of 13.69.

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## **The Effect of Poly(L-Lactic Acid) (PLLA) and Polyethylene Glycol 200 (PEG200) Addition in Cellulose-Based Biocomposite Beads on Adsorption of Methylene Blue in Batch Systems**

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### **ABSTRACT**

Cellulose acetate (CA), poly(L-lactic acid) (PLLA), Polyethylene glycol 200 (PEG200) were successfully blended through solvent blending method followed by solution dropping technique to fabricate cellulose-based biocomposite CA/PLLA/PEG200 beads with the variation of PLLA and PEG content (100/0/0, 70/30/0, 70/15/15, and 70/0/30 wt.%). The obtained biocomposite beads were applied as adsorbent for methylene blue (MB) removal from aqueous solution under various condition of temperature, pH, initial MB concentration, and beads dosage. Batch equilibrium adsorption was carried out to observe the effect of various PLLA and PEG content, temperature, pH, initial MB concentration, and mass of beads on the adsorption performance (adsorption capacity and % dye removal), and to study the adsorption kinetics. The best bead composition in adsorption performance was evaluated for the kinetics using three kinetic models of pseudo-first order, pseudo-second order, and elovich equation. The best adsorption performance in term of adsorption capacity and % removal (%R) was obtained on CA/PLLA/PEG200 (70/15/15) biocomposite cellulose beads at temperature of 40 °C, pH of 11, initial MB concentration (C<sub>0</sub>) of 30 mg/L, and beads dosage (G) of 2 g/L. The kinetic model to describe the adsorption process in this experiment for CA/PLLA/PEG200 (70/15/15) biocomposite beads is the pseudo-second-order model, showing that the adsorption rate is more dependent on adsorption capacity rather than on initial concentration of MB dye.

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## Synthesis and Structure of $[\text{Ni}(\text{4-ampy})_4(\text{dca})_2] \cdot \text{4-ampy}$ (ampy = aminopyridine, dca = dicyanamide ion)

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### ABSTRACT

This study aims to synthesize the complex compound  $[\text{Ni}(\text{4-ampy})_4(\text{dca})_2] \cdot \text{4-ampy}$ . The synthesis was carried out through the reaction between Ni(II) metal ions, 4-aminopyridine (4-ampy) ligands, and dicyanamide (dca) ion ligands with a mole ratio of Ni(II) : 4-ampy : dca = 1 : 4 : 2 in methanolic solution. Reaction was carried out using the solvothermal method at 70 °C. Cube-shaped blue crystals were collected after evaporation for several days at room temperature. Characterization of the as-synthesized crystal showed that the compound has a melting point of 195-200 °C, with monoclinic crystal lattice data, space group  $P2_1/m$ , and crystal lattice parameters  $a = 13.077(6) \text{ \AA}$ ,  $b = 16.927(8) \text{ \AA}$ ,  $c = 15.492(8) \text{ \AA}$ ,  $\alpha = 90^\circ$ ,  $\beta = 109.298(8)^\circ$ . The compound has an octahedral molecular structure with the chemical formula  $[\text{Ni}(\text{4-ampy})_4(\text{dca})_2] \cdot \text{4-ampy}$  and is a molecular compound. The results of FTIR analysis showed vibrations of the  $\text{C}\equiv\text{N}$  group at wave number  $2223 \text{ cm}^{-1}$ , indicating the presence of dicyanamide ligand,  $\text{C-NH}_2$  group at wave number  $1280 \text{ cm}^{-1}$  and N-H group stretching vibrations at wave number  $3370 \text{ cm}^{-1}$ , indicating the presence of 4-aminopyridine ligand. UV-Vis data showed a wavelength shift from 407 nm to 307 nm, indicating a change in the splitting orbital d of Ni(II) ions. Keywords: Solvothermal method, Nickel complexes, Mixed-ligand complexes, mixed 4-aminopyridine-dicyanamide ligand, complex structure.

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# **SYMPOSIUM**

## **Nanomaterials and Nanodevices (NN)**



# Single-step green synthesis of gold-conjugated polyphenol nanoparticles using extracts of *Cajanus cajan* as chemical probes for heavy metal detection and its biological applications

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## ABSTRACT

The utilization of nanotechnology in biomedical and environmental applications has garnered substantial attention, particularly focusing on the green synthesis of gold nanoparticles (AuNPs) through plant-mediated methods. This synthesis is a single step and eco-friendly approach, where phenolic compound from plant extracts act as reducing and capping agents in nanoparticle production. This research aimed to synthesized AuNPs via bioreduction facilitated by extracts from *Cajanus cajan* (Pigeon pea) and subsequently assess their dual functionality-antioxidant activity and potential as chemical probes for heavy metal ion detection in water samples. Phenolic compounds in *C. cajan* extract serve as reducing agents that facilitate the reduction of Au<sup>3+</sup> to Au<sup>0</sup>, which is characterized by a noticeable colour change from clear yellow to reddish-purple. Synthesized gold nanoparticles capped C. cajan extract (CJ-AuNPs) were stabled and evaluated by UV-Visible spectrophotometer ( $\lambda$  SPR at 534 nm), FTIR to examine the functional groups present on the nanoparticle surface (OH groups, Carbonyl groups, alkil groups) and dynamic light scattering (DLS) was applied to measure the hydrodynamic size and dispersity of CJ-AuNPs in solution (5.52 nm, PDI 0.2345), offering valuable information about their physical properties and colloidal stability, SEM and HR-TEM study. The CJ-AuNPs were tested for their radical scavenging exhibited a good antioxidant property with ABTS method. The characterization SPR peak of CJ-AuNPs at 534 nm was red shifted to 560 nm confirm the coordination bonds between CJ-AuNPs and Cr<sup>3+</sup> ion and the colour was changed from reddish purple to blue. This result clearly indicated that CJ-AuNPs can be used as chemical probes for detecting heavy metal ions in water samples.

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## **STABILITY TEST OF NANOGOLD SYNTHESIZED USING ASCORBIC ACID AT ROOM TEMPERATURE AS PREPARATION FOR THE COMMERCIALIZATION NANOGOLD HEALTHY DRINK**

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### **ABSTRACT**

This research aims to determine the stability of nanogold synthesized by reducing ascorbic acid at room temperature. This research was carried out as preparation for marketing nanogold healthy drink. Water containing colloidal nanogold is a healthy drink which has benefits as an antioxidant. In preparation for the commercialization of healthy drinks, data on the colloidal stability of nanogold is needed. Stability is measured from the UV absorption value at a constant maximum absorption wavelength. Nanogold synthesis was carried out at room temperature without heating with ascorbic acid or vitamin C as reducing agents. Synthesis was carried out at a concentration of 2.5; 5, 10, 15 and 20 ppm. UV-visible analysis is carried out every 3 days. Data was collected and analyzed to determine the colloidal stability of nanogold. TEM analysis to determine the diameter of the collection of nanogold atoms at the beginning and end of the study. The results show that there is a change in the size of the atomic group in colloidal nanogold. On the first day the absorption was at a wavelength of 520 nm for all concentration variations except 20 ppm absorption at 522nm. The second measurement after 3 days showed that there was a shift in the absorption wavelength at concentrations of 2.5 ppm and 5 ppm at 524nm and 526nm respectively. The third measurement showed a shift in absorption towards shorter wavelengths, namely absorption from 522 nm to 520 nm, 520 nm to 518 nm, which shows an increase in the diameter of the nanogold atom collection. The absorption price showed no change. This is also supported by the absence of sediment so that the colloid is stable during measurement. The research conclusion is that diameter cluster size was dynamics occur in colloidal nanogold during measurements but are still within the range of nanomaterials. No precipitation occurs, meaning the nanogold colloidal was still stable. Keywords: nanogold, stability, wavelength, absorption and diameter atomic cluster

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## **Synthesis of TiO<sub>2</sub> nanotubes using a two-stage hydrothermal process with variations in the TiO<sub>2</sub>/NaOH molar ratio.**

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### **ABSTRACT**

TiO<sub>2</sub>, a nanomaterial compound with a large surface area, has excellent photocatalytic activity. TiO<sub>2</sub> nanoparticles can be converted into several forms, one of which is TiO<sub>2</sub> nanotubes. TiO<sub>2</sub> nanotubes have a larger surface area than TiO<sub>2</sub> nanoparticles and have more applications. This research synthesizes TiO<sub>2</sub> nanotubes hydrothermally using a TiO<sub>2</sub> micropowder precursor. The synthesis was carried out in two hydrothermal steps: the first hydrothermal to synthesize TiO<sub>2</sub> nanoparticles from the TiO<sub>2</sub> micropowder precursor and the second hydrothermal to synthesize TiO<sub>2</sub> nanotubes from the TiO<sub>2</sub> nanoparticle precursor. The addition of TiO<sub>2</sub> micropowder to the hydrothermal synthesis of TiO<sub>2</sub> nanoparticles with the TiO<sub>2</sub>/NaOH molar ratio of 0.01, 0.025, and 0.04, respectively. The obtained TiO<sub>2</sub> nanoparticles have a morphology of short fibers, with the particle size getting more significant as the molar ratio increases and have an anatase crystal structure at all TiO<sub>2</sub>/NaOH mole ratios. The TiO<sub>2</sub> nanoparticles were then calcined at a temperature of 450°C. The calcined TiO<sub>2</sub> nanoparticles obtained have a morphology of shorter fibers that are less than the sample without calcination and have a larger particle size than the sample without calcination. The calcined TiO<sub>2</sub> nanoparticle has an anatase crystal structure. The obtained TiO<sub>2</sub> nanotubes have an elongated tube morphology with a particle size of 3.93-11.44 nm for the outer diameter, 2.5-4.25 nm for the inside diameter, and a wall thickness of 1.09-3.4 nm. TiO<sub>2</sub> nanotubes have a surface area of 256,744 m<sup>2</sup>/g.

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## **Biosynthesis of TiO<sub>2</sub> Nanoparticle using Aloe Vera for the photodegradation of of Linear Alkyl Benzene sulphonate (LAS)**

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### **ABSTRACT**

Abstract. Biosynthesis of TiO<sub>2</sub> nanoparticle (NPs using plant extract was found to be easy, eco-friendly, and economical. In this study, TiO<sub>2</sub> NPs were synthesis using Aloe Vera in various extract volum. The synthesized TiO<sub>2</sub> NPs were karakterized by Scanning Electron Microscopy (SEM), Fourier Transform InfraRed (FTIR), X-Ray Diffraction (XRD), and Spektrofotometer UV-Vis. The Surface morphology of synthesized TiO<sub>2</sub> NPs samples was found to be 60-140 nm in size and irregular shape by SEM. XRD characterization showed that all samples had anatase phase with a tetragonal structure. FTIR spectra confirmed the presence of Ti-OH, O-H, Ti-O-Ti. The band gap energy decreases as the volume of Aloe Vera flesh extract increases. The band gap energies of TiO<sub>2</sub> NPs(240), TiO<sub>2</sub> NPs(360), TiO<sub>2</sub> NPs(480), and TiO<sub>2</sub> NPs(600) were 3.115 eV, 3.120 eV, 3.069 eV, and 2.980 eV respectively. The degradation of linear alkyl benzene sulphonate (LAS) in the presence of UV light is used to test the photocatalytic activity of the synthesized TiO<sub>2</sub> nanoparticles in various time radiation. The TiO<sub>2</sub> NPs(480) sample degraded LAS the highest with a degradation percentage of 95.14% with an irradiation time of 180 minutes.

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## **The stability of human serum albumin nanocolloid based on the type of sugar molecule and their radiochemical purity**

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### **ABSTRACT**

The nanocolloid human serum albumin (HSA) labeled with radionuclide <sup>99m</sup>Tc has been used extensively for Sentinel Lymph Node (SLN) detection. SLN is the first lymph node to which cancer cells usually spread from a primary tumor. The success of diagnosis with this method is highly dependent on the stability of colloids in the solution. Sugar molecules are one of the important components to establish an HSA nanocolloid. The present study aimed to determine the role of these molecules on nanocolloid formation by evaluating their physical, morphological, and chemical properties. The thermal gelation method was applied for the preparation of an HSA nanocolloid. Then, the effect of three types of sugar (glucose, maltose, and lactose) with different concentrations was identified. The variations of sugar molecules were (a) no sugar, (b) HSA: glucose weight ratio of 1:15, (c-e) HSA: maltose weight ratios of 1:10, 1:15, 1:20, (f-h) HSA: lactose weight ratios of 1:10, 1:15, 1:20. Our results showed the mean particle diameter and zeta potential value in all variations was meets the requirements. However, the polydispersity index, the degree of "non-uniformity" of a distribution, of two variations (without sugar and HSA: lactose weight ratio of 1:20), did not meet the requirements due to the value being greater than 0.4. To get a more detailed image of the size of HSA nanocolloid particles, we also identified their morphology using a transmission electron microscope (TEM). The formula with sugar addition showed a particle size lower than 50 nm, while without sugar showed more than 100 nm. In addition, the radiochemical purity of <sup>99m</sup>Tc-nanocolloid HSA in all variants exhibited good stability (>95%) when stored at RT for 24 hr.

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# **POSTER ABSTRACTS**



## Isolation and Optimization of Incubation Time, pH, and Temperature for Amylase Enzyme Production from Indigenous Bacteria in Sugar Factory Waste

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### ABSTRACT

Enzymes are biocatalysts commonly used in industries. The demand for enzymes in Indonesia has reached 31 thousand tons and continues to increase from 2018 to 2022. However, a significant portion of these enzymes is still imported from China, Turkey, and several other countries. One of these enzymes is amylase, making it necessary to domestically produce indigenous amylase enzymes derived from Indonesian microorganisms to reduce production costs on an industrial scale. This research aims to obtain amylase-producing bacteria from a liquid waste of sugar factories in Jombang, East Java, optimize amylase enzyme production, and identify genotypically the indigenous bacterial isolates with the highest specific amylase activity. This study consists of 7 stages: sample preparation, isolation of amylase-producing bacteria, crude amylase extract production, amylase activity assay, optimization of amylase enzyme production, determining the specific activity of amylase enzyme, and bacterial identification through genotyping. This research successfully identified 3 bacterial isolates (G-7, G-8, and G-12) that positively produce amylase enzymes. The optimal conditions for amylase enzyme production for all three isolates were at 37°C, pH 7.0, and during the exponential growth phase - at 24 hours for isolate G-8 with specific amylase enzyme activity of 0.198 U/mg, and at 48 hours for isolates G-7 and G-12 with specific amylase enzyme activities of 0.108 U/mg and 0.208 U/mg respectively. The 16S rRNA gene identification results showed that isolate G-12 belongs to the species *Pseudomonas nitroreducens*.

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## **Biotransformation of Vanillin from Isoeugenol Using *Pseudomonas aeruginosa* as an Enzyme Biocatalyst Agent: Effect of Substrate Concentration and Incubation Time**

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### **ABSTRACT**

Isoeugenol (2-methoxy-4-[(E)-prop-1-enyl] phenol) is a compound resulting from the isomerization of eugenol contained in clove oil (*Syzygium aromaticum*). Isoeugenol can be used as a precursor for vanillin biosynthesis through the biotransformation pathway. In this research, the biotransformation of isoeugenol was carried out using *Pseudomonas aeruginosa* as an enzyme-producing biocatalyst agent. This research uses several parameters, including the effect of substrate concentrations (0.5, 1; 1.5; and 2% v/v), incubation times (24; 48; 72; and 96 hours), as well as extracting solvents with ethyl acetate and chloroform. Substrate concentration determination was carried out at a 24-hour incubation time, and then the characterization results with the best product concentration were used to determine the incubation time. These research steps include determining the growth curve, biotransformation, extraction, and product identification and characterization, such as identification with Schiff's reagent, TLC, FT-IR, and GC-MS. The results of qualitative identification and characterization show that as the substrate concentration increases, it can cause target biotransformation results to decrease. The 1% concentration treatment with the most concentrated magenta-purple color intensity from the Schiff reagent test and the most concentrated intensity of the TLC stain has more potential to produce vanillin products with chromatogram peak areas of 0.51% (ethyl acetate) and 0.36% (chloroform), as well as vanillyl methyl ketone with an area of 1.38% (ethyl acetate) and 4.91% (chloroform). On the other hand, increasing the incubation time can reduce the target biotransformation product. The 72-hour incubation time treatment produced vanillin 0.19% (ethyl acetate) and 0.74 (chloroform), as well as vanillyl methyl ketone 1.96% (ethyl acetate), and no vanillyl methyl ketone was produced in the chloroform solvent. In this biotransformation, 1% substrate concentration and 24 hours of incubation time in the chloroform extracting solvent became a more potential condition to produce the target biotransformation product with a substrate conversion of 5.27%, which was selective for vanillyl methyl ketone at 93.17% and vanillin at 6.83%. Keywords: Biotransformation, Isoeugenol, *P. aeruginosa*, Vanillin, Vanillyl Methyl Ketone.

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## **Comparative phytochemical analysis of the fresh and fermented leaves of two varieties of *Leucaena leucocephala* L. (Taramba and Wondergraze) using Gas chromatography-mass spectrometry (GC-MS) method**

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### **ABSTRACT**

This study was conducted to identify the phytochemical constituents of *Leucaena leucocephala* leaf extracts between Taramba and Wondergraze varieties using gas chromatography-mass spectrometry (GC-MS). The ethanol leaf extract of *Leucaena leucocephala* was analyzed using GC-MS, while the mass spectra of the compounds found in the extract were matched with the National Institute of Standards and Technology (NIST) library. The result of this study show that major chemical constituents fermented Taramba were squalene (41.02%), phytol (33.80%), 3,7,11,15-tetramethyl-2-hexadecen-1-ol (30.86%) and 3,7,11-tridecatrienitrile, 4,8,12-trimethyl (25.64%), while fresh Taramba were 1,2-benzenedicarboxylic acid, diisooctyl ester (65.7%),  $\beta$ -sitosterol (27.2%), betulin (22.1%), lupeol (21.1%), and 9,12-octadecadienoic acid, methyl ester (8.8%). The study found that the fermentation process increased the hydrocarbon compounds in *Leucaena leucocephala* leaves.

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## Structure analysis of $\text{Ru}_3(\text{CO})_9(\mu\text{-Ph}_2\text{AsCH}_2\text{AsPh}_2)(\text{AsPh}_3)$ : Single crystal X-ray diffraction, thermal analysis, Density Functional Theory (DFT) and Hirshfeld surface analysis.

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### ABSTRACT

The synthesis and characterization of  $\text{Ru}_3(\text{CO})_9(\mu\text{-Ph}_2\text{AsCH}_2\text{AsPh}_2)(\text{AsPh}_3)$  (1) are reported using CHN, IR, <sup>1</sup>H NMR, and <sup>13</sup>C{<sup>1</sup>H} NMR spectroscopy. The structure of 1 was further analysed via single-crystal X-ray diffraction, crystallizing in the monoclinic space group C2/c, where a = 41.564(7) Å, b = 11.603(2) Å, c = 20.338(4) Å, and β = 92.517(3)°. Studies on the thermal behaviour of 1 revealed three stages of decomposition, with a residual rate of Ru atoms at 18.60% (calculated: 18.41%). Theoretical studies using Density Functional Theory (DFT) were performed with the B3LYP hybrid exchange-correlation functional method, employing the LanL2DZ pseudopotential on Ru and a 6-31G basis set for all other atoms. A comparison of bond lengths and bond angles between the experimental and theoretical (DFT) data shows that the majority of values fall within the expected range. Molecular Electrostatic Potential (MEP) study and the energy gap for HOMO-LUMO analysis were also conducted. H···H interactions predominate the total intermolecular interactions, accounting for 38.0%. Hirshfeld Surface Analysis was used to further analyse the interplay of intermolecular C-H···O hydrogen bonds and C-H···π interactions, which were found to be useful in stabilizing the molecular structure.

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## **ANALYSIS OF THE SOURCES AND IMPACTS OF MERCURY CONCENTRATIONS IN SEDIMENTS OF BELAWAN HARBOR WATERS, MEDAN**

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### **ABSTRACT**

Mercury is a non-essential heavy metal, meaning it is not a vital element required by living organisms to carry out crucial biological functions. Instead, mercury can be harmful to organisms and the environment when it accumulates in high concentrations due to its toxic nature. Because of its toxicity, mercury often becomes an environmental and public health concern when released into the environment. The aim of this research is to identify the sources and impacts of mercury concentrations in the sediments of Belawan Harbor waters. Sediment samples were collected using purposive sampling at ten different stations. Composite sediment samples were collected using a Van Veen Grab and analyzed using the Atomic Absorption Spectrophotometer method. Descriptive data analysis was performed using a quantitative comparative method, comparing mercury levels in sediments to the ANZECC/ARMCANZ and CCME guidelines. Mercury concentrations in the water sediments were found to be relatively low, with values below <0.11 ppb. However, mercury concentrations were still detectable and not at zero, indicating the presence of the heavy metal mercury, albeit in small amounts. Therefore, in this context, it can be assumed that mercury does not have a significant impact or contamination of Belawan Harbor waters. The source of mercury in the sediments is attributed to anthropogenic activities along the Deli River and Belawan River.

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## Green Synthesis of *p*-Hydroxychalcones Using FeCl<sub>3</sub>.6H<sub>2</sub>O as A Catalyst Under Solvent-Free Conditions

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### ABSTRACT

Chalcone is a precursor of a group of flavonoid and isoflavonoid compounds that are commonly found in plants in Indonesia. Chalcone compounds and their derivatives are reported to have antibacterial, antioxidant, anti-inflammatory, antimalarial, anticancer, antitumor, analgesic, and antipyretic activities. Chalcones can be synthesized through a Claisen-Smidth condensation reaction between aromatic aldehydes and ketones using an acid or base catalyst followed by a dehydration reaction. This study aimed to synthesize chalcone derivatives using eco-friendly non-toxic FeCl<sub>3</sub>.6H<sub>2</sub>O catalysts under solvent-free conditions. Our experiment was carried out to synthesize some chalcone derivatives at temperature 140°C by stirring process. In this study, the synthesis of chalcone derivatives was started with 10 mmol of *p*-hydroxybenzaldehyde and 10 mmol acetophenone in the presence of 0.1 mmol FeCl<sub>3</sub>.6H<sub>2</sub>O catalysts then the mixture was stirred for 20, 40 and 60 minutes. The product was then investigated by Thin Layer Chromatography (TLC) then characterized by UV-Vis and GC-MS analysis. The result showed that the optimal reaction time was 20 minutes. GC-MS analysis confirmed the product was *p*-hydroxychalcones and have been successfully synthesized in 45.54% yield.

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## **Fractionation of Goat Liver Urikase Based on Carbonate Buffer with Variations in Ammonium Sulfate and Precipitation Time on Urikase Characteristics**

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### **ABSTRACT**

Uric acid is the end product of purine metabolism in humans. If the levels in the blood exceed normal limits (hyperuricemia) it will cause disease. Humans do not have degrading agents such as enzymes to degrade uric acid into simpler substances. This problem can be overcome by administering the enzyme uricase, which is an enzyme that can degrade uric acid from goat liver. Urikase crude extract (crude enzyme) in Carbonate buffer has a specific activity value of 0.0154 U/mg. By purification at the initial stage of fractionation at various levels of Ammonium Sulfate and settling time, the optimum specific activity was obtained in the 0-20% fraction with a time of 16 hours, namely 0.0291 U/mg. This means that the purity of the enzyme increases. Furthermore, the enzyme was characterized by SDS-Page electrophoresis to determine its molecular weight, and a molecular weight range of 40 kDa was obtained. *Keyword : uricase, fractionation, specific activity, molecular weight*

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## **Profile of flavonoid and phenolic compounds from ethyl acetate fraction of *Caesalpinia sappan* heartwood having antioxidant and anti-inflammatory properties**

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### **ABSTRACT**

Dried heartwood of *Caesalpinia sappan*, known as secang in Indonesia is commonly consumed as herbal tea has various medicinal properties, such as antioxidant, anti-inflammatory, antimicrobial, hypoglycemic, anti-allergic, and anti-photoaging. The identified compound from *C. sappan* including phenolic such as brazilin, flavone and flavanone such as narigenin, pinostrobin, alpinone, and cirsimaritin reported as antioxidant. It is found that the position of substituent in flavone and flavanone gave a wide variety of the antioxidant activity. The presence of brazilin in the ethyl acetate fraction has suppressed the nitric oxide (NO) production in RAW 264.7 cells lines induced by LPS. From this result, brazilin supposed to be a lead compound for its activity as anti-inflammatory agent. Further analysis of the constituents from ethyl acetate fraction of *C. sappan* is ongoing.

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## **The Effect of pH and Fe (VI) Concentration on the Coagulation Process of River Water Samples**

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### **ABSTRACT**

The effect of pH and Fe (VI) concentration on the coagulation process of river water samples has been developed. The aim of this research is to study the effect of adding Fe (VI) as a coagulant in the processing of river water samples. The variables of this research include pH and Fe(VI) concentration. The pH variations used were 4, 6, 7, 10 and 12. The Fe (VI) concentration variations used were 0, 3, 5, and 7 mg/L. The variables pH and Fe (VI) concentration were studied as well as determining the quality of river water samples at optimal conditions for the coagulation process. The river water sample processing method used is the coagulation method using Fe (VI) as a coagulant. The research results show that Fe (VI) can remove turbidity simultaneously and effectively. The results of water sample processing performance are influenced by pH and Fe (VI) concentration. The research results showed that the optimum pH for the coagulation process was at alkaline pH, namely pH 12 with a turbidity percentage of 94.22%. The optimum Fe(VI) concentration was obtained by adding 5 mg/L Fe(VI) with a % reduction in turbidity of 86.81%. The results of the analysis of the quality of river water samples obtained that the TDS and pH of the water after the coagulation process were 239.88 and 7.35. Key words: Coagulation, Fe(VI) coagulant, Water Treatment, Brantas River

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## **Biotransformation of Isoeugenol to Vanillin Using *Pseudomonas aeruginosa* in Various pH of Culture Medium**

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### **ABSTRACT**

In this study, biotransformation of isoeugenol was carried out using *Pseudomonas aeruginosa* in various pH of culture medium (4; 5.5; 7; 8.5; and 10). The ability of different solvent (ethyl acetate and chloroform) to extract the product of biotransformation was also studied. The concentration of isoeugenol used is 1% (v/v) and was incubated for 72 hours at 30 °C. The products of biotransformation were identified and analyzed using thin layer chromatography (TLC), FTIR and GCMS. The results have shown that pH 10 gave the highest of vanillin product (4,72%) using chloroform as solvent in extraction step. The value of conversion and selectivity product of vanillin were obtained at 5,95% and 82,70%. *Keyword : biotransformation, isoeugenol, vanillin, Pseudomonas aeruginosa*

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## **The Effect of Chicken Egg shells (*Gallus gallus domesticus*) Addition on the Content of Calcium, Nitrogen, and C-Organic in Eco-Enzyme**

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### **ABSTRACT**

The aim of this study is study the effect of adding the mass of eggshells of purebred chickens and the length of extraction time on the content of calcium, C-Organic, N-total of the eco-enzyme samples, and also the size of particle that was extracted by fermentation process. This study used a completely randomized design (CRD) which consisted of 12 treatments with three repetitions. The treatment was given in the form of adding eggshell mass with variations of 10, 20, and 30 grams and extraction times, which lasted for 3, 5, 7, and 10 days so that there were 36 experimental parameter units in the form of calcium, C-Organic, and N- total. Observational data were analyzed statistically and then tested by DMRT (Duncan's Multiple Range Test) with a level of 5%. The study's results stated that adding purebred hen eggshell mass and extraction time could affect the calcium, C-Organic, and N-total content in the eco-enzyme samples. The distribution of particle size that had extracted by fermentation process in nanometer distribution.

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## **Permeation Study of Curcumin-Tween 80-Soybean Oil Nanoemulsion on Synthetic Membrane and Shed Snake Skin**

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### **ABSTRACT**

Curcumin is a natural polyphenolic compound that has antiinflammatory, anti-cancer, antioxidant, antibiotic and antiviral properties. Nanotechnology such as nanoemulsion, which consist of two immiscible liquids such as water and oil which are surfactant stabilized, can increase the efficacy of curcumin in the human body. One of the methods for preparing nanoemulsions is PIT (Phase Inversion Temperature) in which the size results obtained are quite uniform and small increasing the active ingredients permeation to the skin. Our study compares the permeation of curcumin nanoemulsion through polyamide-synthetic membrane and shed snake skin which corresponds to the constituent components of the human stratum corneum. The curcumin nanoemulsion permeation on the synthetic membrane was measured based on the intensity of curcumin passing the membrane for 30 minutes using spectrofluorometer NanoDrops. Meanwhile, curcumin nanoemulsion permeation on the surface of shed snake skin was monitored based on the curcumin intensity using CLSM (Confocal Laser Scanning Microscope). The graph of intensity change as a function of time and depth of penetration was drawn and plotted to a third order polynomial regression model to determine the inflection point which represents the changes of permeation rate. The results show that the average percentage of curcumin nanoemulsion permeation is 89.71% on shed snake and 18.32% on synthetic membrane which is much higher than conventional water-solubilized curcumin, which is 0.25%. The difference in permeation percentage proves that the nanoemulsion system can increase skin permeation.

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## Passive samplers for inorganic phosphate measurement in water system

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### ABSTRACT

Eutrophication in waters is caused by increasing nutrients concentrations, in this case inorganic phosphate compounds. In situ monitoring of inorganic phosphate concentrations in water systems is needed to determine the average phosphate concentration over a certain period of time. In this research, inorganic phosphate in the form of orthophosphate was measured using two passive samplers, *i.e.* a Polymeric inclusion membrane (PIM) passive sampler and a Diffusive Gradient in Thin Films (DGT) passive sampler. PIM passive sampler was consisted of a polymeric inclusion membrane embedded in a glass bottle containing NaCl solution as the internal phase. For this research, PIMs was prepared by using PVC as base polymer, Aliquat 336-Cl as carrier, and 1-decanol as plasticizer. The DGT passive sampler used arrangement of cellulose nitrate filter membrane, agarose-citric acid diffusive hydrogel, and ferrihydrite-agarose binding hydrogel that was assembled in a plastic piston. Method validation showed that  $CPIM = 1.1708C_{soln} - 0.032$  ( $R^2 = 0.9914$ ) while  $CDGT = 0.6179C_{soln} + 328.88$  ( $R^2 = 0.9252$ ). This shows that the PIM passive sampler is more linear and sensitive compared to the DGT passive sampler for measuring inorganic phosphate in waters.

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## **Microencapsulation by Spray Drying of *Tithonia diversifolia* Extracts: Design, Characteristics, and Antioxidant Activity**

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### **ABSTRACT**

Spray-drying is a technique used to produce microencapsulated from *T. diversifolia* extracts, the optimum conditions, characteristics, and the antioxidant activities of the microcapsules are investigated. The objectives of the study are to determine the effects of coating agents and stirring time on the encapsulation efficiency and to determine the antioxidant activities of the microcapsules from *T. diversifolia* extracts. Microencapsulation processes were manufactured under the influences of coating agents (chitosan, gum Arabic, and maltodextrin) concentration, and stirring time. The optimum microencapsulation conditions were selected based on the highest encapsulation efficiency. The microcapsules produced in optimum conditions were characterized using FTIR (Fourier Transform Infrared) Spectroscopy and SEM (Scanning Electron Microscopy) technique. The microcapsules were also tested their antioxidant activities using DPPH free radical assay. Chitosan concentration of 0.05% (w/v), gum Arabic concentration of 4% (w/v), and maltodextrin concentration of 0.8% (w/v) with 90 minutes stirring time for each encapsulated agent have resulted in the highest encapsulation efficiency. The encapsulation efficiencies were 76.03%, 80.29%, and 74.16% for *T. diversifolia* extracts encapsulated with chitosan, gum Arabic, and maltodextrin, respectively. Microencapsulation of plant extracts can be one of the strategies for natural product enhancement with preserved biological functions.

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## Quantum Molecular Simulations for Lithium-Ion Transport in Solid Polymer Electrolyte of Layered Cellulose and Its Derivatives

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### ABSTRACT

Li-ion batteries are widely used as energy storage materials in daily life. In commercial Li-ion batteries, polyethylene oxide (PEO) is commonly used as the solid polymer electrolyte. However, PEO is one of the petroleum products and its production cost is relatively high. Therefore, further research into finding alternative materials is necessary. Cellulose-based compounds, which are eco-friendly biomass-derived materials, are promising alternative to PEO. The present study focuses on investigating the Li-ion transport performance of cellulose-modified solid polymer electrolytes in Li-ion batteries using quantum molecular dynamics simulations. Solid polymer electrolyte model structures were created by inserting six LiPF<sub>6</sub> ion pairs into layer of Li-carboxymethyl cellulose (CMC), Li-carboxyethyl cellulose (CEC), cellulose acetate (CA), and non-modified cellulose. CMC and CEC layers contain Li-ion, so the model of CMC and CEC have 60 Li-ions in total, while the model of CA and non-modified cellulose have 6 Li-ions. The simulation models consisting of 1000–2000 atoms were treated quantum mechanically with DCDFTBMD program, developed by Nakai-group. Total 50 ps equilibration was performed at 300 K with a time step of 1 fs. Three independent production runs were performed for each model under microcanonical ensemble for 30 ps with a time step of 0.5 fs. As dynamical and structural properties, diffusion coefficients of Li-ion and coordination number of oxygen of cellulose derivatives and fluorine of PF<sub>6</sub><sup>-</sup> to Li-ion were analyzed. Diffusion coefficients of Li-ion in CMC, CEC, CA, and cellulose were  $1.86 \times 10^{-6}$ ,  $1.65 \times 10^{-6}$ ,  $4.79 \times 10^{-6}$ , and  $4.67 \times 10^{-7}$  cm<sup>2</sup>s<sup>-1</sup>, respectively. The calculated value of CA was approximately three times larger than those of CMC and CEC, and ten times larger than that of non-modified cellulose. The Li-ion coordination numbers of (oxygen, fluorine, total) were (3.90, 0.22, 4.12) for CMC, (3.98, 0.24, 4.22) for CEC, (2.27, 1.25, 3.52) for CA, and (2.83, 1.56, 4.40) for non-modified cellulose. There seems to exist opposite relationship between dynamical and structural properties, namely, the larger coordination number is, the smaller diffusion coefficients are. The obtained results indicate that attractive interaction with surrounding oxygen of cellulose and counter anion contributes to suppression of Li-ion transport.

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## Ionic liquid supported organotelluride

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### ABSTRACT

Oxidation is one of the most important reactions in organic reactions. Various methods have been developed for oxidation reactions of organic compounds. Oxidation reactions using peroxides or transition metal catalysts are excellent methods, but they have problems such as danger and environmental load. We have previously reported photo-oxidation reactions using organotellurium compounds. The advantage of this reaction is that various substrates can participate efficiently using light and atmospheric oxygen. Therefore, this method is non-hazardous and does not require expensive reagents. However, the product obtained using this reaction must be purified, such as by column chromatography, and organotelluride catalyst is not recyclable. To overcome these problems, we investigated the preparation of ionic liquid supported organotelluride and its application for the oxidation of thiol and phosphite esters using ionic liquid supported organotelluride. The ionic liquid supported organotelluride was synthesized through several steps of reactions. Next, we investigated the oxidation reaction using the newly developed ionic liquid supported organotelluride. As a result, this ionic liquid supported organotelluride was effective in various oxidation reactions and able to be recovered. Additionally, this reaction system can be recycled and reused at least five times. This system is advantageous because of its environmental friendliness and good yields.

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## **SYNTHESIS CELLULOSE ACETATE FROM CORN COBS WITH VARYING ACETYLATION TIMES AS A MATERIAL FOR FILTRATION MEMBRANES**

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### **ABSTRACT**

Corn cob is a waste that is classified as a large amount so it has the potential to be utilized properly. Corncobs can be converted into cellulose acetate which is used in the fabrication of filtration membranes. The purpose of this study was to determine the characteristics of the isolated cellulose, to determine the time variation on the characteristics of cellulose acetate and to determine the characteristics of synthetic cellulose acetate membranes. Methods in this research include isolation of cellulose, synthesis of cellulose acetate and fabrication of cellulose acetate membranes. Cellulose isolation produced a yield of 30.05% and a water content of 3.46%. The successful isolation of cellulose was proven by the loss of lignin and hemicellulose peaks in the IR spectra of cellulose at wave number 1731.21 cm<sup>-1</sup>, namely the vibrational absorption band C=O stretching, the C=C group of aromatic rings 1511.31 cm<sup>-1</sup> and the =C-O-C group at number wave 1244.90 cm<sup>-1</sup>. Synthesis of cellulose acetate through activation, acetylation, de-acetylation and purification processes. Variations in this study is acetylation time 1;1,5;2; and 2.5 hours. The optimum acetylation time is when the acetylation time is 2 hours with an acetyl content of 41.73% and a degree of substitution of 2.6 and dissolves in acetone solvent. Cellulose acetate membranes were prepared using a phase inversion technique. The density of the synthetic CA membrane is lower than that of commercial CA membranes because it has a large pore density while the resulting swelling degree is greater. The physical characteristics of synthetic CA membranes are very wrecked, so alternative to mix CA synthetic and commercial 1:1 to quantify performance. The flux and permeability coefficient produced by synthetic/commercial CA membranes are higher than CA commercial membranes due to the very low solubility in dope solutions. Key words: acetylation times, cellulose acetate, corncobs, and membrane filtration.

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## **Synthesis of Cellulose Acetate Based on Corn Cob as a Membrane Material with Variations in the Amount of Acetic Acid**

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### **ABSTRACT**

The objectives of this study were to analyze the effect of acetic acid volume on the characteristics of cellulose acetate from corn cobs formed and to determine the performance of cellulose acetate membranes. Cellulose is obtained from the process of isolating it from corn cobs by delignification and bleaching. Cellulose acetate is obtained from the synthesis of cellulose acetate. Variations in the amount of glacial acetic acid used are 5 mL; 7.5 mL; 10 mL; and 12.5 mL during the deacetylation process. The characterization of cellulose acetate was carried out by determining the acetyl content, degree of substitution, FTIR, solubility, and molecular weight. The results showed that the volume of acetic acid affected the characteristics of the resulting cellulose acetate. Variation in amount of glacial acetic acid are 5; 7.5; and 10 mL produces cellulose acetate with the type of cellulose diacetate while the amount variation of 12.5 mL glacial acetic acid includes cellulose monoacetate. The molecular weight of the synthesized cellulose acetate decreased with the addition of acetic acid. The FTIR spectrum of the synthesized cellulose acetate showed the same functional group peaks as commercial cellulose acetate. The obtained cellulose diacetate is used in the manufacture of ultrafiltration membranes. Based on the research results, the synthetic/commercial cellulose acetate membrane has a flux value of 36.38 L/m<sup>2</sup>.hour and a permeability coefficient of 5.91 L/hour.m<sup>2</sup>.barr. Keywords: corn cob, acetic acid, acetylation, cellulose acetate, membrane

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## Room Temperature Synthesis of Crystalline Cu(II)-citrate-niacinamide Coordination Compound by Layered Solution Technique

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### ABSTRACT

MOFs or Metal Organic Frameworks-based materials are gaining more attention due to its versatile modification and wide range applications. As a result, new types of MOF, as well as new synthetic approaches are being extensively explored. In this study, crystalline Cu(II)-citrate-niacinamide coordination compound is successfully synthesized at room temperature by layered solution technique using a water-alcohol mixture system. The compound was aimed as part of modification of Cu(II)-citrate based metal-organic frameworks, which can be further developed as potential porous material or other functional materials. The synthesis was done using primary alcohol of methanol, ethanol, and n-propanol as the top layer solvent, and distilled water as the bottom layer solvent with Cu(II):citric-acid:niacinamide molar ratios of 3:2:2; 3:2:4; and 3:2:6. The crystals were isolated after 15 days and then characterized by infrared spectroscopy, powder X-ray diffractometry, melting point analysis, and scanning electron microscopy. Experimental data shows that identical blue crystalline solid was isolated from all variations with the highest yield obtained from the 3:2:6 reactions. IR analysis indicates the presence of characteristic functional groups from the citrate ligand (O-H, C=O, and C-O), and from the niacinamide ligand (N-H, C=O, and C=N). Melting point analysis suggest that the compound was stabled up to 200 C and then it gradually turns into yellow and finally black upon reaching 210-220 C. The crystalline state of the product was confirmed by the powder XRD and SEM analyses. Preliminary analysis suggests that the use of different polarity of primary alcohol may led to different crystallinity degree of the product. Further analyses using DTA-TGA and single crystal XRD are ongoing for more detail characterization of the product.

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# **Electrical conductivity of ionic-liquid electrolytes containing imidazolium-based cation from all atom molecular dynamics simulation with a self-consistent atomic charge determination**

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## **ABSTRACT**

Sodium-ion battery is widely investigated for its potential to be the next-generation secondary battery for a large-scale energy storage grid owing to its abundance, uniform distribution, low cost, and low environmental impacts. The requirement for a sodium-ion battery with a high-energy density and excellent charging-discharging performance then urges the exploration for an effective combination of electrolyte and electrode materials. Recently, ionic liquid (IL) based electrolyte has been actively explored for its advantages such as low volatility, low flammability, high operation temperature, and the ease in tuning its properties through a simple structure modification. In this work, the performance of imidazolium-based cations for ionic liquid based electrolyte is investigated using a self-consistent method of molecular dynamics simulation and density functional theory calculation. The method addresses the effects of intramolecular polarization and intermolecular charge transfer, that characterize a highly concentrated ionic system, while the sampling of dynamics properties is made possible over hundreds of nanoseconds.

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## PHOTOESTERIFICATION OF WASTE COOKING OIL USING ZNO DOPED EMPTY FRUIT BUNCHES ASH HETEROGENEOUS CATALYST

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### ABSTRACT

Waste from the palm oil industry, such as empty fruit bunch ash (EFBA) and palm oil mill effluents (POME) is a type of biomass created during the production of palm oil and produced in vast quantities. Due to the massive amounts of empty fruit bunch ash produced because of the exponential rise in worldwide palm oil production, major plantations are having trouble disposing of them. The purpose of this research is to study the effectiveness of the ZnO-EFBA catalyst under visible light irradiation for the photoesterification reaction and its physicochemical properties of the photocatalyst that will be determined using TGA, FTIR, SEM-EDX, XRD and BET. The biodiesel will be produced by using two steps which are photoesterification to reduce the FFA value in WCO and followed by transesterification to produce FAMES. The photoesterification reactions were conducted using WCO under visible light irradiation. Various parameters were examined, including different reaction times of 1 to 4 hours, different methanol to oil molar ratios of 12:1, 14:1, 16:1, and 18:1, and different ZnO-EFBA catalyst loadings ranging from 0 wt.% to 8 wt.%. The obtained results demonstrated that each WCO sample have a different optimum condition in the photoesterification reaction. Moreover, it was observed that lower FFA values correlated with higher biodiesel conversion rates in the transesterification reaction with 79.06%, 77.72% and 73.33% for sample 1, 2 and 3 respectively. By using EFBA as a heterogeneous catalyst doped with ZnO in the manufacturing of biodiesel, it helps to reduce the waste that the palm oil industry creates, limiting the adverse effects on human health and environmental harm. Furthermore, biodiesel is a renewable, clean-burning alternative to petroleum fuel, which is domestically manufactured. The use of biodiesel as a vehicle fuel boosts energy security, enhances the environment and air quality, and offers safety advantages.

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## **Solvothermal Synthesis of Ni(II)-BDC-Pyrazine complex: Effect of solvent toward the yield, surface morphology, and crystallite size of the complex**

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### **ABSTRACT**

Ni(II)-BDC-Pyrazine is one of many metal-organic frameworks (MOF) materials that can be potentially used as catalysts or porous materials. The previously reported Ni(II)-BDC-Pyrazine metal complex was successfully synthesized by hydrothermal reaction at 200°C for 48 hours. However, in order to obtain a mild synthesis condition, a study was conducted by reducing the reaction temperature and reaction time. The effects of the solvent and mol ratio of the precursor were also investigated. The synthesis was done at 150°C for 10 hours in Ni(II):H<sub>2</sub>-BDC:pyrazine mol ratio of 1:1:2 and 1:1:4, using DMF or DMF-water (1:1) solvents, for each mol ratio. Precipitated product was characterized by infrared spectroscopy, powder-XRD, and SEM-EDS to confirm the presence of the targeted Ni(II)-BDC-Pyrazine complex. Experimental data showed that the different type of solvent affects the yield of the Ni(II)-BDC-Pyrazine complex. Reaction with DMF-water (1:1) solvent produced a greenish solid with a smaller yield compared to the reaction with DMF solvent, which resulted in a bluish solid. Infrared spectra of the product show typical functional groups, namely C=O, C-O, C=N, and C-N groups which confirm the presence of both ligands in the product. The p-XRD analysis showed that different solvents produce different diffraction patterns which indicate different compounds. SEM imaging revealed that different solvents form different surface morphology and crystallite size distribution, in which the DMF-water (1:1) reaction produced a solid with a more homogeneous smooth surface and size, while the DMF reaction produced a solid in the form of aggregates. Based on this analysis, the targeted Ni(II)-BDC-Pyrazine was successfully obtained and the use of solvent affected the yield, surface morphology, and crystal size

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## Synthesis and Characterization of Thermoresponsive Hydrogels of P(SPE-ko-NIPAM) as a Carrier for a Model Drug of Metformin HCl

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### ABSTRACT

Thermoresponsive hydrogels are a promising approach in the field of drug carriers. These types of hydrogels are smart materials that can change their physical properties in response to temperature, making them suitable for controlled drug release applications. This study focused on the synthesis of a poly(sulfobetaine methacrylate-co-N-isopropylacrylamide) (P(SPE-co-NIPAM)) which is a thermoresponsive hydrogel through free-radical polymerization by varying monomer composition in the monomer feed and polymerization time. The success of polymerization was proven by the absence of the vinyl peak in the FTIR spectra. The gel content of the hydrogels was determined, and it was observed that hydrogels with 20 mol% SPE had the lowest gel content which corroborate the results of the swelling test, i.e., the highest equilibrium swelling ratio (ESR). Moreover, the gel content increased with increasing polymerization time. It was found that an increase in polymerization time resulted decrease in the ESR. The obtained P(SPE-co-NIPAM) hydrogels exhibited LCST/UCST swelling behaviors, depending on the SPE and NIPAM composition. The deswelling rate was affected by the SPE composition and polymerization time, that is: the higher the SPE composition and the longer polymerization times are, the slower deswelling rates could be obtained. P(SPE20-co-NIPAM80) hydrogel with a polymerization time of 1 hour was able to entrap 2.75% of metformin-HCl. Furthermore, the cumulative release of metformin-HCl from this hydrogel in buffer pH 7.4 at 37°C within 15 hours was 26.33%. Key words: copolymeric hydrogels; poly(sulfobetaine methacrylate); poly(N-isopropylacrylamide); thermoresponsive hydrogels; drug carrier.

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## Magnetite Coated with Oxalic Acid Crosslinked Chitosan Hydrogel for Zn<sup>2+</sup> and Cd<sup>2+</sup> Removal from Aqueous Media

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### ABSTRACT

Magnetite coated with oxalic acid crosslinked chitosan hydrogel was prepared in order to study its adsorption characteristic toward Zn<sup>2+</sup> and Cd<sup>2+</sup>. Crosslinking of chitosan with oxalic acid was carried out to increase its stability at low pH. The crosslinking reaction was done by dissolving 2.5 grams of chitosan powder in 100 mg/mL of oxalic acid. The solution, then, was added to 250 mL of 1 M NaOH solution to obtain oxalic acid crosslinked chitosan hydrogel. Magnetite was made through coprecipitation method with a mole ratio of Fe<sup>2+</sup> : Fe<sup>3+</sup> of 1 : 2. Coating of magnetite with chitosan-oxalic acid hydrogel was prepared with a mass ratio of magnetite and chitosan-oxalic acid hydrogel of 1 : 1. The coated magnetite were characterized using FTIR, XRD, and SEM-EDS. The adsorption experiments were performed at various pH, contact time, and individual adsorbate concentration. FTIR spectra of adsorbent indicate the presence of an oxalic acid carbonyl group (-C=O), a shift in the wave number of a typical magnetite group (Fe-O), and an amide group (-CONH-). The XRD diffractogram shows the presence of a magnetite (Fe<sub>3</sub>O<sub>4</sub>) phase with a crystal size of about 20.55 nm. Based on SEM photos, magnetite coated with oxalic acid crosslinked chitosan hydrogel has an irregular bead and porous structure. The EDS results showed that the main components of adsorbent were Fe, O, N, and C. The adsorption experiment results showed that the optimum conditions for adsorption occurred at pH 5 and contact time of 45 minutes for Zn<sup>2+</sup> and pH 5 and contact time of 75 minutes for Cd<sup>2+</sup>. The highest amount of adsorbed Zn<sup>2+</sup> and Cd<sup>2+</sup> were 71.25 ± 0.56 mg/g and 69.81 ± 1.19 mg/g at an initial adsorbate concentration of 300 mg/L. In this study, the adsorbent capacity toward Zn<sup>2+</sup> and Cd<sup>2+</sup> could not be determined, yet. Keywords: magnetite, chitosan, oxalic acid, crosslinking, heavy metal

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## **Chitosan film incorporated with Sodium Tripolyphosphate (STPP) and glycerol as an active packaging material**

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### **ABSTRACT**

Chitosan films with STPP as a cross-linker and glycerol as a plasticizer were prepared using the solvent casting method for food packaging application. STPP was used as the cross-linker which enhances the stability of the films. Glycerol was used as a plasticizer which imparts flexibility. Successful cross-linking was confirmed by Fourier Transform-Infra Red (FT-IR) spectra and incorporation of glycerol was seen clearly in the 3247.48 cm<sup>-1</sup> (-OH and -NH stretching), 2888.08 cm<sup>-1</sup> (C-H stretching), 1633.01 cm<sup>-1</sup> (C = O stretching), 1257.92 cm<sup>-1</sup> (P=O stretching), 1150.95 cm<sup>-1</sup> (stretching of -PO<sub>2</sub> group), and 894.23 cm<sup>-1</sup> (stretching of the P-O-P bond). The modified films show an improved water resistance, optical properties, and elongation percentage value. An improved moisture barrier was also observed with a 25.78% reduction in water vapor transmission rate and showed a 42.26 % increase in the haze value. Modified films showed a drastic 55.66% increase in the elongation percentage value, hence enhanced flexibility. These films also showed increased antibacterial activity which showed a decrease in the log CFU/mL value of the control group compared to the sample by 6.56 to 4.46 log CFU/mL. Keywords : Chitosan films, Food packaging, Active packaging, Cross linker and plasticizer, Sodium Tripolyphosphate

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