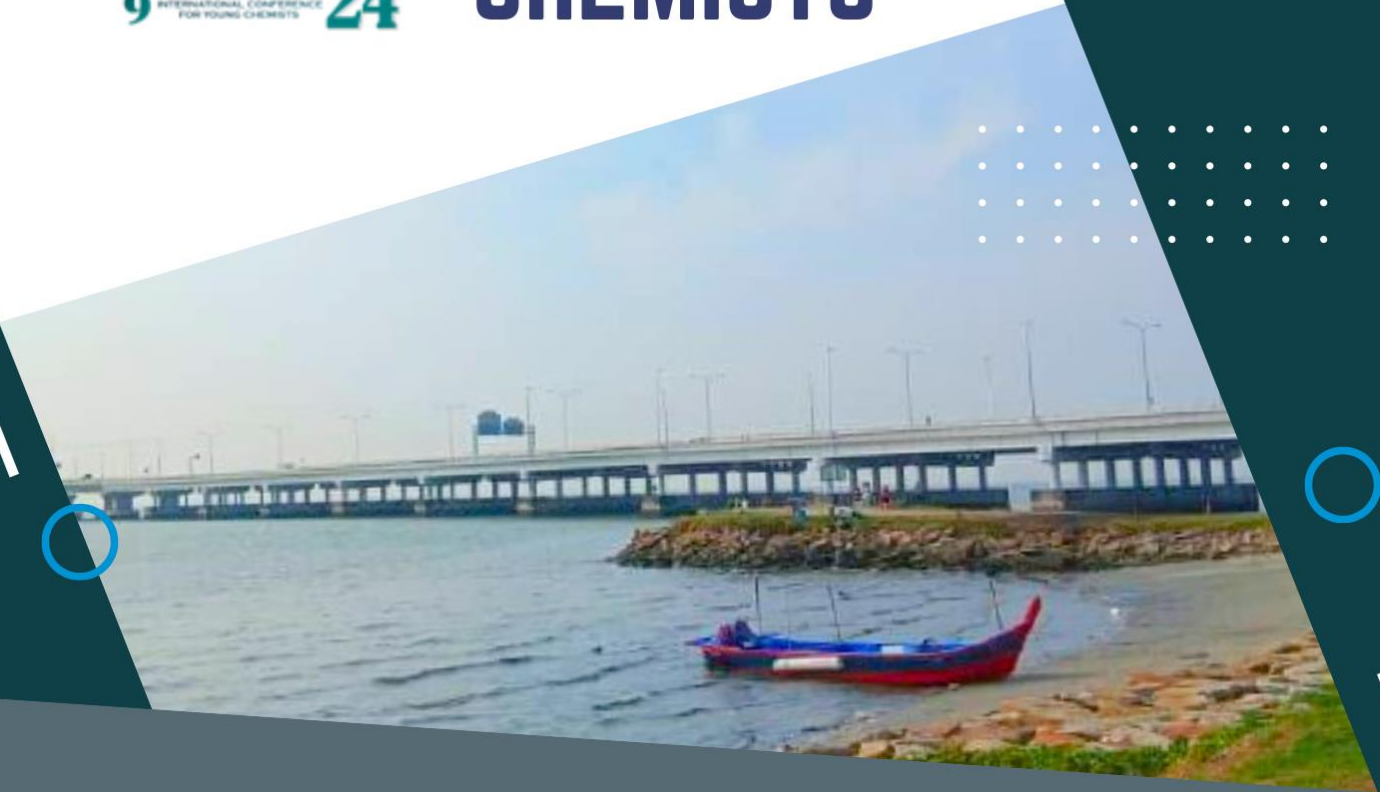
9th INTERNATIONAL Conference FOR YOUNG CHEMISTS

ICYC 2024
9th INTERNATIONAL CONFERENCE FOR YOUNG CHEMISTS

09 - 11th
OCTOBER
2024



GREEN INNOVATION IN CHEMISTRY: CATALYZING SUSTAINABLE SOLUTIONS FOR A GREENER TOMORROW

ORGANIZED BY

School of Chemical Sciences
USM
UNIVERSITI SAINS MALAYSIA
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FOREWORDS

DEAN OF THE SCHOOL CHEMICAL SCIENCES,

UNIVERSITI SAINS MALAYSIA

Assalamualaikum and greetings to all ICYC 2024 participants,

It gives me great pleasure to welcome all of you to the 9th International Conference for Young Chemists (ICYC 2024). Starting in 2001 as the Regional Conference for Young Chemists, ICYC has since evolved into a prominent platform for disseminating the latest knowledge in the field of chemistry.

Organized biennially by the postgraduate students at the School of Chemical Sciences, Universiti Sains Malaysia, ICYC aims to bring together local and international researchers, facilitating interaction and networking, and enabling the sharing and discussion of new findings and applications in chemistry. We hope that this intellectual discourse will lead to future collaborations between universities, research institutions, and industry both locally and internationally.

In line with the theme *"Green Innovation in Chemistry: Catalyzing Sustainable Solutions for a Greener Tomorrow,"* speakers and participants of ICYC 2024 will share their research and knowledge on the advancements and innovations made despite challenges, to solve problems and create a better future for mankind.

Finally, I would like to thank the organizing committee for their tremendous efforts in organizing the conference. I would also like to take this opportunity to express my gratitude to our co-organizer from Institut Pertanian Bogor (IPB) University, all speakers, participants, and sponsors for your full support, cooperation, and contribution to ICYC 2024. I wish you all a fruitful and successful conference.

Sincerely,

PROF. DR. ROHANA ADNAN
Dean,
School of Chemical Sciences,
Universiti Sains Malaysia

CHAIRPERSON OF ICYC 2024,

UNIVERSITI SAINS MALAYSIA

Heartfelt greetings to all attendees of 9th ICYC,

First and foremost, I am honoured and delighted to welcome everyone to the 9th International Conference for Young Chemists (9th ICYC). After our last physical conference in 2019 during the 7th ICYC and the virtual 8th ICYC in 2022 due to the global pandemic, we are excited to return to an in-person format this year. The chemistry community has shown incredible resilience and adaptability during these challenging times, and we can't wait to reconnect with you all in person.

This year, we are excited to continue the legacy of ICYC, a biennial conference that has grown in prominence since its inception in 2001. Embracing the theme "Green Innovation in Chemistry: Catalyzing Sustainable Solutions for a Greener Tomorrow", 9th ICYC highlights our commitment to addressing global environmental challenges through sustainable practices. The conference will serve as dynamic platform for researchers worldwide (a) to present their latest findings, (b) to foster collaboration locally and internationally, and (c) to keep abreast with the latest trends and developments in the field of chemistry. To this end, speakers and presenters from across the globe, including countries such as Spain, France, Indonesia, Japan, Hong Kong, Kazakhstan, Pakistan and others, are expected to gather to share their expertise. Consequently, a captivating array of fields will be featured, including physical chemistry, organic chemistry, inorganic chemistry, biochemistry, analytical sciences, and industrial chemistry.

In light of this, I would like to extend my heartfelt gratitude to Prof. Dr. Rohana Adnan, Dean of the School of Chemical Sciences, and to the advisory board, led by Dr. Oh Wen Da, which includes our esteemed faculty members and technical staff. Their invaluable guidance and support, along with the dedication of our working committee of postgraduate students, have been crucial to the success of ICYC 2024. I wish all participants a rewarding and enriching experience at the conference and hope that the discussions and interactions here will inspire you to continue making impactful contributions to the field of chemistry. If there are any shortcomings, we sincerely apologize and will strive to improve in the future.

Sincerely,

ChM. Ganapaty Manickavasagam
Chairperson,
9th International Conference for Young Chemists 2024,
School of Chemical Sciences,
Universiti Sains Malaysia,
11800 Minden, Penang.

PLENARY SPEAKERS

Prof. Dr. Mohd Hafiz Dzarfan Othman
Advanced Membrane Technology Research Centre
(AMTEC),
Faculty of Chemical and Energy Engineering,
Universiti Teknology Malaysia (UTM),
81310 Johor Bahru, Johor,
Malaysia.
hafiz@petroleum.utm.my

Ts. Dr. Mohd Hafiz Dzarfan Othman is a distinguished Professor in the Faculty of Chemical and Energy Engineering at Universiti Teknologi Malaysia (UTM) and currently serves as the Chair of the Frontier Materials Research Alliance at UTM. He earned his PhD in Chemical Engineering from Imperial College London in 2011. His research focuses on the development of innovative membrane technologies for pollutant removal from water and wastewater, as well as for efficient energy generation. He has filed over 40 intellectual property patents and has published more than 600 indexed articles, achieving an H-index of 64 with citations of around 15,000 according to Scopus.

Prof. Dr. Nicolas Brosse

LERMAB,

Université de Lorraine,

France.

nicolas.brosse@univ-lorraine.fr

Prof. Nicolas Brosse is currently a research group leader in LERMAB (laboratory dedicated to wood material) University of Lorraine. He is a wood chemist. His current interests include lignocellulosic pretreatment by steam explosion, polyphenolics and lignin characterizations and utilizations, natural fibres, bioenergy, wood recycling and fire-proof materials. He has published ~200 reviewed papers, he is Elected fellow at IAWS (International Academy of Wood Science) since 2017 and Concurrent Professor in Nanjing Forestry University (China).

KEYNOTES SPEAKERS

Associate. Prof. Dr. Low Siew Chun

Associate Professor,

School of Chemical Engineering,

Universiti Sains Malaysia.

chsclow@usm.my

Dr. Low Siew Chun is an Associate Professor at the School of Chemical Engineering, Universiti Sains Malaysia. Her research is centered on developing advanced separation and sensing systems, with a particular emphasis on the fundamental transport phenomena in thin films and their applications in mitigating environmental pollution. To date, she has contributed 10 book chapters and published over 150 peer-reviewed journal papers, achieving an h-index of 31, an i10-index of 89, and accumulating over 3,800 citations according to Google Scholar. Dr. Low has presented at more than 30 conferences, including 7 keynote addresses and 5 invited lectures. In her academic role, she serves as a reviewer for prominent publishers such as Springer, ACS, RSC, Elsevier, and Taylor & Francis, and she is the section editor for both the ASM Science Journal and ASEAN Engineering Journal. In recognition of her research impact, Dr. Low was honored as one of Malaysia's Top Research Scientists (TRSM) in 2022.

Prof. Dr. Nobuto Yoshinari
Department of Chemistry,
Osaka University,
1-1 Machikaneyama,
Toyonaka, Osaka 560-0043, Japan
nobuto@chem.sci.osaka-u.ac.jp

Prof. Dr. Nobuto Yoshinari is a professor in the Department of Chemistry at Osaka University. He received his bachelor's degree in 2005 from Osaka University, a master’s degree in 2007 and a PhD in 2010. In 2015, he was honored with the BCSJ award from The Chemical Society of Japan and the Rising-Star award from the Japan Science and Technology Agency, CREST ‘Molecular Technology’. His research focuses on multinuclear metal complex, supramolecular chemistry, S ligands, P ligands, coordination chemistry, metal cluster, magnetic properties, photoluminescence, gas adsorption/desorption, and ion-conducting materials. He actively participates in research publications with a record of 10 original papers, 6 review papers, 1 book chapter, 5 patents, and Web of Science h index = 18.

Dr. Faiz Bukhari Bin Mohd Suah

Associate Professor,

School of Chemical Sciences,

Universiti Sains Malaysia.

fsuah@usm.my

Dr Faiz Bukhari Mohd Suah is an Associate Professor at the School of Chemical Sciences, Universiti Sains Malaysia. He received his tertiary education, including a postdoctoral research position in chemical technology and analytical chemistry, from Universiti Kebangsaan Malaysia, The University of Melbourne, and Imperial College London, respectively. His research interest is in green analytical chemistry, with a focus on the development and application of polymer inclusion membranes, chitosan material, electrogenerative processes, electroanalytical techniques and chemical sensors. He has published more than 100 peer-reviewed articles, one chapter in the research book and one textbook. He has also applied for one patent and granted one copyright. As the main supervisor, he has supervised two postdoctoral researchers, five PhD students, and 20 master's students. Additionally, he was appointed as a grant evaluator for the Nippon Sheet Glass Foundation, the Polish Academy of Sciences, the Austrian Academy of Sciences, the Qatar Foundation, Badan Riset dan Inovasi Indonesia, the Ministry of Natural Resources and Environment of Malaysia, and the Ministry of Higher Education of Malaysia. His academic influence extends to his editorial roles in leading journals such as Advances Applied Sciences (Editor), Journal of Renewable Materials (Guest Editor), Separation Journal (Guest Editor), Eurasian Journal of Analytical Chemistry (Editor), and Bulletin of The School of Chemical Sciences (Editor-in-Chief), where he has contributed significantly to the advancement of the field.

Dr. Mohamad Rafi,

Professor,

IPB University,

Indonesia.

mra@apps.ipb.ac.id

Dr. Mohamad Rafi is a lecturer at Institut Pertanian Bogor (IPB), Indonesia, where he has been teaching since September 2000. With a deep expertise in analytical chemistry, Dr. Rafi specializes in analytical separation and chromatography. He earned his PhD in Material Engineering from Gifu University, Japan, in 2013, after completing his Master of Science in Analytical Chemistry at IPB in 2010. His academic journey began at IPB, where he obtained his Bachelor's degree in Chemistry in 2000. With over two decades of experience in teaching and research, Dr. Rafi is a respected figure in the field of analytical chemistry, contributing extensively to the advancement of chemical sciences in Indonesia.

Dr. Wei Shen Aik,

Assistant Professor,

Department of Chemistry,

Hong Kong Baptist University.

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Dr Wei Shen Aik is an Assistant Professor at Hong Kong Baptist University. He obtained his Bachelor of Arts degree in Natural Sciences at the University of Cambridge. He then received his doctoral training in chemical biology at Prof. Christopher Schofield's laboratory at the University of Oxford. After his D.Phil. studies at Oxford, Dr Wei Shen Aik did his postdoctoral research in Structural Biology with Professor Liang Tong at Columbia University in the United States. As group leader, Dr Wei Shen Aik aspires to combine structural biology and chemical biology to design new solutions for human health problems.

Dr Jalel Labidi,

Professor,

University of the Basque Country (UPV/EHU),

Spain.

jalel.labidi@ehu.eus

Dr Jalel Labidi is Chemical Engineer (National Engineering School of Gabes, Tunisia) with PhD in Chemical Engineering (National Polytechnic Institute of Lorraine, France). He is currently Senior Researcher at the Department of Chemical and Environmental Engineering of the University of the Basque Country (Spain). His research focuses on biorefinery development within a circular economy context. He has published more than 300 papers in peer-reviewed scientific journals and 23 book chapters (H-index: 62). He has supervised 32 PhD thesis. He currently serves as associate editor of 2 international journals: Industrial Crops and Product (Elsevier) and Frontiers in Energy Research: Bioenergy and Biofuel (Frontiers) and member of the editorial board of several journals.

LIST OF SPEAKERS

CODE	PLENARY SPEAKERS
PL-01	**Prof. Ts. Dr. Mohd Hafiz Dzarfan Othman** *"Development of Cost-Effective Ceramic Hollow Fiber Membranes for Sustainable Water Treatment"*
PL-02	**Prof. Dr. Nicolas Brosse** *"Steam Explosion: An Ancient Steam Cracking Process for Innovative Applications"*

CODE	KEYNOTES SPEAKERS
KN-01	**Assoc. Prof. Dr. Low Siew Chun** *"Interface Chemistry of Polymer-Modified Screen-Printed Electrodes for Enhanced Lead Ion Detection"*
KN-02	**Prof. Dr. Nobuto Yoshinari** *"Supramolecular Frameworks of Metal-Organic Carboxylates"*
KN-03	**Assoc. Prof. Dr. Faiz Bukhari Mohd Suah** *"Polymer inclusion membranes in analytical chemistry: progress and potential"*
KN-04	**Prof. Dr. Mohamad Rafi** *"Chemometrics As a Comprehensive Data Analysis in The Context of Natural Product Research"*
KN-05	**Prof. Dr. Aik Wei Shen** *"Distinguishing the Catalytic Mechanisms of RNA N6-Methyladenosine (m^6A) Erasers"*
KN-06	**Prof. Dr. Jalel Labidi** *"Advances in Lignocellulosic Biorefineries"*

CODE	INVITED SPEAKERS
IV-01	**Dr. Kavirajaa Pandian Sambesevam** *“Electropolymerization of Polyaniline: A Versatile Approach for Rapid Deployment of Sensors in Food and Environmental Pollutant Monitoring”*
IV-02	**Assoc. Prof. Dr. Muggundha Raoov** *“Advanced Microextraction Methods for Polycyclic Aromatic Hydrocarbons in Food Using Magnetic Nanoparticle-Ionic Liquid Technology”*
IV-03	**Asst. Prof. Dr. Subhan Salaeh** *“New Crosslinking Routes of Rubber Vulcanizates for Smart and Sustainable Materials”*

LIST OF PRESENTING PARTICIPANTS

CODE	NAME	TITLE
IV-01	DR. KAVIRAJAA PANDIAN SAMBASEVAM	Electropolymerization of Polyaniline: A Versatile Approach for Rapid Deployment of Sensors in Food and Environmental Pollutant Monitoring
IV-02	DR. MUGGUNDHA RAOOV	Advanced Microextraction Methods for Polycyclic Aromatic Hydrocarbons in Food Using Magnetic Nanoparticle-Ionic Liquid Technology
IV-03	DR. SUBHAN SALAEH	New Crosslinking Routes of Rubber Vulcanizates for Smart and Sustainable Materials
ANA-01	DR. ALOYSIUS AKAANGEE PAM	Making The Switch from Traditional Activating Agents to Eco-Friendly Solvents for Activated Carbon: A Step Towards Long-Term Pb(II) Removal from Water
ANA-02	DR. ISA BABA KOKI	The Use of Chemometric Techniques in The Assessment and Source Identification of Toxic Metal Pollutants Along Kano Rivers Nigeria
ANA-03	MR. ZHEN HONG CHANG	Enhanced Stability and Permeability of Graphene Oxide Nanocomposite Membranes Via Glycine and Diglycine Cross-Linking
ANA-04	AISHA HAMID BALOCH	Development of Bimetallic Supported on 3D-Structured Metals Catalysts
ANA-05	MR. NASIR MUAZU	Electrochemical Degradation of Methylene Blue (MB) Using Graphite/PVC Anodes Coated with Nickel Oxide and Zinc Oxide:

		Optimization, Kinetic Analysis and Industrial Application Potential
ANA-06	MR. YAHAYA ALIYU DANMARAYA	Development of Dummy Template Molecularly Imprinted Polymer for The Adsorption of Organophosphorus Pesticides: Preliminary Studies
ANA-07	MUSAB ALGHODRAN	Development of Magnetic Graphene Oxide-Deep Eutectic Solvent for The Determination of Organophosphorus Pesticides: A Preliminary Studies
ANA-08	DR. SAPTONO HADI	Fabrication of Carboximetyl Chitosan-Alginate Polyelectrolyte Complex Membrane for Adsorption of Methylen Blue in Water
ANA-09	NURFARHANIM ABU BAKAR	Innovative Chitosan Hydrogels as A Sustainable Plant Growth Regulator for Resilience Agriculture
ANA-10	ZULHAN ARIF	Simple Detection of Hexavalent Chromium in Solutions Using Optode Membrane
ANA-11	NATALIA MARBUN	Microparticles Zerumbone from Zingiber Zerumbet Rhizome in Chitosan Modified Oleic Acid
ANA-12	DOREEN NB CHANDRA SIRI	Rapid Portable Atmospheric Solids Analysis Probe Mass Spectrometry for On-Site Urine Drug Screening
ANA-13	AMIRUL RAHIMI NORAZMI	Exploration of Potential Application of Natural Deep Eutectic Solvent in Vortex Assisted Liquid-Liquid Microextraction for The Determination of Selected Furanic Compounds in Honey

ANA-14	MR. MAMDOOH QATAN	Trends in Bimetallic Nanomaterials and Methods for Removal of P-Nitrophenol and Its Derivatives from Wastewater
ANA-15	YI HUAN TAN	Environmental Assessment of Single-Use Laboratory Plastic Waste: A Case Study
ANA-16	ZENI RAHMAWATI	Potentiometric Sensor-Based Imprinted TS-1 Zeolite for Selective Detection of Cholesterol
ANA-17	ASSOC. PROF. DR. MATEEN ABBAS	Green Synthesis of Iron Nanoparticles using Tagetes Erecta Flower Extract for The Detoxification of Various Mycotoxins
ANA-18	AR. DR ALIYU MUHAMMAD	Voltammetric Detection of Amoxicillin Residue in Milk at Nanohybrid Modified Screen Printed Electrode
BIOCHEM-01	YEHEZKIEL STEVEN KURNIAWAN	Design and *In Silico* Modelling of Heterocyclic-Based Xanthone Derivatives as Potential Anticancer Agent Through Tyrosine Kinase Inhibition
BIOCHEM-02	HUSNAINI BASIR	Discovery of Indoleninyl-Pyrazolo[3,4-*b*]pyridines as Potent Chemotherapeutic Agents Against Colorectal Cancer Cells
BIOCHEM-03	YONG YONG ONG	*In Silico* Peptidomics in Identifying Novel Bioactive Peptides from Sludge Worm (*Tubifex Tubifex*): A Green Chemistry Approach
BIOCHEM-04	TRIVADILA	In Vitro Kinetics of Cyclooxygenase-2 (COX-2) Inhibition by Spagneticola Tribolata Extract
IND-01	ZHEXUN ONG	Reforming Wood Preservative Delivery: Employment of Tebuconazole-Loaded Self-Emulsifying Drug Delivery System (SEDDS) and Tebuconazole-Loaded Zein Nanoparticles

IND-02	ISABELLE ZIEGLER-DEVIN	Green Approach to Produce Lignin Nanoparticules
IND-03	MS. AFREEN AHTESHAM	Development Of PPy/MnO_2/N-CNT Coated Carbon Felt Anode for Microbial Degradation of Methyl Yellow Dye
IND-04	NOR NAJHAN IDRIS	Enhancing Lignin Properties Via Steam Explosion Pretreatment: A Novel Modification Approach
IND-05	SANI MUHAMMAD GUMEL	Investigation of Chitosan Efficacy as A Good Delivery Biopolymer for Anti-Breast Cancer Drugs Through Molecular Docking
IND-06	MOHAMAD HAMDI ZAINAL ABIDIN	Neoteric Green Solvents for Improved Solubility and Antioxidant Activity of α-Tocopherol
IND-07	LAI YEE LEE	Development of A 3D Reduced Graphene Oxide Aerogel for Treatment of Pharmaceutical Wastewater
INO-01	ADHI DWI HATMANTO	Incorporation of ZnO Nanofillers into Chitosan/Ki/I_2-Based Quasi Solid Electrolytes
INO-02	RATIH LESTARI	Sustainable Recycling of Plastic Bag Waste into Carbon Quantum Dots Using Optimized Pyrolysis-Hydrothermal Methods for Selective Fe(III) Sensing
INO-03	INDRIANA KARTINI	Carbon Dot Nanocomposites from Cajeput Tree Modified with Folic Acid and Chlorophylls as Potential Photosensitizers for Photodynamic Therapy
INO-04	MR. AHMAD ALIF SYAMSUDDIN MOHAMAD NASIR	NiO/CeO_2-Al_2O_3 Mesoporous Catalyst Supported on Alumina Beads for Hydrogen Generation from Ammonia Decomposition

INO-05	MR. HII CHIONG HWEE	Seeking The Potentiality of Phenylphosphonate/HDPE/Graphene Oxide Composite: An Environmentally Friendly Flame Retardant
INO-06	MAS SYAZLIN MASBAH	Microwave-Assisted Synthesis and Characterisation of Zinc Oxide Quantum Dots for Detection of Antibiotics
INO-07	MUHAMMAD AMIR FIRDAUS MOHD ZULKFLY	Microwave-Assisted Synthesis of Carbon Quantum Dots from The Deactivated Cells of Pseudomonas Aeruginosa Usm-AR2
INO-08	MS. HANISAH ZAINAL ABIDIN	Effect of Tin Filler Composition on Porosity in Tin-Polydimethylsiloxane Composites
INO-09	NOVIYAN DARMAWAN	Enhanced Photocatalytic Degradation of Emerging Pollutants by Hybrid Metal-Organic Frameworks and Carbon Dots Composites
INO-10	MR. MUHAMMAD FATHURRAHMAN	Kinetic and Optimization Studies of Methylene Blue Photodegradation Over Fe-PTC MOF and H_2O_2 using Response Surface Methodology
INO-11	SEOW CHING PHOON	Microware-Assisted Synthesised SnO_2 Quantum Dots Photocatalysts for The Removal of Antibiotics
INO-12	MS. NUR AMANINA JUNIASARI TUN NUR ISKANDAR	Sulfone-Centred Systems with Diverse Terminal Alkoxy Chains: Synthesis, Characterization, and Their Mesomorphic and Photoluminescence Behaviors
INO-13	MRS. LUTFIYA RIZQIYANIKA	Fe_3O_4@SiO_2 Modified HDTMS Hydrophobic Coatings as Anti-Corrosion Coating on Steel
INO-14	ZI KANG KOI	Synthesis And Characterization of Layered Double Hydroxide

INO-15	AMAL NAYEF AL-MOMANI	Microwave-Assisted Synthesis of Laccase of *Trametes Hirsuta*-Derived Carbon Dots for Ciprofloxacin Detection
INO-16	DR. NOR HAFIZAH BERAHIM	Catalytic Hydrogenation of CO_2 to Methanol Over Cu/ZnO Based Catalyst Supported on Various Types of Al_2O_3 Pellet
INO-17	MS. JEESICA HERMAYANTI PRATAMA	Catalytic Study of CO/γ-Al_2O_3 on The Deoxygenation of Palm Oil Biodiesel for Green Diesel Production
INO-18	MRS. NURUL ATIKAH NORDIN	Enhanced Photocatalytic Generation of H_2O_2 via a Composite of ZIF-8 and Carbon-Doped g-C_3N_4 Derived from Kapok Fiber
ORG-01	FIA FATHIANA WULAN	Evaluating Antimalarial Properties Via Chemical Modification of Furan-Based Chalcones: Insights from Biological Activity, DFT Calculations, Molecular Docking, and ADMET Study
ORG-02	MS. YAP PUI WING	Synthesis and Properties of Non-Linear Disulphide-Centered S-Shaped Oligomers Armed with Aromatic Azo Moieties
ORG-03	LIM XIN YI	TMPTA Crosslinker UV-Grafted BPADA-BAPP Polyimide Thin Films: Thermos-Chemical Stability and Structural Characterization
ORG-04	MS. NUR FATIN ATIKAH ABDUL MUTALIB	Acid-Activated Natural Zeolite Clinoptilolite Functionalized with Curcumin for Superior Methylene Blue Adsorption: Insights into Optimization, Characterization, and Adsorption Mechanisms
ORG-05	MS. DANA AINAKULOVA	Utilization of Poly(Glycidyl Methacrylate-Co-Butyl Acrylate) Reactive Dilutes to Improve

		The Properties of Epoxy Resin as Anticorrosion Coating
ORG-06	BUDI HASTUTI	Synthesis of Chitosan-Alginate-Montmorillonite Hydrogel Micro Composite for Paracetamol Adsorption in Aqueous Solutions
ORG-07	MR. AIDIEL MOHAMMAD	Isolation, *In-Vitro* Cytotoxicity and Molecular Docking of Polymethoxyflavones from *Kaempferia Parviflora* on Breast Cancer Cell Lines
ORG-08	BUDI ARIFIN	Effect of Solvent Polarity on Side-Chain Rearrangement in Bromination of Methyleugenol with Molecular Bromine
ORG-09	REYMARK EREJE	Synthesis, Molecular Docking and Quantitative Structure-Activity Relationship Analysis of Bioactive 2o-Alkylated Benzofuropyridines
ORG-10	MR. ABRAR MOHAMMAD SAYAF	Evaluation of 2-(1H-1,2,3-Triazol-1-yl)acetic Acid Derivatives as Potential Human Hypoxia Inducible Factor (HIF) Prolyl Hydroxylase Domain-2 (PHD2) Inhibitors
ORG-11	NAFISAH NAFISAH	Anti-inflammatory Activity of Biflavonoid from Genus Araucaria: *In Vitro* and *In Silico* Approach
ORG-12	DR. CHAPUIS HUBERT	Chemical Treatment of Flax Fibre Materials for Biocomposite Applications
PHY-01	MS. EARLY ZAHWA ALHARISSA	Remarkable Enhanced Visible Activity of TiO_2-N CO-DOPED with Cu from Electroplating Wastewater for Degradation of Amoxicillin Residual in Water Media

PHY-02	KELLY LOKE KAH YEE	Enhancing Plastic Pyrolysis: Predictive Analysis Integrated with Machine Learning
PHY-03	MR. GANAPATY MANICKAVASAGAM	Unlocking The Synthesis Tuning of Hydrochar-Based Catalysts for Enhanced Peroxymonosulfate Activation
PHY-04	EKA PRATISTA	Doping TiO_2 with Cu from Electroplating Wastewater for Remarkable Improvement of Its Activity Under Visible Light for *E. Coli* Bacterial Disinfection in Water
PHY-05	MS. MARYAM ABDUL-RAHEEM	Fabrication of KOH Impregnation Pome Sludge Biochar-Based Photocatalyst Via Hydrothermal Synthesis for Photodegradation of Ciprofloxacin Antibiotic Pollutant Under Solar-Simulated Visible Light
PHY-06	MD MOKARRAM BADSHA	Predictive Analyses for The Dark Fermentative Hydrogen Production from Food Waste
PHY-07	MR. AHMAD ALIN BAFFA	Synthesis and Characterization of Graphene Oxide Zinc Metal-Organic Framework (BgO-ZnMOF) for The Removal of Bisphenol-A in Wastewater Via Adsorption Process
PHY-08	SUN YANLI	Enhanced Photodegradation of Ceftazidime by BIOBR(110)/BIOCL(110) Composite: Its Synthesis, Mechanism, and Degradation Pathways
PHY-09	PHILIP JOHN AMEJI	Integrated Ligand and Structure Based Approaches for The Design of Novel Antagonists of Estrogen Receptor Alpha (ERα) from Colchicine Amides and Sulfonamides
PHY-10	YUNG XIN KOH	Optimizing Curing Duration of Self-Healing Chitosan/Polyacrylamide Hydrogel Coating

		on Polyethersulfone Membrane for Enhanced Stability and Filtration Efficiency
PHY-11	MENGNAN WANG	Biosorption of Cu(II) onto Dried Activated Sludge: Equilibrium and Kinetic Studies
PHY-12	HENNY PURWANINGSIH	Characterization Of Food Freshness Indicator from Ganyong Flour Modified with The Addition of Nanocellulose from Corn Husk and Curcumin
PHY-13	RUT NOVALIA RAHMAWATI SIANIPAR	Indonesian Medicinal Plants Used for COPD Treatment Via Inhibition of Inflammatory Rules
PHY-14	RUT NOVALIA RAHMAWATI SIANIPAR	Virtual Screening Using Ensemble Docking Approaches for The Inhibition of Arcangelisia Flava Compounds to Janus Kinase-2 And Cyclooxygenase-2
PHY-15	NURFARHANA MOHD MUSTAFFARIZAN	Nitrogen-Doped Porous Carbon (NDPC) Sorbents from Biomass for Carbon Dioxide Capture
PHY-16	NURUL HUDA ABDUL HALIM	Removal of Rhodamine B Dye utilizing Graphene Oxide-Rubber Based Hydrogel as an Alternative for Water Treatment
ANA-01 (P)	HUI JING CHAM	Co_2 Removal Via Aqueous Methyldiethanolamine-Tetrabutylphosphonium P-Toluene Sulfonate ([MDEA]-[TBP][P-TSA]) Hybrid Solvent
ANA-02 (P)	RAHMAT HIDAYAT	Cutting-Edge Electrodialysis Methods for Analytical Separation
BIOCHEM-01 (P)	MUHAMMAD AZRI FAIZ ABD ZAKI	Design, Synthesis and Mechanistic Studies of Novel Benzimidazoles as A Novel Class of

		Therapeutics Against Drug-Resistant Oral Cancer Cells
IND-01 (P)	EJAZ HUSSAIN	Synthesis, Characterization, and Applications of Ambi-Functional PANI/GO/MOF-FE$_3$O$_4$ Magnetic Nanocomposite for Removing Industrial Dye and Emerging Contaminant
INO-01 (P)	YIXUAN DUAN	Activation of Persulfate by Zeolite Supported CuO Catalysts for Phenol Degradation
ORG-01 (P)	CHEAN HUI NG	Investigating The Potential of Prenylated and Geranylated Acylphloroglucinol-Based Xanthenones as Potent Soybean 15-Lipoxygenase Inhibitors: A Combined *In Vitro* and *In Silico* Approach
PHY- 01 (P)	MR. MUHAMMAD MUJAHID	Palm Oil Mill Effluent (POME): Environmental Challenges and Exploring Sustainable Applications for Eco-Friendly Solutions
PHY-02 (P)	MR. KAMALADDEEN ABDULLAHI	Photoluminescence Studies on Zinc-Neodymium Layered Double Hydroxide

PROGRAM SUMMARY

Day 1: 9th October 2024 (Wednesday)

Time	Programme	Room
0745 – 0855	Registration	Ballroom
0900 – 0905	Welcome Address	Ballroom
0910 – 1010	Plenary Lecture	Ballroom
1015 – 1045	Tea Break	Ballroom
1050 – 1055	Video Presentation	Ballroom
1100 – 1230	Oral Session 1	Sri Perak 1-3
1235 – 1435	Lunch	Coffee House
1440 – 1455	Arrival of VIP	Ballroom
1500 – 1540	Opening Ceremony	Ballroom
1545 – 1900	High Tea	Eating Hall

Day 2: 10th October 2024 (Thursday)

Time	Programme	Room
0745 – 0855	Morning Tea Break	Eating Hall
0900 – 1000	Plenary Lecture	Ballroom
1005 – 1135	Oral Session 2	Ballroom and Sri Perak 1-3
1135 – 1235	Oral Session 3	Ballroom and Sri Perak 1-3
1240 – 1410	Lunch	Coffee House
1415 – 1615	Oral Session 4	Ballroom and Sri Perak 1-3
1620 – 1720	Oral Session 5	Ballroom and Sri Perak 1-3
1725 – 1900	Tea Break	Eating Hall

Day 3: 11th October 2024 (Friday)

Time	Programme	Room
0900 – 1100	Oral Session 6	Sri Perak 1-3
1105 – 1235	Award presentation & Closing Ceremony	Ballroom
1240 – 1355	Lunch	Coffee House
1400 – 2000	Excursion *(Available as an add-on)*	Georgetown, Penang

SCHEDULED OVERVIEW

	Time	**Programme**		
Day 1	0745 - 0855	Registration Arrival of Guest & Participants		
	0900 - 0905	Welcome Address by Vice-Chairperson of ICYC 2024: **Ms. Nur Fatin Atikah binti Abdul Mutalib**		
	0910 - 1010	Plenary Lecture: **Prof. Ts. Dr. Mohd Hafiz Dzarfan Othman** *(Ballroom)*		
	1015 - 1045	Tea Break		
	1050 – 1055	Video Presentation *(Ballroom)*		
		Oral Session – 1 *(Ballroom & Sri Perak 1-3)*		
	ROOM	**Sri Perak 1**	**Sri Perak 2**	**Sri Perak 3**
	1100 – 1230	KN-01	IV-01	BIOCHEM-01
			INO-01	BIOCHEM-02
		PHY-01	INO-02	ORG-01
		PHY-02	INO-03	ORG-02
		PHY-03	INO-04	ORG-03
		PHY-04	INO-05	ORG-04
	1235 – 1435	Lunch		
	1440 – 1455	Arrival of VIP		
	1500 – 1600	Opening ceremony, **WELCOMING SPEECH BY:** Chairman of 9th ICYC 2024 - **ChM. Ganapaty Manickavasagam** **OFFICIATING SPEECH BY:** Dean of School of Chemical Sciences - **Prof. Dr. Rohana Adnan**		

	1605 – 1900	High Tea *(Ballroom)*			
Day 2	0745 – 0855	Morning Tea Break			
	0900 – 1000	Plenary Lecture: **Prof. Dr. Nicholas Brosse** *(Ballroom)*			
		Oral Session – 2 *(Ballroom & Sri Perak 1-3)*			
	ROOM	**Ballroom**	**Sri Perak 1**	**Sri Perak 2**	**Sri Perak 3**
	1005 – 1135	KN-02	PHY-05	IV-02	IND-01
			PHY-06	ANA-01	IND-02
		INO-06	PHY-07	ANA-02	IND-03
		INO-07	IND-04	ANA-09	PHY-08
		-	ANA-18	ANA-02 (P)	-
		Oral Session – 3 *(Ballroom & Sri Perak 1-3)*			
	ROOM	**Ballroom**	**Sri Perak 1**	**Sri Perak 2**	**Sri Perak 3**
	1135 – 1235	KN-03	INO-08	ORG-05	PHY-09
			INO-09	ORG-06	PHY-10
		IV-03	INO-10	INO-12	INO-17
	1240 – 1410	Lunch			
		Oral Session – 4 and **Poster Session – 1** *(Ballroom & Sri Perak 1-3)*			
	ROOM	**Ballroom**	**Sri Perak 1**	**Sri Perak 2**	**Sri Perak 3**
	1415 – 1615	KN-04	ANA-05	ANA-16	ORG-07
			ANA-06	PHY-11	ORG-08
		IND-05	ANA-07	PHY-14	ORG-09
		IND-06	INO-01 (P)	PHY-01(P)	ORG-10
		IND-07	ANA-01 (P)	PHY-02(P)	ORG-11
		ANA-08	IND-01 (P)	BIOCHEM -01 (P)	ORG-12
		-	-	-	ORG-01 (P)
		Oral Session and Poster – 5 *(Ballroom & Sri Perak 1-3)*			

		Ballroom	Sri Perak 1	Sri Perak 2	Sri Perak 3
	1620 – 1720	KN-05	BIOCHEM-04	INO-13	ANA-10
			INO-11	INO-14	ANA-11
		BIOCHEM-03	INO-16	INO-15	ANA-15
	1725 – 1900	Tea Break			
Day 3	0755 - 0855	Morning Tea Break			
		Oral Session – 6 *(Sri Perak 1-3)*			
	ROOM	**Sri Perak 1**	**Sri Perak 2**	**Sri Perak 3**	
	0900 – 1100	KN-06	ANA-03	ANA-04	
			ANA-13	ANA-12	
		PHY-12	PHY-13	ANA-14	
		PHY-15	PHY-16	INO-18	
		-	-	ANA-17	
	1125 – 1235	Award presentation & Closing Ceremony *(Ballroom)*			
	1240 – 1400	Lunch			
	1400 – 2000	Excursion *(Available as an add-on)*			

*Note: Oral presenters will be allotted a maximum of **15 min** to present including Q&A session.*

Research Areas:

Analytical Chemistry (ANA)	**Inorganic Chemistry (INO)**
Biochemistry (BCHEM)	**Organic Chemistry (ORG)**
Industrial Chemistry (IND)	**Physical Chemistry (PHY)**

DETAIL SCHEDULED

Day 1: 9th October 2024 (Wednesday)

PLENARY LECTURE

Ballroom		
Time	**Code**	**Title**
0945 – 1045	PL-01	*Development of Cost-Effective Ceramic Hollow Fiber Membranes for Sustainable Water Treatment*

KEYNOTE LECTURE

Sri Perak 1		
Time	**Code**	**Title**
1100 – 1130	KN-01	*Interface Chemistry of Polymer-Modified Screen-Printed Electrodes for Enhanced Lead Ion Detection*

INVITED SPEAKER

Sri Perak 2		
Time	**Code**	**Title**
1100 – 1230	IV-01	*Electropolymerization of Polyaniline: A Versatile Approach for Rapid Deployment of Sensors in Food and Environmental Pollutant Monitoring*

ORAL SESSION

Sri Perak 1

Time	Code	Title
1100 – 1230	PHY-01	*Remarkable Enhanced Visible Activity of TiO_2-N CO-DOPED with Cu from Electroplating Wastewater for Degradation of Amoxicillin Residual in Water Media*
	PHY-02	*Enhancing Plastic Pyrolysis: Predictive Analysis Integrated with Machine Learning*
	PHY-03	*Unlocking The Synthesis Tuning of Hydrochar-Based Catalysts for Enhanced Peroxymonosulfate Activation*
	PHY-04	*Doping TiO_2 with Cu from Electroplating Wastewater for Remarkable Improvement of Its Activity Under Visible Light for E. Coli Bacterial Disinfection in Water*

Sri Perak 2

Time	Code	Title
1100 – 1230	INO-01	*Incorporation of ZnO Nanofillers into Chitosan/Ki/I_2-Based Quasi Solid Electrolytes*
	INO-02	*Sustainable Recycling of Plastic Bag Waste into Carbon Quantum Dots Using Optimized Pyrolysis-Hydrothermal Methods for Selective Fe (III) Sensing*
	INO-03	*Carbon Dot Nanocomposites from Cajeput Tree Modified with Folic Acid and Chlorophylls as Potential Photosensitizers for Photodynamic Therapy*
	INO-04	*NiO/CeO_2-Al_2O_3 Mesoporous Catalyst Supported on Alumina Beads for Hydrogen Generation from Ammonia Decomposition*
	INO-05	*Seeking The Potentiality of Phenylphosphonate/HDPE/Graphene Oxide Composite: An Environmentally Friendly Flame Retardant*

Sri Perak 3

Time	Code	Title
1100 – 1230	BIOCHEM-01	*Design and In Silico Modelling of Heterocyclic-Based Xanthone Derivatives as Potential Anticancer Agent Through Tyrosine Kinase Inhibition*
	BIOCHEM-02	*Discovery of Indoleninyl-Pyrazolo[3,4-b]pyridines as Potent Chemotherapeutic Agents Against Colorectal Cancer Cells*
	ORG-01	*Evaluating Antimalarial Properties Via Chemical Modification of Furan-Based Chalcones: Insights from Biological Activity, DFT Calculations, Molecular Docking, and ADMET Study*
	ORG-02	*Synthesis and Properties of Non-Linear Disulphide-Centered S-Shaped Oligomers Armed with Aromatic Azo Moieties*
	ORG-03	*TMPTA Crosslinker UV-Grafted BPADA-BAPP Polyimide Thin Films: Thermos-Chemical Stability and Structural Characterization*
	ORG-04	*Acid-Activated Natural Zeolite Clinoptilolite Functionalized with Curcumin for Superior Methylene Blue Adsorption: Insights into Optimization, Characterization, and Adsorption Mechanisms*

Day 2: 10th October 2024 (Thursday)

PLENARY LECTURE

Ballroom		
Time	**Code**	**Title**
0900 – 1000	PL-02	*Steam Explosion: An Ancient Steam Cracking Process for Innovative Applications*

KEYNOTE LECTURE

Ballroom		
Time	**Code**	**Title**
1005 – 1035	KN-02	*Supramolecular Frameworks of Metal-Organic Carboxylates*
Time	**Code**	**Title**
1135 – 1205	KN-03	*Polymer inclusion membranes in analytical chemistry: progress and potential*
Time	**Code**	**Title**
1415 – 1445	KN-04	*Chemometrics As a Comprehensive Data Analysis in The Context of Natural Product Research*
Time	**Code**	**Title**
1620 – 1650	KN-05	*Distinguishing the Catalytic Mechanisms of RNA N6-Methyladenosine (m^6A) Erasers*

INVITED SPEAKER

Sri Perak 2		
Time	**Code**	**Title**
1020 – 1035	IV-02	*Advanced Microextraction Methods for Polycyclic Aromatic Hydrocarbons in Food Using Magnetic Nanoparticle-Ionic Liquid Technology*
Ballroom		
Time	**Code**	**Title**
1135 – 1235	IV-03	*New Crosslinking Routes of Rubber Vulcanizates for Smart and Sustainable Materials*

ORAL SESSION

Ballroom		
Time	**Code**	**Title**
1005 - 1135	INO-06	*Microwave-Assisted Synthesis and Characterisation of Zinc Oxide Quantum Dots for Detection of Antibiotics*
	INO-07	*Microwave-Assisted Synthesis of Carbon Quantum Dots from The Deactivated Cells of Pseudomonas Aeruginosa USM-AR2*
Time	**Code**	**Title**
1415 - 1615	IND-05	*Investigation of Chitosan Efficacy as A Good Delivery Biopolymer for Anti-Breast Cancer Drugs Through Molecular Docking*
	IND-06	*Neoteric Green Solvents for Improved Solubility and Antioxidant Activity Of α-Tocopherol*
	IND-07	*Development of A 3D Reduced Graphene Oxide Aerogel for Treatment of Pharmaceutical Wastewater*

	ANA-08	*Fabrication of Carboximetyl Chitosan-Alginate Polyelectrolyte Complex Membrane for Adsorption of Methylen Blue in Water*
Time	**Code**	**Title**
1620 – 1720	BIOCHEM-03	*In Silico Peptidomics in Identifying Novel Bioactive Peptides from Sludge Worm (Tubifex Tubifex): A Green Chemistry Approach*

Sri Perak 1		
Time	**Code**	**Title**
1005 – 1135	PHY-05	*Fabrication of KOH Impregnation Pome Sludge Biochar-Based Photocatalyst via Hydrothermal Synthesis for Photodegradation of Ciprofloxacin Antibiotic Pollutant Under Solar-Simulated Visible Light*
	PHY-06	*Predictive Analyses for The Dark Fermentative Hydrogen Production from Food Waste*
	PHY-07	*Synthesis And Characterization of Graphene Oxide Zinc Metal-Organic Framework (BgO-ZnMOF) for The Removal of Bisphenol-A in Wastewater Via Adsorption Process.*
	IND-04	*Enhancing Lignin Properties Via Steam Explosion Pretreatment: A Novel Modification Approach*
	ANA-18	*Voltammetric Detection of Amoxicillin Residue in Milk at Nanohybrid Modified Screen Printed Electrode*
Time	**Code**	**Title**
1135 - 1235	INO-08	*Effect of Tin Filler Composition on Porosity in Tin-Polydimethylsiloxane Composites*
	INO-09	*Enhanced Photocatalytic Degradation of Emerging Pollutants by Hybrid Metal-Organic Frameworks and Carbon Dots Composites*

	INO-10	*Kinetic and Optimization Studies of Methylene Blue Photodegradation Over Fe-PTC MOF and H_2O_2 Using Response Surface Methodology*
Time	**Code**	**Title**
1415 – 1615	ANA-05	*Electrochemical Degradation of Methylene Blue (MB) Using Graphite/PVC Anodes Coated with Nickel Oxide and Zinc Oxide: Optimization, Kinetic Analysis and Industrial Application Potential*
	ANA-06	*Development of Dummy Template Molecularly Imprinted Polymer for The Adsorption of Organophosphorus Pesticides: Preliminary Studies*
	ANA-07	*Development of Magnetic Graphene Oxide-Deep Eutectic Solvent for The Determination of Organophosphorus Pesticides: A Preliminary Studies*
Time	**Code**	**Title**
1620 – 1720	BIOCHEM-04	*In Vitro Kinetics of Cyclooxygenase-2 (Cox-2) Inhibition by Spagneticola Tribolata Extract*
	INO-11	*Microware-Assisted Synthesised SnO_2 Quantum Dots Photocatalysts for The Removal of Antibiotics*
	INO-16	*Catalytic Hydrogenation of CO_2 to Methanol Over Cu/ZnO Based Catalyst Supported on Various Types of Al_2O_3 Pellet*

Sri Perak 2

Time	Code	Title
1005 – 1135	ANA-01	*Making The Switch from Traditional Activating Agents to Eco-Friendly Solvents for Activated Carbon: A Step Towards Long-Term Pb(II) Removal from Water*

	ANA-02	*The Use of Chemometric Techniques in The Assessment and Source Identification of Toxic Metal Pollutants Along Kano Rivers Nigeria*
	ANA-09	*Innovative Chitosan Hydrogels as A Sustainable Plant Growth Regulator for Resilience Agriculture*
	ANA-02 (P)	*Cutting-Edge Electrodialysis Methods for Analytical Separation*
Time	**Code**	**Title**
1135 – 1235	ORG-05	*Utilization of Poly(Glycidyl Methacrylate-Co- Butyl Acrylate) Reactive Dilutes to Improve The Properties of Epoxy Resin as Anticorrosion Coating*
	ORG-06	*Synthesis of Chitosan-Alginate-Montmorillonite Hydrogel Micro Composite for Paracetamol Adsorption in Aqueous Solutions*
	INO-12	*Sulfone-Centred Systems with Diverse Terminal Alkoxy Chains: Synthesis, Characterization, and Their Mesomorphic and Photoluminescence Behaviors*
Time	**Code**	**Title**
1415 – 1615	ANA-16	*Potentiometric Sensor-Based Imprinted TS-1 Zeolite for Selective Detection of Cholesterol*
	PHY-11	*Biosorption of Cu(II) onto Dried Activated Sludge: Equilibrium and Kinetic Studies*
	PHY-14	*Virtual Screening Using Ensemble Docking Approaches for The Inhibition of Arcangelisia Flava Compounds to Janus Kinase-2 And Cyclooxygenase-2*
Time	**Code**	**Title**
1620 – 1720	INO-13	*Fe_3O_4@SiO_2 Modified HDTMS Hydrophobic Coatings as Anti-Corrosion Coating on Steel*
	INO-14	*Synthesis and Characterization of Layered Double Hydroxide*

	INO-15	*Microwave-Assisted Synthesis of Laccase of Trametes Hirsuta-Derived Carbon Dots for Ciprofloxacin Detection*

Sri Perak 3

Time	Code	Title
1005 – 1035	IND-01	*Reforming Wood Preservative Delivery: Employment of Tebuconazole-Loaded Self-Emulsifying Drug Delivery System (SEDDS) and Tebuconazole-Loaded Zein Nanoparticles*
	IND-02	*Green Approach to Produce Lignin Nanoparticules*
	IND-03	*Development Of PPy/MnO_2/N-CNT Coated Carbon Felt Anode for Microbial Degradation of Methyl Yellow Dye*
	PHY-08	*Enhanced Photodegradation of Ceftazidime by BIOBR(110)/BIOCL(110) Composite: Its Synthesis, Mechanism, and Degradation Pathways*
Time	**Code**	**Title**
1135 – 1235	PHY-09	*Integrated Ligand and Structure Based Approaches for The Design of Novel Antagonists of Estrogen Receptor Alpha (ERα) from Colchicine Amides and Sulfonamides*
	PHY-10	*Optimizing Curing Duration of Self-Healing Chitosan/Polyacrylamide Hydrogel Coating on Polyethersulfone Membrane for Enhanced Stability and Filtration Efficiency*
	INO-17	*Catalytic Study of CO/γ-Al_2O_3 on The Deoxygenation of Palm Oil Biodiesel for Green Diesel Production*
Time	**Code**	**Title**
1415 – 1615	ORG-07	*Isolation, In-Vitro Cytotoxicity and Molecular Docking of Polymethoxyflavones from Kaempferia Parviflora on Breast Cancer Cell Lines*

	ORG-08	*Effect of Solvent Polarity on Side-Chain Rearrangement in Bromination of Methyleugenol with Molecular Bromine*
	ORG-09	*Synthesis, Molecular Docking and Quantitative Structure-Activity Relationship Analysis of Bioactive 2o-Alkylated Benzofuropyridines*
	ORG-10	*Evaluation of 2-(1H-1,2,3-Triazol-1-yl)acetic Acid Derivatives as Potential Human Hypoxia Inducible Factor (HIF) Prolyl Hydroxylase Domain-2 (PHD2) Inhibitors*
	ORG-11	*Anti-inflammatory Activity of Biflavonoid from Genus Araucaria: In Vitro and In Silico Approach*
	ORG-12	*Chemical Treatment of Flax Fibre Materials for Biocomposite Applications*

Time	**Code**	**Title**
1620 – 1720	ANA-10	*Simple Detection of Hexavalent Chromium in Solutions Using Optode Membrane*
	ANA-11	*Microparticles Zerumbone from Zingiber Zerumbet Rhizome in Chitosan Modified Oleic Acid*
	ANA-15	*Environmental Assessment of Single-Use Laboratory Plastic Waste: A Case Study*

POSTER SESSION

Sri Perak 1		
Time	**Code**	**Title**
1415 – 1615	INO-01 (P)	*Activation of Persulfate by Zeolite Supported CuO Catalysts for Phenol Degradation*
	ANA-01 (P)	*Co$_2$ Removal Via Aqueous Methyldiethanolamine-Tetrabutylphosphonium P-Toluene Sulfonate ([MDEA]-[TBP][P-TSA]) Hybrid Solvent*
	IND-01 (P)	*Synthesis, Characterization, and Applications of Ambi-Functional PANI/GO/MOF-FE$_3$O$_4$ Magnetic Nanocomposite for Removing Industrial Dye and Emerging Contaminant*

Sri Perak 2		
Time	**Code**	**Title**
1415 – 1615	PHY-01 (P)	*Palm Oil Mill Effluent (POME): Environmental Challenges and Exploring Sustainable Applications for Eco-Friendly Solutions*
	PHY-02 (P)	*Photoluminescence Studies on Zinc-Neodymium Layered Double Hydroxide*
	BIOCHEM-01 (P)	*Design, Synthesis and Mechanistic Studies of Novel Benzimidazoles as A Novel Class of Therapeutics Against Drug-Resistant Oral Cancer Cells*

Sri Perak 3		
Time	**Code**	**Title**
1415 – 1615	ORG-01 (P)	*Investigating The Potential of Prenylated and Geranylated Acylphloroglucinol-Based Xanthenones as*

		Potent Soybean 15-Lipoxygenase Inhibitors: A Combined In Vitro and In Silico Approach

Day 3: 11th October 2024 (Friday)

KEYNOTE SPEAKER

Sri Perak 1		
Time	**Code**	**Title**
0900 – 0930	KN-06	*Advances in Lignocellulosic Biorefineries*

ORAL SESSION

Sri Perak 1		
Time	**Code**	**Title**
0900 – 1100	PHY-12	*Characterization Of Food Freshness Indicator from Ganyong Flour Modified with The Addition of Nanocellulose from Corn Husk and Curcumin*
	PHY-15	*Nitrogen-Doped Porous Carbon (NDPC) Sorbents from Biomass for Carbon Dioxide Capture*

Sri Perak 2		
Time	**Code**	**Title**
0900 – 1100	ANA-03	*Enhanced Stability and Permeability of Graphene Oxide Nanocomposite Membranes Via Glycine and Diglycine Cross-Linking*
	ANA-13	*Exploration of Potential Application of Natural Deep Eutectic Solvent in Vortex Assisted Liquid-Liquid Microextraction for The Determination of Selected Furanic Compounds in Honey*
	PHY-13	*Indonesian Medicinal Plants Used for COPD Treatment Via Inhibition of Inflammatory Rules*

	PHY-16	*Removal of Rhodamine B Dye utilizing Graphene Oxide-Rubber Based Hydrogel as an Alternative for Water Treatment*

Sri Perak 3		
Time	**Code**	**Title**
0900 – 1100	ANA-04	*Development of Bimetallic Supported on 3D-Structured Metals Catalysts*
	ANA-12	*Rapid Portable Atmospheric Solids Analysis Probe Mass Spectrometry for On-Site Urine Drug Screening*
	ANA-14	*Trends in Bimetallic Nanomaterials and Methods for Removal of P-Nitrophenol and Its Derivatives from Wastewater*
	INO-18	*Enhanced Photocatalytic Generation of H_2O_2 via a Composite of ZIF-8 and Carbon-Doped g-C_3N_4 Derived from Kapok Fiber*
	ANA-17	*Green Synthesis of Iron Nanoparticles using Tagetes Erecta Flower Extract for The Detoxification of Various Mycotoxins*

PLEANARY SPEAKERS

INTERNATIONAL CONFERENCE OF YOUNG CHEMISTS

PLENARY SPEAKER

Prof. Dr Mohd Hafiz Dzarfan Othman

DEVELOPMENT OF COST-EFFECTIVE CERAMIC HOLLOW FIBER MEMBRANES FOR SUSTAINABLE WATER TREATMENT

Mohd Hafiz Dzarfan Othman

Advanced Membrane Technology Research Centre (AMTEC), Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia (UTM), 81310 Johor Bahru, Johor, Malaysia.
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With the increasing demand for clean and safe water, membrane technology has become an essential tool in water and wastewater treatment. Polymeric membranes are widely used due to their affordability and market availability, but their performance is often limited by chemical and thermal resistance issues. Ceramic membranes, while offering superior mechanical strength and longevity, are traditionally constrained by high production costs. Our research has pioneered the development of high-performance ceramic hollow fiber membranes utilizing cost-effective and readily available materials such as natural clays, agricultural, industrial waste, and animal bones. These membranes exhibit remarkable chemical and thermal resistance, making them suitable for a variety of applications including microfiltration, photocatalysis, and membrane distillation. We have achieved significant advancements by optimizing the fabrication process, utilizing phase inversion techniques to create asymmetric structures in a single step, and designing hollow fiber configurations to maximize surface area. These improvements have reduced production costs, making ceramic membranes a more viable option for large-scale applications. Our findings demonstrate that these newly developed ceramic hollow fiber membranes not only meet but exceed the performance of traditional polymeric membranes, offering a sustainable and economical solution for water treatment. This research opens the door to broader adoption and application of ceramic membranes in the industry, contributing to global efforts in addressing water scarcity and promoting environmental sustainability.

Keywords: Ceramic membrane, hollow fiber, water treatment and purification, surface modification, cost-effective materials

PLENARY SPEAKER

Prof. Dr Nicolas Brosse

STEAM EXPLOSION: AN ANCIENT STEAM CRACKING PROCESS FOR INNOVATIVE APPLICATIONS

Nicolas Brosse

LERMAB, Université de Lorraine, France

The steam explosion process is an environmentally-friendly, energy-efficient hydrothermal treatment. The process has also been used since the first half of the 20th century for the production of high-density panels (Hardboard, Isorel®). It is not only an ancient process, but also one of today's most mature technologies for the industrial production of cellulosic bioethanol and black pellets. Technically, a batch steam explosion pilot plant comprises a steam generator feeding a closed reactor into which biomass is introduced. The biomass is then steamed for a few minutes (2 to 15 min) at temperatures ranging from 160°C to 270°C, followed by rapid depressurization (< 300 ms). The combined effect of the hydrolysis stage (steaming phase) and the explosion stage (explosive decompression phase) leads to chemical (hydrolysis) and morphological (defibration, separation of constituents due to shear forces) changes in the plant material. In addition to the traditional application sectors mentioned above, the research work carried out at the LERMAB laboratory over the past 8 years in this area is focused on developing innovative, unconventional and credible technological solutions for industrial developments in various fields:

- Extraction of polymers (especially hemicellulose and lignin) and high-value-added molecules for cosmetics, as well as active extracts.
- The refining of natural fibers (or "cottonization") such as hemp and flax for textile and composite applications, and the production of cellulose micro/nano-fibers.
- Materials: advanced functionalization and properties, glueless panels and materials, fireproofing of fibers and materials
- Recycling of waste wood (B-wood) to produce panels.

The latest advances and prospects for this promising process for adding value to plant resources will be presented.

KEYNOTE SPEAKERS

INTERNATIONAL CONFERENCE OF YOUNG CHEMISTS

KEYNOTE SPEAKER

Associate. Prof. Dr. Low Siew Chun

INTERFACE CHEMISTRY OF POLYMER-MODIFIED SCREEN-PRINTED ELECTRODES FOR ENHANCED LEAD ION DETECTION

[1] Chyh Shyang Ong, [1,*] Siew Chun Low, [2,3] Qi Hwa Ng

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Heavy metal contamination, particularly lead, poses a significant threat to environmental and public health. To address this issue, electrochemical sensors have been developed as effective tools for lead detection. This study investigates the impact of various polymer modifiers, including cellulose acetate, chitosan, nylon 6, and Nafion, on the performance of screen-printed electrodes (SPEs) for lead sensing. Anodic stripping voltammetry is employed to assess how different polymer concentrations (1–5 wt.%) influence the electrode's surface morphology and electrochemical properties. Among the tested configurations, the 1 wt.% Nafion-modified SPE (Naf/SPE) exhibited the highest sensitivity, achieving a detection limit of 8.4 ppb, which complies with the World Health Organization's guidelines for lead in drinking water. The study found that an optimal polymer layer promotes effective lead ion interaction through metal-attracting SO_3^{2-} functional groups and surface charge properties. In contrast, higher polymer concentrations (5 wt.%) increased electrochemical resistance, reducing sensor sensitivity. These findings highlight the critical role of polymer composition and surface characteristics in enhancing the performance of SPE-based sensors for reliable lead detection.

Keywords: Heavy metal ions; Screen-printed electrode; Stripping voltammetry; Polymer; Nafion

KEYNOTE SPEAKER

Prof. Dr Nobuto Yosinari

SUPRAMOLECULAR FRAMEWORKS OF METAL-ORGANIC CARBOXYLATES

***Nobuto Yoshinari**

[1] *Department of Chemistry, Graduate School of Science, Osaka University, Toyonaka, Osaka, Japan*
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Organic carboxylates are fundamental building units for constructing coordination and hydrogen-bonded frameworks in supramolecular chemistry. Recently, discrete metal complexes with non-coordinating carboxy moieties (Metal-Organic Carboxylates; MOCs) have attracted increasing attention as alternatives to organic carboxylates because of their simple synthetic procedures and structural diversity, as well as the functionality due to transition metal centers.[1] Inspired by the historically important Cu_{14} cluster with D-penicillamine, which is the first MOC,[2] we have developed a variety of metallosupramolecular aggregates based on MOCs using metalloligand approach.[1,3] In my talk, I will describe our recent achievements about the migration and condensation reaction of aqua metal species in the supramolecular frameworks.[4]

Keywords: Metal-organic carboxylates; Metalloligands; Ionic conductor; Cluster synthesis

KEYNOTE SPEAKER

Assoc. Prof. Dr. Faiz Bukhari Mohd Suah

POLYMER INCLUSION MEMBRANES IN ANALYTICAL CHEMISTRY: PROGRESS AND POTENTIAL

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This presentation underscores the growing interest in polymer inclusion membranes (PIMs) in analytical chemistry, particularly as they are adapted for new and innovative applications. PIMs, liquid membranes based on polymers, have a rich history spanning five decades. They were initially introduced as sensing membranes in ion-selective electrodes. However, their recent diversification into other analytical chemistry applications, including sample separation, sample pre-concentration, electro-driven extraction, passive sampling, chemical sensors, electroanalysis, and integration into online and automated analysis systems, marks a significant shift. This presentation offers a comprehensive overview of the analytical chemistry applications of PIMs, showcasing their remarkable adaptability in solving complex chemical analysis problems and their potential outlook.

Keywords: Analytical chemistry, liquid membranes, polymer inclusion membranes

KEYNOTE SPEAKER

Prof. Dr. Mohamad Rafi

CHEMOMETRICS AS A COMPREHENSIVE DATA ANALYSIS IN THE CONTEXT OF NATURAL PRODUCT RESEARCH

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Chemometrics analyses are robust and comprehensive tools in analytical chemistry and other disciplines. Chemometrics uses statistical methods to deal with analytical data from a system or chemical process. Chemometrics maximizes the extraction of information and knowledge from chemical data. The application of chemometrics is increasing continuously because instrumentation technology and data analysis are more advanced in exploring new issues, etc. Advancements in chemical instrumentation make us deal with big data, so chemometrics has gained more attention and uses in many fields, such as natural product research, to identify biomarkers, contaminants, metabolite profiles, and authentication methods with metabolomics approaches. In this presentation, we would like to briefly introduce chemometrics and its application in natural product research, especially using chemometrics analysis for Indonesian biodiversity, such as plants, animals, and microbes.

Keywords: analytical chemistry, big data, chemometrics, metabolomics, natural product

Research area: *Analytical Chemistry*

KEYNOTE SPEAKER

Prof. Dr. Aik Wei Shen

DISTINGUISHING THE CATALYTIC MECHANISMS OF RNA N6-METHYLADENOSINE (m^6A) ERASERS

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AlkB homologue 5 (ALKBH5) is a ferrous iron and 2-oxoglutarate dependent oxygenase that demethylates RNA N^6-methyladenosine (m^6A), a post-transcriptional RNA modification with an emerging set of regulatory roles. Along with the fat mass and obesity-associated protein (FTO), ALKBH5 is one of only two identified human m^6A RNA oxidising enzymes and is a potential target for cancer treatment. Unlike FTO, which produces a mixture of products including the N^6-hydroxymethyladenosine (hm^6A) hemiaminal species, ALKBH5 efficiently catalyses fragmentation of its proposed nascent hemiaminal intermediate to give formaldehyde and a demethylated nucleoside. A detailed analysis of the molecular mechanisms used by ALKBH5 for substrate recognition and m^6A demethylation is lacking. We reported three crystal structures of ALKBH5 in complex with an m^6A-ssRNA 8-mer substrate and supporting biochemical analyses. These results provided insights into the catalytic mechanisms of ALKBH5, which is different from that of FTO.

KEYNOTE SPEAKER

Prof. Dr. Jalel Labidi

ADVANCES IN LIGNOCELLULOSIC BIOREFINERIES

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Lignocellulosic biomass, abundant in nature, plays a pivotal role in the transition to a green economy by serving as a valuable source of energy, chemicals, intermediates, and commodities. However, realizing its full potential requires fractionation to separate its primary components—cellulose, lignin, and hemicellulose—using a biorefinery approach. While the biorefinery approach shares similarities with fossil oil refineries, the complexity and heterogeneity of biomass present unique challenges. This complexity demands intricate processes involving multiple transformations and separation steps. The adoption of biorefineries raises concerns regarding product sustainability and cost competitiveness when compared to conventional fossil-derived counterparts. Effective fractionation and conversion of biomass into desired products are crucial prerequisites for addressing these concerns. This presentation highlights recent advancements in biomass fractionation and conversion through biorefinery processes, emphasizing efficient feedstock utilization, adherence to green chemistry principles, and minimization of energy and water consumption.

INVITED SPEAKERS

INTERNATIONAL CONFERENCE OF YOUNG CHEMISTS

INVITED SPEAKER

Dr. Kavirajaa Pandian Sambasevam

ELECTROPOLYMERIZATION OF POLYANILINE: A VERSATILE APPROACH FOR RAPID DEPLOYMENT OF SENSORS IN FOOD AND ENVIRONMENTAL POLLUTANT MONITORING

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The utilization of conducting polymers in sensor applications has garnered significant attention due to their versatility and potential for various sensing functionalities. Among these, polyaniline stands out, often synthesized through chemical oxidative methods or electropolymerization techniques. Electropolymerization offers distinct advantages, particularly in producing uniform coatings of conducting polyaniline, facilitating its seamless integration into sensing devices for environmental monitoring. This study focuses on the electropolymerization of polyaniline-chitosan composites onto screen-printed electrodes, aiming to monitor environmental and food pollutants such as 3 MCPD and TBBPA. The facile electropolymerization process yields PANI-CHT coatings suitable for immediate deployment by regulatory authorities, streamlining monitoring efforts. Notably, 3-MCPD contamination poses a significant challenge to the vegetable oil industry, particularly affecting Malaysia's prominent oil palm commodity. In response, molecularly imprinted polymer (MIP) sensors tailored for 3-MCPD detection were developed and optimized using Response Surface Methodology (RSM), effectively reducing elution times, thus enhancing practical applicability. Furthermore, TBBPA detection was addressed through the development of electropolymerized PANI-CHT sensors, optimizing detection parameters via RSM analysis. This multifaceted approach underscores the versatility and efficacy of electropolymerization in sensor fabrication. Compared to traditional bulk synthesis methods, electropolymerization offers several advantages. Firstly, it enables precise control over film thickness and morphology, ensuring uniformity critical for sensor performance. Additionally, it allows for facile integration with microfabrication techniques, enhancing scalability and miniaturization potential. Moreover, electropolymerization offers tunable properties through parameter adjustments, enabling tailored sensor designs for specific applications. These benefits collectively underscore the superiority of electropolymerization over conventional synthesis routes, positioning it as a preferred method for conducting polymer sensor fabrication in diverse sensing environments.

Keywords: polyaniline, 3-MCPD, cypermethrin, chitosan, RSM

Research area: *Analytical Chemistry*

INVITED SPEAKER

Assoc. Prof. Dr. Muggundha Raoov

ADVANCED MICROEXTRACTION METHODS FOR POLYCYCLIC AROMATIC HYDROCARBONS IN FOOD USING MAGNETIC NANOPARTICLE-IONIC LIQUID TECHNOLOGY

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Food contamination, particularly by polycyclic aromatic hydrocarbons (PAHs), presents a significant global health concern. This study involves advanced magnetic nanoparticles as a sorbent material for extracting PAHs in food samples. The first study introduces Poly(B-Cyclodextrin functionalized Ionic Liquid) coated magnetic nanoparticles (poly(βCD-IL)@Fe_3O_4) for magnetic micro solid phase extraction (µ-SPE) of low and high molecular weight PAHs in rice. The poly(βCD-IL)@Fe_3O_4 was thoroughly characterized and applied successfully in µ-SPE coupled with gas chromatographic-flame ionization detection (GC-FID). The method demonstrated excellent linearity (0.1-500 $\mu g\ kg^{-1}$), low detection limits (0.01–0.18 $\mu g\ kg^{-1}$), and satisfactory precision and reproducibility. Real sample analysis of commercial rice in Malaysia confirmed the method's effectiveness in ensuring food safety. Additionally, the nanoparticles were further utilized in ferrofluid-based dispersive liquid-phase microextraction (FF-DLPME) for PAH extraction from various food and beverage samples, showing promising results. In the second study, Poly(methyl methacrylate-vinyl imidazole bromide) coated with magnetic nanoparticles (poly-(MMA-MNP-IL)) was synthesized and employed in magnetic µ-SPE for the determination of 16 types of PAHs in fried food, grilled food, and tea samples as an improvement to the previous works. Extensive characterization confirmed the nanoparticles' suitability for µ-SPE. The method was optimized using Response Surface Methodology (RSM) and demonstrated good linearity (0.2 $\mu g\ L^{-1}$- 500 $\mu g\ L^{-1}$ for water, 0.5-1000 $\mu g\ kg^{-1}$ for fried and grilled food, and 0.5-1000 $\mu g\ L^{-1}$ for tea samples), low detection limits, and acceptable precision and recovery values. Real sample analysis of various commercial foods in Malaysia validated the method's efficacy in ensuring food safety. Both studies contribute to advancing analytical techniques for PAH analysis in food samples, offering sensitive, efficient, and reliable methods for monitoring and ensuring food safety on a global scale. The innovative use of nanomaterials in magnetic µ-SPE techniques holds promise for enhancing food safety regulations and protecting public health.

Keywords: Polycyclic aromatic hydrocarbons, ionic liquid, sample preparation method

Research area: *Analytical Chemistry*

INVITED SPEAKER

Asst. Prof. Dr. Subhan Salaeh

NEW CROSSLINKING ROUTES OF RUBBER VULCANIZATES FOR SMART AND SUSTAINABLE MATERIALS

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The high elasticity of rubber makes it a versatile material for applications like tires, seals, damping, and even aerospace. However, traditional vulcanization methods using sulfur or peroxides pose limitations for the development of advanced and environmentally friendly rubber with tailored properties. This highlights the crucial role of cross-linking in rubber elasticity, achieved through a network structure. Recent advancements in dynamic covalent and non-covalent interactions offer a promising solution for thermoset recycling and addressing plastic pollution. These approaches exploit the inherent reversibility of the bonds during reprocessing, enabled by dynamic exchange reactions and thermos-responsive characteristics. Vitrimer chemistry utilizes dynamic covalent bonds to transform permanent covalent networks into reversible, adaptable ones. This enables polymer recycling and reprocessing while preserving their initial properties over multiple cycles. A common approach to enhance damping in carboxylic rubbers involves the use of metallic oxides to create ionic crosslinks. This reaction forms a distinct microphase of ionic bonds within the elastomeric matrix. These ionic aggregates, acting as both a reinforcing agent and a physical crosslink network, improve mechanical properties and introduce shape memory functionality. Additionally, the unique thermal transition associated with these ionic domains allows for precise control over the shape memory effect.

Keywords: Cross-linking, rubber vulcanizates, dynamic bonds, sustainability, smart rubber

Research area: *Organic Chemistry*

ORAL : ORGANIC CHEMISTRY

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EVALUATION OF 2-(1H-1,2,3-TRIAZOL-1-YL)ACETIC ACID DERIVATIVES AS POTENTIAL HUMAN HYPOXIA INDUCIBLE FACTOR (HIF) PROLYL HYDROXYLASE DOMAIN-2 (PHD2) INHIBITORS

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The hypoxia-inducible factor (HIF) prolyl hydroxylase domain (PHD) inhibitors have potential for treating ischemic and hypoxic-related diseases, as demonstrated by their use in anemia treatment. Docking studies showed that 2-(1H-1,2,3-triazol-1-yl)acetic acid (TA) derivatives could bind to the PHD2 active site iron in a bidentate manner and form hydrogen bond interactions with Arg 383. Molecular dynamic simulation analysis revealed that derivative **14** exhibits stable dynamic features, with some flexible regions stabilized upon binding to PHD2, similarly but not identically to the positive control inhibitor bicyclic isoquinoline (BIQ). The total binding energies were calculated to be -42.90 kcal/mol and -36.08 kcal/mol for BIQ-PHD2 and **14**-PHD2, respectively, indicating that the binding affinity of **14** is comparable to BIQ. The TA derivatives were synthesized using copper(I)-catalyzed azide–alkyne cycloaddition, and their PHD2 inhibition was evaluated using an AlphaScreen assay. Most of the derivatives were not inhibitors, but one (**14**) demonstrated weak inhibition at 100 µM (>50%). In conclusion, although most TA derivatives did not exhibit strong inhibitory activity against PHD2, structural modifications of **14** may lead to the development of a potent PHD2 inhibitor.

Keywords: Hypoxia-inducible factor, HIF, prolyl hydroxylase domain, PHD inhibitors, 1,2,3-triazole.

Research area: *Organic Chemistry, Computational chemistry*

ISOLATION, *IN-VITRO* CYTOTOXICITY AND MOLECULAR DOCKING OF POLYMETHOXYFLAVONES FROM *KAEMPFERIA PARVIFLORA* ON BREAST CANCER CELL LINES

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Polymethoxyflavones (PMF) are a secondary metabolite that offers various health benefits, including potential application in cancer treatment, particularly breast cancer. PMF are abundant in *Kaempferia parviflora* (*K. parviflora*), an herbaceous plant species native to Thailand characterized by distinct methoxylated and hydroxylated positions. Given the rising incidence of breast cancer particularly in Asia, exploring the therapeutic potential of PMF from *K. parviflora* is crucial for drug discovery. In this study, we screened the cytotoxic activity of PMF isolated from *K. parviflora* on breast cancer cell lines and conducted a structural activity relationship (SAR) analysis based on cytotoxic activity and molecular docking. PMF was isolated from ethanolic extract of *K. parviflora* using fractionation and gravitational column chromatography, followed by structural characterization with ^{1}H-NMR and ^{13}C-NMR. The PMF were screened against hormone-dependent breast cancer cell lines MCF-7, triple-negative MDA-MB-231, and NIH/3T3 mouse fibroblast cells using 3-(4,5-Dimethylthiazol-2-yl)-2,5-Diphenyltetrazolium Bromide (MTT) colorimetric assay for 24- and 48-h. Nine PMF were successfully isolated from *K. Parviflora*, with 5-hydroxy-3,7-dimethoxyflavone (PMF 1) as a major compound. A concentration- and time-dependent decrease in cell viability was observed, particularly with PMF 8 and 9. At the highest concentration (100 µM), PMF 8, identified as 5,7-dimethoxyflavone was the most potent reducing MCF-7 cell viability to 43.85% and 30.05% in 24- and 48-h, respectively, while maintaining over 75% viability in NIH/3T3 cells at 48h. PMF 1 to 7 demonstrated moderate to low cytotoxic effects on both cancer cell lines and mouse fibroblast cells. Molecular docking analysis revealed strong binding energies of PMF 8 with the apoptotic markers BCL-xL (-8.7 kcal/mol) and BCL-2 (-7.2 kcal/mol), suggesting that the hydrophobic effect of the methoxy group on ring A of flavones is a key marker in inducing apoptotic cell death. This research was supported by the Ministry of Higher Education, Fundamental Research Grant Scheme, FRGS/1/2021/SKK0/MSU/02/1.

Keywords: *Kaempferia parviflora*, isolation, polymethoxyflavones, breast cancer, molecular docking

Research area: *Organic Chemistry*

SYNTHESIS OF CHITOSAN-ALGINATE-MONTMORILLONITE HYDROGEL MICRO COMPOSITE FOR PARACETAMOL ADSORPTION IN AQUEOUS SOLUTIONS

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In this study, chitosan beads incorporated alginate and montmorillonite were prepared and employed for paracetamol adsorption from an aqueous solution. The materials were characterized by Fourier transform infrared spectroscopy, Scanning Electron Microscopy, X-Ray Diffraction, DTA-TGA, and Particle Size Analysis. Optimization studies revealed that the highest adsorption capacities were obtained at pH 5 with 60 minutes of contact time, and paracetamol concentration of 80 mg l^{-1}. The adsorption capacity reached 36,62 mg g^{-1} with the adsorption efficiency of paracetamol being 85,60%. The micro composite beads with alginate and montmorillonite proved to be better adsorbents than those without alginate and clay minerals. Both chitosan-alginate-montmorillonite adsorbents and pure chitosan adsorbents fit the Langmuir model and followed the pseudo-second-order kinetic model. The micro composite demonstrated higher efficiency of paracetamol removal and increased stability than pure chitosan beads. They can be promising candidates for paracetamol removal from aqueous solution.

Keywords: Chitosan 1, alginate 2, montmorillonite 3, paracetamol 4

Research area: *Organic Chemistry*

EVALUATING ANTIMALARIAL PROPERTIES VIA CHEMICAL MODIFICATION OF FURAN-BASED CHALCONES: INSIGHTS FROM BIOLOGICAL ACTIVITY, DFT CALCULATIONS, MOLECULAR DOCKING, AND ADMET STUDY

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Malaria remains endemic in tropical regions, with *Plasmodium falciparum* being the most prevalent and deadly species. Control efforts are hindered by increasing drug resistance, particularly to chloroquine. Chalcones have shown significant antimalarial potential, enhanced by structural modifications. This study synthesizes furan bioisosteric chalcone derivatives with methoxybenzene and furan moieties, evaluating their efficacy against *P. falciparum* FCR3 strains. Chalcones were synthesized via a condensation reaction using 2-acetylfuran or furfuraldehyde with dimethoxy counterparts in base conditions at room temperature, yielding 73-81%. Among the six (6) chalcones tested, compounds using 2-acetylfuran (compounds **2** and **3**) exhibited superior antimalarial activity (1.51 μM and 1.04 μM, respectively) compared to those using furfuraldehyde (compound **6**, 6.28 μM). The DFT study elucidated structural information utilizing diverse chemical descriptors and molecular electronic potential maps. Molecular docking at the P*f*DHFR-TS active site highlighted interactions with the Asn108 residue through hydrogen bonding, suggesting potential as an antimalarial agent similar to chloroquine. Evaluation of drug-likeness based on Lipinski's and Veber's rules, coupled with ADMET studies, shows their promise as oral drugs. Hence, furan-chalcones derived from 2-acetylfuran exhibit encouraging selective antimalarial activity and deserve further investigation.

Keywords: chalcone, furan, antimalaria, *P.falciparum*, FCR3, P*f*DHFR-TS.

Research area: *Organic Chemistry*

TMPTA CROSSLINKER UV-GRAFTED BPADA-BAPP POLYIMIDE THIN FILMS: THERMOS-CHEMICAL STABILITY AND STRUCTURAL CHARACTERIZATION

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Polyimide is widely used as a membrane construction material in gas separation, fuel cell, and desalination applications. Nevertheless, excessive crosslinking in polyimide can lead to brittleness, compromising its performance. Hence, this study focuses on the thermos-chemical stability properties of TMPTA grafted BPADA-BAPP polyimide thin film, prepared from BPADA and BAPP monomer via conventional two step method, followed by UV-crosslinked by UV irradiation using 2,4,6-trimethylbenzoyl-diphenyl-phosphine oxide (TPO) as photo-initiator and trimethylolpropane tri-acrylate (TMPTA) as crosslinker. The structural characterization of TMPTA grafted BPADA-BAPP polyimide by Fourier Transform Infra-Red (FT-IR) showed the presence of TMPTA crosslinker at 1725cm^{-1} (C=O) and a slight decrease in intensity at 1635cm^{-1} (C=C), suggesting successful grafting of TMPTA. Furthermore, the ^{1}H NMR signals at regions around 4.1 ppm. and 5.5-6.5 ppm indicated that the BPADA-BAPP PI backbone was grafted with TMPTA. Thermogravimetric Analysis (TGA) showed no significant changes in thermal degradation temperature (T_{max}) (177.09 ˚C, 479.40 ˚C, 179.62 ˚C, 480.26 ˚C) as the exposure time increases (0.5 min, 5 min, 15 min & 30 min) but the decrement can be seen in glass transition temperature (Tg) (218, 178, 173, 164, 170 ˚C). The TMPTA grafted BPADA-BAPP PI series demonstrated high chemical stability, being insoluble in strongly acidic (HCl, H_2SO_4), polar aprotic (Acetone, DMSO), polar protic (Distilled water, Methanol) and non-aprotic (Hexane) solvent respectively. Moreover, water uptake percentage showed decrement in values (4.75%, 3.17%, 3.88%, 1.60%) with the increment of exposure time in UV-irradiation. These findings suggested that TMPTA had been grafted to the BPADA-BAPP PI backbone along with the enhancement of thermos-chemical stability while maintaining its flexibility.

Keywords: Crosslinker, grafted polyimide, thermal stability, chemical stability, TMPTA grafted BPADA-BAPP PI

Research Area: *Organic Chemistry*

UTILIZATION OF POLY(GLYCIDYL METHACRYLATE-CO- BUTYL ACRYLATE) REACTIVE DILUTES TO IMPROVE THE PROPERTIES OF EPOXY RESIN AS ANTICORROSION COATING

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Anticorrosion coatings protect metal surfaces from environmental factors including moisture, oxygen, and gases that caused corrosion to the metal. Various types of anticorrosion coatings are available, with different properties and application methods. Many researchers have been developing methods to prevent corrosion, and epoxy polymers are one of the wide methods due to their excellent adhesion, chemical resistance, and durability. In this study, synthesis reactive dilute based on glycidyl methacrylate (GMA) with butyl acrylate (BuA) to improve the performance of epoxy resin and anticorrosion coating. The copolymers were synthesized with composition 30/70, 50/50, 70/30 (w/w) ratio by bulk polymerization technique using benzoyl peroxide as a catalyst and 1-dodecanthiol as a chain transfer aging at the temperature of 90◦C for 2 hours and at 120◦C for 30 minutes to complete the polymerization process. The obtained copolymers were characterized by FTIR, viscosity and thixotropic index. The effect of copolymers as reactive dilute on the physical and mechanical properties of epoxy resin was investigated. Metal plates coated by the modified epoxy resins with different contents of copolymers were tested using alkali and salt test methods, and the copolymer based on GMA and BuA in the 50/50 (w/w) ratio showed the best protection efficiency due to the barrier effect of the polymer layer.

Keywords: Epoxy, Coating, Dilute, Corrosion, Reactive

***Research area:** Chemical Engineering, polymeric materials*

ACID-ACTIVATED NATURAL ZEOLITE CLINOPTILOLITE FUNCTIONALIZED WITH CURCUMIN FOR SUPERIOR METHYLENE BLUE ADSORPTION: INSIGHTS INTO OPTIMIZATION, CHARACTERIZATION, AND ADSORPTION MECHANISMS

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This study investigates the treatment of natural zeolite clinoptilolite (NZC) through acid and base pretreatments, aiming to enhance its adsorption efficiency for methylene blue (MB) dye removal. The results indicate that NZC treated with 3.0M HCl (hydrochloric acid) exhibits superior MB removal efficiency (93.24%) compared to 1.0M NaOH (sodium hydroxide)-treated NZC (91.40%), accompanied by a higher Brunauer–Emmett–Teller (BET) surface area (135.5002 m²/g) in contrast to (43.6059 m²/g). The optimized 3.0M HCl-treated NZC is further functionalized with curcumin, resulting in CUR-HCl-NZC, which demonstrates enhanced MB removal efficiencies of 95.09% at 45 minutes and 83.81% at 90 minutes, surpassing untreated NZC. The adsorption parameters, including concentrations of acid and base pretreatment, contact time, adsorbent dosage, and initial dye concentration, are systematically varied to optimize the conditions for CUR-HCl-NZC. Characterization through Fourier-transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and BET analysis confirms the successful binding of curcumin to HCl-treated NZC, revealing structural and surface modifications. The isotherm analysis identifies the Langmuir isotherm model as the best fit, suggesting monolayer adsorption dominance. This study establishes CUR-HCl-NZC as an effective, low-cost adsorbent for the removal of MB, offering a promising solution for water purification applications.

Keywords: Natural zeolite clinoptilolite; acid-base pretreatments; methylene blue adsorption; curcumin functionalization; water purification

EFFECT OF SOLVENT POLARITY ON SIDE-CHAIN REARRANGEMENT IN BROMINATION OF METHYLEUGENOL WITH MOLECULAR BROMINE

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When activated allylbenzenes such as estragole and safrole are treated with equimolar Br_2, they produce 1,3-dibromopropyl derivatives. Methyleugenol, a more active allylbenzene, is likely to undergo a similar side-chain rearrangement when brominated. The rearranged dibromide product of methyleugenol, namely 4-(1,3-dibromopropan-2-yl)-1,2-dimethoxybenzene (hereafter referred to as **A**) is required as a precursor in our synthetic approach to alpha-alkylstyrene (AAS) derivatives. Therefore, we investigated the bromination of methyleugenol with Br_2 at room temperature in eleven solvents with varying polarity to determine the best solvent for generating **A**. Methyleugenol was no longer detectable after adding 1.13 equivalents Br_2 in chloroform. **A** was the main product, with a lesser amount of the unrearranged dibromide, 4-(2,3-dibromopropyl)-1,2-dimethoxybenzene (hereafter referred to as **B**). The same amount of Br_2 was then utilized for bromination in ten additional solvents. Product **A** also dominated **B** in ethyl acetate ($\varepsilon = 6.02$), which is more polar than chloroform ($\varepsilon = 4.80$), but product **B** became dominant when the solvent polarity further increased in dichloromethane ($\varepsilon = 8.93$). **A** was the only product resulted in diethyl ether ($\varepsilon = 4.33$), a more nonpolar solvent than chloroform. In more nonpolar solvents such as diisopropyl ether, carbon tetrachloride, and *n*-hexane, while product **A** was still dominant, the yield reduced significantly. The reactions in tetrahydrofuran and methanol produced some byproducts, whereas in acetone neither **A** nor **B** was produced. Based on these findings, diethyl ether is the most effective solvent for producing **A** from methyleugenol and Br_2. Nonpolar solvents facilitate side-chain rearrangement while polar solvents prevent it. In subsequent experiments, we shall employ greater equivalents of Br_2 in diethyl ether, to consume the reactant that still remains after using 1.13 equivalents of Br_2.

Keywords: allylbenzene; bromination; eugenol; methyleugenol; rearrangement

Research area: *Organic Chemistry*

SYNTHESIS, MOLECULAR DOCKING AND QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP ANALYSIS OF BIOACTIVE 2*O*-ALKYLATED BENZOFUROPYRIDINES

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Heteroaromatic systems of small molecules have long been known for its wide application in drug discovery. Benzofuropyridines (BFP) are polycyclic compounds with known applications in neuronal diseases. However, its derivatization patterns and anticancer potential remains unexplored. We developed a highly efficient synthetic route for BFP to increase the library of available analogs producing diverse derivatives by alkylating the 2*O*-position of the BFP. The breadth of the anticancer activity of the compounds was assessed against SH-SY5Y (neuroblastoma), HepG2 (hepatocellular carcinoma), Kb (human oral epidermoid), HeLa (cervical) and MCF-7 (breast) cancer cell lines. The assay revealed the potent bioactivity of the BFP with the *m*-methoxybenzyl (**5c**) 2*O*-alkylated derivative having 14 µM and 10 µM IC_{50} against Kb and HeLa cells, respectively. In the series, the *m*-bromobenzyl (**5b**), methylcyano (**5g**) and propargyl (**5h**) 2*O*-derivatives demonstrated excellent selectivity towards cancer cells with selectivity index (SI) of >71 for **5g** against HeLa over the normal cells, as compared to the standard drug, Doxorubicin (SI = 6.7). To suggest a plausible inhibition target, molecular docking study was performed against CDK-5 kinase enzyme, and the results revealed an improvement in binding energy for all derivatized compounds with top value of -9.45 kcal/mol as compared to -7.69 kcal/mol for the underivatized BFP compound **3**. The quantitative structure-activity relationship (QSAR) analysis showed an impressive correlation of the identified descriptors with the actual bioactivity having an R^2 value of 0.971 and 0.893 for Kb and HeLa, respectively. Overall, this work highlighted the potential of the BFP moiety as an anticancer regimen while revealing key information on the future rational design of more potent analogs using computational tools.

Keywords: Benzofuropyridines; Cancer; Molecular Docking; QSAR analysis

Research area: *Organic Chemistry*

MESOMORPHISM AND PHOTOISOMERIZATION OF NON-LINEAR DISULPHIDE-CENTERED S-SHAPED OLIGOMERS ARMED WITH AROMATIC AZO MOIETIES

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The synthesis and characterization of a series of non-linear S-shaped liquid crystalline oligomers, [*bis*-*n*-(2-(6-(4-{4-acetylphenylazo}phenoxy)hexyloxy)phenoxy)alkyl]disulphide containing aromatic azo moieties are reported. In this series, the length of the two outer alkyl spacers is retained at six methylene units while the length of the inner alkyl spacer, *n*, varies from six to eleven methylene units. The structural elucidation of the oligomers is confirmed using spectroscopic methods such as CHN, FT-IR and NMR (^{1}H, ^{13}C). The series of oligomers exhibit a uniform orange colour with increasing melting points as the series ascends. UV-vis is employed to confirm the presence of azo moiety and to study the photoisomerization properties of the oligomers. In texture optical analysis by POM, all oligomers exhibit monotropic nematic phase upon cooling. In the thermal study by DSC, the odd-even effect is verified at the Cr-I and I-N transition temperatures, as well as entropy change associated with the I-N transition. It is observed that oligomers with odd-numbered inner alkyl spacers display higher transition temperatures compared to their even-membered analogous compounds. Meanwhile, oligomers with even-numbered inner alkyl spacers show higher average entropy change values than the odd-numbered analogous compounds. In the photoisomerization study, the oligomers demonstrate a long duration of thermal back relaxation, indicating their potential use in the optical storage devices. A molecular modeling study is conducted to further understand the structure-property relationship.

Keywords: Non-linear, central disulphide, liquid crystal, photoisomerization, molecular model study.

Research area: *Organic Chemistry*

ANTIINFLAMMATORY ACTIVITY OF BIFLAVONOID FROM GENUS *Araucaria*: IN VITRO AND IN SILICO APPROACH

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The research focused on the potential of biflavonoids from the genus *Araucaria* as anti-inflammatory agents by inhibiting the phosphodiesterase 4 (PDE4) enzyme. PDE4 is a promising drug target for treating inflammatory conditions. The study investigated twenty-six biflavonoid compounds from the genus *Araucaria*, including six biflavonoids isolated from *A. hunsteini* and *A. cunninghamii* derived from Bogor Botanical Garden, Indonesia, as PDE4B and PDE4D inhibitors using in silico and in vitro methods. The six biflavonoids were tested in vitro on MCF-7 breast cancer cells to measure their anti-inflammatory activity against the PDE4B enzyme and PDE4B with the ELISA technique. Ochnaflavone and 7,7″-di-*O*-methylamentoflavone showed the highest affinity and selectivity for PDE4B over PDE4D based on in silico analysis. Additionally, in vitro results showed that 7,7″-di-*O*-methylamentoflavone and 7,4‴-di-*O*-methylcupressuflavone showed inhibitory activities against PDE4B with IC_{50} values 10.65 ± 2.28 and 58.31 ± 2.29 µM, and against PDE4D with IC_{50} values 12.69 ± 5.82 and 105.15 ± 41.79 µM, respectively. Therefore, the study concludes that biflavonoids are prospective PDE4 inhibitor agents and should be considered when developing candidates for new anti-inflammatory medicines.

Keywords: Biflavonoid, *Araucaria*, Antiinflammatory, In Vitro, In Silico.

Research area: *Organic Chemistry*

CHEMICAL TREATMENT OF FLAX FIBERES MATERIALS FOR BIOCOMPOSITES APPLICATIONS

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Flax is a renewable and natural resource, degradable and having has a very positive environmental assessment, compared to synthetic fibres. Indeed, among all plant fibres, flax fibre exhibits a high potential as composite material reinforcement: low density, damping properties higher than carbon and glass fibres, and stiffness close to the glass. Unfortunately, depending on the applications that are being targeted, the hydrophilic nature of plant fibres can hamper the final properties of the materials. The work presented here therefore deals with eco-friendly chemical methods available to allow modification of the flax fiber and/or flax biocomposites in order to make them less sensitive to ambient humidity variations and, if possible, fire-resistant. Studies were led on several types of samples: epoxy flax composites, flax fabrics, combed and non-combed flax fibers. First, samples were processed using organosilane reagents, a class of chemical compounds that has have been previously used for similar purposes.[1,2] Organosilanes are indeed capable of establishing covalent bonds with the natural fibers taking advantage of the large amounts of -OH groups available. Silanes such as APTMS, GPTMS, VTMS, showing aminopropyl, glycidyloxypropyl and vinyl functional groups, respectively, have been used at various concentrations (1, 5, 9, 13 wt%). Then another method combining both water-repellence and flame-retardancy, has also been assessed, based on previous results obtained in our group.[3] This treatment involves the phosphorylation of lignocellulosic fibers by an aqueous mixture of phytic acid and urea, which are both biobased chemicals. Properties of the resulting treated fibers/materials were evaluated, among others, by IR spectroscopy, AFM, SEM and contact angle measurements. Mechanical performances, such as tensile strength and Young's modulus, were also assessed for the different kinds of treated materials. Our work is therefore primarily dealing with the optimization of biocomposites, in terms of sustainability, and mechanical performances under various storage or use conditions, while trying to reach a maximum amount of plant fibers within the polymeric materials that are being studied.

ORAL : PHYSICAL CHEMISTRY

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OPTIMIZING CURING DURATION OF SELF-HEALING CHITOSAN/POLYACRYLAMIDE HYDROGEL COATING ON POLYETHERSULFONE MEMBRANE FOR ENHANCED STABILITY AND FITLRATION EFFICIENCY

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Membrane filtration is a well-established technology extensively employed in diverse industries especially in wastewater treatment plants. However, maintaining membrane integrity remains a crucial challenge in filtration system. Damage to filtration membrane during installation and backwashing can significantly affect the separation efficiency, deteriorate permeate quality and reduce membrane lifespan. A membrane with self-healing ability has been introduced to address this challenge. Herein, a self-healable chitosan/polyacrylamide (CS/PAM) hydrogel is coated onto polyethersulfone (PES) membrane to restore the membrane separation performance. Upon physical damage, the membrane exhibits water-responsive in-situ self-healing ability, restoring its properties when flushed with water. The CS/PAM hydrogel absorbs water and swells, facilitating the connection of the fracture interface and the formation of reversible hydrogen bonding between amide group in PAM and hydroxyl group in CS. In this context, the stability of polymer chain is vital to prevent flux reduction after healing. The CS/PAM hydrogel further entangles and crosslinks throughout the preparation, filtration and healing process due to instability of the polymer chain. This study investigated the curing condition of the coated CS/PAM hydrogel on the PES membrane to ensure a more stable polymer network, avoiding detachment of the coating and over-healing condition. The effect of curing duration was assessed by measuring the pure water flux of pristine, damaged and healed membrane to ensure complete crosslinking between polymers. The CS/PAM-coated PES membrane with a one hour curing duration exhibited instability in permeation flux. With an incomplete crosslinking process, the flux after healing had appeared to be lower than the flux before damage as the polymer network continued to entangle throughout filtration process. Conversely, for curing duration more than two hours, the flux of membranes after healing was found to be higher than the flux of pristine membranes as further crosslinking of polymers was prevented due to the sufficient curing duration.

Keywords: Self-healing Coating; Curing Duration; Stability; Polymeric Membrane; Filtration

Research area: *Physical Chemistry*

ENHANCING PLASTIC PYROLYSIS: PREDICTIVE ANALYSIS INTEGRATED WITH MACHINE LEARNING

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The extensive use of plastic in daily life poses significant risks to the environment in recent years. Thus, transforming plastic waste into a valuable resource is essential to accomplish Sustainable Development Goals (SDGs) 11 (Sustainable Cities and Communities) and 12 (Responsible Consumption and Production). Pyrolysis process as an alternative solution is proposed for the conversion of plastic waste into products such as oils, gases, and chars. A search on the Scopus database yielded 28 studies since 2021 on plastic pyrolysis using machine learning (ML). This study highlights the application of ML techniques to enhance predictive modelling in plastic pyrolysis processes. Various ML methods such as regression, decision trees, artificial neural networks (ANN), support vector machines (SVM), Random Forest (RF), Gradient Boosting Regressor (GBR), eXtreme Gradient Boosting (XGBoost), AdaBoost, and Stochastic Gradient Descent (SGD) are reviewed in terms of their effectiveness in predicting pyrolysis outcomes, considering different feedstock types, dataset sizes, and input/output variables. The study also addresses current challenges and future prospects, focusing on refining ML models with larger datasets and optimizing pyrolysis conditions. In conclusion, integrating ML into plastic pyrolysis processes enhances both process efficiency and economic viability.

Keywords: Plastic Waste , pyrolysis, machine learning, optimization

UNLOCKING THE SYNTHESIS TUNING OF HYDROCHAR-BASED CATALYSTS FOR ENHANCED PEROXYMONOSULFATE ACTIVATION

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Conventional pyrolysis of biomass feedstock has garnered significant interest in the preparation of biochar-based catalysts for environmental remediation. However, this method typically produces lower yield, results in secondary char formation, necessitates high temperatures, and requires an inert atmosphere. In contrast, hydrothermal carbonization (HTC) has been proposed as an alternative method for synthesizing hydrochar-based catalysts aimed at removing emerging pollutants in wastewater treatment. A literature search across Google Scholar, ScienceDirect, Web of Science, PubMed, SpringerLink, and Scopus databases using the Preferred Reporting Items for Systematic Review and Meta-Analysis Protocols (PRISMA-P) from 2015 to 2025 identified fewer than 20 published papers on hydrochar-based catalysts used as peroxymonosulfate activators for environmental remediation. Despite possessing advantageous properties such as a higher heating value and abundant oxygen-containing functional groups compared to biochar-based catalysts, hydrochar-based catalysts suffer from drawbacks including lower resistance to oxidative environments, poor porosity, and a lower specific surface area, which have limited their popularity among researchers. Furthermore, due to variations in the polarity, aromaticity, hydrophobicity, and molecular structure of pollutants, a single type of hydrochar-based catalyst may not effectively remove all types of emerging pollutants. Therefore, tuning the synthesis conditions of hydrochar-based catalysts is pivotal to develop catalysts capable of enhancing peroxymonosulfate activation and efficiently removing a broad spectrum of emerging pollutants.

Keywords: Hydrochar-based catalysts, Peroxymonosulfate, Hydrothermal carbonization, Synthesis strategies, Environmental remediation

Research area: *Physical Chemistry*

DOPING TiO_2 WITH CU FROM ELECTROPLATING WASTEWATER FOR REMARKABLE IMPROVEMENT OF ITS ACTIVITY UNDER VISIBLE LIGHT FOR *E. COLI* BACTERIAL DISINFECTION IN WATER

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The use of electroplating wastewater as a source of Cu dopant to improve TiO_2 activity under visible irradiation for disinfection of *E.coli* bacterial in water is addressed in this research. Synthesis of the Cu-doped TiO_2 was conducted by using sol-gel method by interacting titania tetra isopropoxide and Cu(II) ion in the electroplating wastewater. In this step, the concentration of Cu(II) was varied to get TiO_2-Cu with Cu content alteration. The doped photocatalysts produced were characterized by operating X-ray diffraction (XRD), Fourier Transform infrared (FTIR), specular reflectance UV/visible (SR-UV/Visible) and scanning electron microscope (SEM) equipped with electron dispersed X-ray (EDX) machines. The effect of Cu doping on the TiO_2 activity under visible light was evaluated through disinfection of the total *E.coli* bacteria in water under visible light exposure. The results of the research assigned that doping Cu into TiO_2 has successfully narrowed the gap that shifted into visible regime, allowing TiO_2 to be more visible responsive. The reducing gap of the Cu doped TiO_2 was found to be controlled by Cu fraction, and the most effective decreasing was shown by 0.60% Cu (Eg =2.88 eV) from Eg = 3.20 eV belonged to the undoped TiO_2. In accordance with that gap or Eg value, TiO_2−Cu (0.60%) posed the best performance in the bacterial killing under visible light irradiation, that was 96.68% in 30 min, which was much higher compared to the un-doped TiO2, that was 38.42%. This discovery highlights that priceless electroplating wastewater is a valuable resource for elevating TiO_2 photocatalyst performance in the providing clean consumable water through a low cost operation.

Keywords: TiO_2, doping, Cu, electroplating wastewater, antibacterial

Research area: *Physical Chemistry*

INTEGRATED LIGAND AND STRUCTURE BASED APPROACHES FOR THE DESIGN OF NOVEL ANTAGONISTS OF ESTROGEN RECEPTOR ALPHA (ERα) FROM COLCHICINE AMIDES AND SULFONAMIDES

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The rising mortality and morbidity rates associated with breast carcinoma calls for global concern. This unpleasant situation is aggravated by the declining efficacies of existing drugs due to multi-drug resistance, high toxicities and poor pharmacokinetic profiles, necessitating the discovery of newer drugs. In search of potent and non-toxic drug candidates against breast carcinoma, a data set of colchicine amides and sulfonamides with established in vitro anti-proliferative activities against MCF-7 cell line was subjected to QSAR modelling. The validated tri-parametric model ($R^2_{train} = 0.989$, $R^2_{adj} = 0.986$, $Q^2_{CV} = 0.984$, $R^2_{test} = 0.664$) was used to optimize the potency of the most active member of the dataset selected as lead molecule (Tm) to form new analogues; DC-1, DC-2, and DC-3 having better potency than Tm and Tamoxifen (Ta), a standard anti-breast cancer drug used herein for comparison. Also, molecular docking simulation studies and molecular mechanics-generalized Born surface area (MM/GBSA) binding energy (ΔG_{bind}) calculations on the interactions of the ligands against the active sites of estrogen receptor alpha (ERα) supports the findings of the QSAR modelling as ΔG_{bind} values of -44.71, -44.14, and -47.67 kcal/mol were obtained for DC-1, DC-2, and DC-3, respectively, against the binding energies of -39.56 and -38.66 kcal/mol computed for Tm and Ta, respectively. The thermodynamic stabilities of complexes of the designed ligands with ERα were confirmed by coarse-grain based molecular dynamic simulations while their kinetic stabilities were affirmed by density functional theory B3LYP/6-31G* calculations. In addition, the new ligands were found to have comparable oral bioavailability potentials with Ta but with better pharmacokinetic and toxicity profiles. Hence, DC-1, DC-2, and DC-3 might be novel sources of potent and non-toxic ERα antagonists and as such could be subjected to further preclinical and clinical investigations.

Keywords: Colchicine, ERα, DFT, MMGBSA, breast carcinoma

Research area: *Physical Chemistry*

SYNTHESIS AND CHARACTERIZATION OF GRAPHENE OXIDE ZINC METAL-ORGANIC FRAMEWORK (bGO-ZnMOF) FOR THE REMOVAL OF BISPHENOL-A IN WASTEWATER VIA ADSORPTION PROCESS.

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Bisphenol A (BP_A) is widely used in the manufacturing of many current household products and plastic bottles. Human exposure to BP_A may take place mainly via food, but air, dust or water are also possible sources for BP_A exposure. BP_A is well-known to disrupt endocrine activities, especially in humans. It has been found to alter multiple oncogenic pathways and cause changes in both male and female human reproductive systems. It was also found to distort the function of a group of cells responsible for the reception and transmission of vital signals in human cerebrospinal activities. This presentation reports the synthesis of graphene oxide from oil palm empty fruit bunch and the fabrication of graphene oxide zinc metal-organic framework (bGO-ZnMOF) nanocomposite as adsorbent for the removal of BP_A from aqueous solution. The physicochemical properties of the nanocomposite were characterized using FTIR, XRD, TGA, SEM-EDX, and $pH_{PZC.}$ The effects of BP_A initial concentration, adsorbent dosage, contact time, pH of the solution, temperature and stirring speed on the removal efficiency were examined using UV-vis spectroscopy. Under optimum conditions of pH = 2, dosage = 20 mg, concentration = 60 mgL^{-1}, time = 30 min, temperature = 25 -30 ^{o}C, and stirring speed = 200 rpm, removal of up to 95% was achieved. The kinetic data was best described by the pseudo-second-order kinetics model ($R^2 = 0.9917$). The isotherm data fitted better with the Langmuir model with an R-square value of 0.9982 with a maximum adsorption capacity of 153.69 mgg^{-1}. Based on the thermodynamic properties obtained ($\Delta G < 0$, $\Delta H = +22.04 kJ\ mol^{-1}$ and $\Delta S = +80.07\ J\ mol^{-1}K^{-1}$) it is concluded that the adsorption of BP_A onto bGO-ZnMOF is a spontaneous and endothermic process, and the mechanism of the adsorption process was physisorption.

Keywords: Bisphenol-A, Biomass, Graphene Oxide, Metal-Organic-Framework.

Research area: *Physical Chemistry.*

REMARKABLE ENHANCED VISIBLE ACTIVITY OF TiO_2-N CO-DOPED WITH Cu FROM ELECTROPLATING WASTEWATER FOR DEGRADATION OF AMOXICILLIN RESIDUAL IN WATER MEDIA

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The development of photocatalysts together with wastewater management has drawn attention of many scientists, particularly in environmental chemistry field. This research investigates the enhancement activity of TiO_2 photocatalyst co-doped with N and Cu from urea and electroplating wastewater respectively as sources, for photodegradation of amoxicillin (AMX) residual in water media. The synthesis of co-doped TiO_2 photocatalyst has been done through sol-gel process with titanium tetraisopropoxide (TTIP) as TiO_2 precursor and determined the optimal concentration for each single dopant of Cu and N based on the the highest band gap energy (E_g) narrowing as well as their improving performance in photodegradation of AMX. The successful synthesis was also investigated by material characterization using XRD, FTIR, SEM-EDX, TEM, and DRUV-Visible spectrophotometer. The effect of the double dopants on the photocatalyst activity was examined through photodegradation of AMX with varying operational conditions (time, photocatalyst dose, solution pH). It can be inferred that both doping N and Cu into TiO_2 can considerably decrease the E_g level. The optimum N and Cu dopant concentrations were found to be 30%wt and 0.60%wt, giving E_g values of 2.88 eV and 2.93 eV with photodegradation percentages obtained as much as 64.50% and 68.50% respectively, while only 40% degradation over pristine TiO_2 with 3.20 eV E_g level. Furthermore, the co-doping Cu into TiO_2-N has significant reduction of E_g in 2.74 eV compared to the single-doped TiO_2 with AMX photodegration reaching 95.76%. It indicated that the co-doping TiO_2 photocatalyst agreed with the combination of interstitial and substitution mechanisms. This dwindling of band-gap energy in co-doping photocatalyst could be wider application in visible light exposure with an ideal condition for the photodegradation of AMX having 20 mg/L and 50 mL over TiO_2-N,Cu (30:0.6) is 1 g/L of the photocatalyst dose, solution pH 5, and 120 min of the irradiation time.

Keywords: TiO_2, co-doping, electroplating wastewater, sol-gel, amoxicillin

Research area: *Physical Chemistry*

ENHANCED PHOTODEGRADATION OF CEFTAZIDIME BY BIOBR(110)/BIOCL(110) COMPOSITE: ITS SYNTHESIS, MECHANISM, AND DEGRADATION PATHWAYS

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A simple and economical precipitation process was used to synthesize a heterojunction of BiOBr(110)/BiOCl(110) *in situ.* Numerous techniques, such as SEM, XRD, HRTEM, BET, FTIR, and XPS, confirmed the successful creation of the heterostructure. In this study, the heterostructures exhibited significantly enhanced photocatalytic degradation efficiency towards ceftazidime (CFZ). The degradation kinetic constant of CFZ by BiOBr(110)/BiOCl(110) (5:5) was three times higher than those of BiOBr and BiOCl. A type I heterojunction was also proposed following the UV-vis DRS and VB-XPS investigations. DFT calculations indicated that an internal electric field (IEF) was created when electrons (e^-) on the BiOBr surface were transferred to BiOCl in the dark. Upon visible light illuminated, photoinduced-e^- was transferred from the conduction band (CB) of BiOCl to that of BiOBr under the action of IEF. In contrast, holes (h^+) moved in the opposite direction, realizing the separation of e^-/h^+ pairs. Three degradation pathways were deduced based on intermediate products (IPs) detection by HPLC-MS. More importantly, the heterojunction catalyst exhibited efficient catalytic performance across solutions with different pH and maintained great reusability during four cycles of photodegradation. Overall, the work revealed distinctive insights concerning the mechanism of antibiotic degradation with BiOBr(110)/BiOCl(110) heterojunction structures.

Keywords: BiOBr(110)/BiOCl(110), Type I heterojunction, Photocatalysis, Ceftazidime degradation

Research area: *Physical Chemistry*

FABRICATION OF KOH IMPREGNATION POME SLUDGE BIOCHAR-BASED PHOTOCATALYST VIA HYDROTHERMAL SYNTHESIS FOR PHOTODEGRADATION OF CIPROFLOXACIN ANTIBIOTIC POLLUTANT UNDER SOLAR-SIMULATED VISIBLE LIGHT

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In the quest for an economical and eco-friendly solution for the effective degradation of ciprofloxacin (CIP) antibiotic pollutant, this study explores the utilisation of biochar (BC) derived from palm oil mill effluent sludge (POMES) to fabricate biochar-based BiOBr composites (BBC) via hydrothermal method. A series of BBC composites were synthesised and characterised by varying the BC to BiOBr mass ratio. The prepared BBC composites exhibited the features of a crystal plane that could be assigned to tetragonal BiOBr, as shown by XRD and supported by HR-TEM results. Additionally, BET surface area analysis demonstrated the porous nature of biochar, significantly enhancing the surface properties of BiOBr. This augmentation resulted in a notable reduction of BiOBr's band gap, as evidenced by UV-Vis DRS, and a decrease in the recombination rate of electron-hole pairs, as indicated by PL spectra. The synergistic effect between BC and pure BiOBr notably increased the degradation efficiency of CIP, with the BBC-1:1 composite displaying the highest efficiency of 97.49%, surpassing that of pure BiOBr under optimized conditions. Furthermore, the scavenging experiments confirmed the contribution of the active radicals h^+ and O_2^- as main photoactive species, while the $OH^{\cdot}$ effect remained negligible. The study delves into the photocatalytic degradation kinetic and BBC-1:1 composite rate was 2.75 times that of BiOBr. The regeneration test confirms the remarkable stability of the BBC composites, retaining an efficiency of 77% over seven cycles. These findings show the viability of the BBC composite as a scalable and environmentally benign photocatalyst, promising widespread practical applications.

Keywords: POMES, BiOBr, Ciprofloxacin, Photodegradation

Research area: *Physical Chemistry*

PREDICTIVE ANALYSES FOR THE DARK FERMENTATIVE HYDROGEN PRODUCTION FROM FOOD WASTE

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Dark fermentation is becoming more attractive as an environmentally friendly technology for generating hydrogen from renewable sources. This paper focused on the influences of household food waste and activated sludge ratios on hydrogen production at ambient temperature. It was found that the ratios of food waste and activated sludge influenced the hydrogen production yield. The highest hydrogen yield (45.26 mL/g.d VS) was achieved with a 1:1 ratio of food waste and activated sludge. The predictive analyses on hydrogen production from food waste were conducted using mixed-effects models. The finding of the present study reveals that household food waste has the potential to be used as a feedstock for hydrogen production.

Keywords: Food waste (FW), Bio-hydrogen, Activated sludge (AS), Dark fermentation

Research area: *Biochemistry*

CHARACTERIZATION OF FOOD FRESHNESS INDICATOR FROM GANYONG FLOUR MODIFIED WITH THE ADDITION OF NANOCELLULOSE FROM CORN HUSK AND CURCUMIN

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This research aimed to characterize food freshness indicator made from modified ganyong flour with the addition of Nanocellulose from corn husk and curcumin as bioindicator. This research was conducted at the Laboratory of Physical Chemistry, Faculty of Mathematics and Natural Sciences, IPB University, Bogor. The research started with the isolation of cellulose using microwave-assisted cellulose isolation (MAE). Food freshness indicators are produced by mixing ganyong starch, nanocellulose, glycerol, bioindicator and producing a product in the form of a biofilm. The biofilm characterized for mechanical (tensile strength and elongation), and physical properties such as thickness, density, moisture content, water vapor transmission rate (WVTR), and solubility. There were reducing moisture content, water vapor transmission rate, solubility, and elongation in physical and mechanical properties of biofilms. However, the tensile strength, density, and thickness were increased. The performance as food freshness indicator was evaluated from increasing of pH and total volatile base nitrogen values. The research results showed the food freshness indicator produced by modified ganyong flour with the addition of Nanocellulose from corn husk and curcumin as bioindicator is a promising innovation for food packaging technology and its application.

Keywords: food freshness indicator, ganyong starch, microwave-assisted extraction, nanocellulose

BIOSORPTION OF Cu(ll) ONTO DRIED ACTIVATED SLUDGE: EQUILIBRIUM AND KINETIC STUDEIS

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This study investigates the biosorption capabilities of dried activated sludge (DAS) of different sludge age for the removal of copper ions from aqueous solutions. The DAS used in this study was derived from a sequencing batch reactor, operated in time-sequenced steps including fill, react, settle, draw, and idle at a ratio of 2:12:2:2:6 for a cycle time of 24 hours. Factors affecting the Cu(II) removal efficiency, such as contact time (0-7 hours), initial concentration (10-100 mg/L), biosorbent dosage (1.25-10 g/L), and pH (2-5), were investigated. The results showed that the optimum adsorption time to achieve equilibrium was 2 hours. The adsorption capacity was significantly reduced when the pH was lower than 3. Both equilibrium and kinetic studies were conducted, with equilibrium data best fitted into the Langmuir isotherm model ($R^2 > 0.9949$), with the maximum monolayer adsorption capacities DAS-5 (40.3226 mg/g) > DAS-20 (37.0370 mg/g) > DAS-40 (24.2718 mg/g). The biosorption was found to follow pseudo-second-order ($R^2 > 0.9992$, $k_2 > 0.0193$ g/(mg·min)). From the Fourier Transform Infrared Spectrometer analyses, it was deduced that the biosorption of Cu(II) onto DAS involved various functional groups on the DAS, including hydroxyl (–OH), amino (–NH2), and carboxylic (–COOH). The results demonstrate that DAS is a cost-effective and environmentally sustainable biosorbent for copper ions.

Keywords: Dried Activated sludge; biosorption; heavy metal; copper.

Research area: *Physical Chemistry*

REMOVAL OF RHODAMINE B DYE UTILIZING GRAPHENE OXIDE-RUBBER BASED HYDROGEL AS AN ALTERNATIVE FOR WATER TREATMENT

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This study aims to synthesize and evaluate a hydrogel nanocomposite composed of liquid natural rubber/poly(acrylic acid)/reduced graphene oxide (LNR-g-AAc/rGO), with a specific focus on its effectiveness in adsorbing the dye rhodamine B (RhB). Copolymerization of acrylic acid (AAc) onto liquid natural rubber (LNR) was conducted to synthesize the LNR-g-AAc/rGO hydrogel using N,N-methylene-bis-acrylamide (MBA) and potassium persulfate (KPS) as cross-linker and initiator, respectively. Optimization of hydrogel synthesis parameters was performed to achieve maximum swelling capacity. Structural, thermal stability, and morphological characteristics of LNR-g-AAc and LNR-g-AAc/rGO were examined using Fourier transform infrared (FT-IR), X-ray diffraction analysis (XRD), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM). The LNR-g-AAc hydrogel, enhanced with incorporated reduced graphene oxide, exhibited significant adsorption efficiency. The addition of rGO improved the mechanical strength of the hydrogel, allowing the LNR-g-AAc/rGO hydrogel to maintain dye adsorption-desorption processes for up to 11 cycles with an 86% adsorption rate. In contrast, the LNR-g-AAc hydrogel achieved only 55% adsorption over 4 cycles. We suggest the use of LNR-g-AAc/rGO as a sustainable and easily recyclable material with remarkable adsorption capabilities suitable for dye removal applications.

Keywords: Reduced graphene oxide, hydrogel composite, dye adsorption, reusability

Research Area: *Physical Chemistry*

NITROGEN-DOPED POROUS CARBON (NDPC) SORBENTS FROM BIOMASS FOR CARBON DIOXIDE CAPTURE

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In response to the escalating environmental crisis caused by climate change and the increasing concentration of carbon dioxide (CO_2), researchers are actively seeking solutions to mitigate this issue. One prevalent method for removing CO_2 is adsorption using solid adsorbents, which offer high adsorption capacity, low corrosion, and easy regeneration. Among various solid adsorbents, porous carbon (PC) derived from biomass is considered an ideal choice for CO_2 capture due to its large surface area, good thermal and chemical stability, eco-friendliness, and low manufacturing costs. The addition of nitrogen-containing functional groups can further enhance CO_2 adsorption, as the physicochemical properties of PC play a crucial role in CO_2 uptake. This review aims to provide a comprehensive understanding of the production and performance of nitrogen-doped porous carbon (NDPC) derived from biomass for CO_2 adsorption. By consolidating key scientific findings from the published literature and offering critical commentary, the review seeks to shed light on the advancements and challenges in this field. It includes a thorough comparison of various types of nitrogen-doping in biomass-derived porous carbon, highlighting their effectiveness and differences. Additionally, the review explores the potential applications of NDPC, emphasizing its viability for large-scale commercial development as a low-cost, high-performance CO_2 adsorbent.

Keywords: Porous carbon, CO_2 capture, biomass, nitrogen functionalities, pyrolysis

Research area: *Physical Chemistry*

VIRTUAL SCREENING USING ENSEMBLE DOCKING APPROACHES FOR THE INHIBITION OF *Arcangelisia flava* COMPOUNDS TO JANUS KINASE-2 AND CYCLOOXYGENASE-2

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Arcangelisia flava is an herbal plant that has various bioactivities, such as anti-inflammatory. This study aimed to predict the compounds from this plant that have roles as anti-inflammatory and immunosuppressant agents through the inhibition to the activity of the enzymes for regulating the immune responses and cell inflammation, namely janus kinase-2 (JAK-2) and cyclooxygenase-2 (COX-2) *in silico*. The ensemble docking technique was conducted by tethering the compounds (ligands) to several different protein structures, then the binding information of the test ligands were compared to several commercial JAK2 and COX-2 inhibitors. The results indicated that the compounds from *A. flava*, namely pachybasin and talifendin, had a potency as JAK-2 inhibitors because they showed lower binding energy values than commercial inhibitors, such as baricitinib, ruxolitinib, and decernotinib. Meanwhile, for the COX-2 binding, both compounds showed allosteric binding to COX-2. These compounds also showed good results on ADMET predictions and had met Lipinski's rule. Therefore, pachybasin and talifendin have a potency as immunosuppressant agents.

Keywords: anti-inflammatory, *Arcangelisia flava*, ensemble docking, inhibition, immunosuppressant.

Research area: *Physical Chemistry*

ORAL : INORGANIC CHEMISTRY

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EFFECT OF TIN FILLER COMPOSITION ON POROSITY IN TIN-POLYDIMETHYLSILOXANE COMPOSITES

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A weak structure and high porosity in radiation shielding material led to radiation penetrating and dispersing, raising the risk of exposure for radiation workers, patients, and the public. Thus, this study is designed to observe and evaluate the morphology and structure of a composite material using Field Emission Scanning Electron Microscopy (FESEM) image analysis and image processing using ImageJ software. Tin-PDMS-based composite is prepared by dispersing pure tin powder into PDMS polymer liquid at different weight percentages of tin powder, such as 20%, 30%, 40%, 50%, and 60% (w/w). It was then analysed under FESEM to observe the cross-sectional structure inside the composite. The porosity of the composite was evaluated using ImageJ software. Energy dispersive X-ray (EDX) analysis has also been used to evaluate the oxygen content in the composite. As a result, increasing the composition of the tin filler causes a decrease in oxygen content and an increase in porosity or air bubbles, which was confirmed using ImageJ software. This may be due to the reduced and insufficient polymer as a matrix for the tin particles to bind, which causes insufficient polymer to fill the gaps. Low PDMS content causes low viscosity of the mixture, making it harder to achieve a compact structure. However, the percent of porosity was not higher than 0.34% for the sample with 60% tin filler and the highest pore size was only 0.031 µm for the sample with 20% tin powder, which highlights the composites' low porosity. In conclusion, the sample showed low porosity within the composite. However, to ensure that the composite is compact and can attenuate the radiation beam, a crucial step such as a slow stirring or degassing procedure must be carried out to minimise the formation of air bubbles and porosity.

Keywords: Composite, metal-polymer, porosity, ImageJ

Research area: *Inorganic Chemistry*

SEEKING THE POTENTIALITY OF PHENYLPHOSPHONATE/HDPE/GRAPHENE OXIDE COMPOSITE: AN ENVIRONMENTALLY FRIENDLY FLAME RETARDANT

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High-density polyethylene (HDPE) is a well-known polymer due to its versatility, durability, and low cost, making it economically appealing for a wide range of applications. However, HDPE attains high flammability, which causes serious fire safety concerns. To solve this issue, phosphorus-based flame retardants have emerged as a possible alternative because of their capacity to improve HDPE fire resistance. These retardants function by halting the combustion process, lowering the material's flammability and preventing fire spread. Studies have shown that integrating phosphorus flame retardants into HDPE can greatly increase its flame-retardant efficacy, resulting in slower burning rates and greater limiting oxygen index (LOI). Existing research lack comprehensive investigation of the effects of phosphorus flame retardant additives on HDPE, particularly the synergistic effects with graphene oxide (GO). This study explores the development of bis(4-acetylphenyl) phenylphosphonate (**BAP-PP**) as novel phosphorus flame retardant to enhance fire resistance of HDPE. **BAP-PP** was synthesised and characterised through ^{1}H-, ^{13}C-, and ^{31}P- nuclear magnetic resonances (NMR) and Fourier-transform infrared (FTIR) spectroscopy analyses, using triphenylphosphine-PPh_3 as a comparative model. Geometrical optimisation was performed with B3LYP/6-311G(d,p) in Gaussian 09w software. The flame retardancy of HDPE composites with **BAP-PP** was assessed using thermogravimetric analysis (TGA/DTG), LOI, and UL 94 vertical burning tests. Results showed that incorporating **BAP-PP** into HDPE significantly enhanced its fire resistance, achieving an LOI of 21% and a V-0 rating in the UL 94 test. Besides, cytotoxicity testing has demonstrated that BAP-PP is a non-toxic additive. The hybrid filler approach effectively enhanced both the thermal properties and fire safety of the composites. BAP-PP has potential to enhance fire safety in polymer composites. Further research is needed to explore its long-term stability, environmental impact, and effectiveness in various polymer matrices.

Keywords: Phosphorus Flame Retardant, High-Density Polyethylene (HDPE), Fire Safety, Graphene Oxide, Fire Resistance Materials

Research area: *Inorganic Chemistry*

$Fe_3O_4@SiO_2$ MODIFIED HDTMS HYDROPHOBIC COATINGS AS ANTI-CORROSION COATING ON STEEL

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Steel is the primary material used in ship construction due to its strength and durability. However, it is highly vulnerable to corrosion damage. Consequently, an effective coating method is essential to enhance the corrosion resistance of steel surfaces. This research aimed to investigate the synthesis and characterization of a $Fe_3O_4@SiO_2$ modified HDTMS hydrophobic coating layer. The $Fe_3O_4@SiO_2$-HDTMS hydrophobic coating was synthesized using the sol-gel method. The characteristics of the coatings were analyzed, encompassing aspects of their structure, chemical composition, particle morphology, contact angle, adhesion strength, flexibility, and resistance to shock loading. To evaluate the performance of $Fe_3O_4@SiO_2$-HDTMS coatings on steel, anti-corrosion properties were evaluated using salt spray and salt immersion methods. FTIR analysis demonstrated that the $Fe_3O_4@SiO_2$-HDTMS coatings have chemical similarities with HDTMS, as indicated by the absorption band at 1462 cm^{-1}, which signifies the presence of C-O bonds in silicon-ether groups. Additionally, absorption bands at 2921 and 2850 cm^{-1} were observed, corresponding to C-H sp^3 stretching bonds. XRD analysis revealed peaks in diffraction patterns at $2\theta = 20.08, 30.23, 35.56, 43.24, 53.63, 57.05$, and $62.84°$, suggesting a combination of crystalline Fe_3O_4 and amorphous SiO_2 structures. TEM imaging of the $Fe_3O_4@SiO_2$ nanocomposite showed a silica shell with a thickness of 9.04 nm coating an Fe_3O_4 core with a thickness of 8.26 nm, forming a core-shell structure. The $Fe_3O_4@SiO_2$-HDTMS coating was applied using a spray coating method with an optimal mole ratio of Fe_3O_4: SiO_2: HDTMS of 0.002: 0.006: 0.003, resulting in a hydrophobic surface with a water contact angle (WCA) of 142.33°. The coating demonstrated excellent adhesion strength, flexibility, and impact resistance. The corrosion rate of steel was recorded at 0.0059 mpy in the salt spray test and 0.5267 mpy in the salt immersion test, suggesting that the hydrophobic coating offers effective anti-corrosion protection.

Keywords: $Fe_3O_4@SiO_2$-HDTMS, sol-gel, steel, hydrophobic, anti-corrosion.

Research area: *Inorganic Chemistry*

KINETIC AND OPTIMIZATION STUDIES OF METHYLENE BLUE PHOTODEGRADATION OVER Fe-PTC MOF AND H_2O_2 USING RESPONSE SURFACE METHODOLOGY

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A novel iron-based Metal-Organic Framework (MOF), synthesized via a solvothermal method using iron (Fe) and perylene-3,4,9,10-tetracarboxylate (PTC), was selected for its effective visible light absorption properties. Characterization confirmed the MOF's features through FTIR, XRD, DRS, SEM, EDS, and BET analyses as well as cyclic voltammetry. FTIR analysis showed Fe-O bonding, XRD indicated a crystallinity of 46.6% with an average crystal size of 51 nm, and DRS revealed a bandgap of 1.94 eV. SEM displayed a cylindrical morphology while EDS confirmed iron content at 21.6%. BET analysis reported a surface area of 15.36 m^2/g and cyclic voltammetry demonstrated an onset oxidation potential of 0.641 V versus NHE with a LUMO of -1.299 V. The kinetic study of methylene blue photodegradation using MOF Fe-PTC and hydrogen peroxide under visible light followed pseudo-first-order kinetics with a reaction rate constant of -0.7213 per minute. Optimization using response surface methodology identified the best conditions for maximum degradation efficiency, which included 1.35 mg of photocatalyst, 0.22 M concentration of H_2O_2, and a contact time of 135 minutes.

Keywords: Metal-Organic Frameworks (MOF), Photodegradation, Methylene Blue, Visible Light Catalysis, Response Surface Methodology

Research area: *Inorganic Chemistry*

CARBON DOT NANOCOMPOSITES FROM CAJEPUT TREE MODIFIED WITH FOLIC ACID AND CHLOROPHYLLS AS POTENTIAL PHOTOSENSITIZERS FOR PHOTODYNAMIC THERAPY

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Folic acid-modified carbon dot nanocomposites with chlorophyll derivatives have been successfully synthesized. This study investigates the properties of these carbon dot nanocomposites, particularly with chlorophyll and its derivatives, as potential photosensitizers for photodynamic therapy. The carbon dots were synthesized hydrothermally using Cajeput tree bark at various temperatures. The resulting samples were then combined with chlorophyll (Chl) and chlorophyll derivatives (Chlide) through stirring. The carbon dot samples were characterized using UV-Vis, fluorescence, FTIR, Raman, XRD, and TEM. Reactive Oxygen Species (ROS) generation was analyzed using 1,3-Diphenylisobenzofuran (DPBF) and measured with UV-Vis spectroscopy. The results showed that both folic acid-modified carbon dots (FACD) and non-modified carbon dots (CD) were synthesized, with an optimal hydrothermal temperature of 100°C (FACD-100), and remained stable for up to 20 days. The carbon dots were identified as graphene quantum dots (GQD), with the highest relative quantum yield (QY) observed in FACD-Chlide at 8.57%. The carbon dots with the highest QY also exhibited the highest ROS generation activity, indicating their potential as sensitizers for photodynamic therapy.

Keywords: Graphene carbon quantum dots, hydrothermal, cajeput tree, reactive oxygen species (ROS), nanocomposite

Research area: *Inorganic Chemistry*

SUSTAINABLE RECYCLING OF PLASTIC BAG WASTE INTO CARBON QUANTUM DOTS USING OPTIMIZED PYROLYSIS-HYDROTHERMAL METHODS FOR SELECTIVE FE(III) SENSING

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Environmental pollution from plastic bag waste has emerged as a critical issue demanding urgent solutions. Here, an innovative and sustainable approach to recycling plastic bag waste into carbon quantum dots (CQDs) using a low concentration of H_2O_2 oxidant (<7 wt%) was explored. A combination of pyrolysis and hydrothermal methods was employed to accelerate the synthesis time. Several parameters, including pyrolysis product mass, hydrothermal time, and H_2O_2 concentration, were investigated to reach optimal CQDs production conditions. The optical properties of the CQDs were characterized using UV-Vis and fluorescence spectrophotometers, while their structure and composition were analyzed using IR spectroscopy, Raman spectroscopy, XRD, zeta potential analysis, elemental analysis, HR-TEM, SAED, and EDS. The shortened synthesis time was achieved (10 h) using 4 h of pyrolysis time, 0.25 g of pyrolysis product mass, and 6 h of hydrothermal time. Moreover, a low concentration of H_2O_2 was used to produce CQDs (5 wt%). Bright blue fluorescence of CQDs under UV light with a high quantum yield of up to 10.04% was obtained. In addition, remarkable fluorescence stability of CQDs was acquired under UV light exposure, in various ionic strengths, and during prolonged storage. The size distribution of CQDs is 1.5–4.5 nm with a defected graphitic structure caused by incorporating oxygen-containing functional groups such as hydroxyl, carbonyl, and carboxyl, enhancing their functionality to interact with metal ions. Notably, these CQDs showed high selectivity for Fe^{3+} ions, with a good correlation coefficient (R^2) of 0.9983 and a low detection limit (LOD) of 9.50 µM. This research underscores the potential of converting plastic waste into valuable nanomaterials, presenting a cost-effective, eco-friendly solution for advanced sensing applications of metal ions.

Keywords: Carbon quantum dots, hydrothermal, plastic recycling, pyrolysis, Fe (III) sensing

Research area: *Inorganic Chemistry*

INCORPORATION OF ZnO NANOFILLERS INTO CHITOSAN/KI/I_2-BASED QUASI SOLID ELECTROLYTES

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This research explores the use of quasi solid polymer electrolytes as a substitute for liquid electrolytes in dye-sensitized solar cells to mitigate issues such as leakage and counter electrode corrosion. Chitosan, known for being biodegradable, non-toxic, odorless, and having high mechanical strength, has shown promise for this application. To enhance the electrochemical performance of chitosan-based polymer gel electrolytes, zinc oxide (ZnO) nanofillers, including ZnO nanorods and ZnO nanoalmonds synthesized through hydrothermal methods, were incorporated into the chitosan PGE matrix mixed with potassium iodide and iodine to create a redox couple. Characterization of the polymer gel electrolyte was conducted using cyclic voltammetry (CV), Fourier-transform Infrared (FTIR) spectroscopy, X-ray Diffractometry (XRD), Scanning Electron Microscopy (SEM), and Transmission Electron Microscopy (TEM). Adding ZnO nanoparticles improves ionic conduction by creating additional pathways. The study's findings indicate that incorporating 0.25%wt of ZnO nanorods into the polymer matrix results in the highest intensity of anodic and cathodic peak currents, suggesting that it is one of the excellent candidates to replace the liquid electrolyte.

Keywords: Chitosan, electrolyte, nanofillers, ZnO

Research area: *Inorganic Chemistry*

NiO/CeO_2-Al_2O_3 MESOPOROUS CATALYST SUPPORTED ON ALUMINA BEADS FOR HYDROGEN GENERATION FROM AMMONIA DECOMPOSITION

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The development of non-noble metal catalysts for ammonia (NH_3) decomposition to produce CO_x-free hydrogen (H_2) has received significant attention due to its potential for clean energy generation. This research investigates a new method for creating efficient catalysts for hydrogen production from ammonia decomposition. The method incorporates a triblock copolymer, Pluronic F-127 to fabricate NiO/CeO_2-Al_2O_3 mesoporous catalyst supported on alumina beads via a hybrid method of self-assembly, solvothermal treatment, and calcination for deposition onto alumina beads. By controlling the composition, these catalysts exhibit improved performance. Various characterization techniques such as XRD, FESEM, and BET were used to investigate the physical and chemical properties of the prepared catalysts. Their activity was tested at temperature range of 450 to 650 °C and GHSV of 500 to 2500 $mL.g_{cat}^{-1}h^{-1}$. The optimized catalyst is expected to remain highly active below 550 °C. This approach, using non-noble metals, offers a promising and practical way to utilize ammonia as a source of hydrogen for on-board fuel cell applications.

Keywords: NiO/CeO_2-Al_2O_3, ammonia, decomposition, hydrogen, solvothermal

Research Area: *Inorganic Chemistry, Material Sciences, Catalysis*

MICROWAVE-ASSISTED SYNTHESIS AND CHARACTERISATION OF ZINC OXIDE QUANTUM DOTS FOR DETECTION OF ANTIBIOTICS

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In this study, zinc oxide quantum dots (ZnO QDs) fluorescent sensor was developed through a microwave-assisted synthesis method by hydrolysing zinc acetate dihydrate with lithium hydroxide in ethanol, for rapid tetracycline (TC) detection. The ZnO QDs exhibited a strong yellow emission under 365 nm UV light. Transmission electron microscopy (TEM) analysis revealed a spherical surface morphology with an average particle size of 3.17 nm. X-ray diffraction (XRD) analysis shows a broad peak in 2θ range of 27 to 32°, corresponding to ZnO’s hexagonal close-packed (hcp) wurtzite structure. The quantum yield (QY) of the ZnO QDs was determined to be 35%. Fluorescence behaviour was studied at an excitation wavelength of 340 nm, showing an optimal emission peak at 560 nm. The particle size remained constant across various excitation wavelengths. The fluorescence response of the ZnO QDs was linear with TC concentration over a range of 2-112 μM, with a detection limit of 3 μM. The emission colour under 365 nm UV light gradually changed to green when the concentration of TC was increased. The simplicity, cost-effectiveness, and rapid detection capability of ZnO QDs make them a promising tool for trace antibiotic determination in various matrices.

Keywords: zinc oxide, quantum dots, microwave-assisted, fluorescent sensor, tetracycline, fluorescence response.

Research area: *Inorganic Chemistry*

MICROWAVE-ASSISTED SYNTHESIS OF CARBON QUANTUM DOTS FROM THE DEACTIVATED CELLS OF *Pseudomonas aeruginosa* USM-AR2

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In this research, a novel class of carbon quantum dots (CQDs) is synthesised from the deactivated cells of *Pseudomonas aeruginosa* USM-AR2 (PA USM-AR2/CQDs) using the microwave-assisted synthesis method. The average particle size of the PA USM-AR2/CQDs, as estimated by transmission electron microscopy (TEM), was 5.64 nm. The X-ray diffraction (XRD) pattern displayed a broad diffraction peak in the 2θ range of 27° to 31° attributed to a disordered graphitic-like structure. The PA USM-AR2/CQDs exhibited strong blue emission radiation with a quantum yield of 48%. The photoluminescent properties of the PA USM-AR2/CQDs were found to be excitation-dependent, with the highest emission peak at 480 nm when excited at 410 nm. However, the fluorescence intensity stability gradually decreased over five months of storage. These findings suggest potential applications for PA USM-AR2/CQDs in various fields, especially bioimaging and optoelectronics.

Keywords: carbon quantum dots (CQDs), *Pseudomonas aeruginosa*, *Pseudomonas aeruginosa* USM-AR2 , microwave irradiation

Research area: *Inorganic Chemistry*

ENHANCED PHOTOCATALYTIC DEGRADATION OF EMERGING POLLUTANTS BY HYBRID METAL-ORGANIC FRAMEWORKS AND CARBON DOTS COMPOSITES

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The development of efficient photocatalysts for the degradation of emerging pollutants is crucial due to the increasing variety of new pollutants from various industries and their negative impacts on human health. In this study, we reported the synthesis and characterization of hybrid composites composed of metal-organic frameworks (MOFs), specifically MIL-100(Fe), and carbon dots (CDs) derived from palm kernel by-products. The integration of carbon dots into the MIL-100(Fe) matrix was achieved through a facile hydrothermal synthesis and was confirmed by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), transmission electron microscopy (TEM), Brunauer-Emmett-Teller (BET) surface area analysis, thermogravimetric analysis (TGA), and photoluminescence (PL) spectroscopy analysis. The photocatalytic activity of the composite was assessed under visible light irradiation, and it demonstrated superior degradation efficiency of a model dye pollutant, Auramine O, compared to the pristine MIL-100(Fe) and CDs.

MICROWARE-ASSISTED SYNTHESISED SnO_2 QUANTUM DOTS PHOTOCATALYSTS FOR THE REMOVAL OF ANTIBIOTICS

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In this study, NaCl/SnO_2 quantum dots (NaCl/SnO_2 QDs) were synthesised by microwave synthesis method using $SnCl_4{\cdot}5H_2O$, at 600 W and 3 min of irradiation time for the photodegradation of tetracycline (TC). The particle size of the NaCl/SnO_2 QDs was estimated using transmission electron microscopy (TEM) were 2.7 nm. The X-ray diffraction (XRD) analysis detected phases related to amorphous SnO_2 and cubic NaCl. The X-ray photoelectron spectroscopy (XPS) and energy dispersive X-ray (EDX) detected the presence of Sn, O, Na and Cl elements. The N_2 adsorption-desorption analysis showed Type IV with H3 hysteresis loop typical for mesoporous materials. The Brunauer–Emmett–Teller (BET) surface area was estimated to be 111.62 m^2/g, and the density functional theory (DFT) pore size distribution was estimated to be 2.20 nm. The ultraviolet visible (UV-Vis) analysis detected a single peak at 330 nm attributable to strong absorption edge. The calculated valence band edge potential (E_{VB}) and conduction band potential (E_{CB}) were 3.46 eV and 0.02 eV, respectively. The NaCl/SnO_2 QDs were able to completely remove TC under the optimum conditions (100 mg of catalysts, 10 mg/L of TC solution, pH of 8.5 within 90 min under fluorescent light irradiation (39 mW/cm^2)). However, the removal was reduced to 35% during reuse due to loss of NaCl. The role of NaCl is important in enhancing the photodegradation of TC.

Keywords: Microwave synthesis, SnO_2 quantum dots, photodegradation, tetracycline

Research area: *Inorganic Chemistry*

SULFONE-CENTRED SYSTEMS WITH DIVERSE TERMINAL ALKOXY CHAINS: SYNTHESIS, CHARACTERIZATION, AND THEIR MESOMORPHIC AND PHOTOLUMINESCENCE BEHAVIORS

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A new architectural structures of liquid crystalline materials based on sulfone-centred multisubstituted phenyl derivatives have been isolated and characterized. The members of this series differ by the length of terminal alkoxy chains ($-OC_nH_{2n+1}$), with n ranging from 5 to 10. The purity and molecular structures of all compounds were thoroughly validated by CHN analysis, FT-IR, UV-Vis and NMR spectroscopic techniques. The mesomorphic and thermal behaviors of all target compounds were probed using polarizing optical microscope (POM) and differential scanning calorimetry (DSC). The homologues with odd-numbered terminal chains displayed enantiotropic smectic B (SmB), smectic A (SmA) and nematic (N) phases, whereas the even members only showed enantiotropic SmA and N phases. The phase transition temperatures demonstrated an odd-even effect, with the odd members having lower transition temperatures than their equivalent even counterparts. This indicated that the odd members had difficulty to pack efficiently into liquid crystalline structure than the elongated conformation of even members. The photoluminescence (PL) study revealed that varying the length of the terminal alkoxy chains had a significant effect on the PL intensity, wherein the PL intensity of target compounds increases as the terminal alkoxy chain length increases. The particle sizes of target compounds were determined using dynamic light scattering (DLS), and an odd-even effect was identified, with the odd members having smaller diameters than the even members. Additionally, the molecular model analysis on target compounds was performed utilizing MM2 method.

Keywords: Sulfone, mesomorphic, enantiotropic, odd-even effect, photoluminescence

Research area: *Inorganic Chemistry*

SYNTHESIS AND CHARACTERIZATION OF LAYERED DOUBLE HYDROXIDE

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Layered double hydroxides (LDHs) are a class of advanced inorganic 2D materials, commonly known as hydrotalcite-like ionic lamellar compounds which encompass positively charged brucite-like layers coupled with interlayer anions. The LDH general formula is $[M_{1-x}^{2+}M_x^{3+}(OH)_2]^{x+}[(A^{n-})_{x/n}\cdot mH_2O]$, in which M represents bivalent and trivalent metal cations whereas An– represents interlayer anion, and x is the molar ratio of $M^{3+}/(M^{2+} + M^{3+})$. Such material has received global attention mainly due to its flexible tunability of the cation anion composition, high chemical stability, high specific surface area, nontoxicity and low-cost. Among the benefits, the composition tunability has led to an increase in interest by using LDHs in the field of catalysis, adsorption of organic and inorganic species, electrochemistry, medicine and biochemistry. There are several synthesis methods that have been widely studied such as co-precipitation, hydrothermal and ion-exchange. In this work, hydrothermal method coupled with urea hydrolysis has been used to synthesize magnesium-aluminium (Mg-Al) LDH under various experimental conditions such as different reactant ratios, pH value, temperature, stirring rate and reaction duration. The characterization techniques used to confirm the formation of LDH crystals and their modification include XRD, FE-SEM and BET. The optimal synthesis parameters have been deduced based on the structural formation as well as crystallinity of the Mg-Al LDH.

Keywords: layered double hydroxide, hydrothermal, magnesium, aluminum, tunability

Research area: *Inorganic Chemistry*

MICROWAVE-ASSISTED SYNTHESIS OF LACCASE *Trametes hirasuta* -DERIVED CARBON DOTS FOR CIPROFLOXACIN DETECTION

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This study presents the green and rapid synthesis of carbon dots (CDs) derived from the laccase of *Trametes hirsuta* (Lac-CDs) as a fluorescent probe for detecting ciprofloxacin. Transmission electron microscopy (TEM) analysis reveals that the Lac-CDs are highly agglomerated and spherically shaped, with an average size of 4.42±1.77nm. Fourier-transform infrared spectroscopy (FTIR) and X-ray photoelectron spectroscopy (XPS) confirm the presence of various functional groups on the Lac-CDs surfaces. The Lac-CDs exhibited a blue emission under 365 nm UV light, a quantum yield of 12%, and excitation-dependent emission behaviour. A linear response was achieved in the range of 0 to 15µM, with a limit of detection (LOD) of 2.65µM. These findings indicate that the laccase from *Trametes hirsuta* has the potential for further development as a fluorescent probe for antibiotic detection and other applications.

Keywords: Carbon dots, Laccase, *Trametes hirsute*, Ciprofloxacine, Fluorescent, Microwave.

Research area: *Inorganic chemistry*

TITLE CATALYTIC HYDROGENATION OF CO_2 TO METHANOL OVER Cu/ZnO BASED CATALYST SUPPORTED ON VARIOUS TYPES OF Al_2O_3 PELLET

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CO_2 management is vital for ensuring the economic and environment viability especially for monetization of high CO_2 field. In view of this outstanding challenges, CO_2 is not seen any more as a waste but as an alternative carbon feedstock to transform this stable molecule into useful chemicals and energy carriers. Conversion of CO_2 to valuable product is a challenging contemporary issue, but with the development of optimized process catalyst, the challenges can be overcome. CO_2 catalytic conversion to fuel (methanol) has been studied as one of the strategies to reduce CO_2 emission and can be considered as a complementary technology to CCS, serving similar goals, while additionally providing economic benefits. The study focused on catalytic conversion of CO_2 to methanol over promoted Cu/ZnO based catalyst supported on various shapes and physicochemical properties of Al_2O_3 pellets support (spherical, hollow extrudate and trilobe extrudate). The catalysts were synthesized by impregnation method with fixed metal loading. The aqueous precursor solution was impregnated on the Al_2O_3 pellets support, maintained at pH 7, continuously stirred, filtered and washed. It was then dried, grinded and calcined at 350°C. The synthesized catalysts were characterized using H_2-TPR, FESEM, N_2 adsorption desorption and XRD. The performance of the synthesized catalysts in a CO_2 hydrogenation reaction was evaluated in a fixed-bed reactor. The reaction temperature, pressure, GHSV and H_2: CO_2molar ratio were fixed to study the effect of different shapes of Al_2O_3 pellets support on the catalytic performance. The experimental findings indicate that, the shape of Al_2O_3 pellet gave significant impact on CO_2 conversion and MeOH selectivity. The catalyst with spherical shape resulted in highest CO_2 conversion and MeOH selectivity at 11.83% and 51.84% respectively. The two catalysts samples with the same shape (hollow extrudate) but different dimensions resulted in CO_2 conversion at 11.46% and 11.00% and MeOH selectivity at 45.58% and 40.84%. The trilobe extrudate gives out lowest CO_2 conversion at 10.30%, however higher MeOH selectivity as compared to one of the hollow extrudate at 43.43%. It can be concluded that, the shape of the catalysts influences the catalytic performance significantly.

Keywords: CO_2 conversion, methanol, Cu catalyst, Al_2O_3 support, selectivity

Research area: *Inorganic Chemistry*

CATALYTIC STUDY OF $Co/\gamma\text{-}Al_2O_3$ ON THE DEOXYGENATION OF PALM OIL BIODIESEL FOR GREEN DIESEL PRODUCTION

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This study explains the production of green diesel with alkane structure through the deoxygenation of palm oil biodiesel over supported cobalt catalysts. The $Co/\gamma\text{-}Al_2O_3$ catalyst was prepared via wetness impregnation method, exhibited phase compatibility as confirmed by XRD diffractograms. SEM-EDX analysis revealed random and irregular morphology with evenly distributed elements in the catalysts. EDXRF analysis confirmed the percentage of metal impregnated on the $\gamma\text{-}Al_2O_3$ support. The reducibility of the catalysts, analyzed through H_2-TPR profiles, showed increased reduction with higher metal loading, indicating an increase in active sites on the catalysts. The catalysts were characterized as mesoporous based on the support characteristics. The catalytic activity of $Co/\gamma\text{-}Al_2O_3$ was tested in the deoxygenation reaction of palm oil biodiesel with specific studies on the influence of reaction time, metal loading, and catalyst mass. Cobalt catalysts successfully converted palm oil biodiesel into green diesel within the range of C8-C20 alkanes. The highest conversion and alkane selectivity inferred the optimized reaction conditions of 3 h reaction time, cobalt loading of 10.00 wt%, and catalyst mass of 1.00 wt%. The stability test exhibited a gradual decline in conversion after three reaction cycles and a regeneration treatment allowed partial recovery of conversion up to 34%. The overall result implied that $Co/\gamma\text{-}Al_2O_3$ is a promising catalyst for green diesel production. This project supports the Sustainable Development Goals especially the Affordable and Clean Energy (Goal no. 7) and Climate Action (Goal no. 13).

Keywords: cobalt catalyst, deoxygenation, green diesel, biodiesel, SGDs

Research area: *Inorganic Chemistry*

ORAL : ANALYTICAL CHEMISTRY

INTERNATIONAL CONFERENCE OF YOUNG CHEMISTS

DEVELOPMENT OF MAGNETIC GRAPHENE OXIDE-DEEP EUTECTIC SOLVENT FOR THE DETERMINATION OF ORGANOPHOSPHORUS PESTICIDES: A PRELIMINARY STUDIES

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In this work, a smart material called ferrofluid (FF) was developed for the removal of organophosphorus pesticides (OPPs). FF was synthesized by combining magnetic graphene oxide (MGO-DES) as magnetic nano composite and deep eutectic solvent (DES) as carrier solvent. The synthesized materials were characterized using Fourier Transform-infrared spectroscopy (FTIR), transmission electron microscopy (TEM), scanning electron microscopy (SEM), X- ray diffraction analysis (XRD), thermogravimetric analysis (TGA), and vibration sample magnetometer (VSM). The adsorption performances of methidathion (MET) and malathion (MAL) were evaluated based on kinetic, isotherm, and thermodynamic models. A pseudo-second-order kinetic model, Freundlich and Halsey isotherm model were best fitted the adsorption performance of MGO-DES FF for OPPs. Based on the results on thermodynamic study, the ΔG and ΔH proved that the adsorption processes were exothermic and spontaneous at 298 K. The developed MGO-DES FF adsorbent showed exceptional adsorption performances which can be promising alternative for the removal of the selected OPPs.

Keywords: Ferrofluid, magnetic graphene oxide, deep eutectic solvent, adsorption performances, organophosphorus pesticides.

Research Area: *Analytical Chemistry/ Separation Chemistry*.

DEVELOPMENT OF DUMMY TEMPLATE MOLECULARLY IMPRINTED POLYMER FOR THE ADSORPTION OF ORGANOPHOSPHORUS PESTICIDES: PRELIMINARY STUDIES

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In this study, a novel adsorbent based on a dummy-template molecularly imprinted polymer (DMIP) together with a non-imprinting polymer (NIP) was synthesized using the bulk polymerization method and employed as sorbents for the removal of organophosphorus pesticides (OPPs). The synthesized polymers were characterized using FTIR, nitrogen adsorption-desorption analysis, SEM, XRD, and TGA. The adsorption performances of both DMIP and NIP for chlorpyrifos (CPF), dimethoate (DMT), and parathion-methyl (PM) were evaluated based on the adsorption parameters, kinetic, isotherm, and thermodynamic models. Under optimum conditions, the results revealed that the maximum removal efficiencies of the DMIP (87% CPF, 75% DMT, and 83% PM) were achieved at the optimized conditions of pH 7 (for CPF and PM) and 4 (for DMT), 10 mg adsorbent dosage, and 10 mL of 10 mg/L of adsorbate solution at 30 min contact time, which were higher than the corresponding NIP (53% CPF, 49% DMT, and 51% PM). The adsorption of DMIP and NIP can be best described by a pseudo-second-order kinetic model and Freundlich isotherm, with maximum adsorption capacities ranging from 24.36 to 55.31 mg/g for all the selected OPPs. The values of ΔG and ΔH from thermodynamic studies established that the reactions were spontaneous and exothermic at 298K. The reusability studies indicated that there was no substantial loss of removal efficiency while using the DMIP/NIP for up to five cycles. Hence, the developed DMIP has demonstrated to be a green, cheap, and promising alternative for the removal of the selected OPPs.

Keywords: MIP, adsorption, dummy template, OPPs, Removal efficiency, selectivity.

Research Area: *Analytical Chemistry/ Separation Chemistry.*

DEVELOPMENT OF BIMETALLIC SUPPORTED ON 3D-STRUCTURED METALS CATALYSTS

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Catalysts play a crucial role in various chemical processes, and their design and optimization are essential for efficient reactions. Owing to their decent performance and low cost, nickel (Ni) based catalysts have been widely studied for different application. Herein, we study the potential of Co-Ni bimetal as the catalysts through electrodeposition techniques. The catalysts were prepared by electrodeposition technique on the 3D structured metal and were characterized by using FESEM, EDX, XRD, TGA, TPR, BET, XPS, and HRTEM. The FESEM image revealed the Co-Ni bimetal, and particle distribution, size, shape, and dispersion on the 3D structured metal. EDX confirms the presence of Co-Ni bimetal on the 3D-structured metals and provides a mass of Co 52% Ni 47%, Furthermore, XRD proves the crystal structure of Co-Ni bimetal on the 3D structured metal and TGA confirms the catalyst stability and thermal decomposition also BET confirms the accessibility of active sites and the porosity of the catalyst. In contrast, TPR confirms the redox properties, reduction temperatures, and strength of metal-support interactions of Co-Ni bimetal. These characteristics confirm the Co-Ni bimetal formation on the 3D structured metal.

Keywords: Catalysis, electrodeposition, characterization, Bimetallic, 3D-structure

Research area*:* *Catalysis development*

EXPLORATION OF POTENTIAL APPLICATION OF NATURAL DEEP EUTECTIC SOLVENT IN VORTEX ASSISTED LIQUID-LIQUID MICROEXTRACTION FOR THE DETERMINATION OF SELECTED FURANIC COMPOUNDS IN HONEY

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In this study, a vortex assisted liquid-liquid microextraction (VALLME) method was developed using a three-component natural deep eutectic solvent (NADES) for the determination of furanic compounds, specifically 5-hydroxymethylfurfural and furfural from honey. The extracted furanic compounds were analyzed using high performance liquid chromatography with UV detection. The NADES, synthesized from lauric acid, decanoic acid, and thymol in a 1:2:1 molar ratio through controlled heating and stirring, with thymol as the hydrogen bond acceptor and lauric acid and decanoic acid as hydrogen bond donors. The NADES was characterized using Fourier transform infrared spectroscopy, thermogravimetric analysis, differential scanning calorimetry, and Karl Fischer titration to determine the water content. Key extraction parameters, including the volume of NADES, sample pH, vortex time, and choice of desorption solvent were optimized. The optimal conditions were found to be 800 µL of NADES, pH 2, 4 minutes of vortexing and acetonitrile as the desorption solvent. Under these conditions, the NADES-based microextraction achieved high recovery ranging from 72% to 130% with detection limits between 0.19 and 1.88mg/L and quantification limits between 0.584 and 32.74mg/L. This study demonstrates the effectiveness of a NADES-based VALLME approach for the efficient extraction and analysis of furanic compounds in honey, offering a green, sensitive, and reliable method with high recovery and low detection limits.

Keywords: NADES, VALLME, furanic compounds, honey.

Research area: *Analytical Chemistry*

RAPID PORTABLE ATMOSPHERIC SOLIDS ANALYSIS PROBE MASS SPECTROMETRY FOR ON-SITE URINE DRUG SCREENING

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Atmospheric pressure solids analysis probe (ASAP) is an ambient pressure mass ionization technique that offers rapid analysis of both liquid and solid samples without necessitating sample preparation. This study explores the application of a portable ASAP−mass spectrometry (ASAP−MS) system, operated under the positive ion mode for the rapid screening of nine illicit substances (amphetamine, methamphetamine, oxycodone, methadone, morphine, 3,4-methylenedioxymethamphetamine, ketamine, and 6-monoacetylmorphine) in water and urine matrices. Being portable, the ASAP−MS system accommodates on-site analysis, and real-time results can be generated within 30 seconds. Tentative identification of these psychoactive drugs was achieved by matching their mass fragmentation patterns to an in-house MS spectral library, with matching thresholds of ≥ 800 to ensure decisive identification. The applicability of the proposed ASAP−MS method for the screening of the targeted illicit compounds in United Nations Office on Drugs and Crime interlaboratory urine test samples will be presented.

Keywords: atmospheric pressure solids analysis probe, illicit substances, ambient ionization mass spectrometry

Research area: *Analytical Chemistry/Toxicology*

ENHANCED STABILITY AND PERMEABILITY OF GRAPHENE OXIDE NANOCOMPOSITE MEMBRANES VIA GLYCINE AND DIGLYCINE CROSS-LINKING

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Surface coating of graphene oxide (GO) on membrane surfaces often suffers from low stability, with the GO layer prone to swelling and detachment during filtration. This study introduces glycine (Gly) and diglycine (diGly) as cross-linking agents to improve the stability and performance of GO nanocomposite membranes. FESEM images revealed that amino acid-crosslinked GO formed a thick pile structure on membrane surface. The chemical bonding between GO and glycine derivatives was confirmed by FTIR and XRD analyses. Stability test showed that glycine derivatives reduce the tendency of GO detachment from the self-fabricated polyethersulfone (PES) membrane surface. Ultrafiltration tests demonstrated that water permeability of nanocomposite membranes increased in the order of diGly-GO (14.70 LMH bar^{-1}) > Gly-GO (8.66 LMH bar^{-1}) > GO (4.57 LMH bar^{-1}), without compromising bovine serum albumin (BSA) rejection efficiency (82-84%). However, the reduction of hydroxyl groups in Gly-GO and diGly-GO nanocomposite membranes made them more susceptible to BSA fouling. Consequently, the pristine GO nanocomposite membrane exhibited the lowest flux declination rate and the highest flux recovery rate among the membranes. Overall, the results indicate that cross-linking GO nanosheets with glycine derivatives enhances membrane permeability and stability by improving the staking of GO nanosheets.

Keywords: amino acids, graphene oxide, membrane stability, cross-linking, ultrafiltration

Research area: *Analytical Chemistry*

FABRICATION OF CARBOXIMETYL CHITOSAN-ALGINATE POLYELECTROLYTE COMPLEX MEMBRANE FOR ADSORPTION OF METHYLENE BLUE IN WATER

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The excessive use of synthetic dyes in various industries, including textiles and pharmaceuticals, has led to environmental pollution issues. The synthetic dyes are known as highly toxic and potentially carcinogenic compounds. One commonly used dye is methylene blue. Various methods have been used to overcome this dye pollution problem, one of them is the adsorption. In this study, carboxymethyl chitosan (CMC) and alginate were combined into a polyelectrolyte complex (PEC) membrane, that can function as a dye adsorbent. CMC-Alginate membrane was synthesized with a variation of the mole composition of 2:1; 1:1; and 1:2 and characterized using FTIR, XRD, and SEM. The optimum CMC-Alginate membrane composition was found to be 1:2. FTIR analysis revealed absorption peaks corresponding to –OH groups at 3441.01 cm^{-1}; $–NH_2$ at 1620.20 cm^{-1} and –C=O at 1604.77 cm^{-1}. XRD results indicated changes in the crystallinity of the CMC-Alginate membrane compared to its constituent materials. While from SEM showed that the membranes have porous and homogeneous surfaces. The optimal adsorption conditions occurred at pH 8 with the highest adsorption percentage and a contact time of 120 minutes to reach adsorption equilibrium. The adsorption process followed a pseudo-second-order kinetic model. The Freundlich isotherm was found to be appropriate, indicating a physical adsorption process, supported by a $\Delta G°$ value of 17.27 kJ/mol. However, a relatively high percentage of desorption in NaCl media suggested the presence of ionic bonds in the adsorption process.

Keywords: Adsorbent, carboxymethyl chitosan, CMC-Alginate, methylene blue, PEC

Research area: *Analytical Chemistry*

ELECTROCHEMICAL DEGRADATION OF METHYLENE BLUE (MB) USING GRAPHITE/PVC ANODES COATED WITH NICKEL OXIDE AND ZINC OXIDE: OPTIMIZATION, KINETIC ANALYSIS AND INDUSTRIAL APPLICATION POTENTIAL

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In the quest to mitigate the ecological and health risks posed by synthetic dyes in water systems, this study explores the electrochemical degradation of Methylene Blue (MB) using novel graphite/polyvinyl chloride (graphite/PVC) anodes. These anodes were enhanced with Nickel Oxide (NiO) and Zinc Oxide (ZnO) coatings via electrochemical deposition to boost catalytic activity. The study examined the impact of variables such as dye concentration (10, 20, 50, 100 ppm), pH (4, 6, 8, 10), applied voltage (4, 8, 10, 12 V), and NaCl electrolyte concentration (0.05, 0.1, 0.5, 1.0 M) on the degradation kinetics of MB in aqueous solutions. UV-Vis spectroscopy was employed for monitoring of degradation, while FESEM-EDX, XRD, and BET surface analysis were utilized to evaluate the morphology and chemical stability of the electrodes pre- and post-experiment. The findings revealed that lower MB concentrations (10 – 20 ppm) and higher NaCl electrolyte concentrations (1.0M) generally favoured first-order reaction kinetics, with degradation rates being directly proportional to reactant concentrations. Optimal degradation was achieved at higher voltages and acidic conditions (pH 4), with ZnO-coated anodes demonstrating superior efficiency across various parameters. For example, ZnO-coated anodes achieved up to 99.90% degradation efficiency at 100 ppm MB concentration within 120 minutes, while NiO-coated anodes reached 94.85% efficiency at 100 ppm under the same duration. Applied voltage optimization indicated peak performance for both anodes at 12V, with NiO and ZnO achieving degradation efficiencies of 99.02% and 99.13%, respectively. COD removal studies confirmed maximum efficiencies at higher voltages (12V), with both anode types showing nearly complete removal at 12V. Kinetic studies demonstrated that the degradation followed first-order kinetics for both NiO and ZnO anodes under various conditions, with high correlation coefficients (R^2 values). The results showed that ZnO-coated anodes exhibited superior performance compared to NiO-coated anodes in the degradation of MB. The study underscores the robustness and reusability of these anodes, presenting them as viable solutions for industrial wastewater treatment applications. The high degradation efficiency, coupled with electrode stability, confirms the potential of graphite/PVC anodes coated with NiO and ZnO for efficient and environmentally friendly MB removal from wastewater. This approach complements existing wastewater treatment technologies, offering scalable and effective solutions for dye pollution mitigation.

Keywords: Electrochemical degradation, Graphite/PVC anodes, Nickel Oxide, Zinc Oxide, Electrochemical deposition

***Research area**: Analytical Chemistry*

THE USE OF CHEMOMETRIC TECHNIQUES IN THE ASSESSMENT AND SOURCE IDENTIFICATION OF TOXIC METAL POLLUTANTS ALONG KANO RIVERS NIGERIA

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The continuous utilization of contaminated river water for drinking, irrigation and other domestic purposes is of great concern in recent times, resulting in health complications in most cases. In this study, water and vegetable samples from two main rivers in Kano state were analyzed for the presence of Pb, Cd, Cr, Co, and Mn using atomic absorption spectrophotometer (AAS), in addition to the pH, electrical conductivity (EC), suspended solid (SS), and dissolved oxygen (DO). The variations in the studied parameters were evaluated using multivariate statistical analysis. The findings of principal component analysis (PCA) and linear discriminant analysis (LDA) suggested that pollution due to industrial activities significantly contributed to the heavy metal loads of the rivers while the physico chemical parameters were associated with domestic input and other anthropogenic activities. The PCA and LDA showed a clear separation of the river water samples in which Getsi River water samples were much associated with Cr, Pb, Cd, and Co while DO, SS, pH, EC and Mn were associated with Tatsa warki River. Consumption of water from both rivers was found to be unsafe based on metal index analysis, while the average daily intake (ADI) of the vegetables grown along the river bank identified Cr to be of more health concern. The findings of this research work would be of relevance considering the high population that use the water, and increased rate of industrial discharges along the rivers with frequent consumption of vegetables by the neighboring communities.

Keywords: Chemometric, Heavy metal, Pollution, River, Water quality

Research area: *Analytical Chemistry*

MAKING THE SWITCH FROM TRADITIONAL ACTIVATING AGENTS TO ECO-FRIENDLY SOLVENTS FOR ACTIVATED CARBON: A STEP TOWARDS LONG-TERM Pb(II) REMOVAL FROM WATER

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In this work, we describe the production of activated carbon from biomass using low ecological footprint solvents (urea and choline chloride/orthophosphoric acid) for the remediation of lead(II) in water. We believe activated carbon made from solvents with negligible environmental impact may be used to remediate wastewater.

The activated carbon was produced by chemical method using deep eutectic solvent(urea and choline chloride)/ orthophosphoric acid as low ecological foot print solvents FTIR, BET, XPS, and FESEM were among the techniques employed to characterise the optimal adsorbent sample, AC_6-DES_2/H_3, ratio 2:3.

Based on the results, the optimal adsorbent has a specific surface area of 1413 m^2/g, a pore volume of 0.618 g/cm3, and a pore diameter of 0.8 nm. The influence of kinetic variables, pH, and isotherm models were investigated. The adsorption followed Langmuir model and the pseudo-second order kinetic model. Compared to other biosorbents described in the literature, the AC6-DES2/H3 has a much greater maximum monolayer adsorption capacity of over 90 mg/g at pH 5, indicating strong removal capability. More crucially, Pb(II) from wastewater can be repeatedly treated using activated carbon made from biomass using sustainable activating chemicals.

Keywords: Activated carbon, adsorbent, adsorption, XPS, pH

Research area: *Analytical Chemistry/ Environmental Chemistry*

SIMPLE DETECTION OF HEXAVALENT CHROMIUM IN SOLUTIONS USING OPTODE MEMBRANE

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Hexavalent chromium (Cr (VI)) is a toxic and carcinogenic heavy metal that poses significant health risks, including cancer, respiratory issues, and skin irritation. Therefore, monitoring its levels in water is crucial to ensure they do not exceed the maximum safe limit of 0.1 ppm. One effective method for detecting Cr (VI) is by using an optical sensor, or optode.

The optode is constructed by blending cellulose triacetate polymer with plasticizers such as oleic acid and acetophenone, aliquot 336, and 1,5-diphenylcarbazide. This composition makes the sensor highly effective in detecting Cr (VI). It displays a linear response within the concentration range of 0.02-0.40 ppm, with a determination coefficient (R^2) of 0.9979, indicating a strong correlation between Cr (VI) concentration and the sensor's output. The sensor also has a detection limit of 0.0108 ppm and a quantitation limit of 0.0328 ppm, demonstrating its sensitivity at low concentrations.In terms of performance, the optode offers precision with a relative standard deviation of 4.458% and an accuracy of 97.51%, making it reliable for consistent readings. The sensor exhibits high sensitivity, with a molar absorptivity of 1.139×10^{7} $M^{-1}cm^{-1}$, allowing effective detection even at minimal concentrations. It also demonstrates excellent selectivity against interfering ions like Fe^{3+}, Pb^{2+}, and Zn^{2+}, which could otherwise compromise the results.The optode's color complex remains stable until the 9th day, suggesting good durability. When applied to water samples, the optode detected a Cr (VI) concentration of 0.0664 ppm with good precision and accuracy, although this differed slightly from the UV-Vis spectrophotometer result of 0.0881 ppm. This discrepancy highlights the need for calibration to ensure consistency across different methods.

Keywords: Cellulose triacetate, hexavalent chromium, optode, performance test.

Research area: *Analytical Chemistry*

MICROPARTICLES ZERUMBONE FROM *ZINGIBER ZERUMBET* RHIZOME IN CHITOSAN MODIFIED OLEIC ACID

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Zerumbone is a marker compound of *Zingiber zerumbet* that has antioxidant and anticancer properties. It exhibits low solubility in water, necessitating methods to enhance its solubility, such as creating microparticles with chitosan in oleic acid. Therefore, the research aimed to isolate zerumbone from *Z. zerumbet* rhizome and determine the formation of its microparticles in chitosan in oleic acid. Zerumbone isolated by recrystallization the *Z. zerumbet* essential oil. Six different formulations of microparticle with chitosan (2,5 – 3%), TPP as cross-linker, oleic acid as surfactant, and zerumbone. The formation of microparticles was determined using FTIR. The results showed a zerumbone yield of 0,11% db. The particle size of the best microparticle is 5516 µm, absorptive efficiency is 47%, and amide linkages between the chitosan and oleic acid were confirmed based on FTIR. The microparticles have a value lower than LC_{50} compared to only zerumbone. The microparticles of zerumbone in chitosan modified oleic acid have great potential for the delivery of zerumbone as its activity.

Keywords: Absorption efficiency test, BSLT test, microparticles, *Zingiber zerumbet*

Research area: *Analytical chemistry*

TRENDS IN BIMETALLIC NANOMATERIALS AND METHODS FOR REMOVAL OF P-NITROPHENOL AND ITS DERIVATIVES FROM WASTEWATER

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The current study aims to identify the extent to which bimetallic nanoparticles (NPS) are considered highly effective in removing p-nitrophenol (PNP) and its derivatives from wastewater by using various bimetallic NPS. Many previous studies have been conducted to determine the conversion rate and reduction cycles of all types of bimetallic NPS. The findings indicated that PNP is removed by using bimetallic NPS to help reduce it into p-aminophenol (PAP). Besides, noble metals are considered the most effective metals that can be used in bimetallic NPS for their high conversion rate, ranging from 95 to 100%. It was concluded that bimetallic NPS of transition metals can serve as efficient catalysts that help to reduce PNP into PAP in the presence of sodium borohydride (NaBH4) as a reducing agent. In addition, a critical analysis of various types of bimetallic NPS were also reported.

Keywords: Bimetallic nanomaterials, organic pollutants, p-nitrophenol, wastewater

Research area: *Analytical Chemistry*

ENVIRONMENTAL ASSESSMENT OF SINGLE-USE LABORATORY PLASTIC WASTE: A CASE STUDY

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The fast-paced nature of scientific research often leads to a reliance on convenient single-use plastic consumables due to its noncytotoxicity, sterility, affordable price, shatterproof and durable feature. Plastics have been causing serious environmental issues such as climate change due to greenhouse gases (GHGs) emission. Hence, this study investigated the environmental impact of single-use laboratory plastic waste in a Biological Sciences laboratory of a private university in Malaysia, serving as a case study for Southeast Asia. The information related to the waste management methods and waste data from 2014 to 2023 were collected from the laboratory manager. The environmental impact analysis evaluated the GHGs emissions associated with the end-life management of single-use laboratory plastic waste, including collection, transportation, and final disposal at designated facilities. The GHGs emissions was calculated manually based on the guidelines provided by the Intergovernmental Panel on Climate Change (IPCC), and emission factors provided by the Department for Energy Security and Net Zero (DESNZ) of the United Kingdom, and Malaysia Energy Commission. As a result, a total of 29,180.11 kg of single-use laboratory plastic waste underwent treatment and disposal through three consecutive methods, i.e. incineration (5.66 kg CO_2eq/kg waste), landfilling with microwave pre-treatment (0.80 kg CO_2eq/kg waste), and landfilling with ozone pre-treatment (0.94 kg CO_2eq/kg waste), over the past decade. This resulted in a total of 29,707.52 kg CO_2eq of GHGs emissions, with the main contribution from transportation emission. Disposal methods, transportation distances, waste collection frequency, and source of energy were found to influence the GHGs emissions. Recognising the environmental impact, universities should actively encourage a shift towards reducing and reusing single-use plastic consumables in the laboratories, especially for practical sessions that usually involve non-hazardous laboratory works.

Keywords: laboratory waste; incineration; landfill; environmental impact; single-use plastic

Research area: *Analytical sciences*

INNOVATIVE CHITOSAN HYDROGELS AS A SUSTAINABLE PLANT GROWTH REGULATOR FOR RESILIENCE AGRICULTURE

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Innovative chitosan hydrogels represent a significant advancement in sustainable agriculture as effective plant growth regulators (PGRs). These hydrogels are derived from chitin and offer high water retention, biodegradability, and biocompatibility. This study examines their potential to enhance plant growth resilience in arid environments by assessing their effects on shoot elongation and nutrient uptake efficiency. The chitosan hydrogel crosslinked with sodium alginate (CS/Al-Na) was synthesized and characterized using Fourier transform infrared spectroscopy (FT-IR), nuclear magnetic resonance (NMR), and field emission scanning electron microscopy (FESEM). Results indicate that CS/Al-Na effectively supports crops under abiotic stresses, particularly in drought-prone areas. Furthermore, its ability to incorporate bioactive compounds positions it as a multifunctional growth enhancer, reducing reliance on synthetic fertilizers and chemical growth regulators. The adoption of chitosan hydrogels as sustainable PGRs has significant potential to enhance resilient agricultural systems, addressing challenges in food security and environmental sustainability.

Keywords: Chitosan, alginate, hydrogel, shoot elongation, swelling

Research area: *Analytical Chemistry*

POTENTIOMETRIC SENSOR-BASED IMPRINTED TS-1 ZEOLITE FOR SELECTIVE DETECTION OF CHOLESTEROL

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This study explains the modification on imprinted zeolites with cholesterol molecules to enhance the selectivity of potentiometric sensors in cholesterol analysis. The cholesterol as the target molecule was incorporated into the conductive and feasibly modified zeolite structures during preparation. The TS-1 zeolite was synthesized through hydrothermal method and characterised with XRD and FTIR-ATR. The diffractogram confirmed the presence of the mobile five I (MFI) zeolite structure with high crystallinity that in line with FTIR spectra which implied the Si-O-Si as well as TiO4 tetrahedral vibrations. The imprinted zeolite (IZ) was then assembled in the sensor together with activated carbon and paraffin with the optimum mass ratio of 11 : 7 : 2 respectively. The sensor performance was tested based on the Nernst factor of 30.92 mV/decade within measurement range of 10-6 – 10-3 M and produced linearity of 0.9895, detection limit of 4.36 x 10-6 M, and 7 weeks stability. In range of 10-6 – 10-3 M, the electrode produced a precision of 99.49 – 99.89% and an accuracy of 66 – 134%. In addition, the IZ electrode exhibited excellent robustness despite the presence of glucose. This project addresses the supports the Sustainable Development Goals (SDGs) especially The Good Health and Wellbeing (Goal no. 3).

Keywords*:* Imprinted zeolite, potentiometry, sensor innovation, cholesterol analysis, SDGs

Research area*: Analytical Chemistry*

GREEN SYNTHESIS OF IRON NANOPARTICLES USING *TAGETES ERECTA* FLOWER EXTRACT FOR THE DETOXIFICATION OF VARIOUS MYCOTOXINS

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The development of eco-friendly and green processes for synthesizing metal nanoparticles with a high surface-to-volume ratio is becoming a crucial branch of nanotechnology due to their remarkable properties and diverse applications. Among various approaches, biosynthesis using plant extracts has emerged as a promising area of research. This study focuses on the rapid and scalable biogenic synthesis of iron nanoparticles (FeNPs) using marigold (*Tagetes erecta*) flower petals as a natural reducing agent, performed at room temperature. The phenolic content in the marigold flower extracts was determined using the Folin-Ciocalteu reagent method. Iron nanoparticles were synthesized from ferric chloride, iron sulfate, and Mohr's salt solutions. Characterization of the synthesized nanoparticles was conducted using UV-visible spectroscopy, Fourier Transform Infrared (FTIR) spectroscopy, and X-Ray Diffraction (XRD) techniques. Both the marigold extracts and the iron nanoparticles derived from them were utilized to detoxify various mycotoxins, including aflatoxin, ochratoxin, and fumonisin. The efficiency of mycotoxin removal was quantitatively analyzed using reverse phase High-Performance Liquid Chromatography (HPLC) with a fluorescence detector (FLD). The results indicated significant degradation of fumonisin, with removal efficiencies ranging from 52.11% to 59.8% using iron nanoparticles. Additionally, the marigold petal extracts alone achieved a 71% to 74% removal of aflatoxins, while a 24% to 26% removal of ochratoxin was observed. This study confirms the effectiveness of marigold-derived iron nanoparticles and petal extracts in mycotoxin removal, highlighting their potential as eco-friendly alternatives for agricultural applications. Further research is recommended to explore the application of other plant materials and to evaluate their environmental and economic viability.

Keywords: Biogenic synthesis, nanoparticles, *Tagetes erecta*, mycotoxins, detoxification.

Research area: *Analytical Chemistry*

VOLTAMMETRIC DETECTION OF AMOXICILLIN RESIDUE IN MILK AT NANOHYBRID MODIFIED SCREEN PRINTED ELECTRODE

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Abstract

Here in, nanohybrid containing gold nanoparticles (AuNPs) and multi-walled carbon nanotubes (MWCNTs) is synthesized. Morphology of the synthesized nanohybrid was characterized by Field Emission Scanning Electron Microscopy and Transmission Electron Microscopy while the elemental composition and crystallography of the composites were investigated by Energy Dispersive X-ray, X-ray Diffraction, Ultraviolet Visible, Thermal Gravimetric Analysis and Raman spectroscopic techniques. The nanohybrid was used to modify a screen printed electrode by drop casting method. Electrochemical characterization of the electrode revealed that the nanohybrid have increased the electro-active surface area and conductivity of the screen printed electrode. The modify electrode was applied for the voltammetric detection of amoxicillin in Bovine milk samples by adsorptive stripping voltammetry (AdSV). Under optimized experimental conditions, AdsV measurements of amoxicillin showed a wide linear dynamic range within the concentration range of 0.2-30 µM. Two linear calibration ranges from 0.2-10 µM and 10-30 µM were observed with equations of I_{pa} (µA) = 2.88 C (µM) + 1.2017; r = 0.9939 and I_{pa} (µA) = 0.88 C (µM) + 22.97; r = 0.9973 respectively. The limit of detection (LOD) and limit of quantification (LOQ) were calculated as 0.015 µM and 0.149 µM, respectively.

Keywords: Voltammetry, Residue, Detection, Nanohybrid, Amoxicillin.
Research Area: *Analytical Chemistry*

ORAL : INDUSTRIAL CHEMISTRY

INTERNATIONAL CONFERENCE OF YOUNG CHEMISTS

INVESTIGATION OF CHITOSAN EFFICACY AS A GOOD DELIVERY BIOPOLYMER FOR ANTI-BREAST CANCER DRUGS THROUGH MOLECULAR DOCKING

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Breast cancer remains a significant global health challenge, necessitating the development of innovative drug delivery systems to enhance treatment efficacy and reduce side effects. Chitosan, a biocompatible and biodegradable polysaccharide, holds promise as a delivery vehicle for anti-breast cancer drugs due to its favourable properties. This study employs molecular docking techniques to assess the effectiveness of chitosan as a carrier biopolymer for therapeutic agents targeting breast cancer. A selection of anti-breast cancer drugs, tamoxifen along with relevant target estrogen receptor alpha (Erα) protein implicated in breast cancer progression are subjected to molecular docking simulation. The interactions between the tamoxifen and chitosan derivatives (**1** and **2**) along with their corresponding target ERα protein have been examined which clarify potential binding energies and affinity as -11.52, -5.92 and -5.40 kcal/mol. Some common amino acids interactions like Ala350, Glu353, Leu346, Leu384, Leu387, Leu525, Met343 were also observed. This indicates both the drug and the two chitosan derivatives follow the route to tissue delivery. However, the chitosan efficacy is effective as it demonstrated high binding energy below -6.00 kcal/mol. This is an index of a good medium for drug delivery. Through computational analysis, this study offers valuable insights regarding the viability and efficiency of chitosan as a biopolymer for delivering anti-breast cancer drugs. This research establishes the foundation for future empirical validation and the enhancement of chitosan-based drug delivery systems for the treatment of breast cancer.

Keywords: Chitosan, biopolymer, anti-breast cancer, drug delivery, molecular docking

DEVELOPMENT OF PPy/MnO_2/N-CNT COATED CARBON FELT ANODE FOR MICROBIAL DEGRADATION OF METHYL YELLOW DYE

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This work on innovative anode modifier nanocomposites by utilizing polypyrrole (PPy), manganese dioxide (MnO_2) and carbon nanotubes (CNT) was conducted to address the dual challenge of environmental pollution and energy scarcity. The advanced anode modifier nanocomposites, specifically PPy/MnO_2, PPy/MnO_2/CNT and PPy/MnO_2/N-doped CNT was designed for the microbial degradation of methyl yellow dye while concurrently harnessing energy in a Microbial Fuel Cell (MFC) system. The nanocomposites were meticulously crafted, integrated into MFC anodes and nanocomposites were characterized using scanning electron microscopy (SEM), X-ray diffraction (XRD), and Fourier-transform infrared spectroscopy (FTIR) to evaluate the morphological, structural, and chemical properties of the anode modifier nanocomposite. Furthermore, their electrochemical behaviour was analysed through cyclic voltammetry and chronoamperometry, showcasing heightened catalytic activity and stability. The MFCs, equipped with the innovative anode modifier nanocomposites, were employed for microbial degradation of the azo dye. Energy recovery was monitored simultaneously and a symbiotic relationship between environmental remediation and sustainable energy generation was established. Results revealed that the PPy/MnO_2, PPy/MnO_2/CNT, and PPy/MnO_2/N-CNT nanocomposites significantly enhanced dye degradation and energy recovery compared to the traditional anode materials. This research contributes to the development of multifunctional anode materials capable of efficient dye degradation and concurrent energy harvesting in MFCs. The nanocomposites showcase promising environmentally friendly and energy- efficient applications, bridging the gap between pollution remediation and sustainable energy production.

Keywords: Nanocomposites, Microbial Fuel Cell (MFC), Dye degradation, Energy recovery

DEVELOPMENT OF A 3D REDUCED GRAPHENE OXIDE AEROGEL FOR TREATMENT OF PHARMACEUTICAL WASTEWATER

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The discharge of pharmaceutical wastewater containing diclofenac has caused adverse effects on human health and the environment. Graphene oxide is an innovative adsorbing material that poses superior adsorption efficiency, but its nano-sized scale restricts its application in large scale wastewater treatment. This project aims to address the issue by developing a three-dimensional (3D) reduced graphene aerogel via ice-templating method. The 3D graphene aerogel exhibited desirable properties such as lightweight (20.39 mg/cm^3), relatively large surface area (132.19 m^2/g) and different pore sizes (2 – 90 nm) formed by interconnected graphene nanosheets. The effectiveness of the aerogel in removing diclofenac from wastewater was evaluated through column adsorption mode. It was found that the breakthrough time for the column increases (30, 75, 130 min) with increasing bed height (10, 12.5, 15 cm), but decreases with increasing concentration (25, 50, 75 mg/L) and feed flowrate (1, 2, 3 cm/min). The bed-depth-service-time (BDST) model properties were evaluated and applied to generate the mathematical expression to describe the column operation time based on bed height. The bed height and column operation time exhibited a linear trend, and the mathematical equation developed by the BDST approach demonstrated high correlation coefficient, R^2 (>0.99). The highest adsorption capacity was found to be 84.50 mg/g, with 50% bed saturation attained within 397.13 min, as predicted by the Thomas model. Overall, the results of this study indicate the high effectiveness of the 3D graphene aerogel in the removal of diclofenac pharmaceutical from wastewater.

Keywords: Adsorption, reduced graphene oxide, pharmaceutical residue, wastewater

Research area: *Material Chemistry & Advanced Materials*

NEOTERIC GREEN SOLVENTS FOR IMPROVED SOLUBILITY AND ANTIOXIDANT ACTIVITY OF α-TOCOPHEROL

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Conventional organic solvents in pharmaceutical formulations pose environmental and health risks due to their toxicity and volatility, prompting the need for greener alternatives. Deep eutectic solvents (DESs) have gained prominence as versatile green solvents, offering tailorability in physiochemical properties through their initial components and molar ratio adjustments. This study addresses the underexplored application of DESs in the dissolution of bioactive compounds like α-tocopherol (vitamin E), known for its potent antioxidant properties. This study synthesized hydrophilic DES-1 (choline chloride:acetic acid, 1:2), hydrophobic DES-2 (choline chloride:sucrose:water, 4:1:4), DES-3 (tetraoctylammonium bromide:decanoic acid, 1:2), and DES-4 (decanoic acid:dodecanoic acid, 3:1). The synthesized DESs were characterised through FTIR spectroscopy, viscosity and density analyses. DES-4, being hydrophobic, exhibited the lowest density and viscosity, while hydrophilic DES-2 displayed the highest. The solubility study of α-tocopherol in DESs revealed varying degrees, with DES-4 exhibited the highest solubility, with a value of 102×104 mg/L, attributed to its hydrophobic nature and low viscosity. α-tocopherol dissolved in DESs demonstrated superior reducing capacity compared to hexane, though DES-1 and DES-2 exhibited notable radical scavenging activity. Overall, DESs enhanced the solubility and antioxidant properties of α-tocopherol compared to conventional organic solvents. This study highlights the potential of DESs for customized drug formulations, illustrating their adaptability within the realm of sustainable chemistry. The findings underscore the importance of exploring green and sustainable solvents in pharmaceutical applications, contributing to the global effort towards environmentally friendly and effective drug development.

Keywords: Deep eutectic solvent (DESs), α-tocopherol, Solubility, Antioxidant, Pharmaceutical

Research area: *Industrial Chemistry*

ENHANCING LIGNIN PROPERTIES *via* STEAM EXPLOSION PRETREATMENT: A NOVEL MODIFICATION APPROACH

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This study investigates the effects of different delignification processes on oil palm frond (OPF) biomass and focuses on the structural characteristics and antioxidant properties of lignin isolated with and without pretreatment. The pretreatment involves steam explosion (SE) followed by ethanol organosolv pulping, while the direct method uses ethanol organosolv pulping alone. Functional groups in organosolv lignin (OL) and steam explosion organosolv lignin (SEOL) were analyzed and compared using multiple complementary analyses such as FTIR spectroscopy, NMR spectroscopy, GPC chromatography, HPLC chromatography, CHN and thermal analyses, lignin antioxidant activity *via* reducing power assay and dissolution test. The findings reveal that SEOL achieved the highest solid recovery at 11.50 % yield, surpassing OL, which yielded 8.66 %. Both isolated lignin types predominantly feature non-condensed G-type and S-type units, with relatively fewer H-type units, consistent with existing research. Moreover, this study confirms that modification of lignin with SE pretreatment reduces its molecular weight (Mw) and generates smaller fragments, enhancing its water solubility relative to unmodified lignin (D_{SEOL}: 37.43 % > D_{OL}: 17.50 %). This demonstrates that SEOL exhibits enhanced antioxidant properties with superior reducing power compared to OL. Therefore, modifying lignin polymers has improved their antioxidant properties and structural features, paving the way for various innovative approaches in lignin-based applications.

Keywords: Oil palm frond, steam explosion, organosolv pulping, lignin

Research area: *Industrial Chemistry*

GREEN APPROACH TO PRODUCE LIGNIN NANOPARTICULES

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Lignocellulosic biomass is a complex and resistant plant material, composed mainly of the three highly entangled polymeric fractions cellulose, hemicellulose and lignin. In this work, we are particularly interested in the under-valued lignin polymer, which is mainly used for thermal upgrading, even though it contains high-value-added monomers. Lignin is in fact a generic term for a large family of biopolymers with aromatic skeletons. It is renewable, biodegradable, very abundant (it is the second most abundant biopolymer on earth after cellulose), and accounts for 30% of non-fossil organic carbon in nature. Thanks to their aromatic structure, these lignins possess numerous properties (biocides, antioxidants, UV light blockers...) that could be useful in a wide range of technical applications. To date, most of the work published in the literature has focused on the recovery of lignins from the Kraft process, which are waste products from the paper industry. In this work, another approach is developed ('lignin first' method), where lignin is considered as a resource and not as a waste product. To this end, lignin is extracted from forestry (hardwood and softwood) and agricultural (grass) waste using eco-friendly processes such as steam explosion or organosolv. In a second stage, we optimized macrolignin size reduction using anti-solvent precipitation. The technique used generates particles of controlled size (between 60 and 150 nm) that are stable over time when in aqueous suspension. An experimental design has also been developed to predict the particles size. Finally, various lignin valorizations were considered: 1) to improve the UV resistance of PVA-based plastic materials, 2) to replace non-biosourced and poorly biodegradable nanoparticles in cosmetic applications (sunscreens) and 3) to formulate Pickering emulsion.

Keywords: Lignin, nanoparticles, biorefinery, organosolv process, steam explosion pretreatment

Research area: *Biorefinery*

REFORMING WOOD PRESERVATIVE DELIVERY: EMPLOYMENT OF TEBUCONAZOLE-LOADED SELF-EMULSIFYING DRUG DELIVERY SYSTEM (SEDDS) AND TEBUCONAZOLE-LOADED ZEIN NANOPARTICLES

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Wood preservation found its importance to protect the wood from deterioration and new technology has emerged to improve current preservative usage under the vacuum pressure system. In this research, tebuconazole-loaded self-emulsifying drug delivery system (TEB-SEDDS) and tebuconazole-loaded zein nanoparticles were synthesised. The SEDDS consists of palm oil as oil, Tween 80 as surfactant and PEG as co-surfactant. The preferred ratio of palm oil, Tween 80 and PEG was determined by constructing the pseudo-ternary phase diagram using the water titration and light penetration method. The optimised SEDDS formulation consisted of 0.04% palm oil, 0.06% S_{mix}, and 99.9% water. The formulation was kinetically stable for up to 3 days and visually translucent. The loading efficiency of TEB in the system was between 103.54 to 115.17 %, determined through UV-Vis spectrophotometry method. On the other hand, tebuconazole-loaded zein nanoparticles (TEB-zein NP) were synthesised via pH nanoprecipitation method, using Tween 80 as surfactant. Optimised nanoparticles were synthesised, producing nanoparticles with hydrodynamic particle size at 146.4 ± 10.66 nm. Both approaches treated rubberwood *Hevea brasiliensis* and tested for anti-fungi assays using brown rot fungi *Trametes versicolor*. Preliminary results are expected to display good antifungal activity against brown rot fungi and can be a potential alternative for industrial wood treatment.

Keywords: Wood preservation, tebuconazole, nanotechnology, encapsulation, SEDDS, zein, palm oil

Research Area: *Industrial Chemistry*

ORAL : BIOCHEMSITRY

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IN SILICO PEPTIDOMICS IN IDENTIFYING NOVEL BIOACTIVE PEPTIDES FROM SLUDGE WORM (*TUBIFEX TUBIFEX*): A GREEN CHEMISTRY APPROACH

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Recently, there has been a growing interest in using peptides as treatments because of their specificity, i.e., targeted therapy, and safety, i.e., minimal side effects compared to other treatments. The traditional peptidomic analysis typically requires extensive *in vitro* laboratory tests, which can be time-consuming and resource-intensive and lead to the generation of substantial chemical waste. The study aimed to utilize bioinformatics to discover novel bioactive peptides and explore their potential bioactivity in an aquatic organism, the sludge worm (*Tubifex sp.*). The work introduced a workflow incorporating a sustainable, cost-effective, and quick *in-silico* method for sludge worm peptidomic studies. Firstly, *Tubifex sp.* protein was found in the UniProt database. *In silico* proteolysis was performed using digestive enzymes (trypsin, chymotrypsin, pepsin, and combinations) to produce a list of 398 novel bioactive peptides. These peptides were then screened through PeptideRanker and BIOPEP for potential bioactivity. HPEPDOCK 2.0 and PDBSUM were used for docking to predict the bonding interactions and identify the number of hot-spot residues that contribute to the interaction for angiotensin-I-converting enzyme (ACE) inhibitory and dipeptidyl peptidase-IV (DPP-IV) activities. The peptide's toxicity, allergenicity, hydrophobicity, and Lipinski Rule were characterized (ToxinPred, AllerTOP v.2, Peptide 2.0, and ADMETlab 2.0). Validation was further conducted using Mass spectrometry analysis. There were 5 out of 6 proteins that matched the PEAKS database of *Tubifex sp.* A list of 398 novel peptides was produced from *in silico* proteolysis. A total of 53 peptides were selected at a threshold of 0.5 using the PeptideRanker. 34 out of 53 were determined to be non-allergenic and non-toxic and chosen to conduct docking analysis. Overall, the top 8 hits of novel bioactive peptides from the pool of 398 peptides were selected based on their highest importance: Docking score > number of hotspots > toxicity and allergenicity > hydrophobicity and Lipinski Rule. The study showcased that bioinformatics helps with sustainable development by simulating in vitro laboratory experiments, which offer an alternative to peptidomic research. The application of *in silico* methods for high-throughput screening improves the efficiency of the bioactive peptide discovery process. This facilitates more targeted research, which in turn cuts down on research time and chemical usage that harms the environment. Overall, bioinformatics is in line with the green chemistry principle, making it a suitable and sustainable solution for peptidomic analysis.

Keywords: green technology, sustainable, peptidomic analysis, bioinformatics, bioactive peptide

Research area: *Biochemistry*

DESIGN AND *IN SILICO* MODELLING OF HETEROCYCLIC-BASED XANTHONE DERIVATIVES AS POTENTIAL ANTICANCER AGENT THROUGH TYROSINE KINASE INHIBITION

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Cancer is one of the deadliest diseases nowadays, and tyrosine kinase receptors play crucial roles in cancer cell survival, differentiation, proliferation, and migration. In this work, we designed and developed a new inhibitor from heterocyclic-based xanthone derivatives to target two tyrosine kinase receptors, i.e., epidermal growth factor receptor (EGFR) and platelet-derived growth factor receptor (PDGFR) through in silico screening. Eighteen heterocyclic-based xanthone derivatives were optimized using density functional theory (DFT) and evaluated through molecular docking for both EGFR and PDGFR receptors. All heterocyclic-based xanthone derivatives gave the root-mean-square deviation (RMSD) value lower than 2.00 Å. Xanthone with isobenzothiazole substituent (iBzThio) was found as the most potential inhibitor with binding energy of -10.60 and -12.61 kcal/mol against EGFR and PDGFR, respectively. Further investigation has been performed through molecular dynamics simulations for 100 ns. From the results of molecular dynamics simulations, i.e., RMSD, RMSD, root-mean-square fluctuation (RMSF), radius of gyration (RoG), solvent accessible surface area (SASA), and binding energy parameters, as well as secondary structure fraction, dictionary of protein secondary structure (DSSP), and Ramachandran plot, the iBzThio demonstrated good stability to interact with the active site of both EGFR and PDGFR receptors. The binding energy of iBzThio against EGFR and PDGFR receptors at the final simulation time was -12.58 and -12.90 kcal/mol. These findings revealed that iBzThio is a potential candidate as anticancer agent through tyrosine kinase inhibition mechanism.

Keywords: anticancer; drug design; molecular docking; molecular dynamics; xanthone

Research area: *Medicinal Chemistry / Computational Chemistry*

DISCOVERY OF INDOLENINYL-PYRAZOLO[3,4-*b*]PYRIDINES AS POTENT CHEMOTHERAPEUTIC AGENTS AGAINST COLORECTAL CANCER CELLS

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New series of indoleninyl-pyrazolo[3,4-*b*]pyridines derivatives were synthesized *via* a condensation between substituted 1,3-dialdehyde indolenines and 3-aminopyrazoles. The structures were characterized by NMR (^{1}H, ^{13}C), FTIR, mass spectroscopy, and single X-ray crystallography. In order to obtain efficient method to access pyrazolo[3,4-*b*]pyridines, a few entries have been optimized. By applying the optimized reaction conditions, it was found that the presence of a 37% hydrochloric acid catalyst proceeded smoothly and gives conversion yield **4a-o** up to 96% yields. The present method enables the versatile formation of the pyrazolo[3,4-*b*]pyridine framework, tolerating a broad range of electronic substituents on both precursors. X-ray crystallography of a representative derivative, **4n**, revealed two nearly planar conformations, with the *N*-atom of the pyridyl residue either *syn* or *anti* to the pyrrole-*N* atom in the two distinct molecules within the asymmetric unit. In molecular docking stimulation compounds containing a phenyl group (**4k–o**) exhibit greater binding. Out all these compounds, **4n** has the strongest ability to bind with DNA. *In vitro* antitumor activity against human colorectal cancer cell lines (HCT 116 and HT-29) and normal colon fibroblasts (CCD-18Co) were assessed by using MTT cytotoxicity assay. Some of the tested compounds displayed a good anticancer activity on HCT 116, whereas compounds **4k** and **4n** exerted higher cytotoxicity against both cancer cell lines. These fundamental outcomes offer opportunities in structural functionalization in drug development.

Keywords: Indoleninyl, X-ray crystallography, MTT assay, HCT 116, HT-29, CCD-18Co

Research area: *Bioorganic Chemistry*

IN VITRO KINETICS OF CYCLOOXYGENASE-2 (COX-2) INHIBITION BY *SPAGNETICOLA TRIBOLATA* EXTRACT

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Inflammation is a local response to cellular injury marked by redness, swelling, pain, tenderness, heat, and disturbed function of an area of the body causing discomfort for patients. Inflammation is usually treated by taking anti-inflammatory drugs, one of which is an inhibitor of the cyclooxygenase-2 (COX-2) enzyme. *Spagneticola tribolata* or *wedelia* is an Indonesian medicinal plant that has been reported to have the potential as an anti-inflammatory. However, its activity to inhibit COX-2 is still unknown. This study aims to investigate its ability in inhibiting COX-2 activity *in vitro*. Dry leaves of *S. tribolata* was extracted with water and ethanol 70% (EtOH70). The 25 mg/L of water extract gave the COX-2 inhibition activity more than 90% while the EtOH70 extract showed the increasing inhibition activity up to 99% from 25 to 1000 mg/L of EtOH70 extract. Based on Lineweaver-Burk analysis, the water extract of *S. tribolata* had a competitive inhibition type, where there was a change in the enzyme-substrate affinity (K_M) value to be greater than without an inhibitor, but the maximum reaction rate remains relatively constant, with the *K*i value of 135.19 µM. This result shows that *S. tribolata* water extracts has a potential to be further developed as an anti-inflammatory agent.

Keywords: Anti-inflammatory, cyclooxygenase-2, *Spagneticola tribolata*, *wedelia*

Research area: *Biochemistry/Physical Chemistry*

POSTER: PHYSICAL CHEMISTRY

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PALM OIL MILL EFFLUENT (POME): ENVIRONMENTAL CHALLENGES AND EXPLORING SUSTAINABLE APPLICATIONS FOR ECO-FRIENDLY SOLUTIONS

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Malaysia is the second largest producer of palm oil in the world. Palm oil mill effluent (POME), an industrial waste of the palm oil manufacturing process, poses significant environmental and management challenges. The environmental consequences of POME are intensified by its significant organic load, results in increased chemical oxygen demand (COD) and oxygen demand (BOD). The variability of its composition and its large volume further complicates the challenges associated with its environmental discharge. Because of its abundant availability and composition, POME also offers a cost-effective and environmentally friendly raw material for various applications. This review analyzes the environmental challenges associated with palm oil mill effluent (POME) and explores sustainable alternatives for POME. A comprehensive literature search was conducted using PubMed, Google Scholar, Scopus, and Web of Science databases, specifically focusing on studies within the last ten years. The assessment highlighted the utilization of POME as a sustainable resource for the production of biogas, bioethanol, biodiesel, biohydrogen, and microbial fuel cells. Despite the potential applications, significant research gaps remain, especially in enhancing the effectiveness and cost-efficiency of advanced treatment technologies and in establishing sustainable practices that provide a balance between economic sustainability and environmental protection.

Keywords: Palm oil mill effluents (POME), applications, environmental challenges

Research area: *Environmental Chemistry*

PHOTOLUMINESCENCE STUDIES ON ZINC-NEODYMIUM LAYERED DOUBLE HYDROXIDE

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The development of stable and inexpensive materials for industrial applications is a central problem in modern materials science. The main requirements for such materials are high stability, eco-friendly, simplicity and repeatable synthetic procedures. Zinc-neodymium layered double hydroxide (LDH) materials fulfill many of these requirements and have potential application in luminescent fields. This work is aimed at preparing a novel ZnNd-LDH by coprecipitation method to investigate the luminescence property of the prepared sample. The characterization was carried out using X-ray diffraction (XRD), Fourier transform infrared (FTIR) spectroscopy, Scanning electron microscopy (SEM), Energy dispersive X-ray spectroscopy (EDX), Thermogravimetric analysis (TGA), Brunauer-Emmett-Teller (BET) analysis and fluorescence spectroscopy. XRD analysis demonstrates expanded interlayer spacings confirming successful intercalation of the rare earth ions. FTIR indicates the major functional groups which correspond to the layered nature of the material, where the peaks at 451, 513 and 822 cm^{-1} affirm the formation of the ZnNd-LDH. The peaks correspond to the Nd–O stretching frequencies due to the incorporation of Nd^{3+} ions within the LDH matrix. SEM reveals the structural morphology, high-resolution images and the synthesized sample present a structure with hexagonal symmetry and high crystallinity of ZnNd-LDH framework. The ZnNd-LDH were further characterized by the luminescence emission spectra where the fluorescence spectroscopy of as-prepared LDH excited at the wavelength of 280 nm, which suggest that incorporation of rare earth into LDH enhances the surface charge separation and lower the bandgap by high charge injection efficiency.

Keywords: Layered double hydroxide, zinc, neodymium, characterization, luminescence property.

Research area: *Material Chemistry*

POSTER: ANALYTICAL CHEMISTRY

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CO_2 REMOVAL VIA AQUEOUS METHYLDIETHANOLAMINE-TETRABUTHYLPHOSPHONIUM P-TOLUENE SULFONATE ([MDEA]-[TBP][p-TSA]) HYBRID SOLVENT

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The presence of acid gases in natural gas (NG), particularly carbon dioxide led to issues such as pipelines corrosion and reduce quality of NG. In traditional methods of carbon dioxide removal in natural gas processing, such as scrubbing technology, commercial aqueous amine solutions are commonly used as absorbents. However, one disadvantage of these solutions is their high energy requirement for regeneration. An alternative to commercial aqueous amine solution is ionic liquids, which generally have lower heat capacity and higher CO_2 removal capacity. However, the use of ionic liquid possesses challenges such as expensive and high viscosity. The main purpose of this project is to investigate the solubility of carbon dioxide (CO_2) in an aqueous methyldiethanolamine-tetrabutylphosphonium p-toluene sulfonate ([MDEA]-[TBP][p-TSA]) new hybrid solvent. In this study, the density, viscosity and refractive index of aqueous [MDEA]-[TBP][p-TSA] hybrid solvents containing different weight percentage of MDEA and [TBP][p-TSA] were determined. Raman spectroscopy was employed to identify carbamate formation and the presence of CO_2 in aqueous [MDEA]-[TBP][p-TSA], demonstrating that CO_2 is chemically absorbed by MDEA, converting it to carbamate, while [TBP][p-TSA] physically adsorbs CO_2. Response Surface Methodology (RSM) based on face centered-central composite design (FC-CCD) was used to design the experiments and explore the effects of four independent parameters in predicting the removal of CO_2 by aqueous [MDEA]-[TBP][p-TSA]. These four independent parameters are concentration of MDEA, (30–50 wt.%), concentration of [TBP][p-TSA], (2–20 wt.%), pressure of CO_2 (2–30 bar) and temperature (30–60 ℃). The experimental data was analysed by the analysis of variance (ANOVA) within the RSM-FCC-CCD framework to predict the CO_2 removal capacity. An attempt was made to validate the CO_2 removal predicted by RSM. Based on a validation study, the experimental data showed a percentage error between 0.18% and 2.71% as compared to the predicted value of CO_2 removal by RSM.

Keywords: Carbon dioxide, ionic liquid, absorption, Response Surface Methodology (RSM)

Research area: *Analytical Chemistry*

CUTTING-EDGE ELECTRODIALYSIS METHODS FOR ANALYTICAL SEPARATION

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Abstract

The rise of industrialization and human activities has led to critical challenges in environmental sustainability, food safety, and public health. It is crucial to produce pure products with minimal contamination that could harm humans. Various advanced separation techniques, including electrodialysis, have been developed to achieve high product purity and reduce processing time. This review comprehensively explores the application of electrodialysis techniques in separation processes such as matrix removal, chiral separation, speciation analysis, and macro-to-micro scale analysis. This work also summarizes studies on parameter optimization and membrane fabrication to enhance separation efficiency. Lastly, the review discusses strategies to enhance membrane dialysis performance and presents future industrial-scale electrodialysis applications. This comprehensive work provides valuable insights into the use of electrodialysis for separation in process analysis and offers guidance for its future application.

Keywords: purification, separation, electrodialysis, membrane

Research area: *Analytical Chemistry*

POSTER: INORGANIC CHEMISTRY

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ACTIVATION OF PERSULFATE BY ZEOLITE SUPPORTED CUO CATALYSTS FOR PHENOL DEGRADATION

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In this study, by taking the advantages of the characteristics of zeolite materials such as abundant surface sites and rich electrons, zeolite-supported copper oxide (Cu-Zeolite) was successfully prepared by impregnation and calcination method. Afterwards, activation of persulfate (PDS) by Cu-Zeolite for phenol degradation and the related reaction mechanism was systematically studied. It was found that the Cu-Zeolite/PDS system could effectively degrade phenol under neutral conditions without the dissolution of Cu^{2+}. Different from the conventional sulfate radicals based advanced oxidation processes (AOPs), Cu-Zeolite/PDS could selectively degrade aromatic compounds with hydroxyl and chlorinated groups, suggesting that Cu(III) would be the main active species. Zeolite could effectively improve the catalytic activity of CuO by two aspects: (a) the formed Al-O-Cu bonds could enrich electrons on Cu sites to improve of the catalyst, and (b) the abundant hydroxyl groups on the zeolite surface would favour the adsorption and subsequently activation of PDS. Effects of parameters on the phenol degradation in the system, such as initial pH, PDS concentration, and catalyst dosage, were also investigated. Inorganic anion Cl^- presented marginal effect on the degradation, while $H_2PO_4^-$ almost completely inhibited the reaction. Besides, continuous-flow column test of the Cu-Zeolite/PDS system was conducted in effectively treating a simulated phenolic wastewater with the background of coking wastewater.

Keywords: Copper-based catalyst, zeolite, Fenton-like reaction, persulfate, phenol

Research area: *Inorganic Chemistry*

Enhanced Photocatalytic Generation of H_2O_2 via a Composite of ZIF-8 and Carbon-Doped g-C_3N_4 Derived from Kapok Fiber

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Recently, g-C_3N_4 has demonstrated significant potential as a sustainable, non-metal photocatalyst capable of harnessing visible light to drive a wide variety of photocatalytic processes. However, the inherent limitations of the bulk g-C_3N_4 photocatalyst, such as its limited light-harvesting capacity, small surface area, and low efficiency in photogenerated charge separation, have significantly impeded its photocatalytic activity, especially in the production of hydrogen peroxide (H_2O_2). In this study, we successfully developed a chemically bonded nanocomposite photocatalyst by constructing an association between zeolitic imidazolate frameworks (ZIF-8) and carbon-doped g-C_3N_4 (CCN), which was derived from kapok fiber via a facile hydrothermal approach, resulting in the formation of the ZIF-8/CCN composite. ZIF-8 and CCN were chemically bonded through π–π stacking and hydrogen bond interactions, as confirmed by X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR), and X-ray photoelectron spectroscopy (XPS) analyses. Significant advancements have been achieved in charge separation and photon absorption within the chemically bonded nanocomposite photocatalyst through the combined effects of in-situ carbon doping and the microtubular structure of CCN, which is derived from kapok fiber. The synthesized ZIF-8/CCN successfully enhanced the photocatalytic production of H_2O_2 to 3481 μMg^{-1} h^{-1} compared to pristine g-C_3N_4. The combination of facile preparation and highly efficient photocatalytic performance demonstrates that the modified photocatalyst has the potential to be a highly promising alternative for H_2O_2 production in practical applications.

Keywords: Composite, in-situ carbon doping, hydrogen peroxide, chemically bonding

Research area: *Inorganic Chemistry*

POSTER: INDUSTRIAL CHEMISTRY

INTERNATIONAL CONFERENCE FOR YOUNG CHEMISTS

SYNTHESIS, CHARACTERIZATION, AND APPLICATIONS OF AMBI-FUNCTIONAL PANI/GO/MOF-Fe_3O_4 MAGNETIC NANOCOMPOSITE FOR REMOVING INDUSTRIAL DYE AND EMERGING CONTAMINANT

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Discharging industrial dyes and emerging contaminants (ECs) into water resources has become a serious environmental concern. A novel PANI/GO/MOF-Fe_3O_4 nanocomposite has been synthesized to remove Methyl Orange (MO) and Naproxen Sodium (NAP) from the wastewater. FTIR, XRD, SEM, TGA, BET, and XPS techniques have been exposed to identify nanocomposites’ morphology, composition, and thermal stability. Langmuir and Freundlich’s models revealed that the Langmuir model better describes adsorption ($R^2 = 0.999$ for MO and 0.998 for NAP). Moreover, the findings of kinetic studies established a pseudo-second-order model with good agreement with the experimental results ($R^2 = 0.995$ for MO and NAP), indicating the dominance of chemisorption. The pseudo-first-order reaction model provided reasonable fits ($R^2 = 0.892$ for MO and 0.872 for NAP). Thermodynamic analysis indicated exothermic ($\Delta H^o = -17.72$ kJ $mol^{-1}$for MO and -28.28 kJ $mol^{-1}$for NAP) and spontaneous ($\Delta G^o = -3.877$ kJ mol^{-1} for MO and -5.416 kJ mol^{-1}) nature of dye and ECs. The PANI/GO/MOF-Fe_3O_4 nanocomposite exhibited significant adsorption for MO (239.78 mg g^{-1}) and NAP (40.64 mg g^{-1}), respectively. Furthermore, the ease of recovery (up to 4 cycles) of the nanocomposite enhances its sustainability, offering a viable approach to industrial dye and emerging using ambi-functional nanocomposite.

Keywords: Adsorption, wastewater treatment, magnetic nanocomposite, industrial dyes, emerging contaminants

Research area: *Industrial Chemistry*

POSTER: BIOCHEMISTRY

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DESIGN, SYNTHESIS AND MECHANISTIC STUDIES OF NOVEL BENZIMIDAZOLES AS A NOVEL CLASS OF THERAPUETICS AGAINST DRUG-RESISTANT ORAL CANCER CELLS

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Utilising compounds which are of a different class than the current oral cancer drugs targeting novel cancer targets such as sirtuins is one of the promising strategies in combating drug-resistant oral cancer. Although benzimidazoles have consistently attracted interest as anticancer agent, they have not been greatly explored as oral cancer therapeutics and none of the current treatments for oral cancer bear the benzimidazoles moiety. This makes benzimidazoles which are active against novel cancer targets such as sirtuins an interesting scaffold for exploration as oral cancer therapeutics. Following the anticancer property exhibited by our previously reported benzimidazole-based sirtuin inhibitor **BZD9Q1**, we have carried out several structural modifications at position 5 and evaluated these derivatives primarily against oral squamous carcinoma cells (OSCCs). The synthesised compounds exhibited weak to good inhibitory activities in reducing the viability of the tested OSCC cell lines. Currently, we have identified one derivative with remarkable anticancer activity and equipotent to cisplatin against the tested oral squamous carcinoma cell lines (OSCC) such as cisplatin-sensitive (H103) cells. One of the advantages of the novel compound is that it demonstrates significant anticancer activity against cisplatin-resistant (H103cisD2, H314) cell lines. To further understand the mechanism of action exerted by the **BZD9Q1** derivative in inhibiting the viability of the OSCC cells, flow cytometry-based analyses (cell cycle, apoptosis), and transcriptomic studies (mRNA, miRNA sequencing) were carried out. The lead derivative arrested H103cisD2 cells at G2/M checkpoint and induced late apoptosis to reduce the viability of H103cisD2 cells. The differential gene analysis revealed that the cell death conferred by lead compound may be induced through endoplasmic reticulum (ER) stress. The ER stress-related cell death will be further validated using qPCR and immunoblotting assays.

Keywords: Benzimidazole, anticancer, oral cancer, resistant, ER stress

Research area: *Biochemistry*

POSTER: ORGANIC CHEMISTRY

INTERNATIONAL CONFERENCE FOR YOUNG CHEMISTS

INVESTIGATING THE POTENTIAL OF PRENYLATED AND GERANYLATED ACYLPHLOROGLUCINOL-BASED XANTHENONES AS POTENT SOYBEAN 15-LIPOXYGENASE INHIBITORS: A COMBINED *IN VITRO* AND *IN SILICO* APPROACH

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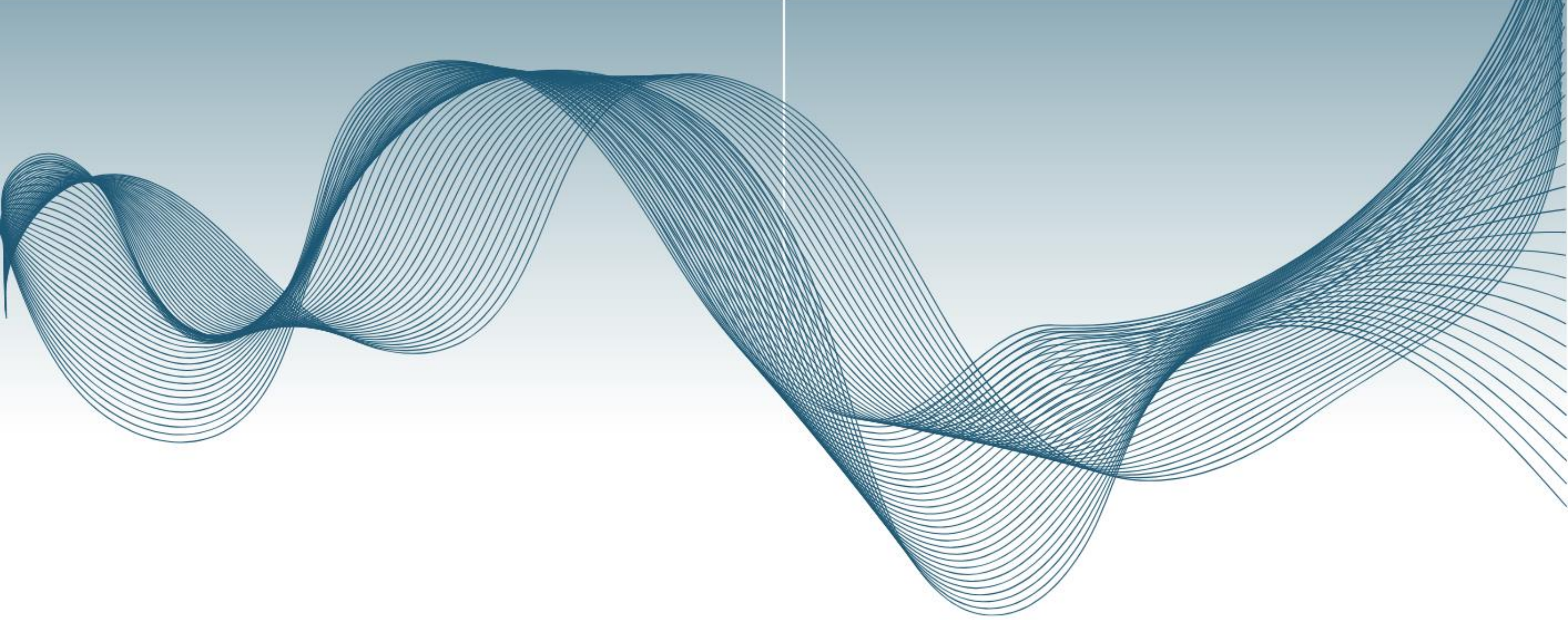
Abstract

Molecular hybridization (MH) has emerged as a novel synthetic approach that combines the pharmacophoric moieties of different bioactive compounds to create hybrids with enhanced affinity and efficacy compared to the parent compounds. In our previous study, a novel series of prenylated and geranylated acylphloroglucinol-based xanthenones hybrid compounds were synthesized using an eco-friendly and facile LiHMDS-induced *in situ* cyclocondensation reaction. To investigate the effect of hybridization on the lipoxygenase (LOX) properties of the natural lead compound 2,4,6-trihydroxy-3-geranylacetophenone (tHGA, **1b**), the soybean 15-lipoxygenase (15-sLOX) inhibitory activity of the hybrids was evaluated, followed by *in silico* docking simulations to study their binding mechanisms with the biological target. Results indicated that all synthesized hybrids **3(a-f)** inhibited 15-sLOX with an IC_{50} value ranges from 0.04 ± 0.1 µM to 5.27 ± 1.7 µM. In comparison to the parent compound tHGA (**1b**, IC_{50}: 23.6 ± 1.7 µM), hybrids are therefore 4.5 to 590-fold more active. Structure activity relationships (SARs) study revealed that introduction of electronic aromatic substituent (-Cl and $-N(C_2H_5)_2$) at ring C of xanthenone improved the inhibitory activity. Molecular docking results were correlated with the *in-vitro* 15-sLOX assay results in which the most active xanthenone hybrid of tHGA (**3e**) exhibited the highest dock score (-10.67 kcal/mol). MD simulation (100ns) confirmed the docking results and provides insights into the 15s-LOX inhibitory profile of the potential lead. This study demonstrates that optimizing tHGA through hybridization with natural pharmacophore such as xanthenone can produce a promising lead compound with enhanced bioactivity and pharmacokinetic properties, offering a new, safe, and effective anti-inflammatory treatment.

Keywords: Molecular hybridization, acylphloroglucinol-based xanthenones, tHGA, 15-sLOX, docking simulations.

Research area: *Organic Chemistry*



THANK YOU

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