MOLECULAR DOCKING AND ADME PROFILING OF XANTHORRHIZOL DERIVATIVES AS HYALURONIDASE INHIBITORS

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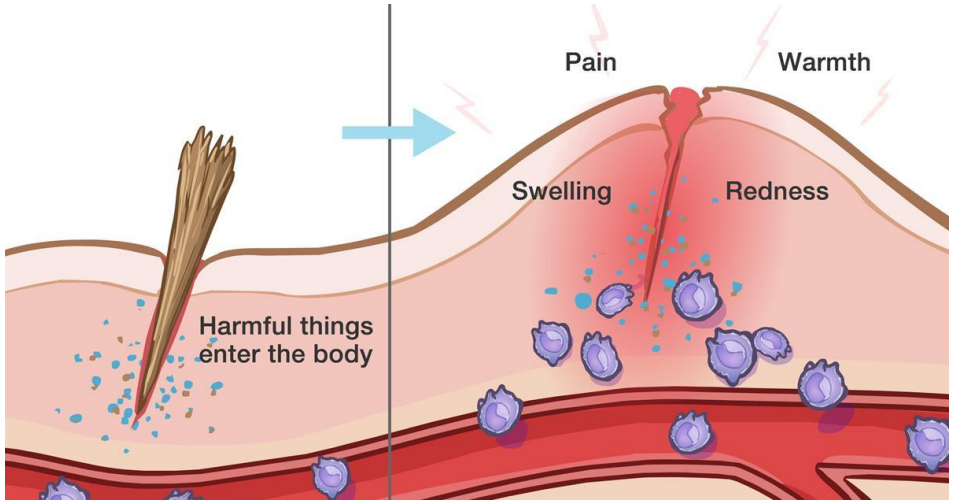
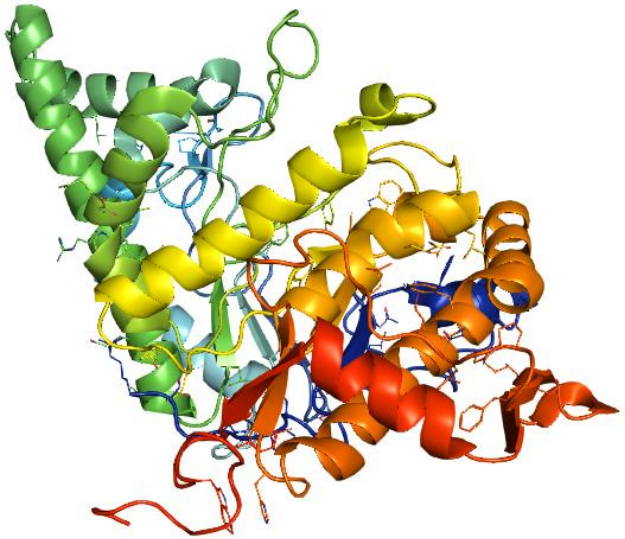
Inflammation



Immune system's response **to maintain the integrity** of human body after exposure to pathogens or external injury[1]

Hyaluronidase

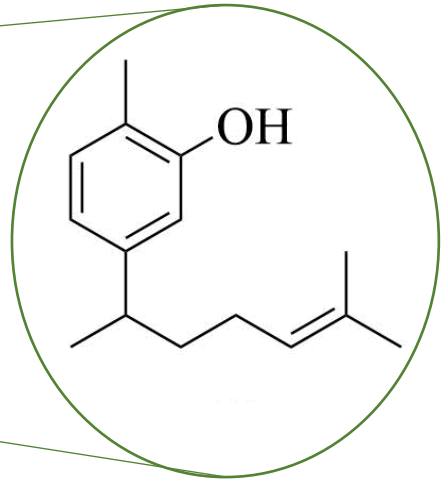


Crystal structure of human hyaluronidase-1 deposited in PDB[5] (PDB ID: 2PE4)

- HA metabolism can result in production of **low molecular weight HA (LW-HA) fragments**[2]
  - Increased expression of **chemokines** and **iNOS**[3]
  - stimulate dendritic cell signaling pathways to produce IL-1β, IL-12, and TNF-α[3]
- **hyaluronidase-1 and 2** are the key enzymes in degradation of HA[4]

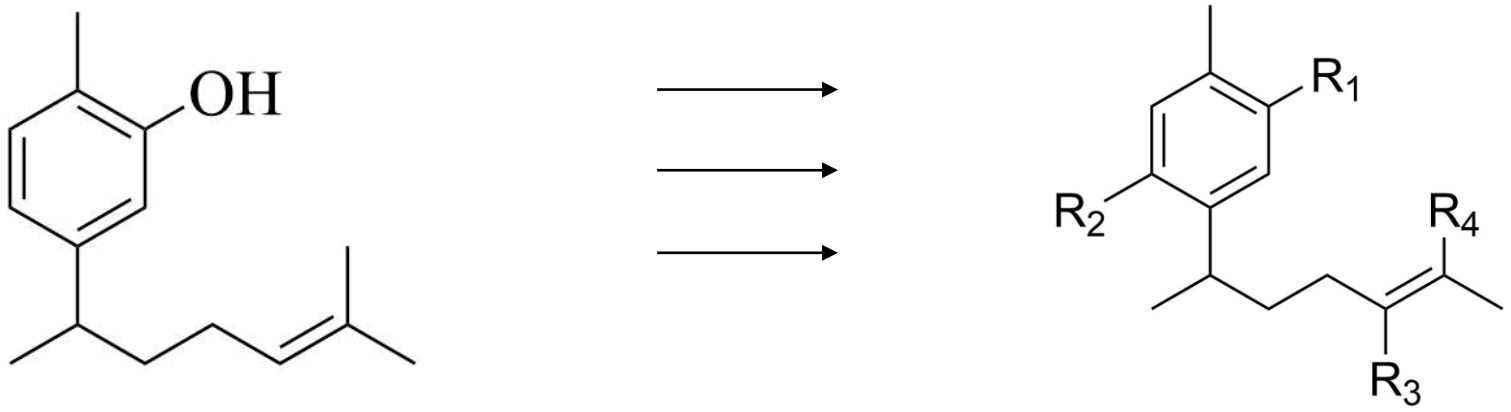
Xanthorrhizol

Curcuma xanthorrhiza (Stock photos)



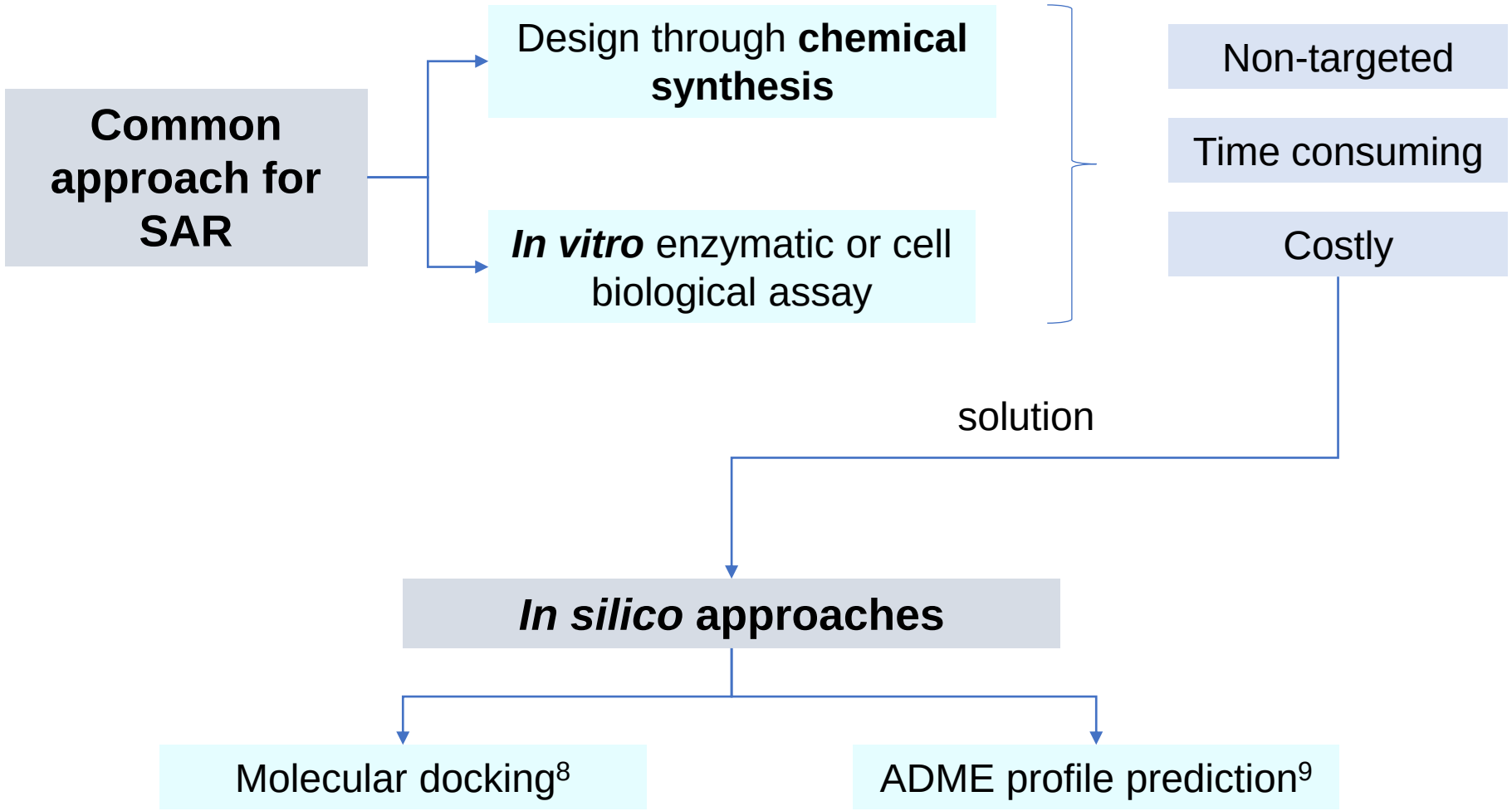
92 % in *Curcuma xanthorrhiza* essential oil[6]

Exhibit anti-inflammatory activities through **inhibition of enzymes** involved in inflammatory response i.e. cyclooxygenase (COX) and inducible nitric oxide synthase (iNOS)[7]



No study has been reported on the structure-activity relationship (SAR) of these derivatives towards the Hyal enzyme

Structure Activity Relationship (SAR)



In this study...

1. A small library containing 26 xanthorrhizol derivatives was virtually screened using molecular docking targeting the Hyal enzyme
2. The SAR of the selected derivatives at R_1 - R_4 positions were determined
3. The ADME profiles and drug-likeness properties of the derivatives were assessed

Methodology

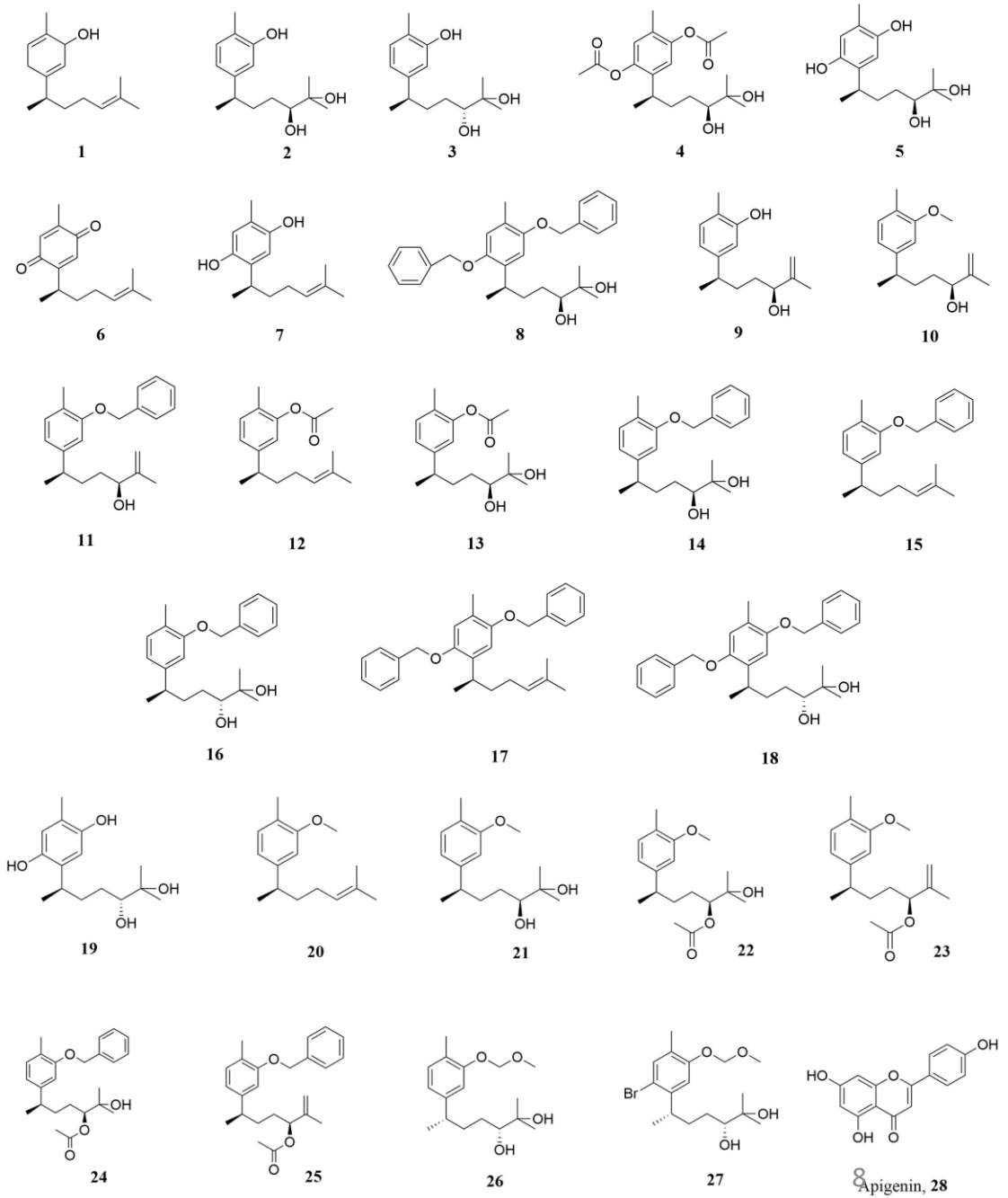
Ligand Preparation

Xanthorrhizol, apigenin and 26 derivatives were sketched using **ChemDraw**

Optimization using AutoOptimize tool in **Avogadro 2.0**

Gastegier charge were computed into the ligands in **AutoDockTools 1.5.6.**

All ligands were saved as PDBQT format



Protein Preparation

Human hyaluronidase-1 (PDB ID: 2PE4)

Retrieved from Protein Data Bank (https://www.rcsb.org)

Bound ligands and water molecules were removed using **PyMOL**

Kollman charge and polar hydrogen atoms were added in ADT and saved as **PDBQT** format

Molecular Docking

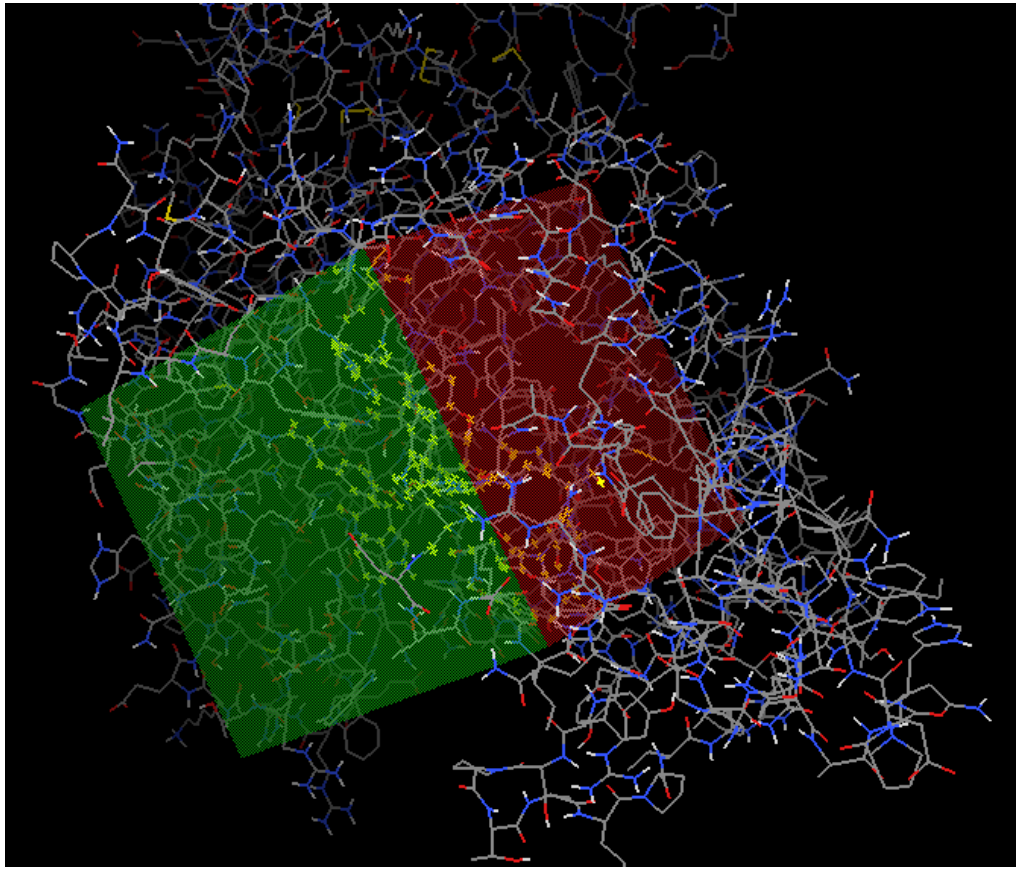
AutoDock Vina was used as docking program

↓

The grid box dimensions were specified at 62, 58 and 58 Å (x, y, z axes respectively) and centered on 37.045, -17.292, -11.844 (x, y, z axes, respectively) to cover all the amino acid residues in active site[5]

↓

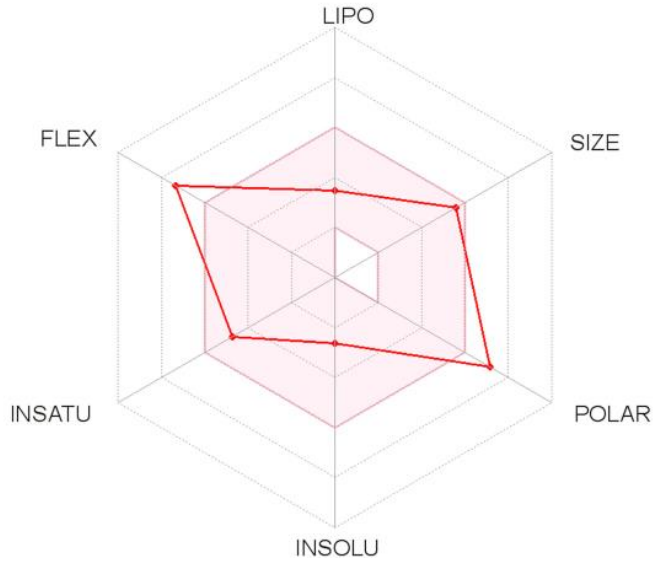
Docking result were visualised in 3D and 2D representations using **PyMOL** and **BIOVIA Discovery Studio**, respectively



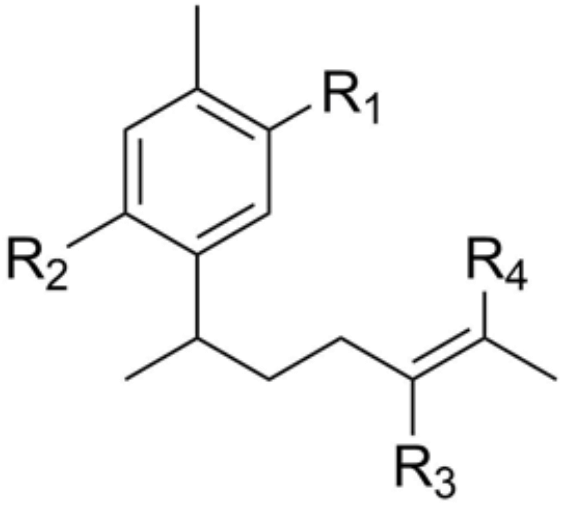
In silico drug-likeness and ADME profiling

All compounds were submitted to **SwissADME** server[9]

Descriptors	Range
Lipophilicity (LIPO)	-0.7 ≤ XLOGP3 ≤ +5.0
Molecular weight (SIZE)	150 g/mol ≤ MW ≤ 500 g/mol
Topological polar surface area (POLAR)	20 Å^2 ≤ TPSA ≤ 130 Å^2
Solubility (INSOL)	Log S ≥ -6
Carbon bond saturation (INSAT)	Fraction of carbons in the sp^3 hybridization not less than 0.25
Flexibility (FLEX)	0 < Number of rotatable bonds < 9

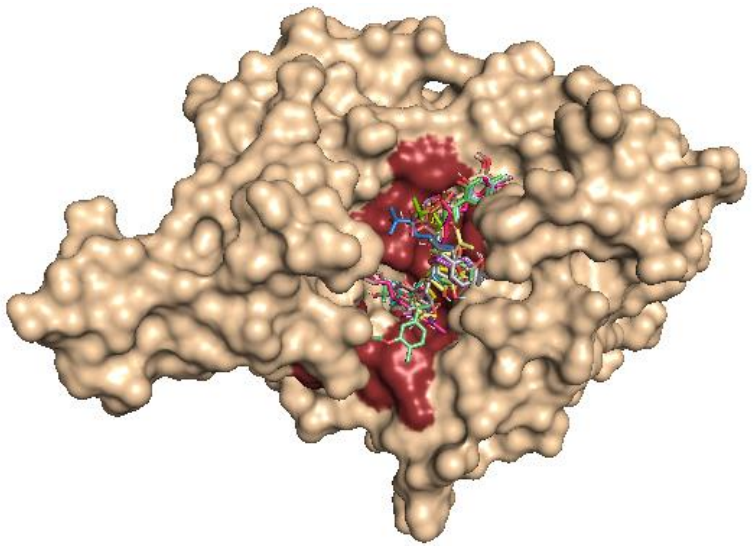


Result and Discussion

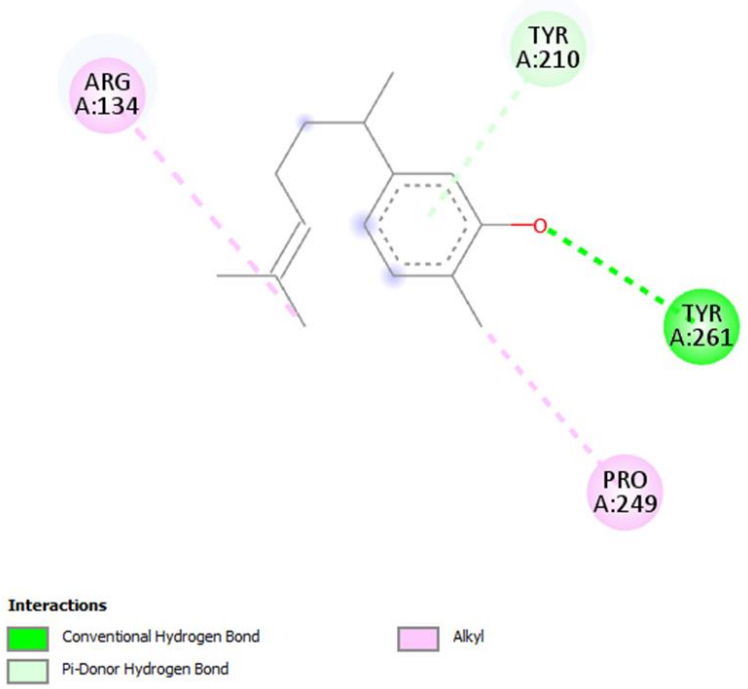


Derivatives	Substituent	Free binding energy (kcal/mol)	Interacting amino acid residues
17	R_1-OBz, R_2-OBz, R_3-H, R_4- CH_3,	-8.5	Ile73, **Asp129**, **Glu131**, Tyr247, Tyr286, Trp321
8	R_1-OBz, R_2-OBz, R_3-(*S*)-OH, R_4-OH	-8.3	**Asp129**, **Glu131**, Tyr202, Tyr210, Tyr286, Trp321
18	R_1-OBz, R_2-OBz, R_3-(*R*)-OH, R_4-OH	-8.3	Ile73, **Asp129**, **Glu131**, Tyr286, Trp321
24	R_1-OBz, R_2-H, R_3-OH, R_4-Ac	-8.3	Ile73, **Asp129**, **Glu131**, Gly203, Tyr210, Ser245, Tyr286, Trp321
25	R_1-OBz, R_2-H, R_3-H, R_4-Ac	-8.2	**Asp129**, **Glu131**, Tyr247, Arg265, Tyr286, Trp321
11	R_1-OBz, R_2-H, R_3-OH, R_4-CH_2	-8.0	Ile73, **Asp129**, **Glu131**, Tyr202, Tyr286, Trp321
15	R_1-OBz, R_2-H, R_3-H, R_4-CH_3	-8.0	Pro62, Ile73, **Asp129**, **Glu131**, Tyr247, Tyr286, Trp321
14	R_1-OBz, R_2-H, R_3-(*S*)-OH, R_4-OH	-7.9	Ile73, **Asp129**, **Glu131**, Tyr202, Ser245, Tyr286, Trp321
28 (Apigenin)	-	-7.9	Trp130, **Glu131**, Tyr202, Tyr210, Ser245, Arg265, Tyr261
1 (Xanthorrhizol)	R_1-OH, R_2-H, R_3-H, R_4-CH_3	-6.5	Arg134, Tyr210, Pro249, Tyr261

a)

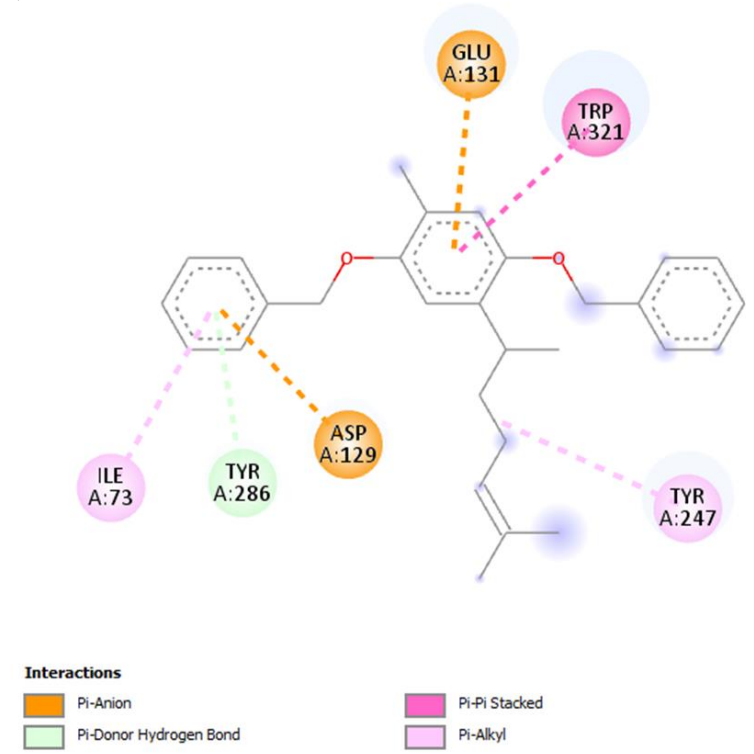


b)



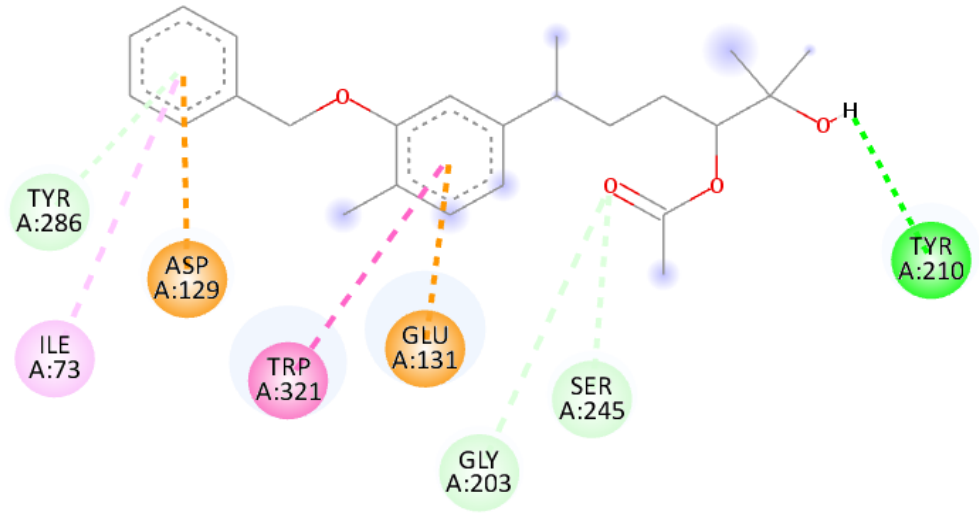
Xanthorrhizol, **1**
Binding energy = -6.5 kcal/mol

c)



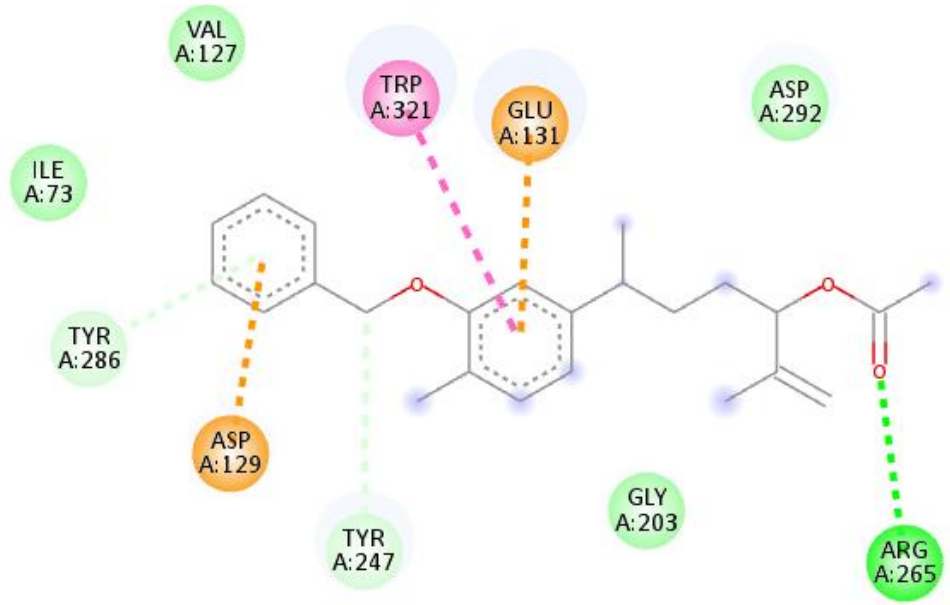
Derivative **17**
Binding energy = -8.5 kcal/mol

24



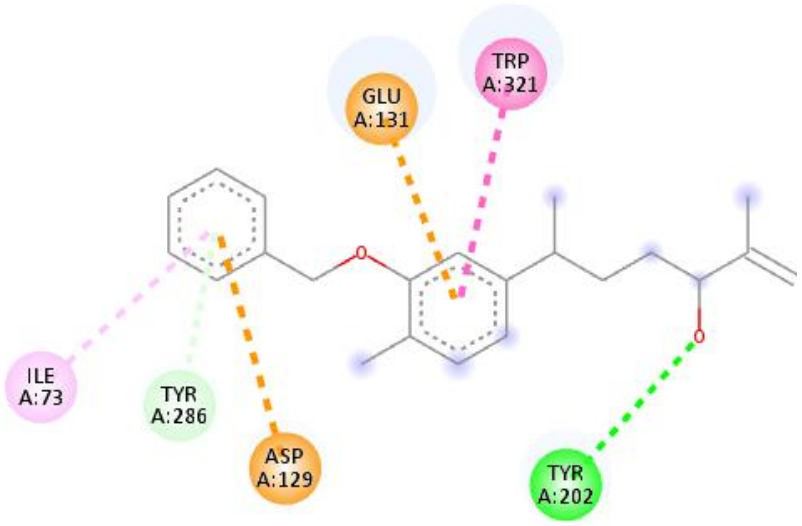
Binding energy = -8.3 kcal/mol

25



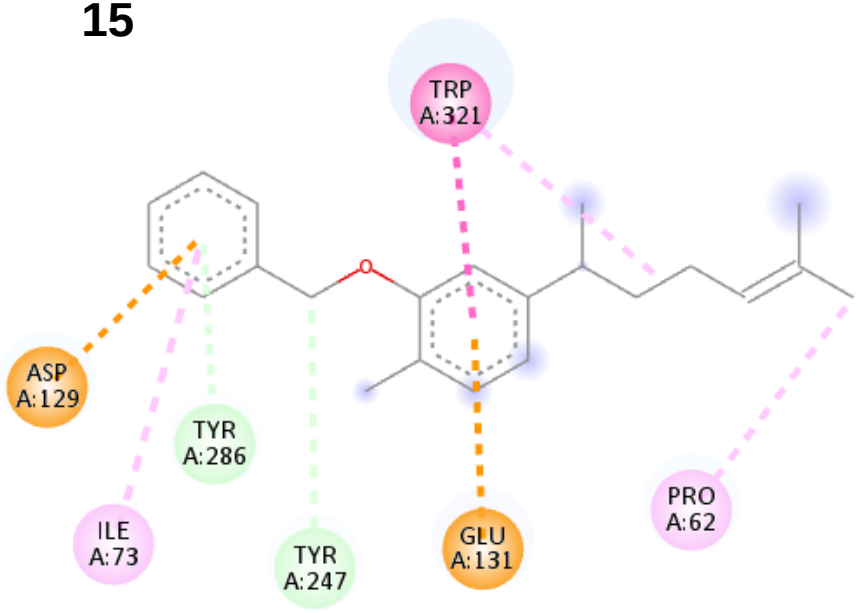
Binding energy = -8.2 kcal/mol

11



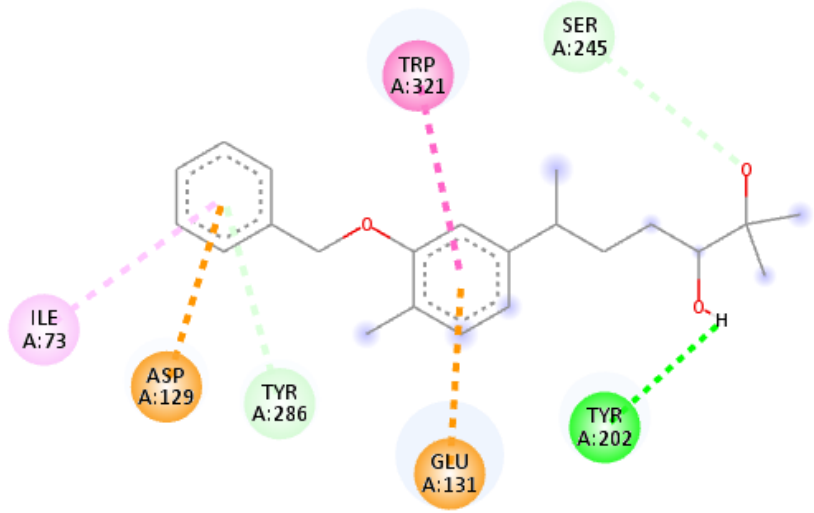
Binding energy = -8.0 kcal/mol

15

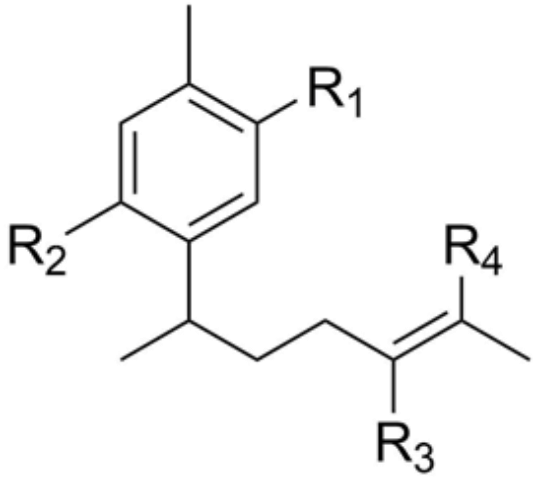


Binding energy = -8.0 kcal/mol

14

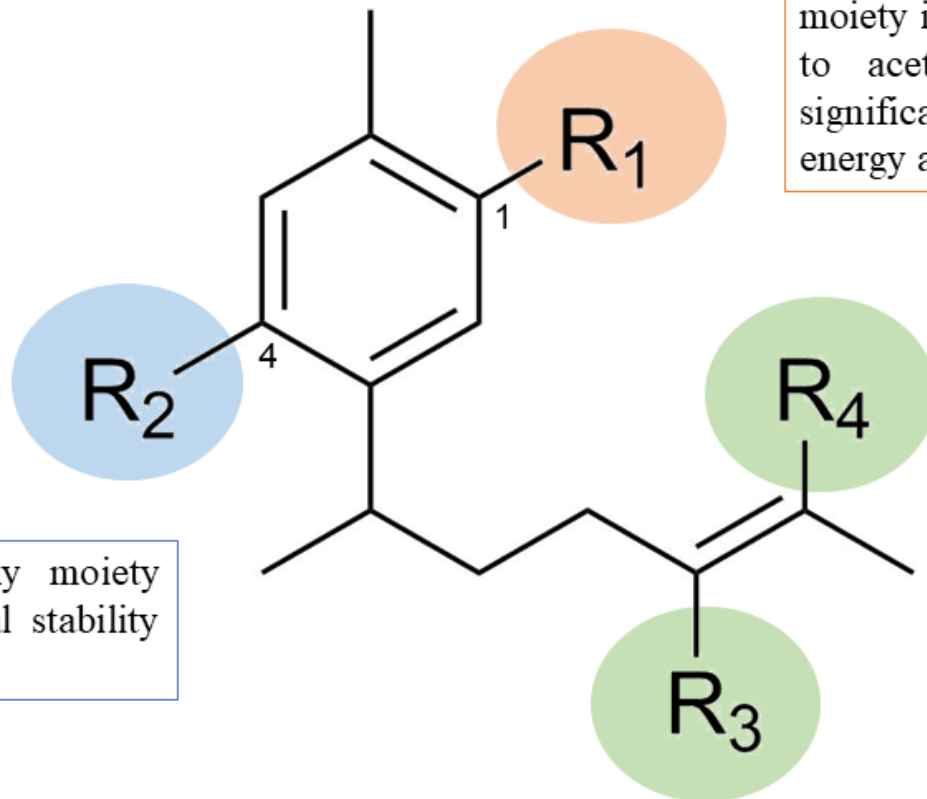


Binding energy = -7.9 kcal/mol



Derivatives	Substituent	Free binding energy (kcal/mol)	Interacting amino acid residues
12	R_1- Ac, R_2-H, R_3-H, R_4-CH_3	-6.9	Tyr75, **Asp129**, **Glu131**, Tyr202, Trp321
13	R_1- Ac, R_2-H, R_3-OH, R_4-OH	-6.7	Tyr75, **Asp129**, **Glu131**, Trp321
3	R_1-OH, R_2-H, R_3-(*R*)-OH, R_4-OH	-6.6	Asn37, Ile73, Tyr75, Val127, **Asp129**, Tyr202, Tyr286, Trp321
4	R_1- Ac, R_2-Ac, R_3-OH, R_4-OH	-6.6	**Glu131**, Tyr202, Ser245, Tyr247
7	R_1-OH, R_2-OH, R_3-H, R_4-CH_3	-6.6	Pro62, Tyr202, Tyr286, Trp321, Val322, Trp324
1 (Xanthorrhizol)	R_1-OH, R_2-H, R_3-H, R_4-CH_3	-6.5	Arg134, Tyr210, Pro249, Tyr261
2	R_1-OH, R_2-H, R_3-(*S*)-OH, R_4-OH	-6.5	Ile73, Tyr75, Val127, **Asp129**, **Glu131**, Tyr202, Tyr286, Trp321
6	R_1- CO, R_2-CO, R_3-H, R_4-H	-6.5	Tyr202, Tyr286, Trp321, Trp324
9	R_1-OH, R_2-H, R_3-OH, R4-CH_2	-6.5	Ile73, Tyr75, **Asp129**, Tyr202, Tyr286, Asp292, Trp321
19	R_1-OH, R_2-OH, R_3-OH, R_4-OH	-6.4	**Asp129**, **Glu131**, Tyr202, Ser245, Tyr247, Trp321
20	R_1-OMe, R_2-H, R_3-H, R_4-CH_3	-6.3	Tyr75, **Asp129**, Tyr202, Trp321
22	R_1-OMe, R_2-H, R_3-Ac, R_4-OH	-6.3	Pro62, **Glu131**, Tyr247
23	R_1-OMe, R_2-H, R_3-Ac, R_4-CH_2	-6.3	Pro62, Trp321
26	R_1-OMOM, R_2-H, R_3-OH, R_4-OH	-6.2	Arg134, Gly203, Asp206, Tyr210
21	R_1-OMe, R_2-H, R_3-OH, R_4-OH	-6.4	Tyr75, **Asp129**, **Glu131**, Tyr202, Asp292, Trp321
10	R_1-OMe, R_2-H, R_3-OH, R_4-CH_2	-6.1	Tyr75, **Asp129**, **Glu131**, Asp292, Trp321
27	R_1-OMOM, R_2-Br, R_3-OH, R_4-OH	-6.1	Tyr75, **Asp129**, **Glu131**, Tyr202, Tyr286, Trp321
5	R_1-OH, R_2-OH, R_3-OH, R_4-OH	-5.7	Asn37, Tyr75, **Asp129**, **Glu131**, Tyr247, Tyr286

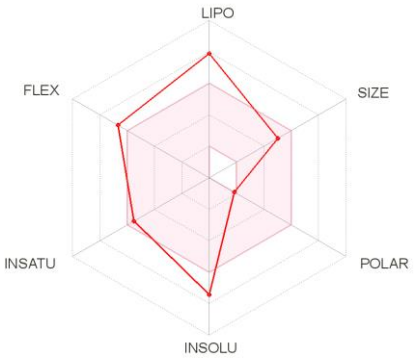
Substitution of hydroxyl group to benzyloxy moiety improve binding energy. Substitution to acetate or methoxy did not have significance difference towards binding energy against Hyal1.



Addition of benzyloxy moiety provide conformational stability to the molecule

No significant difference to binding energy observed in changing to enol or diol functionalities.

In silico drug-likeness and ADME profiling



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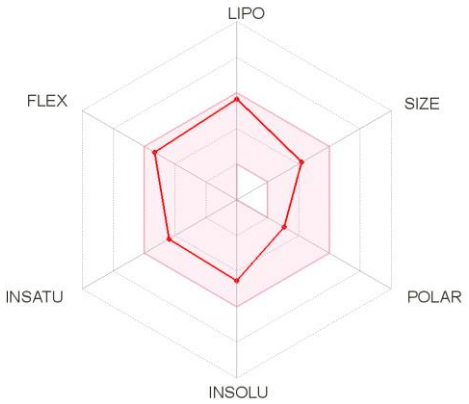
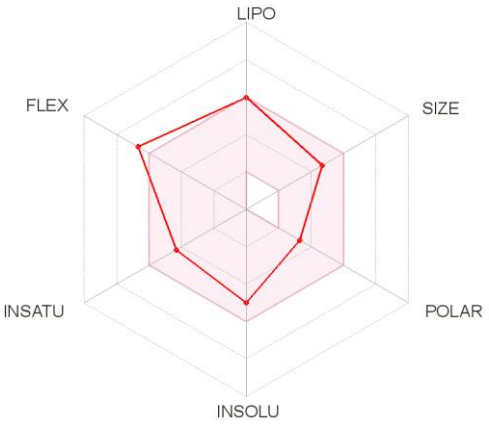


14



24

Derivatives	Molecular weight	Fraction sp^3	Number of rotatable bonds	TPSA	XLOGP	ESOL Log S
1 (Xanthorrhizol)	218.33	0.47	4	20.23	5.46	-4.65
14	342.47	0.45	8	49.69	4.37	-4.54
17	414.58	0.31	10	18.46	8.31	-7.42
24	384.51	0.46	10	55.76	4.94	-4.99

Conclusion

The presence of **two benzyloxy moieties** at R_1 and R_2 positions each, significantly **enhancing the binding activity** against the Hyal1 enzyme but contributed to **poor ADME profile**

Derivatives **14** and **24** which ranked among the most favorable binding energies in the docking studies conformed with all ADME parameters

The presence of **polar functional groups** especially at R_3 and R_4 locations in the xanthorrhizol scaffold are crucial for good absorption in the body

This study served as a **starting point** for further development and optimization of xanthorrhizol as scaffold for the Hyal1 enzyme inhibitor

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Welcoming Message

On behalf of the IKMPB Online Symposium organizing committee, I am honored to welcome you to the 2022 IKMPB Online Symposium. This is the 2nd symposium by IKM Pahang Branch and we have to hold it virtually due to the COVID 19 pandemic.

This year, our symposium is enriched with the theme "Sustainability & Diversity Through Chemistry". We are living in the era of paradigm shift. In the last two years, one can observe the digitalization is growing rapidly, partly due to the COVID19. We can also witness the exponential growth of electric vehicle where internal combustion engine is controversially said to be replaced by electric-powered vehicle. In this context, chemistry plays a vital role in ensuring the sustainability and diversity of this transportation evolution roadmap. This is only one of the example of how chemistry role in shaping a sustainable and diversified world.

This year, the organizing committee received overwhelming response for the participation and carefully reviewed and selected the papers to be presented virtually. The participation consists of chemists around Malaysia and the selected papers will be published in Malaysian Journal of Chemistry as Special Issue. Besides, I would like to thank our co-organizers (Universiti Malaysia Pahang & International Islamic University Malaysia) as well as sponsors (Water Analytical instruments) for their generous support. Not to forget our organizing committee who are so committed to make IKMPB Online Symposium into a great success. Thank you!

The IKMP Online Symposium represents an opportunity to inspire chemists with a perspective of ideas in shaping a sustainable world in chemistry way. We hope all of you find this symposium stimulating, rewarding and meaningful!

Thank you & Terima Kasih!

Best regards,

Prof. ChM Dr. Chong Kwok Feng

IKMPB Online Symposium 2022, Chairman

Welcoming Message

بِسْمِ ٱللَّهِ ٱلرَّحْمَٰنِ ٱلرَّحِيمِ

اَلسَلامُ عَلَيْكُم وَرَحْمَةُ اَللهِ وَبَرَكاتُهُ

It is my great pleasure to welcome you to the 2nd Institut Kimia Malaysia Pahang Branch Online Symposium 2022. The event is organized by Institut Kimia Malaysia, co-organized by the Faculty of Industrial Sciences and Technology, Universiti Malaysia Pahang, and International Islamic University Malaysia. This year IKMPB brings us the latest theme: "Sustainability & Diversity Through Chemistry"; which provides an excellent platform for exchange of ideas in various fields e.g., material synthesis, material characterizations, biological sciences, environmental sciences, food sciences and pharmaceutical, green technology and renewable energy, advanced materials, composite, nanotechnology, natural products, industrial biochemistry, functional materials, catalysts, and separation and purification process.

The symposium is timely and relevant. Participations of professors and researchers representing IKM, UMP and IIUM would trigger exchange of views and experience sharing for sustainability and betterment of mankind. I hope that this symposium will increase the number of collaborations and opportunities between institutions.

I congratulate the organizing committee for their hard work, and my sincere appreciation to the participants, speakers and Waters Analytical Instruments Sdn Bhd as the main sponsor for making this symposium a successful event.

Dr. Saifful Kamaluddin bin Muzakir @ Lokman

Dean

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Program

Time	Session
8:30 – 9:00 AM	Registration (online)
9:00 – 9:05 AM	Welcoming Remarks by the Program Chair
9:05 – 9:10 AM	Welcoming Message by Dean - Faculty Industrial Sciences and Technology, UMP
9:10 – 9:30 AM	Session I
9:30 – 10:30 AM	Parallel Sessions (II & III)
10:30 – 10:45 AM	Break
10:45 – 12:15 PM	Parallel Sessions (IV & V)
12:15 – 2:00PM	Lunch Break
2:00 – 3:15 PM	Parallel Sessions (VI & VII)
3:15 – 3:30 PM	Closing Remark

Scan here to join: **Welcoming Session** **Session I , II, IV, VI** **Closing Remark**	https://meet.google.com/ktn-tqvj-nxn
Scan here to join: **Session III, V, VII**	https://meet.google.com/uzy-tgmh-xkh

IKM PAHANG BRANCH Online Symposium 2022

Welcoming Session		
8:30-9:00 AM	Registration (online)	
9:00-9:05 AM	Welcoming Remarks by the Programme Chair	
9:05-9:10 AM	Welcoming Message: Dean - Faculty Industrial Sciences & Technology, UMP	
Session I		
Chairperson: Asst. Prof. Dr. Mohamad Wafiuddin bin Ismail		
9:10-9:30 AM	Waters Analytical Instruments Sdn. Bhd., Malaysia	
	Session II	**Session III**
	Chairperson: ChM Dr. Nurlin Abu Samah	**Chairperson: Asst. Prof. Dr. Mohamad Wafiuddin bin Ismail**
9:30-9:45 AM	MJC-IKMP-2 Utilisation Of Coconut Shell Ash (Cocos Nucifera) As Lime Replacement In Agricultural Soil	MJC-IKMP-7 Lawn Grass as A Sustainable Adsorbent for Nickel (II) Removal
9:45-10:00 AM	MJC-IKMP-4 Optimisation Of Reaction Parameters In Transesterification Of Waste Cooking Oil Using Response Surface Methodology	MJC-IKMP-9 Utilization of Sodium Hydroxide (NaOH) to Treat Used Tyres as Crumb Rubber in Engineered Cementitious Composites
10:00-10:15 AM	MJC-IKMP-5 Application Of Novel Magnetic Eggshell Membrane Functionalized Waste Palm Fatty Acid For Selective Adsorption Of Emulsified Oil	MJC-IKMP-11 One-pot Sol-Gel Synthesis of Zinc Oxide-Reduced Graphene Oxide Composite: Photocatalytic, Kinetic and Fuzzy Inference System
10:15-10:30 AM	MJC-IKMP-6 Eggshell Membrane Functionalized With Waste Palm Cooking Oil For Removal Of Alizarin Red Dye In Aqueous Solution	MJC-IKMP-12 Enhanced adsorption of carbon dioxide by phosphoric acid modified soybean curd residue biochar
10:30-10:45 AM	**Break**	
	Session IV	**Session V**
	Chairperson: Dr. Nazikussabah Zaharudin	**Chairperson: Asst. Prof. Dr. Rosliza Binti Mohd. Salim**
10:45-11:00 AM	MJC-IKMP-1 DNA Extraction From Fabric Samples Exposed Under Different Environmental Conditions	MJC-IKMP-13 Antibacterial Activity of Metal-Natural Extract Complexes
11:00-11:15 AM	MJC-IKMP-3 Assessment Of Water Quality In Temenggor Forest Reserve Based On Physicochemical Data And Selected Elements Content	MJC-IKMP-15 Photocatalysis of Propanol Synthesis from Glycerol over Fluorine-doped Oxide (FTO) Catalyst

11:15-11:30 PM	MJC-IKMP-10 Comparative Water Quality Analysis Between Tahan River and Sat River in Taman Negara Pahang, Malaysia	MJC-IKMP-16 The Treatment of Acidic Petroleum Crude Oil Assisted by CaO/Al2O3 Catalyst
11:30-11:45 PM	MJC-IKMP-17 RSM-Optimization Approach for Dispersive Micro Solid Phase Extraction for the Determination of Tetracycline Antibiotics in Water Samples	MJC-IKMP-20 Synthesis And Characterization Of Eggshell Membrane (Esm) Functionalized Free Fatty Acids (Ffas) As Potential Adsorbents For Removal Of Anionic And Cationic Dyes Pollutants
11:45-12:00 PM	MJC-IKMP-19 Multi-Trace Metals Determination of Peninsular Malaysia Stingless Bee Honeys from Different Regions and Seasons Using Inductively Coupled Plasma-Optical Emission Spectrometry and Chemometric Techniques	MJC-IKMP-25 Fabrication And Characterisation Of Recycled Polyethylene Terephthalate / Graphene Oxide Nanofibers As Potential Adsorbent Of Methylene Blue
12:00-12:15 PM	MJC-IKMP-28 Optimization of Thin-film Microextraction using Polyelectrolyte Multilayers Sorbent Combined with HPLC-UV for Separation and Determination of Tricyclic Antidepressant Residues	MJC-IKMP-29 Effect of the Molar Ratio of Sodium Hydroxide on Bentonite Support for the Transesterification of Waste Cooking Oil into Fatty Acid Methyl Ester
12:15-2:00 PM	**Lunch Break**	
	Session VI	**Session VII**
	Chairperson: ChM Dr. Norshahidatul Akmar Mohd Shohaimi	**Chairperson: ChM Nur Syamimi Zainudin**
2:00-2:15 PM	MJC-IKMP-8 In vitro Pharmacological Evaluation of the Leaves of Malaysian Mitragyna spesioca Korth.	MJC-IKMP-23 Bio-Nanohybrid Composite Sorbent-Based Microextraction for Acid Drugs in Aqueous Samples: Box-Behnken Design Approach
2:15-2:30 PM	MJC-IKMP-14 Inhibition Of Staphylococcus Epidermidis Biofilm By A Bacteriocin-Like Peptide From The Frog Fejerverya Cancrivora	MJC-IKMP-24 Utilisation of Cationic Surfactant Modified Grated Coconut Residue for the Removal of Reactive Orange 16 from Aqueous Solutions: Fixed Bed Column Study
2:30-2:45 PM	MJC-IKMP-18 Enhanced Extractability of Phenolic Compounds and Antioxidant Activity of Fermented Rice Straw using Aspergillus oryzae	MJC-IKMP-26 A Review On Application Of Carrageenan Extract From Red Seaweed (Rhodophyta) In Cosmetics
2:45-3:00 PM	MJC-IKMP-21 Molecular Docking And Adme Profiling Of Xanthorrhizol Derivatives As Hyaluronidase Inhibitors	MJC-IKMP-27 Preliminary Phytochemical Analysis of Malaysian In Vitro Cultured Aromatic Rice (Oryza sativa L. Cv. MRQ 74)
3:00-3:15 PM	MJC-IKMP-22 Effect Of Carboxymethyl Cellulose (Cmc) As A Plasticizer On Starch/CMC Biocomposites	MJC-IKMP-30 Synthesis, Characterization And Anti-Triple Negative Breast Cancer (TNBC) Activites Of Non-Symmetric Curcumin Derivatives
3:15-3:30 PM	**Closing Remark + Photo Session**	

ID: MJC-IKMP-1

DNA EXTRACTION FROM FABRIC SAMPLES EXPOSED UNDER DIFFERENT ENVIRONMENTAL CONDITIONS

Ayu Syaheera Binti Mohd Shahidi[1], Ain Khairunnisa Binti Rusli[1], Sharifah Nurfitriyani Binti Syed Zubir[1] and Kavitha Rajagopal[1]*

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This research was conducted to identify the type of fabrics retained a highest concentration of DNA when exposed under different environmental condition such as sunlight, high humidity, and heavy rain. There are different locations used in this study namely jungle, abandoned building and construction site to mimic the real crime scene. Ten different types of fabrics used for this study are satin, chiffon, linen, polyester, cotton, crepe, argenti, valentro, lycra and georgette. Ten types of fabric samples are stained with fresh human blood and are exposed for a week under different environmental condition. Sample collection is made for every 24 hours. The type of fabric that retained the highest concentration of DNA when exposed under three different environmental conditions is Crepe. The concentration of DNA retained by the fabric samples in an indoor abandoned building are higher compared to the concentration of DNA retained by the fabric samples in the outdoor jungle area and outdoor construction site. The possibility for contamination or loss of the DNA is high as the period before the evidence collection is increases. Therefore, by reduce the time for the evidence collection can decrease the possibility for the contamination of DNA occurred.

Keywords: Fabrics DNA; Abandoned Building; Jungle; Construction Site; Environmental Exposure

ID: MJC-IKMP-2

Utilisation of Coconut Shell Ash (*Cocos Nucifera*) as Lime Replacement in Agricultural Soil

Wan Noni Afida Ab Manan[1*], Anis Iz'zati Ghazali[1], Fatin Nasuha Mohd Yusoff[1]

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Utilisation of coconut shell ash (CSA) might improve plant growth especially in agricultural activities. This study aims to discover the potential of CSA in decreasing the acidic soil especially one that uses chemical fertilizers or pesticide for crop production. Coconut shell from coconut tree (*Cocos nucifera*) was collected and CSA was produced by pyrolysis process. Fourier-transform infrared (FTIR) analysis was then used to determine the chemical composition of CSA. Three different portions of CSA (1.0, 3.0 and 5.0 g) were added into 10 g of acidic soil (pH 3.81) and control soil (pH 7.1). The usage of coconut shell was proven to be effective in increasing (reduce acidity) the pH of the soil. The highest increment of soil pH; up to pH 7.12, was achieved when 5.0 g of CSA was added. This result suggests that utilisation of CSA on acidic soil will benefit to both soil pH and plant and therefore can possibly be used as an alternative to the usage of lime at a reasonable cost.

Keywords: Acidic soil; Coconut Shell Ash; Soil pH.

ID: MJC-IKMP-3

Assessment Of Water Quality In Temenggor Forest Reserve Based On Physicochemical Data And Selected Elements Content

*Nursyairah Arshad[1,2], Ahmad Taufek Abdul Rahman[1,2], Salifairus Mohammad Jafar[2], Nurul Wahida Aziz[2] and Rozita Osman[1 *]*

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Determination of elemental concentrations in water samples helps in understanding the health conditions of a water system, in addition to their physiochemical parameters measurement. Temenggor area is known as one of the largest reserve forests in Penisular Malaysia. Consequently, the Sustainability Development Goals are significant to imply in this area. This study aims to measure the basic physicochemical parameters as well as the concentrations of selected elements. Measurement of basic physicochemical parameters such as pH, temperature, pressure, dissolved oxygen (DO), electrical conductivity (C), total dissolved solids (TDS), salinity, and oxidation-reduction potential (ORP) of freshwater samples from river streams includes Sungai Gadong Dalam, Sungai Gadong Luar and Sungai Kelam, as well as Tasik Temenggor, were done in situ using YSI multiparameter probe meter. The concentrations of ten elements including As, Cd, Cr, Cu, Ni, Pb, Se, Zn, U and Th were measured using Energy Dispersive X-Ray Fluorescence (EDXRF) Spectrometer. The average elemental concentrations were found to be higher than the threshold level of the National Water Quality Standard for Malaysia (NWQSM) except for Zn. The correlation of the physicochemical data and elemental concentrations to each other were evaluated using SPSS IBM 22 software. Seven strong correlation pairs were observed from the physicochemical data. It includes temperature-pressure, SPC-conductivity, SPC-TDS, SPC-salinity, conductivity-TDS, conductivity-salinity, and TDS-salinity. Meanwhile, the elemental concentrations show a strong correlation between As-Cr, As-Se, Cd-Cr, Cd-Zn, Cr-Pb, Cr-Zn and Pb-Zn. Cluster analysis grouped the 15 sampling locations into two clusters, Cluster 1 (low concentrations) and Cluster 2 (high concentrations) for each element. Heavy metals pollution index (HPI) and metal index (MI) were also calculated to observe the contamination level of water samples in this area. Most of the areas revealed HPI values above 100 showing there is a sign of heavy metals pollution.

Keywords: Heavy metals; Water Sample; Energy Dispersive X-Ray Fluorescence; Metal Index

ID: MJC-IKMP-4

OPTIMISATION OF REACTION PARAMETERS IN TRANSESTERIFICATION OF WASTE COOKING OIL USING RESPONSE SURFACE METHODOLOGY

Noraini Hamzah[1]*, Erma Hafiza Ibrahim[1], Nazrizawati Ahmad Tajuddin[1], Hairul Amani Abdul Hamid[1], Sabiha Hanim Saleh[1], Nursyamsyila Mat Hadzir[1], Rozita Osman[1], Wan Zurina Samad[2] and Mardiana Saaid[3]

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Optimization of reaction parameters for biodiesel production is crucial to develop a more efficient and cost-effective system in the biodiesel industry. The transesterification reaction is affected by several factors which are alcohol to oil molar ratio, reaction temperature, reaction time and catalyst loading. In this study, the Response Surface Methodology (RSM) was utilized to obtain the optimal conditions for maximizing biodiesel yield. RSM using Box-Behnken experimental design that consists of 30 runs (number of the experiment) and three blocks was developed to determine the optimal conditions of key parameters such as (A) Methanol:oil ratio (20-40) ; (B) catalyst loading (0.25-2 %(wt/l); (C) Reaction temperature (50-70 °C) and (D) Reaction time (1-15 hours). The ANOVA analysis suggested that the quadratic model is significant as the p-value for the model is < 0.0001 and large F-value of 37.70. The lack of fit p-value of 0.0928 (p-value is not significant) implies that the model is fitted to all the data. The value of R^2 of 0.9760 indicates that the model fits the experimental data. Based on the F-value and p-value of the significant model terms, methanol:oil molar ratio has the largest effect on biodiesel yield compared to other parameters. The optimum conditions whereby the maximum biodiesel yield of 35.45 % was obtained at methanol to oil molar ratio of 34:1; reaction temperature of at 68.4 ^{0}C ; reaction time of 11.9 h and 1.125 wt% catalyst loading. In terms of interaction, AB, AC, AD, BC, BD and CD were found to be insignificant model terms as their p-values higher than 0.05.

Keywords: Response surface methodology, waste cooking oil, transesterification, biodiesel

ID: MJC-IKMP-5

Application Of Novel Magnetic Eggshell Membrane Functionalized Waste Palm Fatty Acid For Selective Adsorption Of Emulsified Oil

Siti Khalijah Mahmad Rozi[1], Khairul Muzzammil Berhanundin[1], Ahmad Razali Ishak[2*], Fairuz Liyana Mohd Rasdi[2], Nazri Che Dom[2], Nurul Yani Rahim[3], Mohd Yusmaidie Aziz[4], Farah Ayuni Shafie[2]

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Emulsified oil in wastewater is a severe problem in the many treatment steps before being disposed of in a manner that meets environmental standards. One way for dealing with this problem is the adsorption technique. The primary goal of this research is to evaluate the adsorption of three emulsified oils (lubricating oil, corn oil, and olive oil) employing magnetic eggshell membrane functionalized waste palm fatty acid (MNP@ESM-WPFA). This novel adsorbent surface was characterized using SEM, FTIR, and EDX analyses. The porous and fibrous morphological structure of ESM-WPFA was scattered with magnetic nanoparticles across the network, proving that the MNP@ESM-WPFA has been successfully synthesized. Further FTIR analysis on MNP@ESM-WPFA adsorbent confirmed the presence of the alkyl chain of the WPFA and Fe-O band on the surface of MNP@ESM-WPFA. The oil adsorption performance of MNP@ESM-WPFA was optimum at pH 7, 50 minutes contact times, and adsorbent dosage of 50 mg. The oil adsorption capacity (K) for lubricating oil is 4.61 mg/mg, followed by olive oil (2.72 mg/mg) and corn oil (2.00 mg/mg. The MNP@ESM-WPFA adsorbent is also reusable, with a sorption capacity that was maintained after five usage-regeneration cycles.

Keywords: Eggshell membrane, Waste palm fatty acids, Magnetic nanoparticles, Adsorbents, Oil removal.

ID: MJC-IKMP-6

Eggshell Membrane Functionalized With Waste Palm Cooking Oil For Removal Of Alizarin Red Dye In Aqueous Solution

Siti Khalijah Mahmad Rozi[1], Anis Atikah Mohd Zulkifle[1], Ahmad Razali Ishak[2*], Fairuz Liyana Mohd Rasdi[2], Nazri Che Dom[2], Nurul Yani Rahim[3], Mohd Yusmaidie Aziz[4], Siti Rohana Mohd Yatim[2]

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Alizarin Red was reported to be mutagenic and carcinogenic due to its ability to cause oxidative damage in organisms. The utilization of eggshell membrane (ESM) functionalized with waste palm cooking oil (WPCO) as adsorbent (ESM@WPCO) for removal of toxic Alizarin Red from aqueous solution has been investigated. The surface morphology of ESM@WPCO from SEM analysis exhibited an improved and larger microporous network of interwoven and coalescing shell membrane fibers compared to unmodified ESM. FTIR analysis on ESM@WPCO had confirmed the attachment of free fatty acids onto the surface of ESM. The performance of ESM@WPCO as adsorbent was examined at optimum pH, adsorbent dosage, contact time and initial concentration. Alizarin Red was efficiently removed at pH 2 at optimum initial concentration of 50 mg L^{-1}. The optimum dosage and contact time for Alizarin Red removal were 20 mg and 40 min, respectively, with the removal rate of 93%. The adsorption isotherms were analyzed using Langmuir and Freundlich model. It shows that the Freundlich model (R^2 =0.98) is better in describing the adsorption isotherm process with maximum adsorption capacity (K_f) of 8.41 mg g^{-1}. The pseudo-second order is well fitted in the adsorption kinetic analysis, with an R^2 of 0.99. Results clearly reveal that ESM@WPCO acts as an effective adsorbent for the removal of Alizarin Red from aqueous solutions.

Keywords: Eggshell membrane; Waste palm cooking oil; Free fatty acids; Alizarin Red

ID: MJC-IKMP-7

Lawn Grass as A Sustainable Adsorbent for Nickel (II) Removal

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Lawn grass is a waste that potential to be converted as resource for adsorbent to remove nickel (II) from aqueous solution. Methodology involves preparation and characterization of adsorbent, adsorption study for parameters of adsorbent amount, initial pH, contact time, initial nickel (II) concentration and temperature as well as evaluation of isotherm and kinetic studies. Characterization of SEM and EDX also were conducted. The results showed the optimum adsorbent amount, initial pH and time were at 0.35 g, unadjusted pH of 5.62 $\pm$ 0.38 and 30 minutes, respectively. It is well-fitted to Langmuir than Freundlich. The adsorption performance was excellently corresponded to pseudo second-order kinetic than pseudo first-order kinetic. The thermodynamic evaluation revealed it is a non-spontaneous, weak reversible endothermic reaction. SEM and EDX results supported nickel (II) bound on the surface of lawn grass adsorbent in monolayer condition and chemisorption is the rate limiting step. This study provides vital basic information for large scale industrial pilot test. In conclusion, the lawn grass is a potential adsorbent for removal of nickel (II).

Keywords: Adsorbent; Lawn grass; Nickel (II); Sustainable; Waste to Resource

ID: MJC-IKMP-8

In vitro Pharmacological Evaluation of the Leaves of Malaysian *Mitragyna spesioca* Korth.

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This study was to evaluate the hexane and DCM crude extracts from the leaves of *mitragyna speciosa* on antioxidant, antimicrobial, and cytotoxic assay. Evaluation of antioxidant activities were tested against DPPH, ABTS, beta carotene bleaching, FRAP, and total phenolic content (TPC) assays. The antimicrobial activity was investigated by disc diffusion and microdilution methods for determination of zone of inhibition, MIC and MBC, respectively. The cytotoxic activities were performed using MTT assays. The DCM and hexane extract were tested against five cancer cells; two breast cancer cell lines (MCF7 and MDA-MD-231), two colon cancer cell lines (SW948 and HT29), and a lung cancer cell line (A549). The DCM extract of the leaves showed the highest total phenolic content (TPC) (84.63±9.01 μg GE/mg) while hexane extract showed the lowest total phenolic content (74.04±7.07 μg GE/mg). However, the total flavonoid (TFC) content shows that the hexane extract (97.14±1.74 μg QE/mg) is higher than DCM extract (59.88±4.25 μg QE/mg). Both extracts showed DPPH free radical scavenging (EC_{50} >1mg/mL), ABTS (hexane extract: 20.84±0.92 mg/mL; DCM extract: 39.49±2.28 mg/mL) and, the beta carotene bleaching (hexane extract: 78.29 μg/mL; DCM extract: 75.17±3.26 μg/mL), FRAP (hexane extract: 11.45±0.99 μg/mL; DCM extract: 7.94±0.96 μg/mL); and cytotoxic assay for DCM is moderately toxic (IC_{50} value ranging 2.86 to 14.81 ⌈g/mL) on tested cancer cells; while hexane crude showed IC_{50} value more than 100 ⌈g/mL for most of the tested cells. All extracts showed from moderate to weak activity with MIC/MBC values in the ranged of 625-1000 μg/mL. The results revealed that the extracts of *Mitragyna speciosa* has significant activity in various biological studies.

Keywords: *Mitragyna speciosa;* Rubiaceae; antioxidant; antimicrobial; cytotoxic assay

ID: MJC-IKMP-9

Utilization of Sodium Hydroxide (NaOH) to Treat Used Tyres as Crumb Rubber in Engineered Cementitious Composites

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Engineered cementitious composites (ECC) is distinct for the tensile strain-hardening behaviour and tensile ductility contrasting to the quasi-brittle nature of ordinary concrete. The blended materials of ECC only consist of cement, sand, water, fibre, and admixture. The depleting and limited resources of sand in many countries have led to the research on alternative materials to replace sand partially or fully in the concrete mixture. Therefore, this study aims to utilize the crumb rubber (CR) in ECC as a partial sand replacement to enhance the ductility and energy dissipation capacity of the composite. The additional of CR in the ECC cause reduction of compressive strength of the composites due to its smooth surface resulting to less bonding with cement matrix. Hence, the CR is being treated with 10% sodium hydroxide (NaOH) to improve its surface roughness and enhance the adhesion between CR and cement matrix in the composites. The compressive strength results for ECC contained CR treated for duration of 2 days and 4 days were recorded. Two days is the optimum duration of CR treatment using 10% sodium hydroxide (NaOH) to lessen the reduction of the compressive strength of the rubberized engineered cementitious composites (R-ECC).

Keywords: Engineered Cementitious Composites (ECC); Crumb Rubber; Used Tyres; Rubberized ECC; Sodium Hydroxide (NaOH)

ID: MJC-IKMP-10

Comparative Water Quality Analysis Between Tahan River and Sat River in Taman Negara Pahang, Malaysia

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Rivers particularly in the national forest conserve like Taman Negara Pahang, plays an important role in sustaining aquatic lifeforms, besides the livelihood of the locals. In conserving the area, water quality study has been carried out in two tributary rivers namely, Tahan and Sat. Sampling was conducted at 8 sampling locations for each river and the parameters analysed were temperature, pH, Total Suspended Solids (TSS), Dissolved Oxygen (DO), Biochemical Oxygen Demand (BOD), Chemical Oxygen Demand (COD) and ammoniacal nitrogen (AN). Results were then used in calculating the rivers WQI-DOE water quality index. In comparison, through the WQI-DOE indexing, overall Tahan river scores slightly lower water quality then Sat river by obtaining the water quality of Class II while Sat river's water quality is of Class I. However, the one-way Analysis of Variance (ANOVA) with confidence level of 95% shows that all water quality parameters measured exhibited no significant differences between the sampling stations.

Keywords: Water Quality; Taman Negara Pahang; Sat river; Tahan river; WQI-DOE Index

ID: MJC-IKMP-11

One-pot Sol-Gel Synthesis of Zinc Oxide-Reduced Graphene Oxide Composite: Photocatalytic, Kinetic and Fuzzy Inference System

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In this work, zinc oxide/reduced graphene oxide (ZnO/rGO) composites with different ratios, synthesized by the one-pot sol-gel method were tested as photocatalysts for degradation of methylene blue in aqueous phase. The physicochemical properties of the photocatalysts were characterized by FTIR and SEM-EDX. FTIR analysis showed the existence of various functional groups on the ZnO/rGO surfaces indicates strong interactions between the carbonyl, carboxylic, and hydroxyl groups on the rGO with ZnO particles. SEM images revealed a nearly spherical shape of ZnO and homogeneously distributed on the rGO sheets, while EDX result confirmed the presence of C, Zn, and O as increasing amounts of rGO. Based on pseudo first-order kinetic model, the highest degradation rate constant, k of 2.67×10^{-2} min^{-1} was obtained with 85% methylene blue degradation by using ZnO/rGO-10 photocatalyst. The relationship between the amount of rGO loadings, degradation percentage and rate constant are discussed using fuzzy inference system (FIS). The introduction of fuzzy logic controller (FLC) in this work is to provide the future direction and prediction for the construction of the optimum ZnO/rGO photocatalysts for practical water recovery process.

Keywords: Fuzzy Inference System; Photocatalysis; Reduced Graphene Oxide; Water Recovery; Zinc Oxide

ID: MJC-IKMP-12

Enhanced Adsorption Of Carbon Dioxide By Phosphoric Acid Modified Soybean Curd Residue Biochar

Dina Sofiea Zakaria[1,2], Siti Khalijah Mahmad Rozi[1,2*], Hairul Nazirah Abdul Halim[1,2], Ahmad Razali Ishak[3], Sharifah Mohamad[4], Siti Amira Mat Hussin[4]

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In order to preserve environmental quality, biochar is being increasingly applied for the carbon dioxide (CO_2) capture. The used of soybean waste, soybean curd residue (SCR) as CO_2 adsorbents can help to reduce the uncontrolled disposal of SCR all around the world. In this research, biochar based SCR (Biochar@SCR) was prepared by pyrolysis process. For chemical activation, the Biochar@SCR was immersed for 12 hours in 42.5 wt.% H_3PO_4 solution at 1:1 ratio (g precursor/g H_3PO_4) to obtain Biochar@SCR-M1. Biochar@SCR-M2 was produced when Biochar@SCR-M1 was pyrolyzed again at 500 ^{0}C for 2 hours. Elemental and functional groups analyses showed the presence of element Phosphorus (P) and functional groups of P=O or P=OOH for Biochar@SCR-M1 and Biochar@SCR-M2 suggesting the chemical modification using H_3PO_4 was successful. Morphological analysis revealed the formation of pores after pyrolysis process and chemical treatment with H_3PO_4. Analysis of CO_2 adsorption depicts that the adsorption capacity of SCR, Biochar@SCR, Biochar@SCR-M1 and Biochar@SCR-M2 are 3.00 mg/g, 25.21 mg/g, 30.50 mg/g and 36.00 mg/g, respectively. This result proved that the increased CO_2 sorption for H_3PO_4 treated Biochar@SCR suggesting that phosphoric acid modification was an effective method to prepare biochars with a high adsorption of carbon dioxide.

Keywords: Soybean curd residue; Phosphoric acid; Biochar; Pyrolysis; Carbon dioxide

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Antibacterial Activity of Metal-Natural Extract Complexes

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Metal-based compounds are well known for their biological activity. Metal-based compounds consist of a combination of an organic substituent as ligand and inorganic substituent as the metal center. Natural products, in particular natural extract are well known to exhibit excellent biological activities, while the inorganic substituents are usually the metal ions. *Pluchea indica (L.) less*, *Clinacanthus nutans* and *Phyllanthus niruri* are medicinal plants that possess various biological properties. Incorporation of transition metal ions (Cu^{2+}, Ni^{2+}, Co^{2+}, Zn^{2+}) into the crude extracts from these medicinal plants would give metal-natural extract complexes of *Pluchea indica (L.) less*, *Clinacanthus nutans* and *Phyllanthus niruri*. Leaves of *Pluchea indica (L.) less*, *Clinacanthus nutans* and *Phyllanthus niruri* were collected and extracted with either methanol or ethanol and synthesized with various transition metal salts to yield metal-natural extract complexes. The metal-natural extract complexes were assessed for their antibacterial activity using the quantitative and qualitative antibacterial assay against four pathogenic bacteria which are *Staphylococcus aureus* (ATCC 29213), *Bacillus cereus* (ATCC 117788), *Pseudomonas aeruginosa* (ATCC 27853) and *Escherichia coli* (ATCC 25922). The antibacterial assays showed that the biological activities of the metal-natural extract complexes were enhanced and selective towards selected target bacteria. It was found that the identity of transition metal ions played an important role in the enhancement of the bioactivity exhibited by the metal-natural extract complexes. The results showed that these metal-natural extract complexes *of Pluchea indica (L.) less, Clinacanthus nutans* and *Phyllanthus niruri* are potential to be alternative antibacterial agents.

Keywords: *Pluchea indica (L.) less*; *Clinacanthus nutans*; *Phyllanthus niruri*; metal-natural extract complexes; antibacterial agent

ID: MJC-IKMP-14

Inhibition Of *Staphylococcus Epidermidis* Biofilm By A Bacteriocin-Like Peptide From The Frog *Fejerverya Cancrivora*

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Bacterial biofilm is a serious threat to human health as they are resistant against both human defense mechanisms and conventional antimicrobial agents. Biofilm can form on surfaces including medical devices causing chronic infections that are difficult to treat, often requiring the use of large doses of antibiotics or the removal of the contaminated device. Anti-microbial peptides (AMP) isolated from the skin secretion of frogs have been documented as a promising anti-biofilm agent. Malaysia is rich with natural resources, including its rainforest which is a habitat for amphibians. Hence, this study aimed to screen for potential antibiofilm agents from the mucus of local frog *Fejerverya cancrivora* against biofilm former *Staphylococcus epidermidis* ATCC 35984. Antibiofilm activity of the mucus of *F. cancrivora* was recorded at the attachment, maturation and dispersion stage of biofilm formation at 97.67 %, 54.66 % and 11.21 % respectively. The active antibiofilm component was then fractionated and further purified by C18 reverse phase high-performance liquid chromatography column (HPLC) to single peptide with antibiofilm activity. Peptide sequencing revealed a partial amino acid sequence with 67% similarity to the N-terminal bacterial protein belonging to the bacteriocin family. This suggests the potential of a local frog in producing mucus with antibiofilm properties.

Keywords: Antibiofilm, Anti-microbial peptides, *Fejerverya cancrivora*, frog's mucus.

ID: MJC-IKMP-15

Photocatalysis Of Propanol Synthesis From Glycerol Over Fluorine-Doped Oxide (FTO) Catalyst

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Glycerol is the major by-product of biodiesel produced from transesterification process. It is abundantly produced and caused decrease in price market and environmental problem. Because of that, there needs efficiently utilization of glycerol to avoid the glycerol become oversupply without maximizing the benefits. In this study, photocatalytic conversion of glycerol to propanol using fluorine-doped tin oxide (FTO) is proposed for the first time. It aims to produce propanol with high selectivity and glycerol conversion in optimal reaction condition. The surface morphology, composition, reaction yield, and physicochemical state were comprehensively characterized by scanning electron microscope (SEM), Energy Dispersive X-ray (EDX), X-ray diffraction analysis (XRD), X-Ray Photoelectron Spectroscopy (XPS) and high-performance liquid chromatography (HPLC). Optimum glycerol conversion of 86 % and high propanol selectivity of 100 % was achieved under 80 W of light intensity, 90 minutes of reaction time by using 10 wt% glycerol concentrations respectively. It proved that photocatalysis of glycerol reaction using FTO catalyst successfully contributes to formation of free radical and surface of active site to the redox reaction. It was suggested that propanol formation due to amphoteric characteristic of FTO could enhance the C-O and C-H bond dissociation through hydrogenolysis of 1,3-PDO as intermediate substance.

Keywords: Photocatalyst, Fluorine-doped tin oxide (FTO), Free radical, Glycerol conversion, Propanol

ID: MJC-IKMP-16

The Treatment of Acidic Petroleum Crude Oil Assisted by CaO/Al_2O_3 Catalyst

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This study proposes that crude oil processing in petroleum refinery is valuable these days due to an increasing demand in the petroleum by-product. The presence of Naphthenic Acids (NAs)in crude oil lead to great concern to the petroleum industry as it will cause several corrosion problems to the oil refinery process. In this study, (NAs) extraction reaction was conducted by using 2-methylimidazole in ethanol assisted by a heterogeneous catalyst to speed up the reaction. Calcium nitrate ($Ca(NO_3)_2$) loaded at a concentration of 10% on an aluminium oxide (Al_2O_3) support were prepared by Incipient Wetness Impregnation (IWI) method. The feedstock obtained from Petronas Penapisan Melaka with original Total Acid Number (TAN) value of 4.38 mg KOH/g. The operating condition for the extraction reaction were a crude oil and reagent ratio of 0.5:0.5, catalyst loading of 5, 10, 15 and 20 wt%, reaction temperature at 35oC, reaction time at 15 minutes and catalyst calcination temperature at 700,900 and 1000oC. The Total Acid Number (TAN) value of crude oil was successfully lowered to 0.48 mg KOH/g using Ca/Al_2O_3 catalyst at a calcination temperature of 1000oC. The catalyst was extensively investigated by using TGA-DTA, results revealed that calcination temperature above 7000C completely remove all the impurities in the potential catalyst. SEM micrograph showed an inhomogeneous distribution of various particle sizes, which confirm the presented of Ca metals on the prepared catalyst. EDX results confirmed the presence of 6.69% of the weight composition of Ca. This treatment was verified that Ca/Al_2O_3 as a heterogeneous catalyst could be used to extract NAs to lower TAN value of crude oil effectively. Thus, lowering the TAN value to less than 0.5 mg KOH/g.

Keywords: Crude Oil, Extraction, Heterogenous Catalyst, Naphthenic Acid

ID: MJC-IKMP-17

RSM-Optimization Approach for Dispersive Micro Solid Phase Extraction for the Determination of Tetracycline Antibiotics in Water Samples

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Dispersive micro solid phase extraction (D-µ-SPE) using C_{18} for the extraction and pre-concentration of tetracycline antibiotics (TCs) in water samples prior to high performance liquid chromatography ultraviolet/diode array detector (HPLC-UV/DAD) was developed. The selected TCs residues were tetracycline (TC), oxytetracycline (OTC) and doxycycline (DOC). Central Composite Design (CCD) of Response Surface Methodology (RSM) was used for optimization of the mass of sorbent and extraction time. Results show that the coefficient of determination, R^2 value for the extraction of the selected TCs is 0.9980, indicating a good-fitted model. The optimum conditions obtained from the extraction analysis were 75 mg mass of sorbent and 30 min extraction time. Under the optimum conditions, good linearities were obtained over the range of 0.1-10 mg L^{-1} with R^2 of 0.9990-0.9997 and limit of detection of 0.053-0.099 mg L^{-1}. The method was successfully applied to river and tap water samples. The developed method proves to be simple, rapid, and reliable with good extraction efficiencies for the detection of antibiotics in water samples.

Keywords: Dispersive Micro Solid Phase Extraction; Response Surface Methodology; Central Composite Design; Tetracycline Antibiotics; Water Samples

ID: MJC-IKMP-18

Enhanced Extractability of Phenolic Compounds and Antioxidant Activity of Fermented Rice Straw using *Aspergillus oryzae*

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Rice straw is one of the abundantly available agricultural waste materials in Malaysia. Field burning is the major practice used for eliminating the rice straw that increases the air pollution and consequently affects public health. In this study, rice straw was utilized as substrate for solid state fermentation (SSF) by using *Aspergillus oryzae*. Solid state fermentation was conducted at 30°C, with 70% initial moisture content and 10% v/v of inoculum level. The effect of fermentation duration on the total phenolic content, total flavonoid content and antioxidant activity was investigated. It was found that solid state fermentation was able to enhance the extractability of total phenolic content by 104.4% and total flavonoid content by 5.32% after ten days of fermentation. Antioxidant activity of rice straw was increased as the fermentation progressed with 90.01% increment of DPPH radical scavenging activity and 89.24% of FRAP value. The activity of xylanase and β-glucosidase enzymes produced during SSF was also investigated to study the relationship with the polyphenols and antioxidant activity of fermented rice straw extracts. Both enzymes showed increased in activity as fermentation progressed showing that the enzymes might play a significant role in releasing the bound phenolics during SSF.

Keywords: Rice straw, Solid state fermentation, Total phenolic content, Antioxidant activity

ID: MJC-IKMP-19

Multi-Trace Metals Determination of Peninsular Malaysia Stingless Bee Honeys from Different Regions and Seasons Using Inductively Coupled Plasma-Optical Emission Spectrometry and Chemometric Techniques

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Demand for authenticating and distinguishing the provenance of bee honey among consumers is continuously rising. Considering the vast variations in prices attributable to different geographical origins, suitable indication on labelling of honey products is important for consumer protection. Since concentrations of trace metals can be closely related to geographical origin, the use of spectroscopy and chemometric techniques for ascertaining the validity of such a claim may prove relevant. In this study, multi-trace metals in stingless bee honey of *Heterotrigona itama* species, from different regions and seasons in Peninsular Malaysia (Kedah, Johor, Selangor and Pahang) were determined *via* inductively coupled plasma-optical emission spectrometry (ICP-OES). Principal component analysis (PCA) was then applied to recognise the distribution patterns. Subsequently, linear discriminant analysis (LDA) was applied to perform further classification. With the use of LDA, cross-validation was found to be 95.8% and 89.6% during the rainy and less rainy seasons, respectively. The combination of ICP-OES data with PCA and LDA techniques has provided an accurate classification of the Malaysian stingless bee honey samples according to their respective origins. This study provided some elemental information on the distribution of stingless bee honey samples at spatial and temporal levels, and could be used as a reference for their provenance establishment and authenticity.

Keywords: Stingless bee honey; Provenance; Authenticity; Spectroscopy; Chemometric

ID: MJC-IKMP-20

Synthesis And Characterization Of Eggshell Membrane (ESM) Functionalized Free Fatty Acids (FFAs) As Potential Adsorbents For Removal Of Anionic And Cationic Dyes Pollutants

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Dye is a harmful substance to the marine life and aquatic ecology. In this study, eggshell membrane (ESM) was functionalized with free fatty acids (FFAs) from new and used palm cooking oil producing ESM@FFAs-NCO and ESM@FFAs-UCO adsorbents, respectively for removal of selected cationic and anionic dye. The optimum reaction time of ESM with FFAs is 15 minutes while the optimum mass ratio (ESM to FFAs) is 1:4 ratios. both adsorbents were characterized using SEM and FTIR. The surface morphology of functionalized ESM revealed a better and more extensive microporous network of interwoven and coalescing shell membrane fibers compared to non-functionalized ESM. FTIR analysis had confirmed that FFAs were successful attached onto the surface of ESM for both of adsorbents. Using optimum contact time (30 min) and adsorbent dosage (30 mg), the investigation on the adsorption capability of the adsorbents towards alizarin is as following order: ESM < ESM@FFAs-NCO < ESM@FFAs-UCO. The synergistic effect of hydrogen bonding and hydrophobic interaction are caused by the increasing of active site on the functionalized ESM. Moreover, higher removal efficiency was obtained using ESM@FFAs-UCO due to the increasing of hydrophobicity property led by high composition of long alkyl chain. Therefore, ESM@FFAs-UCO was chosen for further investigation as adsorbent for other organic dyes, such as Rhodamine B, Chicago sky blue, and Remazol dye. The removal percentage for the selected dyes was as follows; Alizarin (87.83%), Remazol (84.59%), Rhodamine B (78.34%) and Chicago Sky Blue (65.68%). Based on the results, ESM@FFAs-UCO can be a versatile adsorbent since their potential to adsorb cationic and anionic dyes pollutants in the aqueous solution.

Keywords: Eggshell membrane, free fatty acid, used cooking oil, cationic and anionic dye

ID: MJC-IKMP-21

Molecular Docking And Adme Profiling Of Xanthorrhizol Derivatives As Hyaluronidase Inhibitors

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Hyaluronidase (Hyal) enzyme is one of the potential biological targets for the development of anti-inflammatory agents. Xanthorrhizol, a bisabolene sesquiterpenoid isolated from *Curcuma xanthorrhiza* has been reported showing anti-inflammatory activities against cyclooxygenase (COX), inducible nitric oxide synthase (iNOS), and interleukins (IL). However, the activity of xanthorrhizol as a Hyal inhibitor has not been exploited. In this study, a total of 26 xanthorrhizol derivatives having structural modifications at R_1 - R_4 scaffold were chosen. The molecular docking was performed to virtually screened their SAR activities towards Hyal while the ADME prediction was done to predict their pharmacokinetic profile. All derivatives bind to the active site of Hyal1 with binding energies ranging from -5.7 kcal/mol to -8.5 kcal/mol. Derivatives **24**, and **14** having benzyloxy moiety at R_1 position and polar moieties at R_3 and R_4 position showed lower binding energies (-8.3, and -7.9 kcal/mol, respectively) compared to apigenin, **28** and xanthorrhizol, **1**. These derivatives also fulfilled all ADME and drug-likeness properties suggesting them as potential Hyal inhibitors. Through this work, the activity of xanthorrhizol derivatives against Hyal1 can be predicted and screened as a basis for future modifications of xanthorrhizol as potential Hyal inhibitor.

Keywords: Xanthorrhizol; Hyaluronidase; Molecular Docking; ADME Profile

ID: MJC-IKMP-22

Effect Of Carboxymethyl Cellulose (CMC) As A Plasticizer On Starch/CMC Biocomposites

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Biocomposites/bioplastics can be prepared from agricultural by-products and biodegradable, while conventional plastics which are produced from petroleum are detrimental to the environment. In this research, biocomposites from the mixture of starch solution (extracted from oil palm trunk) and with carboxymethyl cellulose (CMC) (5 wt%, 15 wt% and 25 wt%) were prepared by the solution casting method. The properties of the synthesized starch/CMC biocomposites were realized by Scanning Electron Microscopy, Thermogravimetric Analysis (TGA), Differential Scanning Calorimetry (DSC) and Fourier-transform infrared spectroscopy (FTIR-ATR). SEM images revealed the smooth and compact surface structures for all samples. FTIR-ATR spectra revealed the presence of functional groups such as inorganic phosphate, aliphatic amino acid salt, aliphatic C-H, carbonyl C=O and the ester C-O. For DSC, the spectra proved that the more CMC in the sample, the higher the heat released during the process. TGA analysis exposed the more amount of plasticizer carboxymethyl cellulose in the sample, the lower the sample left after the degradation process. This research proved that the bioplastics prepared from oil palm trunks hold great potential to replace petroleum-based plastics in the future.

Keywords: Biocomposites; Bioplastics; Carboxymethylcellulose; Plasticizer; Thin Film

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Bio-Nanohybrid Composite Sorbent-Based Microextraction for Acid Drugs in Aqueous Samples: Box-Behnken Design Approach

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Biopolymer chitosan was hybridized with tetraethoxysilane via hydrolysis method to obtain bio-nanohybrid composite sorbent. The composite sorbent was then employed for the dispersive solid phase extraction of three non-steroidal anti-inflammatory drugs in aqueous samples. Field Emission Scanning Electron Microscope (FESEM) micrograph showed that the bio-nanohybrid composite consisted of irregular spherical shape nanoscale particles with sizes in the range of 41.1-231.5 nm. Interactive effects of three significant parameters namely extraction time, sample pH and desorption time in determination of naproxen, diclofenac sodium, and mefenamic acid were evaluated systematically by using Box Behnken design (BBD) approach. The predicted response value was found to be in good agreement with the actual value (R^2 > 0.9423). Under the optimum conditions, the method showed low limit of detection, LODs (0.04-0.67 µg/L) and excellent relative recoveries (96.16-101.48%). The results indicated the bio-nanohybrid composite was an excellent sorbent in sorbent-based microextraction that offer fascinating alternatives to synthetic polymer sorbents in the future.

Keywords: Chitosan; Nanohybrid; Dispersive Solid Phase Extraction; Box Behnken design; non-steroidal anti-inflammatory

ID: MJC-IKMP-24

Utilisation of Cationic Surfactant Modified Grated Coconut Residue for the Removal of Reactive Orange 16 from Aqueous Solutions: Fixed Bed Column Study

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The idea of removing reactive orange 16 (RO16) dye using shredded coconut residue as a new low-cost adsorbent was studied. In this investigation, a continuous adsorption technique on a fixed-bed column was used to remove reactive orange 16 using an adsorbent produced from grated coconut wastes that had been chemically treated with the cationic surfactant cetylpyridinium chloride (CPC). The raw and surfactant modified grated coconut (SMGC)were characterised by Fourier Transform Infrared(FTIR) and Field Emission Scanning Electron Microscope(FESEM). The FTIR spectra successfully demonstrate CPC adherence to the SMGC, with two new peaks originating from CPC appearing at 2921.49 and 2853.08 cm-1. Meanwhile, The FESEM image indicates that SMGC has an irregular and uneven surface. It was observed that (SMGC) is an efficient medium for removing colour from an aqueous solution. The findings of the breakthrough column investigation revealed that different column characteristics such as adsorbent bed height and inlet dye flow rate impacted the results. Although the breakthrough time increased as the bed height increased, it was discovered that a greater initial dye input concentration and a quicker flow rate resulted in a shorter breakthrough time. The adsorption data were fitted to the Yoon-Nelson column mathematical model for predicting breakthrough curves and timings. The findings of the Yoon-Nelson model for determining the 50% breakthrough time varied from 5.25 to 35.45 minutes. The findings show that the Yoon-Nelson model is in excellent agreement with the experimental data, as the correlation
coefficient, R2, for all three parameters studied is considerably more than 0.99.

Keywords: Adsorption, coconut residue, fixed-bed column, surfactant modified, Yoon-Nelson model

ID: MJC-IKMP-25

Fabrication And Characterisation Of Recycled Polyethylene Terephthalate / Graphene Oxide Nanofibers As Potential Adsorbent Of Methylene Blue

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Methylene blue (MB) dyes are existed in industrial wastewater and can cause a severe threat to aquatic life. In this study, recycled polyethylene terephthalate/graphene oxide (rPET/GO) nanofibers were fabricated using electrospinning technique. The electrospinning parameters such as concentration, flow rate and voltage had been optimized. The influence of GO amount on the fibers' morphology and diameters, mechanical strength as well as methylene blue and sorption capacity were evaluated using scanning electron microscopy (SEM), tensile strength test, and ultraviolet-visible spectrophotometer, respectively. The Fourier-Transform Infrared Spectroscopy (FTIR) was used to confirm the interaction between rPET and GO. SEM images showed the diameter of rPET/GO nanofibers decreased with increasing GO composition. rPET/GO nanofibers produced the average diameter of 118± 56 nm. FTIR analysis revealed the successful interaction between rPET and GO. The incorporation of GO into rPET nanofibers increased the tensile strength and MB adsorption capacity. The results showed that rPET/GO nanofibers showed a good potential adsorbent for MB thus may be a potential material for water treatment.

Keywords: nanofibers; electrospinning; graphene oxide; adsorption; methylene blue

ID: MJC-IKMP-26

A Review On Application Of Carrageenan Extract From Red Seaweed (Rhodophyta) In Cosmetics

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Cosmetic industries have expanded globally and will continue to increase as long as there are consumers. However, today, concerns arise where consumers become aware of the negative implications on chemical products and the halal status of the cosmetics which is the main concern by the Muslim consumers. Thus, they start to find an alternative by replacing and using cosmetics formulate by using natural products. Marine plants such as seaweed possess numerous natural polysaccharides. Carrageenan is a compound that is extracted from red seaweed (*Rhodophyta*). This natural polysaccharide is widely known to act as thickener, stabilizer and water-binding agent as well as have diverse biological activities that make it a suitable active ingredient in cosmetic products. The review highlights the significant aspects related to carrageenan like describing in details of the source, structure, general and biological properties of carrageenan that make it appropriate to be applied in cosmetics, applications, the extraction method and instrument used.

Keywords: Cosmetic; Carrageenan; Seaweed; Thickener

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Preliminary Phytochemical Analysis of Malaysian *In Vitro* Cultured Aromatic Rice (*Oryza sativa* L. Cv. MRQ 74)

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The present study is aimed at primary screening of the phytochemical contents in aromatic rice stems and leaves of *Oryza sativa* L. Cv. MRQ 74. The plants were subjected to *in vitro* plant tissue culture techniques. The dehusked seeds of *Oryza sativa* L. Cv. MRQ 74 were surface sterilised using 70% (v/v) clorox with two drops of Tween 20, followed by 50%, 30%, 20% and 10% clorox. The sterilised seeds were then cultured on hormone – free MS media for 6 weeks. Stems (basal segment) of 6-week-old aseptic seedlings were approximately excised into 5.0 – 10.0 mm segments. The explants were then cultured onto MS media fortified with 0.1 mg/L BAP and hormone-free MS media as a control. The crude extracts of stems and leaves of raised plantlets were prepared by maceration process. The phytochemical screenings were carried out to detect the presence of flavonoids, alkaloids, saponins, tannins, terpenoids, resins, phenols, reducing sugar and iodine. The results revealed that the crude extracts derived from plantlets grown on MS media with and without BAP were found to be rich in saponins, terpenoids, resins and reducing sugar. There were no presence of flavonoids, alkaloids, tannins, carbohydrates and starch in both crude extracts.

Keywords: Aromatic rice; *In vitro* cultured; BAP hormone; Phytochemical screening

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Optimization of Thin-film Microextraction using Polyelectrolyte Multilayers Sorbent Combined with HPLC-UV for Separation and Determination of Tricyclic Antidepressant Residues

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Thin-film polyelectrolyte multilayers (PEMs) namely poly(allylamine hydrochloride) (PAAH) and poly(styrene sulfonic acid) (PSS) were successfully prepared as a new extraction medium for drugs. Three kinds of tricyclic antidepressant drugs (TCAs) namely imipramine (IMI), amitriptyline (AMI), and chlorpromazine (CHLO) were selected as target model analytes. thin film microextraction (TFME) technique was performed by stacking 7 pieces (ca. 8.4 mg) of circular CA-PEMs (5 mm diameter) through a needle by directly dipping them into a sample solution and agitating the solution during the extraction process. The CA-PEMs were ultrasonicated for analyte desorption using 100 µL of the organic solvent before analysis with high-performance liquid chromatography-ultraviolet detection (HPLC-UV). Several important parameters such as type of desorption solvent, the effect of sample pH, salting-out effect, extraction time, desorption time, the volume of desorption solvent, and stirring speed were evaluated and optimized. Under optimized extraction conditions, the technique demonstrated good linearity in the concentration range of 10-1000 µgL-1 for lake water and river water and 50-1000 µgL-1 for urine samples. The best detection limit was achieved in the range of 3.7 µg L-1 to 40.5 µg L-1. The percentage recoveries were generally achieved in the range of 99% -111.18% with the RSD of 2.6-4.7% (n=3).

Keywords: Drug residues, HPLC-UV, Thin-film microextraction, Tricyclic antidepressant drugs

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Effect of the Molar Ratio of Sodium Hydroxide on Bentonite Support for the Transesterification of Waste Cooking Oil into Fatty Acid Methyl Ester

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Transesterification process using a mono-hydric alcohol and catalyst can generate biodiesel, which is defined as the mono-alkyl esters of vegetable oils or animal fats. In this study, NaOH supported on bentonite was developed with different molar ratio. The impregnation approach was used to make a series of NaOH/bentonite catalysts with molar ratios of 1:1, 1:2, 1:3, and 1:4 between bentonite and NaOH. The synthesized catalyst was characterized using FTIR and XRD analysis. A pre-treatment on the waste cooking oil (WCO) sample was conducted before the transesterification process started. The characteristics of WCO as biodiesel's feedstock, which are free fatty acids (FFAs), saponification, and moisture content were determined. Based on the results, the WCO sample have FFAs value of 0.4902%, saponification value of 206.7 mg KOH/g, and moisture content of 0.22%. Based on the FTIR analysis, the impregnation of NaOH into bentonite can be seen as successful with the presence of stretching band at about 3430 cm^{-1} indicates the presence of Al-O-Na group. The XRD analysis also shows changes in the peaks' intensity indicating the presence of Na_2O crystals. The NaOH/bentonite catalyst with molar ratio 1:3 showed good FFAs conversion (40.7%) at reaction temperature of 60°C and reaction time of 3 hours.

Keywords: WCO; NaOH/bentonite; Molar ratio; Biodiesel

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Synthesis, Characterization And Anti-Triple Negative Breast Cancer (TNBC) Activites Of Non-Symmetric Curcumin Derivatives

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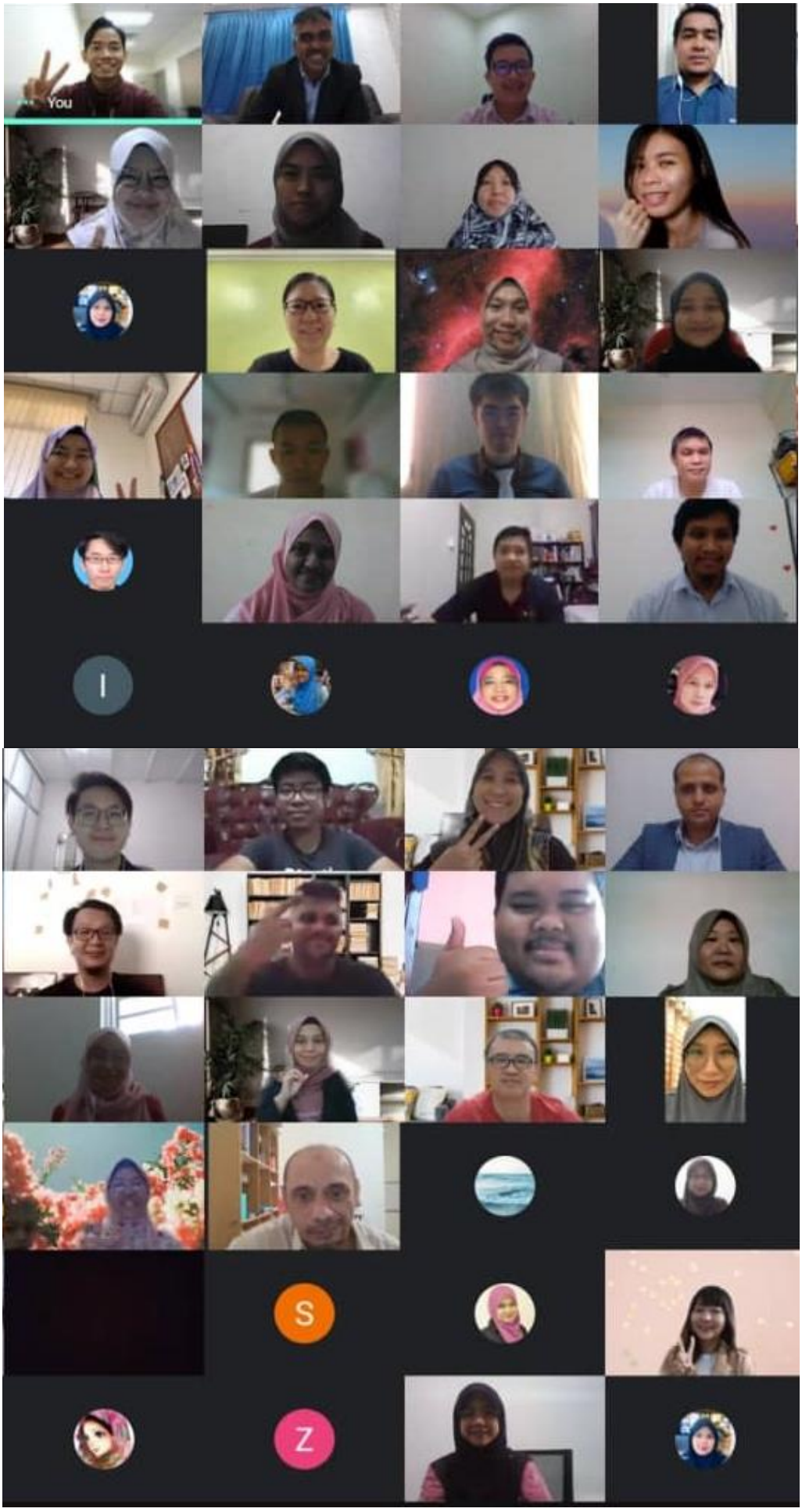
Triple-negative breast cancer (TNBC) is the most aggressive breast cancer subtype with limited treatment options. Of late, curcumin have demonstrated anti-TNBC activity against different cell lines. This study aimed to explore the possibility of developing a new anti-TNBC agent with better activity and selectivity compared to curcumin. Few synthesis methods were explored including Stork enamine aldol condensation of cyclohexanone and 4-nitrobenzaldehyde produced intermediate 4-nitrobenzylidenecyclohexanone, yielded non-symmetric derivatives 1a – d when it was further condensed with various benzaldehyde. Resulted compounds were substituted with allyl bromide and acryloyl chloride to form 2a–2c and 3a-3c, respectively. In a separate reaction, 4-fluorobenzaldehyde and heterocyclic amine reacted to afford intermediates, followed by refluxing with appropriate monoaryl benzylidene to afford compound 4a–4g. Sonication-aldol condensation was used to produce 5a – 5e bearing heterocyclic core linker. All final compounds were characterized using 1H NMR, 13C NMR and HRMS. Compounds cytotoxic activity were tested on various types of cells lines (TNBC MDA-MB-231, HCC-1806; non-TNBC MCF-7; non-cancerous cells Beas-2B, HEK-239, BV-2 and pHMEC). The most active and selective compound (5d and 5e) were further determined with anti-TNBC activities on MDA-MB-231 and HCC-1806 cells, respectively. Findings showed that both compounds arrested G2/M cell cycle progression, induced apoptosis and attenuated proteasome activity in vitro.

Keywords: non-symmetric, curcumin, TNBC, anti-cancer.



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