



# PROGRAMME & ABSTRACT BOOK iCAST2021

7<sup>th</sup> International Conference on Advancement in Science & Technology

24 - 26 August 2021

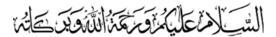
Organised by:
Kulliyyah of Science,
International Islamic University
Malaysia,
Bandar Indera Mahkota, 25200
Kuantan, Pahang
Email: icast@iium.edu.my

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#### **MESSAGE FROM THE ADVISOR OF ICAST 2021**





Praise be to Allah S.W.T. for His grace and benevolence that our Kulliyyah of Science has succeeded in organizing the 7<sup>th</sup> International Conference on Advancement in Science and Technology 2021. I would like to take this opportunity to thank the organising committees who have greatly contributed their time and effort for coordinating this event. Let's thank their undivided commitments and efforts in ensuring this program runs smoothly despite many restrictions due to the current development of Covid-19 cases all around the world.

I would like to also acknowledge everyone at the Kulliyyah of Science for their support towards the accomplishment of this event. This time around, the theme for our conference is 'Physical Sciences for Life'. The Kulliyyah of Science has the pleasure to conduct this conference which focus on the new advancement in the physical sciences in relation to the life sciences.

The core objectives of this conference are to provide a platform for discussion, to promote different applications of physics, mathematics and chemistry to industries relevant to biology and medicine, and to encourage further the multidisciplinary approach for science towards a more comprehensive understanding of nature in general and life sciences in particular. The range of papers comprising this issue exemplifies the diverse experience and knowledge of the worldwide community.

Finally, I would like to welcome all the delegates and participants to the iCAST 2021. I hope that this conference will be useful for you and your scientific activities. I wish that all our delegates and participants will depart from this conference with the satisfaction of having a very fulfilling, pleasant and rewarding experience.

Thank you, wassalam.

"Leading the Way"

#### Prof. Dr. Shahbudin Saad

Advisor

International Conference on Advancement in Science and Technology (iCAST2021)

#### **MESSAGE FROM THE CHAIRMAN OF ICAST 2021**



Assalamualaikum w.b.t. and Greetings!

Please allow me to welcome all to our flagship conference. This conference is the 7th installation since the kulliyyah's inception about two decades ago and this time around, we are committed to a multidisciplinary approach to science.

While many of us tend to work in very specific fields in science, it is undeniable that multidisciplinary scientific research is a more proper approach towards solving realistic problems which tend to be very complex; betraying simple caricatures of models used in specific discipline based textbooks. Rather than isolating a specific element in a given scenario for study, a multidisciplinary approach takes on the problem head on in its entirety and encourages a team of experts in different fields to collaborate towards high impact solutions.

This conference is aimed at creating a platform to encourage conducive discussions between the researchers to better understand the intricacies and details of a given discipline embedded in a multidisciplinary effort while at the same time allowing for constructive criticism and further appreciation of such works.

We hope that this conference, its theme, can only serve as a humble step, one amongst many others in other places and time, for a more coherent effort for such scientific endeavours. I would also like to take this opportunity to thank everyone for their support of the conference, more specifically the participants, our sponsors and of course, our committee who has worked hard to make this event possible.

Thank you.

"Leading the Way"

Assoc. Prof. Dr. Jesni Shamsul Shaari

Chairman

International Conference on Advancement in Science and Technology (iCAST2021)

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# PROGRAMME SCHEDULE

# PROGRAMME SCHEDULE 24 AUGUST 2021 | TUESDAY

Time (GMT +8)	
08:30 am	Registration Open
	OPENING CEREMONY
09:00 — 10:00 am	National Anthem of Malaysia, 'NEGARAKU' and 'Lead the way'
	Doa recitation
	Welcoming Address by Prof. Dr. Shahbudin Saad, Advisor of iCAST 2021
	Officiating Address by Prof. Emeritus Tan Sri Dato' Dzulkifli Abdul Razak, Rector of International Islamic University Malaysia (IIUM)
	SESSION 1
	Chairperson: Assoc. Prof. Dr. Deny Susanti Darnis
10:00 — 11:00 am	PLENARY : Assoc. Prof. Dr. Mohd Firdaus Raih SESSION 1 National University of Malaysia (UKM)
	SUBSTRUCTURE SEARCHING IN BIOLOGICAL MACROMOLECULES - NEW FUNCTIONS FROM OLD FUNCTIONS, NEW TARGETS FOR OLD DRUGS
11:00 — 11:10 am	Break
11:10 — 11:30 am	PRESENTATION 1: COMPUTATIONAL BIOLOGY APPROACH TOWARDS STUDYING PROTEIN-PROTEIN INTERACTION BETWEEN BREAST CANCER CELL PROTEINS AND PLANT COMPOUNDS  Dr. Asita Elengoe Lincoln University College Malaysia
11:30 — 11:50 am	PRESENTATION 2: MOLECULAR BINDING INTERACTION OF ANGIOTENSIN CONVERTING ENZYME AND 1-GALLOYL GLUCOSE, THE MAJOR COMPOUND IN SYZYGIUM POLYANTHUM LEAVES  Mr. Tuan Faiz Tuan Anuar International Islamic University Malaysia (IIUM)
11:50 — 12:10 pm	PRESENTATION 3: GENOME-WIDE COMPARATIVE ANALYSIS OF DROUGHT TOLERANT GENES IN RICE, MAIZE, DATE PALM AND ARABIDOPSIS  Ms. Nurul Asyikin Mohd Zim International Islamic University Malaysia (IIUM)

Time (GMT +8)		
12:10 — 12:30 pm	PRESENTATION 4: IN SILICO DEVELOPMENT OF CRISPR/CAS9 CONSTRUCT FOR ORYZA SATIVA SUBSP. INDICA  Ms. Anis Afuza binti Md Yusof International Islamic University Malaysia (IIUM)	
12:30 — 2:00 pm	Break	
	SESSION 2	
	Chairperson: Asst. Prof. Dr. Siti Fairuz Che Osman	
2:00 — 2:20 pm	PRESENTATION 5: SYNTHESIS AND CHARACTERISATION OF SERIES OF NITRO AND CHLORO 2-ARYLBENZIMIDAZOLE DERIVATIVES  Ms. Mariyah Najihah bt Abdullah International Islamic University Malaysia (IIUM)	
2:20 — 2:40 pm	PRESENTATION 6: IODINE MEDIATED ONE-POT SYNTHESIS OF 3-CARBETHOXYCOUMARINS  Dr. Dinesh Kumar Sharma Kishan Lal Public College, Rewari, India	
2:40 — 3:00 pm	PRESENTATION 7: MULTIFUNCTIONAL LYOTROPIC LIQUID CRYSTALLINE NANOPARTICLES FOR GEMCITABINE AND THYMOQUINONE DELIVERY IN THE TREATMENT OF BREAST CANCER  Ms. Loo Yan Shan University Putra Malaysia (UPM)	
3:00 — 3:10 pm	Break	
3:10 — 4:10 pm	PLENARY SESSION 2: Assoc. Prof. Dr Adérito Araújo University of Coimbra, Portugal  A MATHEMATICAL MODEL FOR THE CORNEAL TRANSPARENCY PROBLEM	
4:10 — 4:30 pm	PRESENTATION 8: POLYMER BLENDED ALGINATE MICROBEADS FOR TARGETED DRUG DELIVERY  Dr. Md. Abul Kalam Azad  AIMST University	
4:30 — 4:50 pm	PRESENTATION 9: GASTROINTESTINAL TRACT DISTRIBUTION OF FLUORESCENCE MODIFIED ALGINATE BEADS  Dr. Md. Abul Kalam Azad  AIMST University	
4:50 pm	End of Day 1	

#### PROGRAMME SCHEDULE 25 AUGUST 2021 | WEDNESDAY

Time (GMT +8)	
08:30 am	Registration Open
	SESSION 3
	Chairperson: Asst. Prof. Dr. Mohd Hazimin Mohd Salleh
9:00 — 9:40 am	PLENARY : Dr. Firdaus Samsudin SESSION 3 : Agency for Science, Technology and Research (A*STAR), Singapore
	MODELLING AND SIMULATION OF SARS-COV-2 SPIKE GLYCOPROTEIN
9:40 — 10:00 am	PRESENTATION 10: EARLIER DENATURATION OF DNA BY USING NOVEL TERNARY HYBRID NANOPARTICLES
	Assoc. Prof. Dr. Akbar John International Islamic University Malaysia (IIUM)
10:00 — 10:20 am	PRESENTATION 11: DEVELOPMENT OF TURBIDITY, PH, TEMPERATURE AND FLOWRATE SENSOR IN WATER AND WASTEWATER BY USING ARDUINO
	Dr. Mohammad Hakim Che Harun University of Malaysia Terengganu (UMT)
10:20 — 10:40 am	PRESENTATION 12: INVESTIGATION ON STRAIN MEASUREMENT USING CARBON ELECTRICAL CONDUCTIVE PAINT
	Mr. Muhammad Nazrul Hisyam Bin Jamaluddin International Islamic University Malaysia (IIUM)
10:40 — 10:50 am	Break
10:50 — 11:10 am	PRESENTATION 13: SECOND HANKEL DETERMINANT OF BI-SUBORDINATE FUNCTIONS
	Assoc. Prof. Dr. Aini Janteng University of Malaysia Sabah (UMS)
11:10 — 11:30 am	PRESENTATION 14: INPAINTING OF DENTAL PANORAMIC TOMOGRAPHY USING DEEP LEARNING
	Dr. Mohd Adli Bin MD Ali International Islamic University Malaysia (IIUM)
11:30 — 11:50 am	PRESENTATION 15: ON SKEW PRODUCT OF QUADRATIC STOCHASTIC OPERATORS
	Prof. Dr. Nasir Ganikhodjaev Institute of Mathematics , Tashkent

Time (GMT +8)	
11:50 — 12:10 pm	PRESENTATION 16: PREPARATION OF SIX ARMS PCL- $b$ -PEG STAR-SHAPED POLYMER HYDROGEL
	Dr. Mohamad Wafiuddin Ismail International Islamic University Malaysia (IIUM)
12:10 — 12:30 pm	PRESENTATION 17: QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) STUDY OF NEWLY SYNTHESIZED CARBONYL THIOUREA DERIVATIVES ON A CANTHAMOEBA SP.
	Dr. Maizatul Akma Ibrahim International Islamic University Malaysia (IIUM)
12:30 — 2:00 pm	Break
	SESSION 4
	Chairperson: Asst. Prof. Dr. Hafizah Bahaludin
2:00 — 2:40 pm	PLENARY : Assoc. Prof. Dr. Yam Wai Keat SESSION 4 Perdana University
	SECOND YEAR INTO THE PANDEMIC ERA – ARE YOU ALREADY IN THE NEW NORM?
2:40 — 3:00 pm	PRESENTATION 18: INVESTIGATING AIR POLLUTION SOURCES USING PRINCIPLE COMPONENT ANALYSIS (PCA)
	Dr. Samsuri Abdullah University of Malaysia Terengganu (UMT)
3:00 — 3:20 pm	PRESENTATION 19: MOLECULAR RECOGNITION OF β-1,4-GLUCOSIDASE FROM TRICHODERMA HARZIANUM T12, ThBg T12 AGAINST MYCELIAL CELL WALL COMPONENTS OF PHYTOPATHOGENIC MACROPHOMINA PHASEOLINA
	Assoc. Prof. Dr. Azzmer Azzar Abdul Hamid International Islamic University Malaysia (IIUM)
3:20 — 3:40 pm	PRESENTATION 20: EFFECT OF DIFFERENT EXTRACTION METHODS ON VITAMIN B12 FROM EDIBLE GREEN SEAWEED, <i>ULVA LACTUCA</i> BY 2-LEVEL FACTORIAL DESIGN
	Ms. Fatin Shazwani Roslan International Islamic University Malaysia (IIUM)
3:40 — 3:50 pm	Break

Time (GMT +8)	
3:50 — 4:10 pm	PRESENTATION 21: ISOCRATIC RP-HPLC METHOD FOR THE SIMULTANEOUS DETERMINATION OF REACTION RATE IN N-PHENYLBENZAMIDE SYNTHESIS AND ITS INTERMEDIATE COMPOUNDS  Mr. Tariqul Islam International Islamic University Malaysia (IIUM)
4:10 — 4:30 pm	PRESENTATION 22: KINETIC MODEL FOR SULFATE RADICAL OXIDATION OF BROMOTHYMOL BLUE  Dr. DJEHICHE Mokhtar  University of Mohamed Boudiaf M'sila, Algeria
4:30 — 4:50 pm	PRESENTATION 23: SCREENING OF SELECTED MICROBES AS BIOCATALYSTS FOR BIOTRANSFORMATION OF CURCUMIN AND XANTHORRIZOL  Ms. Munirah Ridzuan International Islamic University Malaysia (IIUM)
4:50 pm	End of Day 2

# PROGRAMME SCHEDULE 26 AUGUST 2021 | THURSDAY

Time (GMT +8)	
08:30 am	Registration Open
	SESSION 5
	Chairperson: Asst. Prof. Dr. Azaima Razali
9:00 — 9:40 am	PLENARY : Assoc. Prof. Dr. Roswanira Abdul Wahab University of Technology Malaysia (UTM)
	RE-ENGINEERING UNWANTED BIOMASS INTO SMART BIOGENIC COMPOSITES
9:40 — 10:00 am	PRESENTATION 24: RECURSIVE-ADAPTIVE RENTAL SUBSCRIPTION MODEL (R-ARSM) IN THE NEW NORMAL: AM APPLICATION TO THE HOUSING SECTOR Dr. Friday Zinzendoff Okwonu Northern University of Malaysia (UUM)
10:00 — 10:20 am	PRESENTATION 25: REGULARITY OF 2-PARTITION POISSON QUADRATIC STOCHASTIC OPERATOR WITH THREE DIFFERENT PARAMETERS  Ms. Siti Nurlaili Karim International Islamic University Malaysia (IIUM)
10:20 — 10:40 am	PRESENTATION 26: SPATIAL DISTRIBUTION OF CU, ZN, PB AND NI IN SOIL IN BAUXITE MINING AREA USING GEOSTATISTICS AND GEOSPATIAL ANALYSIS  Ms. Mazidah Zulkifli International Islamic University Malaysia (IIUM)
10:40 — 10:50 am	Break
10:50 — 11:10 am	PRESENTATION 27: APPLICATION OF STABILITY INDEX IN CHARACTERIZING THE BASIN OF ATTRACTION IN ECOLOGICAL MODELLING  Dr. Ummu Atiqah Mohd Roslan University of Malaysia Terengganu (UMT)
11:10 — 11:30 am	PRESENTATION 28: OPTIMIZATION OF TOTAL PHENOLIC CONTENT AND ANTIOXIDANT ACTIVITY FROM SUKKARI VARIETY OF DATE PALM (PHOENIX DACTYLIFERA L.) USING SUPERCRITICAL FLUID EXTRACTION METHOD Ms. Nadirah Abd Rahim International Islamic University Malaysia (IIUM)

Time (GMT +8)	
11:30 — 11:50 am	PRESENTATION 29: THE IMPACT OF THE US-CHINA TRADE WAR ON THE MALAYSIAN STOCK MARKET NETWORK  Ms. Sarmita Surantharan National University of Malaysia (UKM)
	CLOSING CEREMONY
11:50 — 12:20 pm	Closing Remarks by Assoc. Prof. Dr. Jesni Shamsul Shaari, Chairman of iCAST 2021
12.20 pm	End of conference

# INVITED SPEAKERS

# SUBSTRUCTURE SEARCHING IN BIOLOGICAL MACROMOLECULES - NEW FUNCTIONS FROM OLD FUNCTIONS, NEW TARGETS FOR OLD DRUGS

Mohd Firdaus Raih Universiti Kebangsaan Malaysia (UKM), Bangi 43600, Selangor, Malaysia.

**Abstract:** The functions of biological macromolecules are dependent on their three-dimensional structures. Although the overall structure of these molecules are important for their functions, only a subset of residues are directly involved in a particular function mechanism. These functionally important residues are usually conserved as 3D substructures or motifs. They are usually involved in molecular interactions such as binding sites or catalytic mechanisms. In our research group, we have developed tools and resources that allow for the searching and comparisons of such 3D substructures in protein and RNA molecules. Recent developments in the field of protein structure prediction have resulted in highly accurate algorithms that can generate the 3D structure of proteins from sequences. Therefore, the capacity to search for similar substructures in protein structures can take on an even larger role in being able to assign a known function to the predicted protein structures that may have little similarity to any known protein structure - thus "giving" these "new proteins" a possible biological function. The same methods can be applied to find the presence of known drug binding sites in proteins that are unrelated, or not known to be the targets of those drugs. This enables new targets to be identified for drugs that have already been approved thus allowing them to be repurposed for other diseases or indications.

#### About the speaker

Dr. Mohd Firdaus Raih is an Associate Professor at the Department of Applied Physics in Faculty of Science and Technology, Universiti Kebangsaan Malaysia. He is currently the President for Malaysian Society of Bioinformatics and Computational Biology: Biophysics and Chair of the Department of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia. He obtained his BSc in Molecular and Cellular Biology - Biochemistry from Universiti Kebangsaan Malaysia and a PhD in Molecular Biophysics from University of



Sheffield. Dr. Mohd Firdaus research is in the field of bioinformatics and molecular biophysics. His research group focuses on the computational analysis of macromolecular structures, and the discovery and characterization of genome encoded non-protein coding elements and regulatory systems. He has published his works in various peer-reviewed journals including Nucleic Acids Research, Science, Scientific Reports and other highly regarded journals.

#### A MATHEMATICAL MODEL FOR THE CORNEAL TRANSPARENCY PROBLEM

Adérito Araújo University of Coimbra, Portugal

**Abstract:** Understanding the physical basis of corneal transparency has been a subject of interest amongst physicists, basic scientists and ophthalmologists. The cornea is the transparent, protective front of the eye and maintaining its curvature and transparency is essential for good vision. This question is relevant because there are several pathologies that increase the scattering of light in the cornea, often requiring surgical intervention. The main objective of our research group is to develop a suitable mathematical model capable of representing the lamellar structure of the cornea and simulating different scenarios that may help to early identify the characteristics that lead to a loss of corneal transparency. In this talk we start with an overview of current and past research on light scattering in the human eye. We will use Maxwell's equations to model the propagation of light in ocular tissues and a discontinuous Galerkin method associated with an explicit Runge-Kutta method to simulate the propagation of light in the human eye. This methodology helped us to assess cell level alterations on the human retina responsible for functional changes observable in Optical Coherence Tomography data in healthy ageing and in disease conditions. Now we are using the same methodology to simulate the propagation of light in normal corneas and corneas that reveal pathologies. The preliminary results obtained so far are very promising and are in line with recent literature. In particular, they allow us to conclude that an increase in the diameter of some collagen fibrils can result in a loss of corneal transparency.

#### About the speaker

Dr Adérito Araújo is an Associate Professor at Department of Mathematics, University of Coimbra, Portugal. He was the President of European Consortium for Mathematics in Industry (ECMI) from 2018 to 2020 and is currently the ECMI Representative in EU-MATHS -IN board. Completed his doctoral degree in Applied Mathematics at University of Coimbra in 1998, Dr Araújo's research is in the field related to numerical analysis, mathematical modelling and industrial mathematics. He has published his works in various journals



including SIAM Journal on Numerical Analysis, Applied Numerical Mathematics and other highly regarded journals.

#### MODELLING AND SIMULATION OF SARS-COV-2 SPIKE GLYCOPROTEIN

Firdaus Samsudin
Agency for Science, Technology and Research (A\*STAR), Singapore

**Abstract:** SARS-CoV-2, the causative pathogen of COVID-19, infects human cells via a spike (S) protein on the surface of the virus. The S protein is therefore a major target for vaccine and drug development. In this study, we used integrative modelling to build a complete model of the S protein with associated glycans using available structural data. Molecular dynamics simulation was used to understand how the protein behaves in its native membrane environment. The dynamic properties displayed by our S protein model are in good agreement with various experimental data. Simulations of S protein model with benzene probes reveal novel and potentially druggable cryptic pockets. We also modelled the binding of S protein with bacterial lipopolysaccharide to elucidate the underlying molecular mechanism of hyperinflammation. Surface accessibility of glycosylation sites was also determined to understand the impact on glycosylation pattern of the S protein. Overall, our study provides valuable information for rational design of therapeutics to combat the COVID-19 pandemic.

#### About the speaker

Dr. Firdaus Samsudin received his B.Sc. in Biotechnology from Imperial College London before completing a D.Phil. in Biochemistry at the University of Oxford. His first postdoctoral work was conducted at the School of Chemistry, University of Southampton. He is currently a postdoctoral research fellow at the Bioinformatics Institute (BII), A\*STAR, Singapore, where he leads a research focusing on understanding the dynamics of SARS-CoV-2 spike protein using molecular modelling and simulation. His research works focus on protein and small



molecule structural analysis, molecular dynamics simulation, homology modelling, docking, and free energy calculation, with a strong track record of collaboration with biophysicists and structural biologists.

# SECOND YEAR INTO THE PANDEMIC ERA – ARE YOU ALREADY IN THE NEW NORM?

Yam Wai Keat Perdana University, Malaysia.

**Abstract:** We are now entering into the second year of the pandemic era and almost getting used to performing teaching, learning and assessment (TLA); and scientific research activities virtually. While some educators and researchers are still having challenges in this area, there are certain perspectives that we could look into to better equip ourselves. There are computational tools and databases that are widely available that would enable this purpose. In this lecture, I would be sharing with you how we could effectively perform TLA and scientific research virtually, especially utilizing computational tools and databases.

#### About the speaker

Dr. Yam Wai Keat is an Associate Professor at the School of Data Sciences in Perdana University, Malaysia. She obtained her Bachelor of Science (Hons) in Bioinformatics from the University of Malaya in 2004 before obtaining a PhD in Structural Bioinformatics from University of Science Malaysia in 2010. Lately, she has started venturing into education research and innovation, with a special interest of reaching out to the community on bioinformatics and data sciences. Over the years, she has obtained several research grants from the Malaysian government and university to conduct



Bioinformatics related works. She is currently an ExCo member for APBioNet (Asia Pacific Bioinformatics Network), actively involved in Bioinformatics education and training. She also serves as Secretary for the Malaysian Society of Bioinformatics and Computational Biology (MaSBiC) and is also the Founding Chairperson for MyBioInfoNet, a virtual networking platform for Malaysian Bioinformatics enthusiasts. She was an affiliated member of the Young Scientists Network - Academy of Sciences Malaysia (YSN-ASM) and was a member of the Royal Chemistry Society.

#### RE-ENGINEERING UNWANTED BIOMASS INTO SMART BIOGENIC COMPOSITES

Roswanira Abdul Wahab Universiti Teknologi Malaysia (UTM), Skudai 81310, Johor, Malaysia.

Abstract: The increasing scarcity of global resources merits the manufacturing community's re-consideration and the change in consumers' mindset to adopt more eco-friendly processes and sustainable lifestyles. The future should involve biocomposite material science and nanotechnology through 'Waste to Wealth' and 'Zero-Waste" initiatives to helm a sustainable world, fully capitalizing renewable carbon and silica feedstocks from biomass for conversion into smart composites. Notwithstanding the low-key repute of biomass-based composites, these materials are profoundly useful starting materials for producing platform chemicals, polymers, and innovative composites of unlimited applications. The repurposing of agro-industrial biomass would, ipso facto, mitigate unwanted surplus biomass while reducing the world's carbon footprint. The archetypical carbonand silica-rich biomass from the agronomic- and industrial activities can be re-engineered into highly functional biogenic polymers using innovatively integrated physical, chemical- and enzymatic processes. The resultant elegant polymer composites have since found applications as enzyme supports, sorbents, fuel cells, and biosensors. Also, the polymers can be re-engineered into materials that promote wound healing and carbon capture. The range of biomaterials/composites has since expanded with the advent of sophisticated machinery, greener solvents, and smarter engineered enzymes. These technologies facilitated better extraction and purification of natural polymers and their nano-sized subunits from different biomass for further treatments. Nevertheless, our ability to actualize these bio-based materials to their fullest greatly hinges on our ardent efforts to consolidate multidisciplinary fields, i.e., material science, enzymology, computational- and engineering science, as well as economics, into the manufacturing process.

#### About the speaker

Dr. Roswanira Abdul Wahab received her BSc. in Industrial and MSc. in Chemistry from Universiti Teknologi Malaysia (UTM) before obtaining her Ph.D. in Enzyme Technology at Universiti Putra Malaysia. She is currently an Associate Professor at the Department of Chemistry, Faculty of Science, UTM. She is the Section Editor (Biochemistry/Biological Chemistry) of the Indonesian Journal of Chemistry and the Journal of Indonesian Chemical Society. She is on the International Editorial Board of Biotechnology and Biotechnological Equipment (Taylor and



Francis) and an Editor of Jurnal Teknologi (UTM). She is also an Associate Research Fellow of the Advanced Membrane Technology (AMTEC) Centre of Excellence (UTM). She is currently an Exco member for the Malaysian Society of Bioinformatics and Computational Biology (MasBiC) and the Assistant Head of Sub-Field (Bio-Analysis) for Persatuan Analisis Malaysia (ANALIS). Her research interest is in biogenic matrices development from biomass, focusing on green hybrid composite for enzyme immobilization and tailoring, nanotechnology, as well as bioinformatics.

# LIST OF ABSTRACTS

# COMPUTATIONAL BIOLOGY APPROACH TOWARDS STUDYING PROTEIN-PROTEIN INTERACTION BETWEEN BREAST CANCER CELL PROTEINS AND PLANT COMPOUNDS

Asita Elengoe<sup>1\*</sup>, Nisha Nadarajan<sup>2</sup>

<sup>1</sup>Department of Biotechnology, Faculty of Science, Lincoln University College, 47301 Petaling Jaya, Malaysia <sup>2</sup>Department of Biotechnology, Manipal International University, 71800 Nilai, Negeri Sembilan Darul Khusus, Malaysia

\*Corresponding author: asitaelengoe@yahoo.com

#### **Abstract**

Breast cancer is the commonest cause of cancer death in women worldwide. Rates vary about fivefold around the world, but they are increasing in regions that until recently had low rates of the disease. Conventional treatment such as chemotherapy, surgery and radiation causes side effects. Therefore, scientists are working to find a better alternative way to treat breast cancer and improve the life quality of patients. Malaysia is rich in biodiversity and has hundreds of florae that are used in traditional medicine and many more used in general folklore medicine. Medicinal plants have played an important role in the treatment of breast cancer. In this study, the three-dimensional (3D) structure of breast cancer cell line proteins (Phosphatase and tensin homolog (pTEN), Breast Cancer Susceptibility Type 1 (BRCA-1) and PALB2 were generated and docking with plant compounds was studied. Swiss model was used to generate the three-dimensional (3D) structure of protein models. The physicochemical characterization of protein models was determined using the ExPASy ProtParam Proteomics server. Then, validation of protein models was evaluated by using ProCheck, ProO, ERRAT and Verify 3D programs. Finally, each target protein was docked successfully with allicin, anonaine, rosmarinic acid, curcumin, lutein, capsaicin, ascorbic acid, catechin and genistein; and visualized with PyMol software. The results show that the binding energy of the protein-phytocompound complexes (pTEN-lutein, BRCA-1-lutein and PABL2-lutein) were -9.17, -8.19 and -8.70 kcal/mol respectively. These target protein-plant compound complexes had the most stable interaction among all the target protein-plant compounds complexes. These protein-protein interactions will help to design substrate (phyto-component) based drugs for breast cancer patients.

# MOLECULAR BINDING INTERACTION OF ANGIOTENSIN CONVERTING ENZYME AND 1-GALLOYL GLUCOSE, THE MAJOR COMPOUND IN SYZYGIUM POLYANTHUM LEAVES

Tuan Ashraf Faiz Tuan Anuar<sup>1\*</sup>, Azlini Ismail<sup>2</sup>, Muhammad Nor Omar<sup>3</sup>, Izzat Fahimuddin Mohamed Suffian<sup>4</sup>, Azzmer Azzar Abdul Hamid<sup>3</sup>

<sup>1</sup>Department of Chemistry, Kulliyyah of Science, International Islamic University Malaysia, 25200 Kuantan, Pahang, Malaysia

<sup>2</sup>Department of Fundamental Dental and Medical Sciences, Kulliyah of Dentistry, International Islamic University Malaysia, 25200 Kuantan, Pahang, Malaysia

<sup>3</sup>Department of Biotechnology, Kulliyyah of Science, International Islamic University Malaysia, 25200 Kuantan, Pahang, Malaysia

<sup>4</sup>Department of Pharmaceutical Chemistry, Kulliyyah of Pharmacy, International Islamic University Malaysia, 25200 Kuantan, Pahang, Malaysia

\*Corresponding author: tuan03faiz@gmail.com

#### **Abstract**

Syzaium polyanthum leaves are traditionally used for treating hypertension. Recently, the plant leaves extract has been demonstrated to exhibit significant angiotensin-converting enzyme (ACE) inhibition activity, and this has further consolidated the evidence for its antihypertensive effect. Previously, 1-galloyl glucose has been suggested as its possible bioactive compound, however, there is no specific study yet on its interaction with ACE enzyme specifically through molecular docking. Therefore, this study aims to investigate the molecular interaction between 1-galloyl glucose (CID 124375) and the ACE protein (PDB: 1086). The standard ACE inhibitor drug captopril (CID 44093) was used as a comparison. Autodock 4 (California, USA) was utilized to prepare the protein and ligand; meanwhile, the docking simulation was conducted in Autodock Vina (California, USA). Molecular docking analysis showed that 1-galloyl-glucose has lower binding energy (-7.7 kcal/mol) with the ACE, as compared to the captopril (-5.6 kcal/mol). Both compounds showed specific interaction mainly towards histidine group, with 1-galloyl glucose specifically bind towards several residues of aspartic acid group. 1-galloyl glucose was shown to have more binding residues than captopril, hence contributed to the binding energy. All these residues were shown to have hydrogen bonds with distance lower than 3.5 Å; indicative of good interaction between 1-galloyl-glucose and the ACE. In conclusion, 1-galloyl glucose has better binding affinity towards ACE enzyme than the standard drug, captopril. This finding further supported the potential of 1-galloyl glucose as one of the possible bioactive compounds responsible for ACE inhibition by *S. polyanthum*.

# GENOME-WIDE COMPARATIVE ANALYSIS OF DROUGHT TOLERANT GENES IN RICE, MAIZE, DATE PALM AND ARABIDOPSIS

Nurul Asyikin Mohd-Zim<sup>1,2</sup>, Suhaila Sulaiman<sup>2</sup>, Siti Habsah Roowi<sup>2</sup>, Nur Sabrina Ahmad Azmi<sup>1</sup>, Zarina Zainuddin<sup>1</sup> and Nurul Hidayah Samsulrizal<sup>1\*</sup>

 Department of Plant Science, Kulliyyah of Science, International Islamic University Malaysia, Jalan Sultan Ahmad Shah, Bandar Indera Mahkota, 25200 Kuantan, Pahang, Malaysia
 FGV R&D Sdn Bhd, FGV Innovation Centre, PT. 23417 Lengkuk Teknologi, 71760 Bandar Enstek, Negeri Sembilan, Malaysia

\*Corresponding author: hidayahsamsulrizal@iium.edu.my

#### **Abstract**

The availability of various comparative genomics tools has allowed the identification of several potential drought-tolerant genes in plants such as wheat, tomato, maize and others. In this study, orthologous drought-tolerant genes in *Oryza sativa* (rice), *Zea mays* (maize), *Phoenix dactilyfera* (date palm) and *Arabidopsis thaliana* (arabidopsis) were identified using InParanoid and SonicParanoid tools. From the 9,952 orthologous proteins found among the four species, 8,573 sequences were annotated and assigned to 5,729 GO terms; classified into the biological process category, molecular function category and cellular component category. Sixty-five OGs were found to be represented under four drought tolerance GO terms; regulation of response to water deprivation (GO:2000070), response to water deprivation, behavioural response to water deprivation (GO:0042630), and cellular response to water deprivation (GO:0042631). The potential drought tolerance genes have been predicted by using sequence homology search against the Drought Stress Gene Database (DroughtDB). Three potential drought-tolerant genes were selected and visualised to compare the gene alignment across the 4 species using the MAUVE software. To assure a satisfactory outcome, this *in silico* study will be confirmed by genome editing studies in rice *via* CRISPR/Cas9 system.

# IN SILICO DEVELOPMENT OF CRISPR/CAS9 CONSTRUCT FOR ORYZA SATIVA SUBSP. INDICA

Anis Afuza Md Yusof<sup>1</sup>, Siti Syafiqa Abdul Sattar<sup>1</sup>, Nurul Asyikin Mohd Zim<sup>1</sup>, Azzmer Azzar Abdul Hamid<sup>2</sup>, Zarina Zainuddin<sup>1</sup> and Nurul Hidayah Samsulrizal<sup>1</sup>

<sup>1</sup>Department of Plant Science, Kuliyyah of Science, International Islamic University Malaysia, 26300, Kuantan, Pahang <sup>2</sup>Department of Biotechnology, Kuliyyah of Science, International Islamic University Malaysia, 26300, Kuantan, Pahang

\*Corresponding author: hidayahsamsulrizal@iium.edu.my

#### **Abstract**

Oryza sativa, which is commonly known as rice, is one of the staple foods consumed by Asian. There are three subspecies of *O. sativa* that are different in their geographical adaptations which are Japonica, Javanica and Indica. Climate change causes increasing greenhouse gas emissions fluctuating rainfall, and drought which is the limiting factors of rice production in Malaysia. In rice, SUMO E2-Conjugating Enzyme (OsSCE1) gene plays a role as a negative regulator in the drought stress response. OsSCE1 gene is a type of small ubiquitin-like modifier (SUMO)-conjugating enzyme involved in a few regulatory processes such as SUMOylation. The crop improvement can be made possible through a genome editing approach which enables the manipulation of targeted genetic traits and Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR) system is one of the genomes editing technologies that are accessible. In this study, the CRISPR construct of drought tolerance of Oryza sativa subsp. indica was developed. The CRISPR construct development involved several stages; OsSCE1 gene prediction, sgRNA design, and vector construction. FGENESH and GeneMarkS were used for OsSCE1 gene prediction. The predicted OsSCE1 gene has been validated using Polymerisation Chain Reaction (PCR) and sequencing. The BLASTN result shows high similarity with Oryza sativa in chromosome 10 with 99% identities. This step followed by sgRNA design which was carried out manually with the help of gRNA prediction tools such as WU-CRISPR, CCTop, Benchling, and CRISPR-P. Lastly, vector construction was executed virtually using Benchling. Overall, the OsSCE1 gene was successfully characterized and validated, and the in silico CRISPR construct for Oryza sativa subsp. indica was developed. To ensure a good outcome, in silico CRISPR construct should be verified through *in vivo* studies in further.

# SYNTHESIS AND CHARACTERISATION OF SERIES OF NITRO AND CHLORO 2-ARYLBENZIMIDAZOLE DERIVATIVES

Mar'iyah Najihah Abdullah<sup>1</sup>, Shafida Abd Hamid<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Kulliyah of Science, International Islamic University Malaysia (IIUM), 25200 Kuantan Pahang

\*Corresponding author: shafida@iium.edu.my

#### **Abstract**

Benzimidazoles have been shown to exhibit various biological activities due to their privileged structure. The benzimidazole scaffold can be designed by adding certain moieties or functional groups to influence its potential in particular or targeted biological activity. Previously synthesised 3-nitrophenyl benzimidazoles and 2,4-dichlorophenyl benzimidazoles were found to show significant antiproliferative activity with MDA-MB 231 cell lines. In continuation of the study, two series of N-sec and tert-butyl-2-arylbenzimidazole were designed and synthesised by substitution of chloro and nitro group at various positions of the aryl ring. All the synthesised compounds were characterised by 1H-NMR, 13C-NMR, IR, and mass spectroscopy.

#### **IODINE MEDIATED ONE-POT SYNTHESIS OF 3-CARBETHOXYCOUMARINS**

Dinesh Kumar Sharma<sup>1\*</sup>

<sup>1</sup>Department of Chemistry, Kishan Lal Public College, Rewari, India-123401

\*Corresponding author: dksharma\_84@rediffmail.com

#### Abstract

2-Hydroxybenzaldehydes on reaction with ethylcyanoacetate in the presence of iodine as catalyst give 3-carbethoxycoumarins in one step under thermal heating as well as microwave irradiations. The latter conditions are much more efficient in terms of time (2-5 minutes) and yield as compared to thermal conditions (2.5-3.0 hours). Following similar procedure, 3-carbethoxy-4-methylcoumarins have also been prepared by the reaction of 2-hydroxyacetophenones with ethylcyanoacetate.

# MULTIFUNCTIONAL LYOTROPIC LIQUID CRYSTALLINE NANOPARTICLES FOR GEMCITABINE AND THYMOQUINONE DELIVERY IN THE TREATMENT OF BREAST CANCER

Yan Shan Loo<sup>1</sup>, Thiagarajan Madheswaran<sup>2</sup>, Armania Nurdin<sup>3,4</sup>, Norazlinaliza Salim<sup>1</sup>, Hong Ngee Lim<sup>1</sup>, and Intan Diana Mat Azmi<sup>1,\*</sup>

Department of Chemistry, Faculty of Science, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia
 Department of Pharmaceutical Technology, School of Pharmacy, International Medical University, Jalan Jalil Perkasa 19, 57000 Bukit Jalil, Kuala Lumpur, Malaysia
 Department of Biochemistry, Faculty of Medicine and Health Sciences, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia
 4UPM-MAKNA Cancer Research Laboratory, Institute of Bioscience, Universiti Putra Malaysia, 43400 Serdang, Selangor, Malaysia

\*Corresponding author: intandiana@upm.edu.my

#### **Abstract**

Lyotropic liquid crystalline nanoparticles (LLCNs) are internally self-assembled (ISA)-somes formed via self assembly process of amphiphilic molecules in a mixture composed of a lipid-based fraction. stabilizer and/or surfactant, and aqueous media/dispersant. LLCNs are capable of phase transitions in response to hydration and/or externally-applied fields to form ordered mesophases. This unique modality presents high tunability of LLCNs for various biomedical functions. Progression on first-line endocrine therapy in a subset of hormone receptor- positive (HR+) breast cancer patients and recurrence caused by invasive lesions is a growing health concern requiring optimal treatment strategies. Importantly, the clinical significance of our research entails the development of a drug delivery system comprising multifunctional and biocompatible LLCNs optimized for gemcitabine e-thymoquinone (Gem-TQ) co-delivery and targeting to HR+ breast cancer cells rendered endocrine resistant, via the expression of vitamin D receptor (VDR). LLCNs prepared using soy phosphatidylcholine (SPC), phytantriol (PHYT), glycerol monostearate (MYV) in pre-determined compositional ratios containing surfactant or citrem, had displayed physicochemical properties i.e. hydrodynamic particle sizes (< 500 nm), negative surface charge, high entrapment efficiency, and controlled drug release. Findings from cytotoxicity analyses in MCF10A and MCF7 cells are also presented herein. We envisage the study to be a first report on Gem-TQ co-encapsulation in lipid and citrem-based LLCNs, and aim to further demonstrate hemocompatibility in human blood, and enhanced anticancer activity and cellular localization of targeted LLCNs.

# LOCALIZATION APPROACH OF ALGINATE MICROBEADS AS A TARGETED DELIVERY CARRIER

Md. Abul Kalam Azad<sup>1</sup> and Abd Almonem Doolaanea<sup>2\*</sup>

<sup>1</sup>Faculty of Pharmacy, AIMST University, Kedah, Malaysia <sup>2</sup>Faculty of Pharmacy, International Islamic University Malaysia

\*Corresponding author: monem@iium.edu.my

#### **Abstract**

Alginate is a biodegradable and biocompatible polymer widely used in biotechnology applications and in the pharmaceutical industry. It can be easily crosslinked with divalent cations such as calcium ions to form microbead hydrogels. The hydrogel properties of calcium alginate microbeads have been proposed for controlling the release of small molecules and macromolecules. In addition, being mucoadhesive, these microbeads are likely to stick to the intestinal mucosa for a prolonged period and have been exploited for the site-specific drug delivery to mucosal tissues. The common method to study the gastrointestinal (GIT) distribution of the microbeads, or particles in general, after ingestion is by sacrificing the animals at specific time points then counting the number of particles in each section of the GIT. However, for alginate microbeads the visibility of the particles in the GIT is difficult especially when particles absorb fluid and swell. The method was modified by adding fluorescent probe to facilitate the detection of the particles. A simple experiment setup using off-shelf materials was enough to clearly observe the particles with high recovery. In this study, the time course of drug distribution of mucoadhesive black seed oil-loaded alginate microbeads was evaluated in rat where stomach and intestinal region were the targeted parts. After 1 h of oral administration of fixed number of microbeads, 90%±4.62% was recovered from stomach, 7.0% ±0.75% was in duodenum followed by 3%±0.35% in jejunum. However, after 3 h of administration, majority of the microbeads moved out from stomach and distributed almost homogenously along the small intestine: duodenum (14%±1.21%) and the lower part of intestine including the sections of jejunum-1 (23%±2.33%), jejunum-2 (21%±1.98%), jejunum-3 (23%±2%), ileum (11%±1%) whereas 8.33%±1.25% passed to the sigmoid colon. After 6 h of administration, less than 10% of the microbeads were recovered from the GIT: 3.33%±1.45%, from the jejunum followed by ileum (1.66±0.38%) and sigmoid colon (3%±1.52%). During the microbead travel in the intestine, more microbeads were started to swell then dissolve. Such studies are needed especially when developing new formulations for targeted delivery in the GIT.

# IN-VITRO DETERMINATION OF TOTAL PHENOLIC AND FLAVONOID CONTENT, AND THROMBOLYTIC, ANTIMICROBIAL AND ANTIOXIDANT ACTIVITIES OF ABROMA AUGUSTA LNN. LEAVES EXTRACT

Md. Abul Kalam Azad<sup>1\*</sup>, Zubair Khalid Labu<sup>2</sup>, Farahidah Binti Mohamed<sup>3\*</sup>

<sup>1</sup>Faculty of Pharmacy, AIMST University, Kedah, Malaysia. <sup>2</sup>Department of Pharmacy, World University of Bangladesh, Dhaka-1205, Bangladesh <sup>3</sup>Faculty of Pharmacy, International Islamic University Malaysia.

 $\hbox{\it *Corresponding author: 01} drazad@gmail.com; farahidah@iium.edu.my$ 

#### **Abstract**

The in-vitro antimicrobial effectiveness of *A. augusta* was shown in (Table S4). Antimicrobic experiment was conducted on four gram positive and five-gram negative bacteria at a conc. of 400 µg/disc. DCMSF exhibited with highest zone of inhibition (19.60  $\pm$  0.12 mm) in *Bacillus subtilis*. a gram-positive bacterium. Other organic soluble fractions such as MSF, PSF and AQSF showed moderate antimicrobial activity ranging from  $11.50 \pm 0.10$  mm to  $18.30 \pm 0.11$  mm respectively compared to the standard antibiotic kanamycin 20 µg/disc ranging from 44.00 ± 0.25 mm to  $48.00 \pm 0.06$  mm of clear zone that characterized the antimicrobial potentials of standard antibiotic. On the other hand, DCMSF faction also displayed the zenithal activity against the growth of *Shigella* dysenteriae (20.00 ± 0.20 mm) which is a gram-negative bacterium. Other Kupchan partitionates of A. augusta barred the proliferation of bacteria in a moderate spectrum from (12.00  $\pm$  0.41 mm to  $18.15 \pm 0.11$  mm) subsequently in resemblance of standard antibiotic (42.00  $\pm$  0.23 mm to 50.00 ± 0.19 mm). But PSF did not show any clear zone which characterized that there was no antimicrobial effectiveness in PSF. The crude methanolic and other partitions of *A.augusta* were subjected to evaluate the probable thrombolytic potentials using streptokinase as positive that demonstrated (69.52%) lysis of blood clot. On the other conditions, sterile distilled water, a negative control, explored a negligible percentage of clot break down (4.24%). The level, expressed as percent, of clot lysis by various fractions were observed in the following order, AQSF (46.58%), PSF (40.79%), DCMSF (39.81%) and MSF (13.54%). It may assume by the apprehension of the results that (considering > 20% moderate); (\*\*p < 0.01; \*\*p < 0.05).

## EARLIER DENATURATION OF DNA BY USING NOVEL TERNARY HYBRID NANOPARTICLES

Jalal Mohammed Zayan<sup>1</sup>, Akbar John<sup>2\*</sup>, Abdul Khaliq Rasheed<sup>3</sup>, Batoul Alallam<sup>4</sup>, Mohammed Khalid<sup>5</sup>, Ahmad Faris Ismail<sup>1</sup>, and Hamzah Salleh<sup>6</sup>

<sup>1</sup>Department of Mechanical Engineering, International Islamic University Malaysia, Gombak <sup>2</sup>Institute of Oceanography and Maritime Studies (INOCEM), Kulliyyah of Science, International Islamic University Malaysia, Kuantan

<sup>3</sup>Department of New Energy Science and Engineering, School of Energy and Chemical Engineering, Xiamen University Malaysia, Jalan Sunsuria, Bandar Sunsuria, 43900 Sepang, Selangor, Malaysia <sup>4</sup>Advanced Drug Delivery lab, Department of pharmaceutical technology, International Islamic University Malaysia, Kuantan

<sup>5</sup>Graphene and Advanced 2D Materials Research Group, Level 4, East Wing - NUB, School of Science and Technology, Sunway University, Sunway City, Petaling Jaya, 47500 Selangor, Malaysia <sup>6</sup>International Institute for Halal Research and Training (INHART), International Islamic University Malaysia, Gombak

\*Corresponding author: akbarjohn50@gmail.com

#### Abstract

Two novel ternary hybrid nanoparticles (THNp) consisting of graphene oxide (GO) and reduced graphene oxides (rGO) were added to samples of DNA. The effect of the addition of nanoparticles on the thermal—denaturation of DNA samples was studied by measuring the absorbance using a temperature-controlled Perkin Elmer UV spectrophotometer. Adding GO-TiO<sub>2</sub>-Ag and rGO-TiO<sub>2</sub>-Ag nanoparticles lowered the denaturation temperature of template DNA significantly. The nanoparticles affect the denaturation rate. The optimal GO-TiO<sub>2</sub>-Ag and rGO-TiO<sub>2</sub>-Ag concentration were found to be  $5 \times 10^{-2}$ , which resulted in 86- and 180-folds augmentation of DNA denaturation (6.5 µg/mL), respectively, while it resulted in 2- and 7-folds augmentation of DNA denaturation (11.5 µg/mL), respectively, at temperature as low as 80 °C. The results indicated that rGO-TiO<sub>2</sub>-Ag nanoparticles exhibited significantly higher DNA denaturation enhancement—than rGO-TiO<sub>2</sub>-Ag nanoparticles, owing to their enhanced thermal conductivity effect. Therefore, these nanoparticles could help to get improved PCR yield, hence enables amplification to be performed for longer cycles by lowering the denaturation temperature.

## DEVELOPMENT OF TURBIDITY, PH, TEMPERATURE AND FLOWRATE SENSOR IN WATER AND WASTEWATER BY USING ARDUINO

Mohammad Hakim Che Harun<sup>1,2\*</sup>, Aisyah Abd Muthalib<sup>2</sup>, Nor Atikah Shahira Binti Razak<sup>2</sup>, Nurafnida Afrizal<sup>2</sup>, Sofiah Hamzah<sup>1,2</sup>, and Asmadi Ali<sup>1,2</sup>

<sup>1</sup>Environmental Sustainable Material Research Interest Group, Faculty of Ocean Engineering Technology and Informatics, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia 

<sup>2</sup>Faculty of Ocean Engineering Technology and Informatics, Universiti Malaysia Terengganu, Kuala Terengganu, Malaysia

\*Corresponding author: m.hakim@umt.edu.my

#### **Abstract**

An Arduino is a single board computer that is open-source hardware. Arduino Development Environment (IDE) software is used to create programs that allow microcontrollers to communicate with various sensors and other hardware. Arduino sensors can be used to track the environment parameters such as water quality. Arduino sensors are designed to simplify complicated task, avoiding miscommunications especially in engineering and environmental sectors. In order to reach the above-mentioned aim, the following objective are established (i) To develop low-cost Arduino sensor system for automatic water monitoring application on pH value, flowmeter, and turbidity. (ii) To compare the competencies of the data generated by Arduino system on water and wastewater quality data are correct and consistent with the high-end instruments. (iii) To measure and monitor the water quality by using Arduino systems. The sensors will be coded according to calibration and measurement standards by the laboratory equipments. Turbidity, pH and flowrate sensor will be equipped at each stage of water treatment. This sensor will measure and monitor the water quality parameters at each stage of water treatment (flocculation, sedimentation, and filtration). The results show that Arduino able to collect and monitor water quality on every water treatment system. The data collection shows maximum competencies data collected with laboratory instruments.

## INVESTIGATION ON STRAIN MEASUREMENT USING CARBON ELECTRICAL CONDUCTIVE PAINT

Muhammad Nazrul Hisyam Bin Jamaluddin<sup>1</sup> and Mohd Hazimin Bin Mohd Salleh<sup>1\*</sup>

<sup>1</sup>BioPhysics Research Laboratory, Department of Physics, Kulliyyah of Science, International Islamic University of Malaysia, Bandar Indera Mahkota, 25200 Kuantan, Pahang, Malaysia

\*Corresponding author: mhazimin@iium.edu.my

#### Abstract

Electrical strain gauge has been used widely in many applications, such as experimental strength of materials and structural health monitoring. This is because of their low cost and durability in making measurements. Recently, few new sensors have been developed using the constantan alloy to enhance the sensor's response and sensitivity. However, researchers have noticed that electrical conductive polymers alternate their electrical resistance when subjected to mechanical strain. This conductivity is given by the conductive network created by the conductive particles in the polymer mixture. The conductive network is then altered as a result of the mechanical deformation, changing the material's electrical properties. This research aims to study the effect of the paper-based strain sensor when the carbon electrical conductive paint is used as a sensor coil in the sensor. We studied the changes of the electrical resistance R as the length of the sensor changed according to the applied strain. The conductive paint was applied on 80gsm A4 printing paper. The I-V graph was plotted first and then the resistance was calculated from the slope of the graph. There are three sensor's designs that has been studied. For the first method, the gauge factor for design one is 0.67, the second design gives 0.33 for the gauge factor, and the gauge factor for the third design is 0.50. The electrically conductive paint can be used to fabricate the strain gauge. However, the sensor's sensitivity must be enhanced by doing more research to produce a better sensor.

#### SECOND HANKEL DETERMINANT OF BI-SUBORDINATE FUNCTIONS

Kiu Shu Huey<sup>1</sup>, Aini Janteng<sup>2\*</sup>

1,2Faculty of Science and Natural Resources, Universiti Malaysia Sabah

\*Corresponding author: aini\_jg@ums.edu.my

#### **Abstract**

Let A be the class of functions which are analytic in the open unit disk  $\mathbb{D}=\{z\in\mathbb{C}:|z|<1\}$  and having the form  $f(z)=z+\sum_{n=2}^\infty a_nz^n$ . Denote S to be the class for all functions in A that are univalent in  $\mathbb{D}$ . Then, let  $\sigma$  denote the class of bi-univalent functions in  $\mathbb{D}$ . In this paper, we obtained the second Hankel determinant for certain classes of analytic bi-univalent function which are defined by subordinations in the open unit disk  $\mathbb{D}=\{z\in\mathbb{C}:|z|<1\}$ . In particular, we determined the initial coefficients  $a_2,a_3$  and  $a_4$  and obtained the upper bound for the functional  $|a_2a_4-a_3^2|$  of functions f in the classes of analytic bi-univalent function which are defined by subordinations in  $\mathbb{D}$ .

#### INPAINTING OF DENTAL PANORAMIC TOMOGRAPHY VIA DEEP LEARNING

Syafie Nizam<sup>1\*</sup>, Mohd Adli Md Ali<sup>1\*</sup>, Ahmad Faisal Ismail<sup>2\*</sup>

<sup>1</sup>Department of Physics, International Islamic University Malaysia <sup>2</sup>Kulliyyah of Dentistry, International Islamic University Malaysia

\*Corresponding author: syafie.nzm@gmail.com, qunox@iium.edu.my, drfaisal@iium.edu.my

#### **Abstract**

The tradition of image inpainting has existed for a long time; it is used to correct old and corrupted images. In recent times, progress in deep learning allows artificial neural networks to perform inpainting on clinical images to reduce image artifacts. In this paper, we demonstrated how various neural network models could perform inpainting on a dental panoramic tomography that was taken by using cone-beam computed tomography (CBCT). Experiments were done to compare the output of three different artificial neural network models: shallow convolutional autoencoder, deep convolutional autoencoder, and U-net architecture. The dataset was taken from an open online dataset provided by Noor Medical Imaging Center. Qualitative assessment of the output shows that the U-net model reproduces the best output images with minimal blurriness. This result is also supported by the quantitative measurement, which shows that the U-net model has the smallest mean squared root error and the highest structural similarity index measure. The experiment results give an early indication that it is feasible to use U-net to fix and reduce any image artifact that occurs in dental panoramic tomography.

#### ON SKEW PRODUCT OF QUADRATIC STOCHASTIC OPERATORS

Nasir Ganikhodjaev<sup>1\*</sup> and Najibakhon Mirkhodjaeva<sup>2</sup>

<sup>1</sup>Institute of Mathematics Academy of Sciences Uzbekistan <sup>2</sup>Tashkent State University of Economics

\*Corresponding author: nasirganikhodjaev@gmail.com

#### Abstract

Let a state space  $X = \{1, 2, \dots, r\}$  be a finite set. Then the set of all probability measures on X has the following form:

$$S^{r-1} = \{ \mathbf{x} = (x_1, x_2, \cdots, x_r) \in R^r : x_i \geq 0 \ \text{ for any } i, \text{ and } \sum_{i=1}^r x_i = 1 \}$$

and corresponding quadratic stochastic operator  $V: S^{r-1} \to S^{r-1}$  has the following form

$$(V\mathbf{x})_k = \sum_{i,j=1}^r P_{ij,k} x_i x_j, \quad i,j,k \in \{1,2,\cdots,r\}$$

where  $i)P_{ij,k}\geq 0;\ ii)P_{ij,k}=P_{ji,k}$  and  $iii)\sum_{k=1}^rP_{ij,k}=1.$  In this paper we consider a product of two quadratic stochastic operators. Let  $V_1:S^{n-1}\to S^{n-1}$  and  $V_2:S^{m-1}\to S^{m-1}$  be the quadratic stochastic operators, where  $S^{n-1}=\{\mathbf{x}=(x_1,x_2,\cdots,x_n)\}$  and  $S^{m-1}=\{\mathbf{y}=(y_1,y_2,\cdots,y_m)\}.$  Then on  $S^{n+m-1}=\{(\mathbf{x},\mathbf{y})=(x_1,x_2,\cdots,x_n,y_1,y_2,\cdots,y_m)\}$  we introduce new operator  $V_1\odot V_2:S^{n+m-1}\to S^{n+m-1}$  as follows:

$$(V_1 \odot V_2({\bf x},{\bf y}))_k = (V_1({\bf x})_k + g_k({\bf x},{\bf y}), \ \ {\rm for} \ \ k \in \{1,2,\cdots,n\}$$

and

$$(V_1 \odot V_2(\mathbf{x}, \mathbf{y}))_{n+l} = (V_2(\mathbf{y})_l + g_{n+l}(\mathbf{x}, \mathbf{y}), \ \ \text{for} \ \ l \in \{1, 2, \cdots, m\},$$

where

$$\sum_{s=1}^{n+m}g_s(\mathbf{x},\mathbf{y})=2(x_1+\cdots+x_n)(y_1+\cdots+y_m) \tag{1}$$

It is evident that there are a lot of  $g_s(\mathbf{x},\mathbf{y})$  satisfying (1). If  $g_k(\mathbf{x},\mathbf{y}) = x_k(y_1+\dots+y_m)$  for  $k=1,\dots,n,$  and  $g_{n+l}(\mathbf{x},\mathbf{y}) = y_l(x_1+\dots+x_n)$  for  $l=1,\dots,m,$  then an operator  $V_1\odot V_2$  is called regular product of operators  $V_1$  and  $V_2$ . The regular product of two quadratic stochastic operators is denoted as  $V_1\otimes V_2$  and for non regular products we will use the same notation  $V_1\odot V_2$  and call such product as skew product. In [T.Bier,Z.Dollah, N. Ganikhodjaev, Construction of non ergodic quadratic stochastic operators. Nonlinear Analysis and Phenomena II (2005), No.1,1-14] have been studied some properties of regular product of two quadratic stochastic operators. In this presentation we will discuss skew products of two quadratic stochastic operators.

#### PREPARATION OF SIX ARMS PCL-b-PEG STAR-SHAPED POLYMER HYDROGEL

Wafiuddin Ismail<sup>1\*</sup>, Siti Hajar Ahmad Sharif<sup>1</sup>, Muhammad Salahuddin Haris<sup>2</sup>

<sup>1</sup>Department of Chemistry, Kulliyyah of Science, International Islamic University Malaysia,
25200 Kuantan, Pahang Darul Makmur, Malaysia
<sup>2</sup>Department of Pharmaceutical Technology, Kulliyyah of Pharmacy, International Islamic University Malaysia,
25200 Kuantan, Pahang Darul Makmur, Malaysia

\*Corresponding author: wafisnj@iium.edu.my

#### **Abstract**

Most new develop drugs are hydrophobic and this property gives drawbacks in delivering the new drugs. An amphiphilic drug delivery cargo may overcome this problem with the features of both hydrophobic and hydrophilic. In this study, 6-arms star-shaped amphiphilic co-polymers with average molecular weight (Mn) of 10000 Da were synthesized and characterized for wound healing application. The 6-arms star-shaped polymer consist of polycaprolactone (PCL) hydrophobics system in the inner segment and poly(ethylene glycol) (PEG hydrophilic system in the outer segment. NMR and FTIR analyses showed that ring opening (ROP) of ε-caprolactone had occurred producing star-shaped homopolymer polycaprolactone (PCL) with di-pentaerythritol as core. Further reaction of these homopolymer with succinilated methoxy poly(ethylene glycol), (mPEG) produced amphiphilic star-shaped polymer consisted of PCL-b-PEG. Thermal analysis of the product using thermogeometric analysis (TGA) shows increased in thermal stability of the star-shaped polymer from 329.7 °C to 377.6 °C after the addition of mPEG. The star-shaped copolymer was incorporated into hydrogel formulation with Carbopol as gelling agent and Ciprofloxacin as drug model to investigate their ability as drug delivery system. The presence of PCL in the formulation showed high drug entrapment efficiency (>95%) via hydrophobic-hydrophobic interaction with the drug.

# QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP (QSAR) STUDY OF NEWLY SYNTHESIZED CARBONYL THIOUREA DERIVATIVES ON ACANTHAMOEBA SP.

Maizatul Akma Ibrahim<sup>1\*</sup>, Nor Hafizah Zakaria<sup>2</sup>, and Mohd Sukeri Mohd Yusof<sup>2</sup>

<sup>1</sup>Department of Plant Science, Kulliyyah of Science, International Islamic University Malaysia, 25200 Kuantan, Pahang

<sup>2</sup>Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu

\*Corresponding author: maizatulakma@iium.edu.my

### **Abstract**

In this study, the effort was to predict and elucidate the molecular structure of newly-synthesized carbonyl thiourea derivatives with their anti-amoebic activities. Therefore, inhibition concentration of 50% the cells population (IC<sub>50</sub>) was determined for 44 carbonyl thiourea derivatives on a pathogenic *Acanthamoeba* sp. (Hospital Kuala Lumpur isolate). Then, quantitative structure-activity relationship (QSAR) analysis was conducted using three QSAR models, namely stepwise-MLR, GA-MLR and GA-PLS. Results showed that these thiourea derivatives are positively active against the *Acanthamoeba* sp. HKL isolate with IC<sub>50</sub> values ranging from 2.56 to 7.81 µg.mL<sup>-1</sup>. From the evaluation of all QSAR models built in this study GA-PLS technique is found to be the best model due to its best predictive ability. The final equation of GA-PLS model gave good statistical output with  $r^2 = 0.827$ , and  $r^2_{cv} = 0.682$  *RMSEC*=0.047, *RMSECV*=0.064,  $r^2_{test}$  =0.790 and *RMSEP*=0.051. Y-randomization confirmed that the model did not occur from chances of correlation with  $r^2 = 0.015$ -0.372. Small residual with values less than 0.25 from prediction in the test set explains robustness of the model. The wealth of information in this study will provide an insight to designing a new thiourea compound with anti-amoebic activity.

# INVESTIGATING AIR POLLUTION SOURCES USING PRINCIPLE COMPONENT ANALYSIS (PCA)

Samsuri Abdullah<sup>1,2\*</sup>, Siti Madihah Mansor<sup>1</sup>, Amalina Abu Mansor<sup>3</sup>, Ku Mohd Kalkausar Ku Yusof<sup>3</sup>, Nazri Che Dom<sup>4</sup>, Ali Najah Ahmed<sup>5</sup>, and Marzuki Ismail<sup>2,3</sup>

<sup>1</sup>Faculty of Ocean Engineering Technology and Informatics, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia

<sup>2</sup>Institute of Tropical Biodiversity and Sustainable Development, Universiti Malaysia Terengganu, 21030 Kuala Nerus, Terengganu, Malaysia

<sup>3</sup>Faculty of Science and Marine Environment, Universiti Malaysia Terengganu, 21030, Kuala Nerus, Terengganu, Malaysia

<sup>4</sup>Faculty of Health Sciences, Universiti Teknologi MARA, UiTM Cawangan Selangor, 42300 Puncak Alam, Selangor, Malaysia

<sup>5</sup>Institute of Energy Infrastructure (IEI), Department of Civil Engineering, College of Engineering, Universiti Tenaga Nasional (UNITEN), Kajang, Selangor Darul Ehsan 43000, Malaysia

\*Corresponding author: samsuri@umt.edu.my

### **Abstract**

Air quality in Malaysia is slowly degrading, resulting from a rapid growth of urban and industrial areas. Poor air quality induces many adverse health effects to human and environment. This study is focusing on investigating the potential sources of air pollution in industrial and urban areas. Data of particulate matter  $(PM_{10})$ , carbon monoxide (CO) and nitrogen dioxide  $(NO_2)$  concentration, and meteorological factors such as wind speed, temperature and relative humidity were obtained from Malaysian Department of Environment for duration of 3 years (2013 until 2015). The data were analyzed by using Principal Component Analysis (PCA). There exists significant difference (p<0.05) of air pollutants at different study areas although the sources analyzer is same but contribution percentage is different. The trend of  $PM_{10}$ , CO and  $NO_2$  in study areas shows that the value of parameter higher in industrial area than urban area. The absolute PCA allowed the quantitative apportionment of the two components observed in industrial area which are vehicular emissions (37.5%) and meteorological factors (35.7%). However, urban area shows that the main contributor is meteorological factors (42.9%) followed by the influences of vehicular emissions (32.6%).

# MOLECULAR RECOGNITION OF $\beta$ -1,4-GLUCOSIDASE FROM TRICHODERMA HARZIANUM T12, ThBglT12 AGAINST MYCELIAL CELL WALL COMPONENTS OF PHYTOPATHOGENIC MACROPHOMINA PHASEOLINA

Mohammad Hakim Mohammad Hood<sup>1</sup>, Azzmer Azzar Abdul Hamid<sup>1,5\*</sup>, Tengku Haziyamin Tengku Abdul Hamid<sup>1,5</sup>, Roswanira Abdul Wahab<sup>2,3</sup>, and Yilmaz Kaya<sup>4</sup>

<sup>1</sup>Department of Biotechnology, Kulliyyah of Science, International Islamic University Malaysia (IIUM), Bandar Indera Mahkota, 25200 Kuantan, Pahang, Malaysia.

<sup>2</sup>Department of Chemistry, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor, Malaysia. <sup>3</sup>Enzyme Technology and Green Synthesis Group, Faculty of Science, Universiti Teknologi Malaysia, 81310 UTM Johor Bahru, Malaysia.

<sup>4</sup>Department of Agricultural Biotechnology, Faculty of Agriculture, Ondokuz Mayis University, Turkey. <sup>5</sup>Research Unit for Bioinformatics and Computational Biology (RUBIC), Kulliyyah of Science, International Islamic University Malaysia (IIUM), Bandar Indera Mahkota, 25200 Kuantan, Pahang, Malaysia.

\*Corresponding author: azzmer@iium.edu.my

### **Abstract**

Efficacy of a β-1,4-glucosidase from Trichoderma harzianum T12 (ThBglT12) in disrupting the cell wall of the phytopathogenic fungus Macrophomina phaseolina was studied, as the underlying molecular mechanisms of cell wall recognition remains elusive. In this study, the binding location identified by a consensus of residues predicted by COACH tool, blind docking and multiple sequence alignment revealed that molecular recognition by ThBglT12 occurred through interactions between the  $\alpha$ -1,3-glucan,  $\beta$ -1,3-glucan,  $\beta$ -1,3/1,4-glucan and chitin components of M. phaseolina, with corresponding binding energies of -7.4, -7.6, -7.5 and -7.8 kcal/mol. The residue consensus verified the participation of Glu172, Tyr304, Trp345, Glu373, Glu430 and Trp431 in the active site pocket of ThBglT12 to bind the ligands, of which Trp345 was the common interacting residue. RMSD, RMSF, total energy and minimum distance calculation from MD simulation further confirmed the stability and the closeness of the binding ligands into the ThBglT12 active site pocket. The hydrogen bond occupancy by Glu373 and Trp431 instated the role of the nucleophile for substrate recognition and specificity, crucial for cleaving the β-1,4 linkage. Further investigation showed the proximity of Glu373 to the anomeric carbon of  $\beta$ -1,3/1,4-glucan (3.5Å) and chitin (5.5Å) indicates the readiness of the nucleophile to form enzyme-substrate intermediate. Plus, the neighboring water molecule appeared to be undeniably correctly positioned and oriented towards the anomeric carbon to hydrolyze the β-1,3/1,4-glucan and chitin, in less than 4.0<sup>o</sup>. In a nutshell, the study verified that the ThBglT12 is a good alternative fungicide to inhibit the growth of M. phaseolina.

# EFFECT OF DIFFERENT EXTRACTION METHODS ON VITAMIN B12 FROM EDIBLE GREEN SEAWEED, ULVA LACTUCA BY 2-LEVEL FACTORIAL DESIGN

Fatin Shazwani<sup>1</sup>, Deny Susanti<sup>1\*</sup>, Normawaty Mohammad Nor<sup>2</sup>, Muhamad Taher<sup>3</sup>, Nurul Iman Aminuddin<sup>1</sup>

<sup>1</sup>Department of Chemistry, Kulliyyah of Science, International Islamic University Malaysia, 25200, Pahang, Malaysia

<sup>2</sup>Department of Marine Science, Kulliyyah of Science, International Islamic University Malaysia, 25200, Pahang, Malaysia

<sup>3</sup>Department of Pharmaceutical Technology, Kulliyyah of Pharmacy, International Islamic University Malaysia, 25200, Pahang, Malaysia

\*Corresponding author: deny@iium.edu.my

### Abstract

*U. lactuca* has been known for its valuable biological properties such as antioxidant and antiviral due to the presence of several bioactive compounds like vitamins, polysaccharides, and lipids. In the present study, different extraction procedures of vitamin B12 were compared. Four types of dried U. lactuca (oven-dried, sun-dried, air-dried, freeze-dried) were subjected to three different extraction methods each (boiling, orbital shaking, and ultrasonic-assisted extraction (UAE)). Also, the effect of solvent:solvent (MeOH:H2O), solute:solvent ratio, and pH on the total vitamin B12 content were screened and statistically analysed using 2-Level Factorial design from RSM. The retention time (RT) from HPLC of all crude extracts were corresponded with the RT of standard cyanocobalamin (CN-Cbl) at 1.9 minutes. The extraction of CN-Cbl by orbital shaking gave insignificant (p > 0.05) result on the yield of CN-Cbl, compared to the boiling and UAE methods when oven-dried *U. lactuca* were extracted (p<0.05). The highest concentration of CN-Cbl (0.0236 mg/mL) was recorded when extracted by UAE method at parameters of 25:75 % MeOH:H<sub>2</sub>O, pH 3, 3 g: 60 mL solute:solvent ratio. Statistically, the concentration of CN-Cbl increased significantly (p<0.05) with decreasing MeOH:H2O, solute:solvent ratios and pH when *U. lactuca* was subjected to oven-dried drying method, and extracted using UAE method. Hence, these factors may be further optimised in the future research to extract a better yield of CN-Cbl.

# ISOCRATIC RP-HPLC METHOD FOR THE SIMULTANEOUS DETERMINATION OF REACTION RATE IN N-PHENYLBENZAMIDE SYNTHESIS AND ITS INTERMEDIATE COMPOUNDS

Tarigul Islam<sup>1</sup>, Md. Zaidul Islam Sarker<sup>1\*</sup>, ABM Helal Uddin<sup>1</sup>

<sup>1</sup>Faculty of Pharmacy, International Islamic University Malaysia, 25200 Kuantan, Pahang, Malaysia

\*Corresponding author: zaidul@iium.edu.my

### **Abstract**

Antiviral activity against Hepatitis C virus (HCV) and Enterovirus 71 (EV 71) has been discovered in a sequence of novel N-phenyl benzamide (Benzanilide) derivatives. Recently, such findings inspired researchers to look for more potent antiviral agents through the N-phenyl benzamide synthesis. A high-pressure liquid chromatography method has been developed to observe the rate of N-phenyl benzamide synthesis. This is the first time reporting the approach has been established together for N-phenyl benzamide and aniline or phenylamine in an amide coupling reaction. These compounds were detected on a reversed-phase column (C<sub>18</sub>) using a 50:50 mobile phase of acetonitrile - 10mM (PH 5) sodium acetate buffer and UV detection is recorded at 254 nm. At a temperature of 30°C, isocratic elution was employed with a flow rate of 0.7 ml/min and an injection volume of 20 µL. The retention time for aniline and N phenyl benzamide was ±4.10 and ±7.60 min respectively. A linear relationship ( $r^2$ =0.9998 for benzanilide and  $r^2$ =0.9992 for aniline) over the concentration range 10-100 µg/ml was found when the peak area was plotted against concentration. The percentage of RSD was also 0.23 and 0.85 for benzanilide and aniline respectively. The method was verified in accordance with the International Conference on Harmonization (ICH) guidelines. The precise, linear, and more accurate method was applied to find out the reaction rate of aniline to produce the N-phenyl benzamide.

### KINETIC MODEL FOR SULFATE RADICAL OXIDATION OF BROMOTHYMOL BLUE

Mokhtar Djehiche<sup>1\*</sup>, Cheikh Mokrani<sup>1</sup>, Azzedine Benyahia<sup>2</sup>, and Nedjma Lahmar<sup>1</sup>

<sup>1</sup>Laboratory of inorganic materials, University of Mohamed Boudiaf, M'sila, Algeria <sup>2</sup>City, Environment, Society and Sustainable Development Laboratory, University of Mohamed Boudiaf, M'sila, Algeria

\*Corresponding author: mokhtar.djehiche@univ-msila.dz

### **Abstract**

The degradation kinetics of bromothymol blue (BBT) in the presence of heated potassium persulfate (KPS) in acidic medium (pH3) was studied. Based on our calculation and simulation methods, we determined, for the first time, the rate constant of the reaction of BBT with sulfate radicals (k6) at 60 °C. By carrying out several experiences at various conditions of concentrations and temperature, we obtain an average value of k6 equal to  $(3.3 \pm 0.3) \times 108 \text{ M-1 s-1}$  and an activation energy equal to 18.84 kJ/mol. On the other hand, we have also calculated the rate constant of the BTB reaction with the hydroxyl radical at 60 °C, equal to  $(1.3 \pm 1) \times 1010 \text{ M-1 s-1}$ . Finally, based on our simulation model, we predicted the dominant radical(hydroxyl or sulfate) at different values of pH.

# SCREENING OF SELECTED MICROBES AS BIOCATALYSTS FOR BIOTRANSFORMATION OF CURCUMIN AND XANTHORRIZOL

Munirah Ridzuan<sup>1</sup>, Nurul Iman Aminudin<sup>1\*</sup>, Zaima Azira Zainal Abidin<sup>2</sup>

<sup>1</sup>Department of Chemistry, Kulliyyah of Science, International Islamic University Malaysia (IIUM), 25200 Kuantan Pahang <sup>2</sup>Department of Biotechnology, Kulliyyah of Science, International Islamic University Malaysia (IIUM), 25200 Kuantan Pahang

\*Corresponding author: nuruliman@iium.edu.my

### **Abstract**

Curcumin is a diarylheptanoid found in *Curcuma longa* while xanthorrizol is a bisabolane-type sesquiterpenoid from *Curcuma xanthorriza* possess numerous biological activities that are beneficial to human health due to their remarkable structure. However, they are available in low concentration with poor water solubility, resulted in low bioavailability thus hindering clinical applications in exploring for novel drug lead. The activities of these compounds can be improved through biotransformation, one of the green methods for structural modifications utilizing ubiquitous biocatalyst. Extracted curcumin from *C. longa* and xanthorrizol from *C. xanthorriza* were purified and characterized through GC-MS and NMR spectroscopy, followed by biotransformation screening performed on the aforementioned compounds through *Streptomyces sp.* previously isolated from Kuantan mangrove and *Aspergillus Niger* as biocatalysts. The promising compound were identified via Thin Layer Chromatography (TLC) before preparative procedure for isolation and characterization purposes.

## RECURSIVE-ADAPTIVE RENTAL SUBSCRIPTION MODEL (R-ARSM) IN THE NEW NORMAL: AM APPLICATION TO THE HOUSING SECTOR

Friday Zinzendoff Okwonu<sup>1,2,3\*</sup>, Nor Aishah Ahad<sup>1</sup>, Zahayu Md Yusof<sup>1,2</sup> and Saadi Ahmad Kamaruddin<sup>2</sup>

<sup>1</sup>School of Quantitative Science, Universiti Utara Malaysia,06010 UUM Sintok, Kedah Malaysia <sup>2</sup>Institute of Strategic Industrial Decision Modeling, School of Quantitative Science, Universiti Utara Malaysia,06010 UUM Sintok, Kedah Malaysia

<sup>3</sup>Department of Mathematics, Faculty of Science, Delta State University, P.M.B.1 Abraka, Nigeria

\*Corresponding author: o.friday.zinzendoff@uum.edu.my; fokwonu@gmail.com

### **Abstract**

The last three decades have witnessed a remarkable transformation from a traditional billing system to a subscription model. Many organizations have adopted the subscription models especially in the service sectors like telecommunication, internet service providers, and satellite television operators. Indirectly, the subscription model has been applied to the air and railways transport system and some other formal sectors. During the lockdown occasioned by the Covid-19 pandemic, many people were forced to subscribe for their daily needs, and lifestyle was altered, and people must reset to cope with the new normal. The new normal era has exposed many people to subscribe to what they could afford based on length of time and limited resources. Unexpected daily economic challenges emerged, and people relocated to affordable places which led to rent default, rent arrears, and refund requests. Although, prior to the Covid-19 era and the new normal, rental default, rent arrears. and refund request delay between landlords and tenants existed. In this paper, we focused on how to solve rent default, rent arrears, and refund request problems in the public and private housing sector in the new normal. Relying on this, we proposed recursive-adaptive rental subscription models (R-ARSM) that could allow tenants options to subscribe for house rent with available resources. The R-ARSM concept mimics the internet subscription, mobile phone subscription, and satellite television subscription models whereby services to customers on annually, monthly, weekly, daily, and hourly rate are terminated when the subscribed amount elapse. The model based on the penalty constant showed that it is a balanced model for both landlords and tenants in the housing sector. The R-ARSM showed promising results, it is time-dependent and indicates the tenant's available balance per period. The analysis revealed that the R-ARSM concept would solve refund requests and rent default problems if implemented.

# REGULARITY OF 2-PARTITION POISSON QUADRATIC STOCHASTIC OPERATOR WITH THREE DIFFERENT PARAMETERS

Siti Nurlaili Karim<sup>1\*</sup>, Nur Zatul Akmar Hamzah<sup>1\*</sup>, Nurfazatul Hazirah A Rahman<sup>1</sup>, Muhammad Fairuz Zulkefli<sup>1</sup>, Nasir Ganikhodjaev<sup>2</sup>

<sup>1</sup>Department of Computational and Theoretical Sciences, Kulliyyah of Science, International Islamic University Malaysia, 25200 Kuantan, Pahang, Malaysia

<sup>2</sup>Institute of Mathematics, Tashkent, Uzbekistan

\*Corresponding author: sitinurlaili.karim@gmail.com, zatulakmar@iium.edu.my

### **Abstract**

Quadratic stochastic operator (QSO) was initiated by Bernstein in the early  $20^{th}$  century as the mathematical investigation on population genetics involving the synthesis of Mendelian law of crossing and Galtonian law of regression. Since then, the study of QSO has been significantly developed for decades to describe dynamical systems in many areas. In this paper, we construct a Poisson quadratic stochastic operator generated by 2-measurable partition with three different parameters defined on countable state space  $X = \{0, 1, 2, ...\}$ . The main objective of this research is to study the trajectory behavior of such operator by reducing the dynamical systems into a one-dimensional setting corresponding to the number of measurable partitions. Some cases of 2-measurable partition generated by singleton and two points with three different defined parameters will be presented. To investigate their trajectory behavior, we may apply the functional analysis within the measure and probability theory. Both computational and analytical results will be provided in such a way that the results show that the Poisson QSO generated by 2-measurable partition with three different parameters is either regular or nonregular transformation for arbitrary initial measures.

## SPATIAL DISTRIBUTION OF CU, ZN, PB AND NI IN SOIL IN BAUXITE MINING AREA USING GEOSTATISTICS AND GEOSPATIAL ANALYSIS

Mazidah Zulkifli<sup>1</sup>, Nur Shuhada Muhamad Tajudin<sup>1\*</sup>, Mohd Fuad Miskon<sup>1</sup>, Mohamad Izzuddin Anuar<sup>2</sup> and Nurul Mayzaitul Azwa Jamaludin<sup>3</sup>

<sup>1</sup>Kulliyah of Science, International Islamic University of Malaysia, Kuantan Pahang

<sup>2</sup>Malaysian Palm Oil Board, Selangor

<sup>3</sup>University Putra Malaysia, Selangor

\*Corresponding author: nurshuhada@iium.edu.my

### **Abstract**

Bauxite mining is one of the most prominent activities because it contains Aluminum (Al), which is in high demand in a variety of industries. However, various adverse consequences have been recorded as a result of this mining activity, which involved towards the environment, socioeconomics, and human health. Soil pollution has long been debated as a serious environmental issue in both developed and developing countries especially in area involving mining activities. This study was carried out to evaluate the level of contamination in soil caused by the bauxite mining activities in selected area in Kuantan district using geostatistics and geospatial analysis. A total of 64 soil samples were collected from the bauxite mining area and were then examined for its pH value and heavy metals constitutions (Cu, Zn, Pb and Ni). The soil samples were evaluated using geostatistical and geospatial techniques; statistical analysis, semi-variogram and ordinary kriging technique. Semivariogram were evaluated by using GS+ software and ordinary kriging were mapped by using ArcGIS software. It can be observed that the pH of the soil is slightly acidic with a range of 3.65 to 4.82. The average content recorded for Cu, Zn, Pb and Ni were 4.18±0.28, 138.94±78.46, 233.55±78.54, 57.58±23.72 and 191.47±159.84 mg kg<sup>-1</sup>, respectively. Semi-variogram has been proved to provide informative spatial structure of heavy metals and information about the processes that influence their distribution. The nugget to sill ratio of pH, Cu, Zn, Pb and Ni were (2.17×10)-3, 0.42,0.08, 0.13 and 0.14 respectively. All variables presented strong spatial dependence (R2>0.5), except for Pb (R<sup>2</sup> =0.01). Mapping using Kriging techniques aid in analyzing spatial distribution of soil heavy metals contents, which it also facilitates in identification of areas with different metal concentrations accordingly. The outcome of this study can be used by respective agencies for recommendation and reference in terms of soil rehabilitation, environmental regulation and replanting activities.

# APPLICATION OF STABILITY INDEX IN CHARACTERIZING THE BASIN OF ATTRACTION IN ECOLOGICAL MODELLING

Ummu Atiqah Mohd Roslan<sup>1\*</sup>

<sup>1</sup>Faculty of Ocean Engineering Technology and Informatics, Universiti Malaysia Terengganu

\*Corresponding author: ummuatiqah@umt.edu.my

### **Abstract**

An approach called the "stability index" was proposed by Podvigina and Ashwin in year 2011 is very useful to characterize the local geometry of riddled basins of attraction for dynamical systems. With the stability index, one can study the dynamics behaviour of a dynamical system. It would be interesting to understand how the stability index behaves on the basin boundary between multiple basins of attraction. In this presentation, the stability index is applied in the case of ecological model. A two-species of competition system will be considered, in which this system contains two attractors with riddled basins. To characterize the local geometry of the riddled basin, the stability index is computed for the attractor in the system. The results show that as a parameter in the system increases, the stability indices vary from infinity down to positive values to minus infinity. The changes in the indices indicate that the attractor loses its stability from being an asymptotically stable attractor (a.s.a.) to riddled basin attractor to chaotic saddle. Thus, it is believed that the stability index has a great potential to become a new study on bifurcation of dynamical system due to its ability to characterize different types of geometry of basins of attraction.

# OPTIMIZATION OF TOTAL PHENOLIC CONTENT AND ANTIOXIDANT ACTIVITY FROM SUKKARI VARIETY OF DATE PALM (*PHOENIX DACTYLIFERA* L.) USING SUPERCRITICAL FLUID EXTRACTION METHOD

Sahena Ferdosh<sup>1\*</sup> and Nadirah Abd Rahim<sup>1</sup>

<sup>1</sup>Department of Plant Science, Kulliyyah of Science, International Islamic University Malaysia (IIUM), 25200 Kuantan, Pahang.

\*Corresponding author: sahena@iium.edu.my

### **Abstract**

Date palm fruit (*Pheonix dactylifera*) is one of the oldest fruit crops that have great nutritional value as well as economically important in many countries. The aim of the study is to assess the total yield, total phenolic content and antioxidant activity from Sukkari variety of date palm (*P. dactylifera* L.) using supercritical carbon dioxide (SC-CO<sub>2</sub>) extraction. Three important operating parameters of SC-CO<sub>2</sub> consist of temperature (40-60 °C), pressure (15-40 MPa) and co-solvent percentage (5-15) were analysed for the interaction effects and optimum condition using the Box-Behken design of response surface methodology (RSM). The antioxidant potential of the extract were evaluated based on total phenolic content (TPC), 2,2,diphenyl-2-picryl-hydrazyl (DPPH) assay and Ferric-Reducing Antioxidant Power (FRAP) assay whereas phenolic compounds (gallic acid, p-coumaric acid, ferulic acid and quercetin) were identified and quantified using High-Performance Liquid Chromatography. In SC-CO<sub>2</sub>, highest yields were recorded 16.06%, TPC 17.88  $\pm$  0.05 mg GAE /g, DPPH at 30.71  $\pm$  0.78 percentage inhibition and FRAP at  $37.03 \pm 0.70$  mg GAE/g. The optimum extraction parameters were pressure 40 Mpa, temperature 602 and Co-solvent 8.056 % whereas expected optimum response value for TPC is 17.88 mg/g GAE, FRAP is 38.57 mg/g GAE and EC50 for DPPH is at 21.81. These data demonstrated the potential of SC-CO<sub>2</sub> with co-solvent as a valuable alternative green processing technology that can provide enhanced result with better selectivity. It indicates the potential of soukari extracts using SC-CO<sub>2</sub> as a source for antioxidant nutraceutical food and useful drug development that can help in free radical related diseases.

# THE IMPACT OF THE US-CHINA TRADE WAR ON THE MALAYSIAN STOCK MARKET NETWORK

Sarmita A/P Surantharan<sup>1\*</sup> and Hafizah Bahaludin<sup>2\*</sup>

<sup>1</sup>Department of Mathematical Sciences, Faculty of Science and Technology,
Universiti Kebangsaan Malaysia, 43600 UKM Bangi, Malaysia

<sup>2</sup>Department of Computational and Theoretical Sciences, Kulliyyah of Science, International Islamic University
Malaysia, Bandar Indera Mahkota Campus, Jalan Sultan Ahmad Shah, 25200 Kuantan, Pahang, Malaysia

\*Corresponding author: sarmita1226@gmail.com, hafizahbahaludin@iium.edu.my

### **Abstract**

A trade war between China and United States began on March 23, 2018, that affecting the Malaysian economy. Basically, China is Malaysia's most essential and largest trading partner. Meanwhile, United States is Malaysia's third-largest export market, accounting for 9.5 percent of total exports, or RM88.7 billion. Any trade liberalisation between these two countries would have a major impact on economic development of Malaysia. Therefore, the first objective of this research is to investigate the effect of the US-China war trade to Malaysian market by using a network analysis. The second objective is to examine the network's topological properties over the specified period. The data is based on FTSE Emas Index on Bursa Malaysia. The duration is divided into three phases in which before trade war, after trade war and overall duration. The threshold network approach is employed to visualize the relationship between the components of FTSE Emas Index. The results shows that the US-China war trade affected the network topology of Bursa Malaysia in which changed the linkages between the stocks.

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# **THANK YOU**