

XXth RENCONTRES
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Gặp gỡ Việt Nam lần thứ 20



INTERNATIONAL SYMPOSIUM OF NANO LIFE SCIENCE:
**NANO BIOTECHNOLOGY,
BIOPHYSICS, COMPUTATION**

HỘI THẢO QUỐC TẾ LẦN THỨ 2 VỀ KHOA HỌC SỰ SỐNG NANO

September 25 - 27, 2024 ICISE Quy Nhon, Vietnam

ABSTRACT BOOK

2nd

SPONSORS

NanoBioCoM2024 is organized and supported by Rencontres du Vietnam, International Centre for Interdisciplinary Science and Education (ICISE), and other institutions, organizations and companies.



Welcome Message from the Organizing Committee of NanoBioCoM2024

Dear Esteemed Participants,

It is our great pleasure to welcome you to "**XX Rencontres du Vietnam: The Second International Symposium of Nano Life Science: Nano Biotechnology, Biophysics, Computation (NanoBioCoM2024)**". This prestigious event brings together leading scientists, researchers, and professionals from around the world to exchange cutting-edge ideas and innovations in the dynamic and interdisciplinary fields of nanobiotechnology, biophysics, and computational science.

NanoBioCoM2024 offers a unique platform for cultivating collaboration and advancing transformative research at the forefront of nano-life sciences. The symposium's comprehensive program includes plenary sessions, keynote and invited talks, oral presentations, poster sessions, as well as panel discussions focused on education, research collaborations, technology transfer, and biophysics activities in Vietnam. These sessions are designed to provide participants with valuable insights, spark new ideas, and encourage fresh approaches to addressing key challenges in these fields.

We encourage you to take full advantage of this opportunity to engage with experts, build new connections, and explore collaborative efforts that will help shape the future of nano life science and technology.

We are confident that your participation will contribute to the success of this symposium, and we eagerly look forward to an inspiring and fruitful event in the beautiful, relaxing circumstances of ICISE, Quy Nhon City, Vietnam.

Thank you for joining us, and welcome to NanoBioCoM2024!

Warm regards,

Quy Nhon, Vietnam, September 25-27, 2024

NanoBioCoM2024's chairmen



A blue ink signature of Trần Quang Huy.

Trần Quang Huy

Chairman



A blue ink signature of Ngô Xuân Kiên.

Ngô Xuân Kiên

Co-Chairman



A blue ink signature of Nguyễn Bảo Quốc.

Nguyễn Bảo Quốc

Co-Chairman

Preface

After the success of the first International Symposium of Nano Life Science: Nano Biotechnology, Biosensor, Computation (NanoBioCoM2023) held from 17-19 September 2023, we continued to organize the second symposium and focused more on the field of biophysics. Biophysics is an interdisciplinary field that combines principles and methods from physics and biology to study the physical aspects of biological systems. The primary function of biophysics is to understand the underlying physical mechanisms and principles that govern the structure, dynamics, function, and behavior of biological molecules, cells, tissues, and organisms. Resolving differences between single molecule experiments and ensemble averaged experiments has fundamental importance in the area of the nano life sciences. The Second International Symposium of Nano Life Science: Nano Biotechnology, Biophysics, Computation (NanoBioCoM2024) is held from 25-27 September 2024 at ICISE, Quy Nhon, Binh Dinh province, Vietnam to provide participants a brilliant insight into new techniques and research trends in life science.

The main aim of this symposium is to introduce a wide range of experimental and computational methods relevant to modern nano life science that are able to comment on these differences. Vietnam, a developing country of nearly 100 million people, is actively creating research programs within the nano life sciences including nano biotechnology (nanomedicine, HS-AFM, FM-AFM, SICM), biophysics (biomolecular nanosystems, nanobio-hybrids, nanosized biostructures, nano-based biosensors), and computation and deep learning (artificial intelligence (AI) in biology). This symposium event is used to further stimulate these research programs by inviting a range of experts from both within Vietnam, and the world, to give structured talks on nano life science topics. The described computational methods range from coarse-grained simulation to molecular dynamic approaches.

The symposium has received 88 abstracts for plenary, keynote, invited, oral and poster presentations. There have been 50 abstracts assigned for oral and 38 abstracts assigned for posters. Presenters come from 19 countries such as Japan, France, Germany, Italy, Poland, USA, Canada, Taiwan, Thailand, Philippines, Malaysia, India, Pakistan, Kazakhstan, and Vietnam as well as 56 universities and research institutes. This symposium has awarded 40 scholarships for young researchers and excellent students to meet, learn and exchange academic topics with worldwide well-known scientists at NanoBioCoM2024.

Honestly, we would like to express our great appreciation to Prof. Jean Tran Thanh Van – President of Rencontres du Vietnam and Prof. Le Kim Ngoc for their generous support to this event. We are truly grateful for the valuable support from WPI Nano Life Science Institute - Kanazawa University, Phenikaa University Nano Institute (PHENA), International Union of Pure and Applied Biophysics (IUPAB), International Centre For Genetic Engineering And Biotechnology (ICGEB), The Japan Society for the Promotion of Science (JSPS), and ADgroup for the success of NanoBioCoM2024.

Wishing you all the best.

The organizing committee of NanoBioCoM2024

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**The second International Symposium of Nano Life Science:
Nano Biotechnology, Biophysics and Computation (NanoBioCoM2024)**
ICISE, Quy Nhon City, Binh Dinh province, Vietnam, September 25-27, 2024

PROGRAMME AT A GLANCE

Date	Time	Program	
DAY 1 Sept. 25 (Wed.)	7:45 – 8:15	Moving to ICISE from Seagull Hotel by Shuttle Buses	
	8:30 – 9:00	Registration	
	9:00 – 10:00	Opening ceremony and group photo	
	10:00-10:30	Coffee break	
		Plenary session, Hall 1 (PL: 40 min; K: 30 min)	
	10:30- 12:10	1 Plenary Lecture (PL-01) + 2 Keynote Lectures (K-01, ,K-02)	
	12:10 – 13:30	Lunch	
		Plenary session, Hall 1 (K: 30 min; I: 25 min)	
	13:30 – 14:55	2 Keynote Lecture (K-03, K-04) + 1 Invited Lecture (I-19)	
		Parallel sessions (I: 25 min; O: 20 min)	
	15:30 – 17:20	Session 1: Nano Biotechnology (Hall 1) 2 Invited Lectures + 2 Oral talks	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) 2 Invited Lectures + 2 Oral talk
	17:30	Moving to hotels by shutter buses	
DAY 2 Sept. 26 (Thu.)	8:00 – 8:45	Moving to ICISE from Seagull Hotel by Shuttle Buses, and hanging posters	
		Plenary session, Hall 1 (PL: 40 min; K: 30 min; I: 25 min)	
	9:00 – 10:35	1 Plenary Lecture (PL-02) + 1 Keynote Lectures (K-05) + 1 Invited Lecture (I-20)	
		Parallel sessions (I: 25 min; O: 20 min)	
	11:00– 12:10	Session 1: Nano Biotechnology (Hall 1) 2 Invited lectures + 1 Oral talk	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) 2 Invited lectures + 1 Oral talk
	12:10 – 13:30	Lunch	
		Parallel sessions (I: 25 min; O: 20 min)	
	13:30 – 15:25	Session 1: Nano Biotechnology (Hall 1) 3 Invited Lectures + 2 Oral talks	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) 3 Invited Lectures + 2 Oral talks
		Plenary session, Hall 1 (K: 30 min)	
	16:00-17:00	2 Keynote Lectures (K-06, K-07)	
	17:00-17:50	Roundtable discussion (Research & education colab., technology transfer)	
	18:00 – 21:30	GALA DINNER	
DAY 3 Sept. 27 (Fri.)	8:00 – 8:45	Moving to ICISE from Seagull Hotel by Shuttle Buses	
		Plenary session, Hall 1 (PL: 40 min; K: 30 min)	
	9:00 – 10:10	1 Plenary Lecture (PL-03) + 1 Keynote Lecture (K-08)	
		Parallel sessions (I: 25 min; O: 20 min)	
	10:40-12:20	Session 1: Nano Biotechnology (Hall 1) 2 Invited Lectures + 1 Oral talk	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) 2 Invited Lectures + 2 Oral talk
	12:20 – 13:30	Lunch	
	13:30 – 14:30	Poster presentation	
		Plenary session, Hall 1 (K: 30 min; I: 25 min)	
	14:30-16:15	1 Keynote Lecture (K-09) + 3 Invited Lectures (I-21; I-22; I-23)	
	16:30-17:00	Roundtable discussion: Biophysics activities (Hall 1)	
	17:00-17:30	IUPAB & Poster awards and Closing ceremony	
	17:30	Moving to Seagull Hotel by Shuttle Buses or Free Excursion	

DETAILED AGENDA

DAY 1 Wednesday, September 25, 2024		
7:45 - 8:15	Moving to ICISE from Seagull Hotel by Shuttle Buses	
8:30 - 9:00	Registration	
9:00 – 10:00	Opening ceremony and group photo Assoc.Prof. TQ Huy (Phenikaa Uni.) Prof. Jean TTV (ICISE) Prof. Takeshi Fukuma (NanoLSI, Kanazawa Uni.)	
10:00-10:30	Coffee break	
	PLENARY SESSION, HALL 1 Chairs: Prof. Wibool Piyawattanametha and Assist. Prof. Ngo Xuan Kien	
10:30 – 11:10	PL-01: Measurements of Nanoscale Dynamics and Mechanics in Living Cells by Nanoendoscopy AFM	Prof. Dr. Takeshi Fukuma Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kakuma-machi, Kanazawa 920-1192, Japan
11:10 – 11:40	K-01: Integrative structural biology of cilia at multiscale resolution by cryo-electron microscopy	Prof. Dr. Khanh Huy Bui Department of Anatomy and Cell Biology, McGill University, Montreal, Quebec, Canada
11:40 – 12:10	K-02: 3D multi-spectral MEMS-based dual-axis confocal microendoscope for clinical applications	Prof. Dr. Wibool Piyawattanametha Department of Biomedical Engineering, King Mongkut's Institute of Technology Ladkrabang, Ladkrabang 10520, Thailand
12:10 – 13:30	Lunch	
	PLENARY SESSION, HALL 1 Chairs: Prof. Dr. Tran Van Nhieu and Prof. Dr. Florence Tama	
13:30-14:00	K-03: A Novel Gate Operating Pathway of Lipopolysaccharide Transport by Bacterial ABC Transporter MsbA and LptC	Assist. Prof. Dr. Kien Xuan Ngo Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan

14:00-14:30	K-04: Structural and functional insights into vinculin supra-activation mediated by Shigella IpaA	Prof. Dr. Tran Van Nhieu Université Paris-Saclay, CNRS UMR 9198, Institute for Integrative Biology of the Cell (I2BC), Gif-sur-Yvette, France.
14:30 – 14:55	I-19: Integrative Modeling Approaches to Characterize Dynamics of Biomolecules: Application to Atomic Force Microscopy	Prof. Dr. Florence Tama Nagoya University, Japan
14:55 -15:30	Coffee break	
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (Hall 1) Chairs: Prof. Dr. N. T. Van-Oanh and Dr. Phuong H. Nguyen	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) Chairs: Prof. Dr. Shigehiko Hayashi and Assist. Prof. Dr. Ayumi Sumino
15:30 – 15:55	I-01: Metal/bimetallic nanoparticles for advanced radiation therapy Prof. Dr. N. T. Van-Oanh , Institut de Chimie Physique (ICP), Université Paris-Saclay, CNRS, UMR8000, Orsay, France	I-02: Atomistically deciphering functional activation processes of proteins with hybrid molecular simulations Prof. Dr. Shigehiko Hayashi , Graduate School of Science, Kyoto University, Kyoto, Japan
15:55 – 16:20	I-03: Nanomedicine: using nanobubbles and ultrasound for enhancing drug delivery Dr. Phuong H. Nguyen , Laboratoire de Biochimie Théorique, Institut de Biologie Physico-Chimique CNRS and Université Paris Cité Paris, France	I-04: High-speed atomic force microscopy studies on the structural dynamics of ion channels at the single molecule level Assist. Prof. Dr. Ayumi Sumino , Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan
16:20 – 16:40	O-01: Developing pharmaceutical nano formulations of <i>Chandamarutha chenduram</i> to combat clinical bacterial resistance and assess its antibacterial efficacy Dr. Muddukrishnaiah Kotakonda ,	O-02: Integration of high-speed atomic force microscopy with in silico modeling for characterizing aptamers targeting METTL3 in cancer cells Assist.Prof.Dr. Madhu Biyani

	Department of Pharmaceutics, Jamia Salafiya Pharmacy College, Pulikkal, Malappuram, Kerala-673637, India	Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Ishikawa, Japan
16:40 – 17:00	O-03: Green bio-fabricated silver nanoparticles from fungal endophyte induces anti-proliferative and apoptotic activities against breast cancer and suppresses in ovo neovascularization PhD stu. Ashish Verma, Centre of Experimental Medicine and Surgery, Institute of Medical Sciences, Banaras Hindu University, Varanasi-221005, India	O-04: Effect of Glu78 on the transport of Cation-Protons across the cell membrane by Ec-NhaA. PhD stu. Anuradha Yadav Amity Institute of Biotechnology, Amity University Uttar Pradesh, Lucknow-226028, India
17:00-17:20	O-05: Antioxidant potential assessment of biosynthesized AgNPs and characterization of hepatoprotective phytoconstituents from Vitis vinifera extract using LC-MS/MS Dr. Muhammad Arshad Biochemistry Section, Jhang campus, University of Veterinary and Animal Sciences Lahore Pakistan	O-06: Exploration and identification of the NPR1 gene mediated plant defense response mechanism in Chili against begomovirus Infection Dr. Muhammad Shafiq, Department of Horticulture University of the Punjab New Campus Lahore, Pakistan
17:30	Moving to hotels by shutter buses, free excursion	
DAY 2 Thursday, September 26, 2024		
8:00 – 8:45	Moving to ICISE from Seagull Hotel by Shuttle Buses, and hanging posters	
	PLENARY SESSION, HALL 1 Chairs: Prof. Dr. Takeharu Nagai and Prof. Dr. Nguyen The Toan	
9:00 – 9:40	PL-02: Trans-scale scope opens up a new horizon in life science research	Prof. Dr. Takeharu Nagai SANKEN, The University of Osaka, Ibaraki, Japan
9:40 – 10:10	K-05: Comparing Receptor Binding Properties of SARS-CoV-2 and of SARS-CoV Virus by Using Unsupervised Machine Learning Models	Prof. Dr. Nguyen The Toan Key Laboratory for Multiscale Simulation of Complex Systems, and Faculty of Physics, University of Science, Vietnam National University

		334 Nguyen Trai Street, Thanh Xuan, Hanoi 11400, Vietnam
10:10-10:35	I-20: Computational simulations supporting observations by atomic force microscopy	Assist. Prof. Dr. Takashi Sumikama, Nano Life Science Institute, Kanazawa University, Kanazawa, Ishikawa, Japan
10:35 – 11:00	Coffee break and Poster visiting	
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (Hall 1) Chairs: Assoc. Prof. Anh T.N. DAO and Dr. Thuy Thi Thu Nguyen	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) Chairs: Prof. Dr. Steven Hayward and Assist. Prof. Duy Phuoc Tran
11:00-11:25	I-05: Fabrication of Silk Protein to Hybrid Nanocarriers for Cancer Therapy Assoc. Prof. Anh T.N. DAO, Graduate School of Integrated Science and Technology, Nagasaki University, Japan	I-06: Interactive flexible receptor docking using DockIT Prof. Dr. Steven Hayward, School of Computing Sciences, University of East Anglia, Norwich, U.K.
11:25 – 11:50	I-07: Nanomaterials in biomedical applications: convergence in fighting against bacterial and virus infections Dr. Thuy Thi Thu Nguyen, Phenikaa University Nano Institute, Phenikaa University, Hanoi, Vietnam	I-08: Ions Permeation through the Stators of Bacterial Flagellar Motors Assist. Prof. Duy Phuoc Tran, School of Life Science and Technology, Tokyo Institute of Technology, Tokyo, Japan
11:50 – 12:10	O-07: Isolation and screening of hydrocarbon degrading bacterial isolated from oil contaminated sites. PhD stu. Hitendra Yadav, Amity Institute of Biotechnology, Amity University Uttar Pradesh, Lucknow Campus, India	O-08: Single fluorescence-based FLIM indicator for observing changes in GTP/GDP ratio in cancer cells PhD stu. Loan Thi Ngoc Nguyen, WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan
12:10 – 13:30	Lunch	

	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (Hall 1) Chairs: Research Assist. Prof. Dr. Thoa Tran and Assist.Prof. Dr. Nguyen Kim Hung	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) Chairs: Assist. Prof. Dr. Shingo Fukuda and Dr. Silvano Piazza
13:30 – 13:55	I-09: Development of Regulable and Targeted Photochemical Internalization Therapy to combat borderline resectable and unresectable locally advanced pancreatic cancer Dr. Thoa Tran, Max Schmidt Indiana University, School of Medicine	I-10: Integrative Analysis of APE1-Mediated MicroRNA Processing and Protein-Protein Interactions in Cancer Prognosis Dr. Silvano Piazza, Group Leader, Computational Biology, International Centre for Genetic Engineering and Biotechnology, Italy
13:55 – 14:20	I-11: Design and Modification of Porous Nanomaterials as Drug Carriers in Cancer Therapy Assoc. Prof. Dr. Doan Le Hoang Tan Center for Innovative Materials and Architectures, Ho Chi Minh City, Vietnam	I-12: Ultra-high-speed atomic force microscopy for visualization of faster biomolecular dynamics Assist. Prof. Dr. Shingo Fukuda WPI Nano Life Science Institute (WPI-NanoLSI), Kanazawa University
14:20 – 14:45	I-13: Viscoelastic Characterization of Soft Materials Using Nanorheological Atomic Force Microscopy Assist.Prof. Dr. Nguyen Kim Hung, School of Materials and Chemical Technology, Tokyo Institute of Technology, 1-12-1 Ookayama, Meguro-ku, Tokyo 152-8552, Japan	I-14: Toward Quantitative Imaging of Cellular Metabolites with Fluorescence Lifetime Biosensors Assist. Prof. Dr. Cong Quang Vu, Nano Life Science Institute (WPI-NanoLSI), Kanazawa University, Kanazawa, Japan
14:45 – 15:05	O-09: Green synthesis, optimization, characterization and exploring the impact of biogenic zinc oxide nanoparticles derived from Lantana camara L. leaf extract on alleviating heat stress in wheat	O-10: The oligomerization and neutralization capabilities of alpha-hemolysin (Hla) toxin from Staphylococcus aureus by mutant Hla proteins Dr. Ngan Thi Phuong Le

	Mr. Neelesh Kapoor Division of Plant Biotechnology, College of Biotechnology, Sardar Vallabhbhai Patel University of Agriculture and Technology, Meerut-250110 (UP) India	Center for Bioscience and Biotechnology, University of Science, Ho Chi Minh City, Vietnam
15:05-15:25	O-11: Unlocking the enhanced Antimicrobial and Anti-biofilm Potential of Microbial Metabolites: A Nanoformulation Approach PhD stu. Shelly Singh, Department of Biological Sciences and Engineering, NSUT, Dwarka Sector-3, New Delhi, India-110078	O-12: High-efficiency Sperm Selection by Microchip Integrated of Electrospun Membrane PhD stu. Huynh-Nhu Luu-Thi, Ton Duc Thang University
15:25 -16:00	Coffee break	
	PLENARY SESSION, HALL 1 Chairs: Assoc. Nguyen Bao Quoc and Assist. Prof. Dr. Ngo Xuan Kien	
16:00 – 16:30	K-06: Twin transition in Vietnam – opportunities for integrating advanced science & technologies in agriculture	Dr. My T. Nguyen RYNAN® Technologies Vietnam JSC
16:30 – 17:00 (online)	K-07: Light Responsive Soft nano- objects: Light Triggered Manipulation of Particle Assembly	Prof. Dr. Svetlana Santer Institute of Physics and Astronomy, University of Potsdam, Germany
17:00 – 17:50	Roundtable discussion (Research & education colab., technology transfer) Chairs: Tran Quang Huy, Ngo Xuan Kien, Nguyen Bao Quoc	
18:00 – 21:30	Gala Dinner	
DAY 3 Friday, September 27, 2024		
8:30 – 9:00	Moving to ICISE from Seagull Hotel by Shuttle Buses	
	PLENARY SESSION, HALL 1 Chairs: Prof. Dr. Akio Kitao; Assoc.Prof. Dr. Tran Quang HUY	
9:00 – 9:40	PL-03: Mechanisms of Conformational Change, Association, and Dissociation of Proteins investigated by Parallel Cascade Selection Molecular Dynamics	Prof. Dr. Akio Kitao School of Life Science and Technology, Tokyo Institute of Technology, Japan

9:40-10:10 (online)	K-08: A Bioactive Disintegrable Polymer Nanoparticle for Synergistic Vascular Anti-calcification and Drug Delivery	Prof. Dr. Hang Thu Ta School of Environment and Science, Griffith University, Brisbane, Queensland 4111, Australia
10:10 – 10:40	Coffee break	
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (Hall 1) Chairs: Assoc. Prof. Huynh Chan Khon and Dr. Nguyen Ba Hung	Session 2: Biophysics and Computation (Hall 2, 2 nd floor) Chairs: Dr. Tri Thanh Pham and Assist. Prof. Dr. Cong Quang Vu
10:40 – 11:10	I-15: The Effect of Shear Stress on Fibronectin Fibrillogenesis: Morphological Properties and Cellular Implications Assoc. Prof. Huynh Chan Khon, International University, Vietnam National University, HCMC, Vietnam	I-16: Applying AI Algorithms to Recognize Important Genes in Cancer Tumors Prof. Turgay Ibrikci Adana Alparslan Turkes Science and Technology University, Adana, Türkiye
11:10 – 11:40	I-17: Development of nanomaterials-based electrochemical biosensors for food safety monitoring Assoc. Prof. Tran Quang Huy Phenikaa University Nano Institute, Phenikaa University, Vietnam	I-18: A combined optical and atomic force microscope for materials and life sciences research Dr. Tri Thanh Pham Department of Biology, School of Sciences and Humanities, Nazarbayev University, Kazakhstan
11:40 – 12:00	O-13: Synergistic Activation of p53 in Cancer Cells Using Zinc Oxide Nanoparticles: A Promising Approach for Cancer Therapy Dr. Samuel Shiferaw Biresaw, Department of Biotechnology, School of Engineering and Technology, Sharda University, Plot No. 32, 34, Knowledge Park III, Greater Noida, Uttar Pradesh 201310, India	O-14: Novel Enzyme- Assisted Cellulose Nanofibre (CNF) Synthesis and its Application in CR Dye Adsorption Using RSM Optimization PhD stu. Twinkle Gupta, Department of Biological Sciences and Engineering, Netaji Subhas University of Technology, Dwarka, New-Delhi, India-110078
12:00-12:20		O-15: Metabarcoding of fish species in mangrove nursery grounds using eDNA (environmental DNA) as a tool for

		conservation and fish stock assessment Tricksie Balatero Department of Biological Sciences, Mindanao State University-Iligan Institute of Technology, Iligan City, 9200 Philippines
12:20-13:30	Lunch	
13:30 – 14:30	Poster presentation	
	PLENARY SESSION, HALL 1 Chairs: Prof. Dr. Florence Tama and Assist. Prof. Dr. Takashi Sumikama	
14:30-15:00 (online)	K-09: Protein Folding and Dimerization on Ribosomes	Prof. Dr. Mai Suan Li Institute of Physics, Polish Academy of Sciences, Poland
15:00-15:25	I-21: Molecular-scale observation of porphyrin derivatives self-assembled at solid-electrolyte interfaces	Assoc. Prof. Dr. Thanh Hai Phan Faculty of Natural Sciences, Quy Nhon University, 170 An Duong Vuong, Quy Nhon, Viet Nam
15:25-15:50	I-22: CM-AFM in biological applications: A correlation of the mechanical properties to the cell membrane composition	Dr. Anh-Dung Nguyen Lemans University, France
15:50-16:15	I-23: Low-cost SmartTrap: An Innovative Pest Observation System Harnessing TinyML and Edge Computing	Dr. Hien Bich Vo, Vietnamese-German University, Binh Duong, Vietnam
16:15 – 16:30	Coffee break	
16:30 – 17:00	Roundtable discussion: Biophysics activities (Hall 1) Chairs: Tran Quang Huy, Ngo Xuan Kien, Nguyen Bao Quoc	
17:00-17:30	IUPAB & Poster awards and Closing ceremony	
17:30	Moving to Seagull Hotel by Shuttle Buses/ Free Excursion	
	Saturday, September 28, 2024	
	Excursion in Quy Nhon (self-paid expenses)	

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PLENARY LECTURES

PL-01 Measurements of Nanoscale Dynamics and Mechanics in Living Cells by Nanoendoscopy AFM

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Abstract: Atomic force microscopy (AFM) has been a powerful tool for imaging nanoscale dynamics of proteins and DNAs in a physiologically relevant liquid environment. However, most of the high-resolution AFM experiments were performed with a biological system reconstructed on a solid substrate. Thus, it has been questioned if the observed behaviors truly represent the phenomena inside living cells. To address this issue, we have recently developed Nanoendoscopy AFM (NE-AFM) [1]. As if we insert a thin camera into a human body in the endoscopic imaging, we insert a thin needle probe into a living cell to perform 2D/3D-AFM measurements. So far, we have successfully visualized 3D structures of the whole cell, nucleus and actin stress fibers, and 2D nanodynamics of cortical actin mesh at the inner surface of a bottom membrane [1]. Now, we are actively exploring possible applications of this novel technique in life science.

For example, we have been investigating the growth and disassembling of focal adhesions (FAs) in living fibroblast cells. With NE-AFM combined with confocal microscopy, we simultaneously visualized paxillin distribution and 3D structural changes of FAs and associated actin fibers during the FA growth and disassembling. The results reveal that the FAs are initially relatively thick but become thinner as they grow. In addition, the actin fiber is initially in contact with the upper cell membrane but detached as it extends towards the growth direction. Meanwhile, the paxillin distribution also extends towards the same direction so that the molecules fill up the gap between the actin fiber and the bottom cell membrane.

Another example is the nuclear elasticity measurements. As we can directly indent the nucleus inside living cells, we can fit a contact mechanics model to the indentation profile to obtain a quantitative value of the nuclear elasticity. As the nuclear envelope is supported by lamin associated domains (LADs) of heterochromatins, the elasticity distribution on the nuclear surface is strongly correlated with the LAD distribution and hence the gene expression activity. Therefore, we are exploring possibilities to apply NE-AFM for investigating nuclear elasticity changes induced by diseases know as nuclear envelopopathy, where gene mutation of nuclear envelope proteins is involved in the pathogenesis. In this presentation, I will present basic principle, experimental setup, applications and future prospects of NE-AFM.

[1] Penedo, M.; Miyazawa, K.; Okano, N.; Furusho, H.; Ichikawa, T.; Alam Mohammad, S.; Miyata, K.; Nakamura, C.; Fukuma, T., Visualizing intracellular nanostructures of living cells by nanoendoscopy-AFM. *Sci. Adv.* 2021, 7 (52), eabj4990.

Keywords: Atomic force microscopy (AFM), nanoendoscopy AFM (NE-AFM), live-cell measurements

PL-02 Trans-scale scope opens up a new horizon in life science research

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Abstract: Conventional scientific approaches generally focus on the major components of the observed sample, therefore, outliers that have unique value are often overlooked. For this reason, only a little information has accumulated on rare components with outlier-like characteristics. On the other hand, in recent years, it has become known that cells that are rarely found in a cell population can have a significant impact on living systems. To understand rare cells with such outlier characteristics, it is necessary to simultaneously observe a very large number of cells and assess how individual cells behave within a multicellular system. However, conventional microscopes are limited by their field of view size (< 0.1 cm) and the pixel count ($<$ several megapixels) on the image sensor, complicating the analysis described above. To overcome this issue, we developed a fluorescence imaging system that combines a 120-megapixel CMOS image sensor and a telecentric macro lens with 2x magnification. This system achieved a field of view greater than 1 cm with a spatial resolution of approximately for 2 μ m, sufficient for single eukaryotic cell analysis. We named this imaging system "AMATERAS" which signifies "illuminate everything". AMATERAS enables the simultaneous imaging of 100,000 to 1,000,000 cells within a single field of view and facilitates the observation of all cell dynamics (displacement, functional expression, state changes, and more) as moving images. This capability allows for the detection of unique cells and events that occur in fewer than 0.01% of one million cells. Furthermore, the integration of a robotic arm and a culture incubator with AMATERAS has enabled automated culturing and imaging of cells and organoids. Such an imaging system, capable of high-throughput acquisition of large-scale data, is expected to have a wide range of applications, not only in life science research but also in drug discovery and medical applications. In this symposium, I will present an overview of the trans-scale scope and demonstrate examples of observation and analysis, focusing on a new scientific approach in life science research.

PL-03 Mechanisms of Conformational Change, Association, and Dissociation of Proteins investigated by Parallel Cascade Selection Molecular Dynamics

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Abstract: Conformational dynamics, dissociation, and association of proteins are closely associated with their biological functions. Molecular dynamics (MD) simulation is a powerful tool to observe such processes, but the scales of functional dynamics are longer than typical MD time. Parallel cascade selection molecular dynamics (PaCS-MD) is an efficient conformational sampling method that can observe relatively slow processes (milliseconds ~ hours) within tens of nanoseconds (1-3). By analyzing trajectories obtained by PaCS-MD with the Markov state model (MSM), we can conduct analysis of pathways of conformational dynamics, and dissociation and association of two molecules (4-6). This combination, PaCS-MD/MSM, enables us to calculate free energy profile of these processes and rates of the processes. In this talk, I will report latest progress of PaCS-MD/MSM and applications, which include the investigation of protein conformational changes, and dissociation and association process (7-12).

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Keywords: *PaCS-MD, MSM, Conformational change, Association, Dissociation*

KEYNOTE LECTURES

K-01 Integrative structural biology of cilia at multiscale resolution by cryo-electron microscopy

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Abstract: In eukaryotes, cilia are ubiquitous organelles contributing to cellular motility and sensory function. In humans, cilia are found in the respiratory tract to clear mucus, in the sperm to propel movement and in the brain to circulate cerebrospinal fluid. The ciliary axoneme is a long microtubule-based cytoskeleton consisting of two central singlets and nine outer doublet microtubules. Understanding the molecular architecture of the axoneme will lead to insights into its assembly and function. We aim to study cilia structures at multiscale resolutions using cryo-electron microscopy, cryo-electron tomography and complementary techniques such as artificial structure prediction, *in situ* cross-linking mass spectrometry and proximity proteomics. We identified and modelled many proteins from proteins inside the lumen to the outside mechano-complexes regulating ciliary beating from low to high resolution. This helps us reveal the importance of ciliary proteins in cilia function and assembly. It also led to the discovery of novel microtubule-binding motifs that might be essential for microtubule stability and function. As a result, our research contributes to the understanding of cilia-related diseases in humans and has the potential to become a powerful tool for disease diagnosis.

Keywords: *cryo-electron microscopy, structural biology, cilia, axoneme, ciliopathy, cytoskeleton, microtubule*

K-02 3D multi-spectral MEMS-based dual-axis confocal microendoscope for clinical applications

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Abstract: At present, precise early cancer diagnosis and precise tumor resection can be achieved through using microendoscopes. Due to various technical challenges, few MEMS-based microendoscopes have been translated to clinics or applied to human patients. However, through synergistic collaborations, we developed a novel MEMS scanner-enabled microendoscopic multispectral (640 nm and 780 nm) three-dimensional (3D) dual-axis confocal fluorescent imaging system for translational applications, including early cancer detection and staging on colorectal cancer, molecular imaging-guided surgical navigation on head and neck cancer. With dual-axis confocal architecture, we have managed to miniaturize the imaging system with a compact form-factor by integrating micro-optics and a gold (as a reflective surface) patterned MEMS scanner, which has been custom-made and mass-produced in the nanofabrication foundry. The metal coating of the scanning mirror provides over 80% high reflectivity over near infra-red range. Both MEMS scanner rotational axes can achieve over 6 degrees mechanical scan angle in both DC and resonant scanning modes. With advanced computational imaging approach, we have achieved real-time cross-sectional imaging in either raster or Lissajous pattern scanning with a fast frame rate (> 10 Hz) with large field-of-view (> 600 microns). An advanced real-time mosaicing algorithm has been developed to achieve a broader view on a millimeter scale. By utilizing molecular contrast probes conjugated with a fluorescence dye, we have successfully demonstrated multi-spectral *ex-vivo* and *in-vivo* imaging on small animal tumor models and human tissue specimens, aimed for both early cancer detection and molecular imaging guided-surgical navigation.

Keywords: MEMS scanner, dual-axis, multi-spectral, microendoscope

K-03 A Novel Gate Operating Pathway of Lipopolysaccharide Transport by Bacterial ABC Transporter MsbA and LptC

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Abstract: All ATP Binding Cassette (ABC) transporters (importers/exporters) that operate in all species from bacteria to human share a common structural organization consisting of two distinct domains: periplasmic Transmembrane Domains (TMDs) and cytosolic Nucleotide Binding Domains (NBDs). This structural arrangement appears to be well-suited for its function of substrate transport across the cell membrane.

The outer membrane (OM) of Gram-negative bacteria contains lipopolysaccharide (LPS) that is essential for their viability and drug resistance. LPS composed of lipid A, core oligosaccharide, and O-antigen is transported from inner membrane (IM) to OM. For this longways transport, bacteria are equipped with ATP-driven MsbA, LptB₂FG and LptC in IM, the periplasmic protein LptA, and LptDE in OM. In the prevailing hypothesis, Lipid A is flipped across IM by bacterial ABC transporter MsbA in a “Trap-and-Flip” mechanism (Mi et al., Nature 2017). Subsequently, LPS is made by attaching lipid A with core oligosaccharide and O-antigen in periplasmic space. LptC, which is anchored to the IM by a single transmembrane helix and contains a periplasmic domain that binds LPS, is thought to play an important role in extracting and transporting LPS via LptB₂FGC to LptADE pathway. Despite the importance of LptC, how it cooperates with MsbA and LptA for this linear transport process has not yet been analysed.

Using high-speed atomic force microscopy (HS-AFM), we observed the TMD side of MsbA embedded in a membrane composed of DOPC/DOPS/ Kdo2 lipid A. In the presence of ATP, a protrusion appeared at the TMD core center, which was possibly formed by the accumulation of Lipid A flipped across the membrane. LptC containing a periplasmic domain that binds lipid A was observed to diffuse in the membrane and enter the large TMD cores of MsbA oligomers containing lipid A, suggesting that LptC can extract lipid A from MsbA and then deliver lipid A to LptA transporter (i.e., MsbA-LptCADE transport channel). These results lead to a completely Novel Gate Operating (NGO) pathway for lipid A/LPS transport from IM to OM in bacteria.

Keywords: ABC transporter, MsbA, LptC, HS-AFM

K-04 Structural and functional insights into vinculin supra-activation mediated by *Shigella* IpaA

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Abstract: Vinculin and talin are cytoskeletal linkers that play a key role in cell adhesion. During integrin-mediated mechanotransduction, stretching of the talin molecule reveals vinculin binding sites (VBSs), otherwise buried in helix bundles of the talin rod domain at the basal state. These exposed VBSs in turn recruit vinculin and promote its activation, leading to the unveiling of the vinculin tail and its binding to F-actin, thereby strengthening the anchoring of integrin receptors to the actin cytoskeleton. *Shigella*, the agent of bacillary dysentery, targets vinculin through the IpaA effector during epithelial cell invasion. We recently showed that IpaA reveals an original mode of vinculin activation, termed supra-activation, associated with major allosteric changes in vinculin leading to its trimerization via its head domain. Vinculin trimers induced by IpaA mediate the bundling of actin filaments and the formation of focal adhesions at a distance from the bacterial invasion sites. We developed a combination of approaches involving structural modelling, electron microscopy and high-speed atomic force microscopy to gain structural insights into the formation of vinculin trimers induced by IpaA. Together, our results support the notion that trimerization of the vinculin D1D2 head subdomains allows the formation of a core domain, while the D3D4 head subdomains are mobile and promote an extension of the region linking the vinculin tail domain. Of interest, the extended exploratory area of Vt associated with D1D2 trimers often appeared somewhat constrained spatially, covering define regions proximal to the core region suggesting some rigidity associated with a D3D4 extension. Finally, we used a mutational analysis of vinculin based on structural modelling to test the function of vinculin supra-activation. Our results suggest that vinculin supra-activation also occurs during integrin-mediated mechanotransduction, but is used by *Shigella* to promote adhesion to the extracellular matrix of cells infected with bacteria in the absence of mechanotransduction.

Keywords: Vinculin, *Shigella*, IpaA, Cell adhesion, bacterial invasion, oligomerization, actin bundling

K-05 Comparing Receptor Binding Properties of SARS-CoV-2 and of SARS-CoV Virus by Using Unsupervised Machine Learning Models

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Abstract: This work continues our recent molecular dynamics investigation of the three systems of the human ACE2 receptor interacting with the viral RBDs of SARS-CoV virus and two variants of SARS-CoV-2 viruses. The simulations are extended and analyzed using unsupervised machine learning models to give complementary descriptions of hidden features of the viral binding mechanism. Specifically, the principal component analysis (PCA) and the variational autoencoder (VAE) models are employed, both are classified as dimensionality reduction approaches with different focuses. The results support the molecular dynamics results that the two variants of SARS-CoV-2 bind stronger and more stable to the human ACE2 receptor than SARS-CoV virus does. Moreover, stronger bindings affect the structure of the human receptor, making it fluctuate more, a sensitive feature which is hard to detect using standard analyses. Unexpectedly, it is found that the VAE model can learn and arrange randomly shuffled protein structures obtained from molecular dynamics in time order in the latent space representation. This result potentially has promising application in computational biomolecules. One could use this VAE model to jump forward in time during a molecular dynamic simulation, and to enhance the sampling of protein configuration space.

Keywords: *Coronaviruses, human ACE2, unsupervised machine learnings, enhanced sampling, molecular dynamics, variational autoencoder*

K-06 Twin transition in Vietnam – opportunities for integrating advanced science & technologies in agriculture

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Abstract: In recent years, the Vietnamese government has been promoting a 'twin transition,' which simultaneously advances digital transformation and green transformation across various sectors. In agriculture, the government encourages stakeholders to adopt digital technologies and green solutions, presenting a great opportunity to integrate advanced science and technology. This can potentially drive sustainable growth and improve productivity, contributing to the country's goal of achieving net zero emissions by 2050.

The brackish water shrimp and rice farming industries are crucial to the Mekong Delta, both in terms of economic output and employment. Together, these industries generate over 7 billion USD annually in export revenues. The brackish water shrimp industry spans about 720,000 hectares, while rice farming covers over 1,500,000 hectares of the delta. These industries significantly contribute to the local economy and provide livelihoods for millions of residents. However, they are also the main contributors to environmental pollutions and greenhouse gas emissions in the region.

In this talk, I will share the objectives, challenges, current progress, and future research directions for the twin transition in the brackish water shrimp and rice farming sectors.

K-07 Protein Folding and Dimerization on Ribosomes

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Abstract: In this talk I will discuss the following problems:

1. Ribosome is a molecular machine for protein synthesis which involves four phases of translation - initiation, elongation, termination and ribosome recycling. This process is an area of intense research due to the essential role of proteins to life. Recently we have shown that electrostatic interactions govern extreme nascent protein ejection times from ribosomes and can delay ribosome recycling [1].
2. The hydrophobic interaction, which plays a key role in protein folding, was well studied in the aqueous environment. However, the water-mediated hydrophobic interaction inside the ribosome exit tunnel has been poorly understood. Using molecular dynamics simulation and umbrella sampling we showed that the hydrophobic effect is weaker in the vestibule. These findings mean that nascent proteins pass through a ribosome vestibule environment that can destabilize folded structures, which has the potential to influence co-translational protein folding pathways, energetics, and kinetics [2].
3. Using coarse-grain simulations of protein synthesis we showed that synonymous mutations can influence the protein dimerization in solution. The structural and kinetic origin of this effect is associated with misfolded states containing non-covalent lasso-entanglements, many of which structurally perturb the dimer interface, whose probability of occurrence depends on translation speed [3]. If time permits, the role of entanglement in the mechanism by which soluble misfolded proteins bypass chaperones at the molecular level will be discussed [4].

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K-08 A Bioactive Disintegrable Polymer Nanoparticle for Synergistic Vascular Anti-calcification and Drug Delivery

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Abstract: We have developed novel polysuccinimide-based nanoparticles (PSI NPs) as prodrug for site-specific treatment of vascular calcification¹ and also as efficient carriers for drug delivery (hydrophobic drug and also hydrophilic molecules such as protein)^{2,3}. Although poly(aspartic acid) (PASP), a strong calcium chelating agent, may be potentially effective in inhibition of vascular calcification, its direct administration may lead to side effects. Therefore, we creatively employed polysuccinimide (PSI), a precursor of PASP, to prepare targeted PSI NPs that not only acted as a prodrug but also functioned as a carrier of additional therapeutics to provide powerful synergistic vascular anticalcification effect¹. We found that chemically modified PSI-NPs serve as effective nanocarriers for loading of hydrophobic drugs, in addition to anti-calcification and anti-ROS activities. Curcumin (Cur), with high loading efficiency, was encapsulated into the NPs. The NPs were stable for 10-16 h in physiological conditions and then slowly dissolved/hydrolyzed to release the therapeutic PASP and the encapsulated drug. Though highly effective in the prevention of calcium deposition, PSI NPs could not prevent the osteogenic trans-differentiation of vascular smooth muscle cells (VSMCs). The presence of Cur addressed this problem. Cur-loaded PSI NPs significantly reduced calcium deposition in the aorta without adversely affecting bone integrity or noticeable side effects/toxicity as examined by organ histological and serum biochemistry analyses.

We also employed PSI NPs to develop theranostic materials for cancer therapy². Here, the NPs function as a carrier for bioactive agents such as Curcumin and IR-780 dye whereby the former exerts its intrinsic anti-cancer abilities, the latter confers photothermal treatment application and bimodal imaging ability using photoacoustic and fluorescence imaging. The NPs exhibited zero burst release. *In vitro* and *in vivo* results establish that administration of folate receptors targeting PSI-NPs in U87MG model effected in a substantial decrease in tumour and photothermal laser exposure at 808 nm further ablated tumours to an almost total eradication. Our dual loaded targeted NPs demonstrated selectivity through enhanced accumulation and retention in tumours as indicated by multi-spectral optoacoustic tomography (MSOT) and fluorescence imaging (FI). Loading of Curcumin and IR-780 into PSI-NPs improved its bioavailability, allowing Curcumin to be administered into the circulation system and retention in tumours which led to the simultaneous application for a successful targeted, synergistic photothermal treatment and bimodal imaging using MSOT and FI.

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K-09 Light responsive soft nano-objects: Light triggered manipulation of particle assembly

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Abstract: Azobenzene molecules are considered as molecular actuators that can convert optical energy into mechanical work under reversible photo-isomerization from a trans- to a cis-configuration. In this talk I will show several interesting examples where azobenzene can be used in order to actuate matter on large time and length scales. I will show how, using azobenzene containing surfactant, consisting of a charged head and a hydrophobic tail into which an azobenzene group is incorporated [1], one can manipulate microparticles and even induce their self-propulsion when trapped at a solid/liquid interface. Depending on the applied wave length one can either disperse/remove or gather particles. The physical origin of this genuine behaviour is related to the phenomenon of light driven diffusioosmosis (LDDO) [2]. During irradiation of a solution containing azobenzene surfactants with focused light, there is a formation of local fluid flow at the solid/liquid interface. The corresponding forces are sufficiently strong to swiftly clean the illuminated area from particles trapped at the interface. The effect of particle displacement is neither limited by the particles' size (at least down to 0.5µm and as large as 100µm) nor by surface type [5].

The phenomenology of light-driven diffusioosmotic flow (LDDO) can be used in a rather flexible way: colloids can be gathered or dispersed and bio-compatibility extends the range of colloid types also to living microorganisms such as soil bacterium *Pseudomonas putida* [3]. We show that DO flow can be considered a versatile method to set hydrodynamic conditions along the sample for investigating the motility of living cells. Further advantages of employing LDDO are the flexibility of flow generation in a reversible way and with spatiotemporal control, without the need to either change the channel geometry by loading a different device, or the periphery of pumps and connectors [4, 6].

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INVITED LECTURES

I-01 Metal/bimetallic nanoparticles for advanced radiation therapy

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Abstract: Gold nanoparticles are of great interest in advanced radiotherapy where these nanoparticles are often used to enhance radiosensitivity. It has been demonstrated by experiments in our lab that interfacial water plays a central role in the production of OH radicals when irradiating solvated gold nanoparticles. Our group has experience simulating these systems using classical potentials [1,2,3]. However, these methods do not predict well the interaction energy between gold nanoparticles and water molecules. Due to the size of the systems and the timescale, direct first principle molecular dynamics simulations of these systems are prohibitively expensive, hence we employ in this work different machine learning strategies to tackle the problem:

- i) the delta-machine learning within the framework of Density Functional based Tight Binding (DFTB) model.
- ii) the Chebyshev Interaction Model for Efficient Simulation (ChIMES), a physics-informed machine learning interatomic potential (ML-IAP)[4,5]
- iii) and the deep neural network ML-IAP of DeepMD model.[6]

The main advantage of these machine learning potentials is that their cost is that of classical potentials but their accuracy is comparable to quantum level calculations.

In this work, we will present the characterization of the interaction energy and structural, dynamical and vibrational properties of the water surrounded gold nanoparticle using these machine learning methods. [7]

A perspective of using these machine learning methods for studying the structure of bismuth-platinum nanoparticles is also presented. [8]

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Keywords: machine learning interatomic potentials, metal nanoparticles, bimetallic nanoparticles

I-02 Atomistically deciphering functional activation processes of proteins with hybrid molecular simulations

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Abstract: Activation processes of protein functions are often fulfilled by dynamic and global molecular conformational changes of complex protein systems which correlate with local molecular events at chemically active sites. Hence the multi-scale functional coupling of local chemical events with protein global molecular dynamics needs to be revealed for understanding of molecular nature of protein functions.

In this talk, I will present our recent studies on activation processes of photo-sensitive ion transporters and bioluminescent proteins by a hybrid quantum mechanical/molecular mechanical (QM/MM) free energy geometry optimization technique, which allows one to optimize electronic wave function and molecular geometry of the chemically active sites at the ab initio quantum chemistry level of theory on a free energy surface constructed with statistically extensive conformational ensemble of the protein environment obtained by long-time MD simulations [1]. Using this method, we succeeded in theoretically predicting photo-activated structural changes of a photo-sensitive cation membrane channel, C1C2 channelrhodopsin, which remarkably differ from previously known conformational changes in other homologous proteins [2] and were verified by a recent time resolved serial femtosecond X-ray crystallography (TR-SFX) measurement [3].

Recently, we simulated photo-activation processes of a photo-sensitive anion membrane transporter, GtACR1, and revealed significant conformational changes of the channels. We first refined molecular conformations of the chemically complex chromophore in the protein by the hybrid QM/MM free energy optimization technique. We observed a spontaneous binding of a chloride anion to the channel in the simulation. We then examined protonation states of carboxy groups in the channel which strongly affect transport properties of ions. Through excitation energy calculations of various mutants, we determined the protonation states which are consistent with experimental evidence. We also succeeded in modeling a photo-activated channel opening structure by the hybrid QM/MM free energy optimization with a long-time MD simulation. Free energy profiles of the ion transport in the channel opening state were obtained by umbrella sampling MD simulations, revealing atomistic dynamics and energetics of the ion transport process.

We also simulated activation processes of a bioluminescent enzymatic reaction of aequorin triggered by binding of Ca^{2+} ions. In collaboration with a TR-SFX experiment, we revealed large protein conformational changes upon Ca^{2+} binding that activate an enzymatic reaction to form a pivotal intermediate state of the bioluminescent reaction.

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Keywords: Hybrid QM/MM free energy optimization, ion channels, photo-receptor proteins, bioluminescent proteins, enzymatic reactions.

I-03 Nanomedicine: using nanobubbles and ultrasound for enhancing drug delivery

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Abstract: Nanobubbles are gas-filled particles with diameters ranging from ~ 100 to 500 nm. When excited by ultrasound, these bubbles can undergo stable oscillation or collapse, phenomena collectively known as cavitation. Stable cavitation generates microstreaming in the liquid, while collapse results in high-speed microjetting or shockwaves. These hydrodynamic effects have been employed for medical applications in both imaging and therapy, such as targeted cancer treatment and intracellular drug delivery. Our research aims to gain insights into bubble dynamics and cellular responses at the submicron scale, where conventional experimental techniques are limited in accuracy. In this talk, I will present our recent results on the development and applications of molecular dynamics simulation methods to study bubble dynamics in both stable and collapse regimes, as well as the mechanisms of cellular responses on nano-to micro-spatiotemporal scales.

Keywords: *nanobubbles, ultrasound, molecular dynamics simulation, drug delivery, cancer*

I-04 High-speed atomic force microscopy studies on the structural dynamics of ion channels at the single molecule level

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Abstract: High-speed atomic force microscopy (HS-AFM) is the powerful tool for observing nanoscale structural dynamics of biomolecules in aqueous solutions. In this study, we utilized HS-AFM to analyze the single-molecule dynamics of 1) the temperature and capsaicin receptor TRPV1 and 2) the voltage-gated Na⁺ channel (Na_v).

1) Previous theoretical studies suggested that changes in the molecular heat capacity during the gating of TRPV1 are crucial for temperature-sensitive gating. Since heat capacity is closely related to structural fluctuations, we analyzed the structural fluctuations of TRPV1 channels in reconstituted membranes using HS-AFM. It was revealed that the structural fluctuations of TRPV1 channels increased and decreased in the presence of agonists and antagonists compared to the unbound state, indicating the importance of structural fluctuations in gating of the TRPV1. ¹

2) Na_v consists of a pore domain (PD) and a voltage-sensor domain (VSD). Previous structural analyses suggested that the VSD is always closely associated with the PD. However, HS-AFM observations of Na_vAb reconstituted in lipid membranes, with different voltage dependence, showed that in the activated state where the gate is open, the VSD was closely associated with the PD. In the resting state, the VSD dissociated from the PD, and the dissociated VSDs dimerized and cross-linked between the channels. Computational analysis suggested that this dimerization is feasible at realistic channel densities at the node of Ranvier and may explain the positive cooperativity observed during the action potential generation. ²

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Keywords: *Ion channel, Voltage-gated channel, TRP channel, High-speed atomic force microscope, Structural dynamics*

I-05 Fabrication of Silk Protein to Hybrid Nanocarriers for Cancer Therapy

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Abstract: This presentation focuses on our recent results in the establishment of multifunctional silk nanocarriers in combination with noble metals for delivery, imaging and targeting in cancer treatment, prepared by a facile co-precipitation method. The synthetic approach is mainly carried out in mild conditions with minimizing residues in the final product. Co-precipitation method showed its potential as one of the most straightforward methods to incorporate inorganic and organic materials into a hybrid system with controllability of the resulting structure and characteristics. The obtained silk NPs are expected to advance the drug nanocarriers to a multifunctional system with tunable drug release and designable targeting. The research also provides a NP library with diverse structures and properties, which can be used to manipulate the drug delivery performance.

Keywords: *silk protein, noble metal, drug delivery, cancer therapy*

I-06 Interactive flexible receptor docking using DockIT

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Abstract: DockIT is an interactive docking tool that enables the user to dock a rigid ligand to a flexible receptor molecule. The conformational change in the receptor due to its interaction with the ligand is modelled using the method of linear response. This is achieved by first performing an explicit-solvent molecular dynamics simulation of the receptor and then performing an eigenvector decomposition of the covariance matrix of atomic displacements. This approach enables us to evaluate the conformational response in real time by: (1) exploiting a feature of protein dynamics whereby most fluctuation occurs within a relatively small subspace; (2) exploiting the power of the modern GPU to achieve maximum efficiency both in memory and computation time [1]. DockIT also has other useful features such as real time molecular surface rendering, which presents a particular challenge in a docking tool that incorporates molecular flexibility. It also can be used in Virtual Reality using a headset and hand-held controllers. This enables particularly intuitive control as movement of the left hand is tied to the receptor and movement of the right hand is tied to the ligand [2].

The talk will introduce DockIT, describe some latest developments, and show results we have obtained with the cancer target protein, histone deacetylase 6, in interaction with the drug molecule belinostat.

DockIT is free for non-commercial use and can be downloaded from <https://dockit.uk>.

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Keywords: *protein conformational change, molecular VR, molecular binding, drug-receptor interaction, HDAC6*

I-07 Nanomaterials in biomedical applications: convergence in fighting against bacterial and virus infections

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Abstract: Bacterial and viral infections are common diseases that people can easily get in daily life, however, these diseases can threaten human health if appropriate treatment is not available. With the development of nanotechnology, more nanomaterials have been used to design novel approaches for treatment of infectious diseases, namely liposomes, polymeric nanoparticles, dendrimers, inorganic nanoparticles, and nanoparticles of natural compounds. The unique physiochemical properties and multivalent nature of nanomaterials provides several therapeutic benefits, such as enhanced pharmacokinetic profile, improved drug solubility, prolonged systemic circulation, decreased toxicity, controllable drug concentration, less amount of dose required, and targeted drug therapy. In this report, we highlight three different types of nanomaterials developed in our laboratory, with their antibacterial activity (against *E. coli* and MRSA) and their antiviral activity (against rotavirus), including:

1. Berberine nanoparticles (BBR NPs) prepared by antisolvent precipitation which can significantly enhance the solubility of BBR. Interestingly, due to the nano-sized efficiency, BBR NPs could completely kill MRSA and *E. coli*, while pure BBR only showed inhibitory activity. Additionally, BBR NPs exhibited antiviral activity against rotavirus (RV) and protecting MA-104 cells from RV invasion, keeping 85% of healthy cells up to 144 h.
2. Gold nanoparticles functionalized with curcumin (GNPs@Cur) showed higher antibacterial activity against MRSA and *E. coli* under laser irradiation in comparison with GNPs and Cur alone, because the plasmonic effect of GNPs released heat and Cur, causing synergic effect that increase the antibacterial activity. Both GNPs and GNPs@Cur could preserve MA-104 cells from RV invasion, remaining more than 60% of the viability of RV-infected cells up to 144 h.
3. BBR NPs-loaded polylactic acid (BBR NPs/PLA) nanofibers could sustain release of 75 wt% of the loaded BBR during the first 24 hours and consequently boosted the antibacterial effectiveness. In case of Cur-loaded PLA nanofibers (Cur/PLA), 50 wt% of Cur was released after 24 hours. Both BBR NPs/PLA and Cur/PLA nanofibers did not exhibit cytotoxic activity. Particularly, Cur/PLA nanofibers could enhance the rate of wound closure *in vivo* in a mouse model.

Keywords: *nanomaterials, nanoparticles, nanofibers, antibacterial activity, antiviral activity, natural compounds*

I-08 Ions Permeation through the Stators of Bacterial Flagellar Motors

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Abstract: Bacterial flagellar motors are among the biomolecular motors responding to the chemotaxis and environmental stimuli. Recently, several structures of the bacterial flagellar motors' stators have been solved by the advance of cryo-EM in 5:2 ratio of the MotA:MotB complexes. We will present our recent data on examining how the stators trigger by the ions flow using molecular dynamics simulations. We found there are unique pathways for the ion permeation through the open channel of MotA/B. In addition, we found the ion type-dependence (sodium, potassium, hydronium) of the free energy difference upon permeation. The MotA/B exhibits a kicking motion during the first ion permeation through the channels.

Keywords: *Flagellar motor, Molecular dynamics simulations*

I-09 Development of Regulable and Targeted Photochemical Internalization Therapy to combat borderline resectable and unresectable locally advanced pancreatic cancer

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Abstract: Pancreatic cancer, the fourth leading cause of cancer-related deaths, is rarely detected early due to nonspecific symptoms, leaving only 15%-20% of patients for potentially curative surgical resection at diagnosis. The rest evolves into locally advanced and unresectable pancreatic cancer (LAPC) due to invasion of adjacent structures. For these cases, chemotherapy and radiotherapy are the main treatments, but their common resistance often leads to poor outcomes, with a 5-year overall survival rate for locally advanced unresectable disease staying below 5%. Researchers at Indiana University Hospital have explored photodynamic therapy (PDT), which has shown promise in phase 1 clinical trials for inducing tumor necrosis and occasionally enabling surgical downstaging. However, the current use of photosensitizers in PDT lacks precise control and selectivity, necessitating high doses and often requiring combination with chemotherapy, which poses risks to healthy cells and may not effectively prevent drug resistance. Thus, it is necessary to develop an approach that not only leverages the therapeutic benefits of PDT in treating LAPC but also includes a tunable and targeted strategy to specifically address drug resistance factors, thereby more effectively combating LAPC. This leads to the concept of a targeted and tunable Photochemical Internalization (PCI).

In pancreatic cancer, the presence of CD133⁺ cancer stem cells (CSCs) strongly associate with drug resistance and oncogenic transformation. Research led by Heeschen's group has demonstrated that the CD133⁺ CSCs subpopulation is detectable and exclusively responsible for tumor metastasis across all examined human pancreatic cancer tumors. Interestingly, CD133 expression in healthy pancreatic tissues is very rare, making it a prime target to combat drug resistance and relapse in pancreatic cancer, as evidenced by clinical trial NCT02541370. Indeed, aptamers, known as advanced chemical antibodies, have been proven significant in therapy by the FDA's approval of the first drug in 2004 and another in 2023. Aptamers efficiently infiltrate cells through aptamer-mediated endocytosis, aligning well with Photochemical Internalization (PCI) strategies. They can also be easily modified to conjugate with other target drugs for combined treatments. Thus, we have selected the CD133 aptamer to target the CD133⁺ subpopulation of cells.

Separately, we have developed an aptamer that regulates the photosensitizer, [Ru(bpy)₃]²⁺, transforms it into a photo-switchable photosensitizer with tunable 1O₂ production capabilities. Moreover, the regulation leads to a four-fold extension of its photo-excited state, integrating in enhance quantum yield to enhance activities, lead to reduced concentration for treatment.

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Keywords: *Unresectable Locally Advanced Pancreatic Cancer , drug resistance, CD133 aptamer, tunable $[Ru(bpy)_3]^{2+}$, targeted and tunable photochemical internalization therapy, generation of singlet oxygen*

I-10 Integrative Analysis of APE1-Mediated MicroRNA Processing and Protein-Protein Interactions in Cancer Prognosis

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Abstract: Apurinic/apyrimidinic endonuclease 1 (APE1) is a multifunctional enzyme that plays a crucial role in DNA base excision repair (BER) and transcriptional regulation, which are pivotal in maintaining genomic stability and modulating tumor progression. Recent studies have uncovered novel post-transcriptional roles of APE1, particularly in the regulation of microRNA (miRNA) processing, exosome-mediated RNA sorting, and interactions within protein-protein networks that contribute to chemoresistance and cancer progression. In this presentation, we delve into the integrative computational analysis and data-driven exploration of APE1's role in cancer. By employing advanced transcriptomic and proteomic analyses, we identified a significant APE1-dependent regulatory mechanism of miRNA loading into extracellular vesicles (EVs), revealing specific RNA sequence motifs enriched in these APE1-dependent miRNAs. Moreover, through systematic bioinformatics analysis of proteomics data from a well-characterized HeLa cell model, we constructed the APE1 protein-protein interaction (PPI) network, identifying key interactors that correlate with poor prognosis across multiple cancer datasets. Our findings indicate that APE1 serves as a central hub in cancer-associated molecular networks, modulating both RNA and protein metabolism in a manner that promotes tumor aggressiveness and chemoresistance. These insights provide a comprehensive view of APE1's dual role in DNA repair and RNA processing, suggesting potential biomarkers for cancer prognosis and therapeutic targets. Further studies will be necessary to elucidate the functional implications of these interactions in cancer biology.

Keywords: APE1, microRNA, protein-protein interactions, cancer prognosis, transcriptomics, proteomics, bioinformatics.

I-11 Design and Modification of Porous Nanomaterials as Drug Carriers in Cancer Therapy

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Abstract: Significant advancements in pharmaceutical research targeting cancer therapies have deepened our comprehension of drug physicochemical properties and cellular absorption mechanisms, leading to more effective treatment strategies. Despite these improvements, current therapies are hindered by challenges such as inefficient drug delivery, necessitating higher dosages, rapid absorption, suboptimal pharmacokinetics, and increased risks of adverse side effects. To address these issues, nanoparticle-based drug carriers have emerged as a promising solution. These carriers—comprising nano-sized particles integrated with active agents—offer critical advantages, including small size, high drug-loading capacity, tunable surface characteristics, controlled drug release kinetics, improved pharmacokinetics, and enhanced biocompatibility. Among the diverse nanomaterials explored for biomedical applications, porous silica nanoparticles and nano metal-organic frameworks (nano MOFs) have shown particular promise. Our research group has successfully developed biodegradable porous organosilica and MOF-based nanoparticles, ranging from 50 to 200 nm in size, with abundant pores. Surface modifications have been optimized to improve tumor targeting and cellular uptake. The porous architecture of these nanoparticles facilitates substantial drug loading, including anti-cancer agents such as doxorubicin, cordycepin, curcumin, and paclitaxel. These nanoparticles enable precise delivery to cancer cells, enhancing therapeutic efficacy. Furthermore, incorporating biodegradable bonds—such as disulfide and tetrasulfide linkages—within the nanoparticle framework enables degradation in the body's reducing environment. Upon degradation, these nanoparticles break down to sizes below 10 nm, allowing for efficient renal clearance. This innovative approach offers a promising pathway to cancer treatment with enhanced drug delivery efficiency and minimized side effects.

Keywords: *porous nanosilica, metal-organic frameworks, anticancer, drug delivery, biodegradable*

I-12 Ultra-high-speed atomic force microscopy for visualization of faster biomolecular dynamics

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Abstract: High-speed atomic force microscopy (HS-AFM) is a powerful technique, which allows us to visualize biological macromolecules at ~100 ms temporal and ~ 2 nm spatial resolutions, without any chemical labelling. Since its establishment around 2008,¹ HS-AFM has been widely used to visualize varieties of biological samples ranging from purified proteins to live-cells; however technical advances are still progressing to broaden potentials of HS-AFM for wider applications.² For instance, temporal resolution of HS-AFM has been recently improved. Unexpectedly, improving response time of instrumental components was not the most effective approach; instead development of a new scanning scheme called only trace imaging (OTI) method greatly contributed to speeding up HS-AFM.³ The OTI method realizes tremendous reduction of the tip-sample interaction, pushing the imaging speed to video rate (30 ms/frame) for visualizations of fragile protein assemblies such as actin filaments and microtubules.³

In this work, we tried to further speeding up HS-AFM. The bottleneck of imaging speed of HS-AFM is a resonant frequency of cantilever.² To increase the resonant frequency, one needs to downsize cantilevers. However, further miniaturized cantilevers have to be stiff, which increases the tapping forces, unsuited for imaging fragile biological samples. To achieve higher resonant frequency without any mechanical modifications of cantilever, we developed a mass (M) - control method, in which we modulate an excitation signal of cantilever using analog electric circuits. The second derivative of deflection signal with gain optimization is appended to the excitation signal. This modulation works as decreasing the cantilever mass, thus increasing the resonant frequency. We achieved two-times improvement of the resonant frequency by the M-control method. In addition to the M-control and OTI methods, we updated components of HS-AFM including a scanner, amplitude detector, and PID controller, and succeeded in HS-AFM imaging of actin filaments and microtubules at 10-ms temporal resolution.

To demonstrate the power of our state-of-the-art HS-AFM, we performed HS-AFM imaging of rotor-less F₁-ATPase ($\alpha_3\beta_3$ complex). We have previously shown that in the presence of ATP, the closed and open conformations cyclically propagate over the three β subunits in the counterclockwise direction when viewed from the C-terminal side.⁴ Here, we challenge to further resolve the conformational states. HS-AFM imaging beyond video rate shows previously undetected intermediate structures. In addition, we performed measurements with various ATP concentrations, ATP γ S, and inorganic phosphate. In the presentation, we will discuss the chemomechanical coupling scheme of F₁-ATPase based on the β subunits' conformations.

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Keywords: HS-AFM, techniques for HS-AFM, single-molecular imaging, F₁-ATPase, Chemomechanical coupling

I-13 Viscoelastic Characterization of Soft Materials Using Nanorheological Atomic Force Microscopy

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Abstract: Atomic Force Microscopy (AFM) has been widely used as a powerful and versatile technique for characterizing nanomechanical properties of numerous soft materials ranging from gels, biological cells to polymer composites, which generally exhibit heterogeneous structures at nanoscale level. However, because of the complex mechanical and dynamic responses of nanoscale structures, it is well recognized that mechanical properties of soft materials are far to be completely quantified using conventional AFM methods in combination with an existing elastic contact model.^{1,2} For such materials, the relationship between stress and strain can be significantly changed over time, which can be attributed to their viscoelastic nature, *i.e.*, combining both solid- and liquid-like responses. In the past decade, several special AFM-based approaches, such as nanorheological AFM and nanoscale dynamic mechanical analysis, have been introduced for characterizing local viscoelastic properties of nanostructures in soft materials at rheologically relevant frequencies from $\sim 10^{-1}$ to $\sim 10^3$ Hz.¹⁻³ However, in most of these approaches, a sample driving system is normally employed for controlling the system oscillation, thus they are mainly suitable for viscoelastic measurements of soft materials in thin films and at room temperature. Recently, a new design in which a piezo based probe-driving system is placed near the base of an AFM probe has been developed, enabling the measurement of viscoelastic properties of materials in complex geometry and over a broad temperature range.^{3,4} In this talk, I will briefly introduce the working principle of nanorheological AFM method and discuss some recent applications of this method for characterizing viscoelastic responses of various soft materials.

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Keywords: *Nanorheological AFM, Soft Materials, Polymers, Viscoelasticity, Nanomechanics,*

I-14 Toward Quantitative Imaging of Cellular Metabolites with Fluorescence Lifetime Biosensors

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Abstract: Fluorescent protein-based biosensors are powerful tools for visualizing the dynamics of cellular metabolites in real time under a fluorescence microscope. These biosensors are genetically encoded, allowing expression in living cells or animals through transfection or infection methods. Typically, genetically encoded fluorescent protein-based biosensors function by altering their fluorescence intensity upon target detection, leading to the so-called intensity-based biosensors. However, the fluorescence intensity readout is susceptible to various factors, such as biosensor concentration, excitation power, photobleaching, pH, and focus drift. These limitations render intensity-based biosensors more suited for qualitative assessments rather than quantitative imaging. To overcome these challenges, fluorescence lifetime-based biosensors present a promising alternative. Unlike intensity-based measurements, fluorescence lifetime is inherently independent of biosensor concentration, excitation intensity, and other factors that typically affect intensity-based biosensors. This feature enables more robust and quantitative imaging of cellular metabolites using fluorescence lifetime imaging microscopy (FLIM). In this presentation, I will introduce our progress in the development and application of fluorescence lifetime biosensors for the precise and quantitative imaging of key metabolites such as calcium ions (Ca^{2+}), adenosine triphosphate (ATP), guanosine triphosphate (GTP) and the ratio of GTP to guanosine diphosphate (GDP). Our approach offer an advancement in the ability to quantitatively assess cellular metabolism, with broad implications for understanding cellular functions and disease mechanisms.

Keywords: *genetically encoded fluorescence lifetime biosensors, fluorescence lifetime imaging microscopy (FLIM), calcium, ATP, GTP, GTP/GDP ratio.*

I-15 The Effect of Shear Stress on Fibronectin Fibrillogenesis: Morphological Properties and Cellular Implications

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Abstract: Fibronectin (FN), a critical extracellular matrix protein, plays a pivotal role in cell adhesion, migration, and proliferation, which are fundamental to various biological processes, including vascular biology. Under different shear stress conditions, FN undergoes fibrillogenesis, resulting in the formation of fibrillar fibronectin (FFN), an active form of FN that supports diverse cellular activities. This talk explores the relationship between shear stress, FFN morphology, and cellular behavior, with a focus on endothelial cells, fibroblasts, and platelets.

Our studies reveal that FN organizes into distinct structural matrices under shear stress, ranging from nodular formations to complex fibrillar networks. Notably, FFN formed at specific shear rates exhibits unique morphologies that significantly influence cellular responses. For example, under a low shear rate of 0.55 s^{-1} , the resulting FFN supports bovine aortic endothelial cell (BAEC) adhesion, spreading, and proliferation more effectively than native FN and other FFN structures. Similarly, fibroblast behavior is closely linked to FFN morphology, with larger, rough-surfaced FFNs enhancing adhesion and spreading but reducing cell migration compared to smaller, smoother FFNs. Furthermore, under high shear stress (4000 s^{-1}), rapid FFN formation leads to a fibrillar matrix that supports robust fibroblast adhesion and stretching, highlighting the morphology-dependent biological activity of FFN.

These findings underscore the importance of FFN morphology in regulating cellular functions and suggest that controlling shear conditions to manipulate FN fibrillogenesis could have significant implications for vascular biology, tissue engineering, and regenerative medicine. Further research is needed to elucidate the underlying mechanisms of FN's shear-induced fibrillogenesis.

I-16 Applying AI Algorithms to Recognize Important Genes in Cancer Tumors

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Abstract: Cancer is one of the deadliest diseases of recent years. It is a genetic disease driven primarily by alterations in genes that control cell growth, repair, and death. This alteration is typically caused by changes or mutations in the deoxyribonucleic acid (DNA) of cells, which is their behavior in ways that promote proliferation and survival. Genetics is a key factor in the development of cancer. An understanding of the genetic basis of cancer has significant implications for the diagnosis, treatment, and prevention of this disease. In light of these considerations, artificial intelligence (AI) algorithms have been employed to categorize cancers and identify genes that may be shared among them. *Tumor RNA* samples were collected from patients with diverse cancer types. This dataset constitutes part of the *RNA-Seq (HiSeq) PANCAN**. The dataset comprises 801 patient samples of tumor types including *BRCA* (breast invasive carcinoma), *COAD* (colon adenocarcinoma), *KIRC* (kidney renal clear cell carcinoma), *LUAD* (lung adenocarcinoma), and *PRAD* (prostate adenocarcinoma). Each patient sample contains 20,531 variables (characteristics) that RNA-Seq gene expression levels measured by the *Illumina HiSeq* platform.

Since the size of the features too much it cannot be processed by the machine learning algorithms and makes the training processed to be hanged, so we have applied *SelectKBest* ($k=500$) algorithm from the *scikit-learn* toolbox, after the feature selection we have had top 500 features.

In conclusion, this type of research will facilitate the reduction of the complexity of the genetic problems that cause cancer, thereby facilitating their resolution. It is reasonable to assume that more effective and targeted strategies will be developed in the future to combat this difficult group of diseases.

* hosted at <https://www.synapse.org/#!/Synapse:syn4301332>

Keywords: *Cancers, Genes, AI, Features, Big Data*

I-17 Advances in the development of screen- printed carbon electrode-based electrochemical biosensors for food safety monitoring

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Abstract: Biosensors have always been an attractive topic for scientists around the world, especially in the biomedical field such as on-site health care, control of infectious diseases, detection of cancer makers, and food safety monitoring. The development of biosensors is still mainly focused on improving selectivity, sensitivity, stability, size, integrating features and reducing production costs. In fact, there are not so many types of biosensors commercialized in the market. Among them, electrochemical biosensors still show to be the most promising. Several trademarks of electrochemical sensors have been commercially available for quick determination of blood sugar levels, which people can buy and use at home easily without requiring complicated operations or sending samples to analytical laboratories. Furthermore, many types of screen-printed electrodes have been commercialized, they are made from different materials such as carbon, platinum, gold for the different purpose of detecting substances through electrochemical methods. However, for biological or small molecules, the working electrode area needs to be functionalized or modified with suitable materials to enhance the sensitivity and selectivity. This presentation introduce the most recent outstanding results of our research group related to the development of electrochemical biosensors based on screen-printed electrodes modified with various nanomaterials for the quick detection of toxic chemicals remaining in food samples as well as agricultural products. Some of these results have been published in peer-reviewed international journals.

Keywords: *Electrochemical sensors; screen-printed electrodes; nanomaterials; food safety*

I-18 A combined optical and atomic force microscope for materials and life sciences research

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Abstract: In this talk, we demonstrated the capabilities of a hybrid optical-atomic force microscope, which has many applications in the fields of materials science and life sciences research. When operating in individual mode, time-lapse imaging, often referred to as live cell imaging, can be utilized to see where a specific organelle or protein of interest is located in a cell or tissue as well as its molecular activity. Membrane fibers and bacterial biofilms can also be observed under an optical microscope by labeling them with a fluorescent dye to determine their shape and size. In contrast to optical microscopy, atomic force microscopy was originally developed to image the morphology of a material surface, using a nano probe to physically scan the surface. Its current capacity, though, far exceeds what was originally intended. It can be used to measure the mechanical, electrical, and magnetic properties of the surface of both living and non-living samples in addition to mapping the surface morphology. In the field of mechanobiology, it has also been utilized recently to measure the biophysical characteristics of cells and tissues in liquid. In a hybrid mode, an atomic force microscope can examine surface characteristics like morphology, adhesion, and stiffness, while an optical microscope provides a clear visualization of the area we are measuring and can reveal the localization or activity of a particular protein of interest through fluorescence emission. We can therefore correlate the molecular activity of the living samples with their biophysical characteristics thanks to this combined setup. During my presentation, I will provide several examples of how this hybrid setup is used extensively in materials and biological sciences research. The study areas include biosensors, gas sensors, photovoltaic solar cells, bacterial biofilms, mechanobiology, nano/biomaterials, metal alloys and their interactions with living cells.

Keywords: *Optical microscope, atomic force microscope, live cell imaging, mechanobiology, biosensors*

I-19 Integrative modeling approaches to characterize dynamics of biomolecules: application to Atomic Force Microscopy

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Abstract: Combining computational molecular mechanics simulations with experimental data has proven useful for elucidating the structure and dynamics of biomolecules. This integrative modeling strategy, which merges theoretical simulations with real-world observations, has been particularly effective in characterizing conformational states identified in 2D cryo-electron microscopy data. Similarly, high-speed atomic force microscopy (AFM) captures biomolecular motions in 2D. Such motions are in real-time and in solutions, presenting a unique opportunity to explore biomolecular function. To capitalize on this, we have developed methods aimed at extracting 3D information from AFM images. Our approach involves representing biomolecules through a coarse-grained model, and we employ various sampling methods to generate candidate 3D models. These models are then evaluated based on their correlation with a given target AFM image. This AFM-based hybrid modeling method could be a valuable tool for extracting 3D information from high-speed AFM experimental data. Even with limited experimental resolution, this approach could aid in annotating distinct conformational states crucial to biomolecular functions.

I-20 Computational simulations supporting observations by atomic force microscopy

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Abstract: Computational simulations are essential tools for understanding the underlying mechanism of phenomena observed by atomic force microscopy (AFM) as well as its principles of imaging. Our institute has developed two cutting-edge AFM techniques: three-dimensional AFM (3D-AFM) and high-speed AFM (HS-AFM). 3D-AFM was originally developed to visualize 3D distribution of solvent molecules on a substrate. It was extended to investigate the 3D structure of soft biomolecules in cells, but the imaging mechanism of such flexible molecules is yet to be clarified. Meanwhile, HS-AFM can visualize dynamics of molecules at video rates. Many movies have been taken especially for biomolecules, but computational analyses and/or simulations are necessary to derive the molecular mechanisms of biological functions from the movies. In this presentation, I will talk about how computational simulations are helpful to understand AFM observations. The first part will focus on 3D-AFM measurements of flexible fibers such as cytoskeleton and carbon nanotube fibers. Comparisons with the polymer simulation revealed that the penetrating probe sometimes pushes fibers away and drags them down, resulting in characteristic shapes appearing in the images. In the latter part, I will present an unprecedented mechanism of AMPA receptor clustering observed by HS-AFM, in which the N-terminal domains split and exchange with the adjacent receptors. The lifetimes of split states were estimated by a theoretical calculation, and the free energy profile toward the exchanged states was calculated by molecular dynamics simulations using umbrella sampling.

Keywords: *atomic force microscopy, polymer simulation, molecular dynamics, umbrella sampling*

I-21 Molecular-Scale Observation of Porphyrin Derivatives Self-Assembled at Solid-Electrolyte Interfaces

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Abstract: Porphyrins, as planar macrocyclic molecules, extensively exist in plants and animals and play an important role in life activities. Naturally, porphyrins exist in the form of nanostructures/aggregations through molecular self-assembly. Observation at the molecular scale these self-assembling processes will provide more comprehensive insights into their key roles in such alive phenomena. Herein, the self-assembly of aqueous soluble porphyrin derivatives on atomically flat surfaces will be investigated systematically upon combined ex-situ and in-situ approaches including cyclic voltammetry (CV), atomic force microscopy (AFM) and electrochemical/scanning tunneling microscopy (EC-STM). The obtained results open such pathways to the design and fabrication of porphyrin-based nano-scale devices towards electronic and sensing applications.

Keywords: *Porphyrins, self-assembly, molecular scale, AFM, EC-STM*

I-22 CM-AFM in biological applications: A correlation of the mechanical properties to the cell membrane composition

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Abstract: The fatty acid membrane constituents play an essential role in mechanical and dynamical features of the cell membrane¹. Vertical and lateral interactions within the membranes change rapidly as new constituents such as the unsaturated fatty acids (*e.g.*, omega-3 and omega-6) are added and/or protein incorporations (*e.g.*, transmembrane protein) are modified. However, it's still challenging to measure the local vertical and lateral interactions of the native cells in one measurement. In this study, we developed a new approach based on the circular mode-AFM² (IMMM, France) to measure directly the mechanical properties (*e.g.*, penetration force and membrane viscosity, young modulus) of the native red blood cells. In parallel, the unsaturated and saturated fatty acid membrane composition was determined by using the gas phase chromatography. Eventually, the relationship between the content of fatty acids (saturated and unsaturated) within RBC membrane and its mechanical properties has been established. This research demonstrates the power of the CM-AFM in studying the physiological cell mechanisms for diagnostic and therapies.

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I-23 Low-cost SmartTrap: An Innovative Pest Observation System Harnessing TinyML and Edge Computing

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Abstract: The threat posed by fruit flies to fruit crops necessitates the development of innovative solutions to protect yields. This study introduces a state-of-the-art approach for safeguarding fruit crops from fruit fly infestations and minimizing excessive pesticide use by employing Tiny Machine Learning on edge devices to monitor fruit fly populations, thereby optimizing both cost and energy efficiency. To this end, we developed an intelligent insect trap system (Low-cost SmartTrap) featuring advanced, high-performance functionalities. The system leverages an ESP-EYE microcontroller running a FOMO MobileNetV2 model, with a peak RAM usage of 2.4MB and an average inference time of 5.694 seconds per image. The device demonstrates high detection accuracy with a recall rate of 0.85 and an F1 score of 0.91 at an IoU threshold of 0.5. This solution not only provides accurate detection and counting but also delivers timely alerts to farmers regarding potential threats via a user dashboard system powered by AWS EC2 and Node-RED. Additionally, the trap operates fully autonomously, eliminating the need for human intervention through an automated sticky trap replacement mechanism driven by an ESP32 microcontroller. Furthermore, we developed a small object detection model based on SSD MobileNetV2 using TensorFlow Lite and TensorFlow Lite Micro, optimized for sustained performance and cost-effectiveness. The resulting TFLite model has an average RAM consumption of 4.6MB per image, facilitating straightforward and efficient deployment on edge devices like Raspberry Pi or Jetson Nano. This flexible and eco-friendly design optimizes resource use and reduces computational costs, showcasing its significant value in agricultural applications and other areas.

Keywords: *fruit fly, TinyML, AIoT, edge computing, FOMO, ESP32, EmbeddedML*

ORAL PRESENTATION

O-01 Developing pharmaceutical nano formulations of Chandamarutha chenduram to combat clinical bacterial resistance and assess its antibacterial efficacy

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Abstract: This study aimed to develop a pharmaceutical nano formulation containing Chandamarutha Chenduram and minerals (CMC-NPs) to treat antibiotic-resistant bacteria. This research involves evaluating the antibacterial efficacy, mechanism of action, and safety dosage of CMC-NPs at a cellular level. This investigation showed promising results. At a concentration of 10 µg, the CMC-NPs demonstrated significant antibacterial activity against drug-resistant bacteria. The drug resistance of clinical bacteria was evaluated using standard antibiotic discs (Himedia Mumbai Pvt). CMC-NPs exhibited zones of inhibition 20 mm against *K. pneumoniae* and *S. aureus*, respectively. Additionally, it showed an inhibition zone of 22 mm against *Enterococcus faecalis*. FE-SEM and TEM observations confirmed the morphological changes in bacterial cells treated with the isolated compounds. The cells appeared to shrink and the cell walls appeared to be damaged. EDAX analysis confirmed the presence of minerals in bacterial cells. This study represents a step toward the development of novel nano formulations for AMR treatment.

Keywords: *Chandamarutha Chenduram (CMC), nanoparticles (NPs), antibacterial activity, FE-SEM, HR-TEM, EDAX*

O-02 Integration of high-speed atomic force microscopy with *in silico* modeling for characterizing aptamers targeting METTL3 in cancer cells

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Abstract: Adenosine N6-methylation (m^6A) is the most common internal RNA modification and is mainly catalyzed by methyltransferase-like 3 and methyltransferase-like 14 (METTL3/14) complex. Accumulating evidence in recent years has revealed the roles of METTL3/14 complex in the progression of various cancer types. Therefore, to catalytically inhibit the METTL3/14 complex as an alternative therapeutic strategy, we identified two METTL3/14 inhibiting DNA aptamers (Apt-LR and Apt-9) by *in vitro* competitive selection method. Both aptamers showed potent inhibition potency of METTL3/14 catalytic activity (>95% inhibition) at a lower concentration of 12.5 nM using an *in vitro* assay. However, to develop the aptamer as a lead candidate for targeted drug designs in cancer, a deeper insight into the conformational dynamics and the search for the most atomistic stable aptamer-target complexes are prerequisites. For this purpose, we utilized high-speed atomic force microscopy (HS-AFM) and molecular docking simulation to directly visualize and analyze aptamer-target binding processes. The docking simulation between the X-ray crystal structure of the METTL3/14 complex and computationally generated 3D structures of aptamers revealed that both aptamers affect the METTL3-METTL14 interface interaction. In parallel, the dynamic interactions of the METTL3/14 complex with and without aptamers were visualized by HS-AFM, and the spatio-temporal analysis of captured images enabled us to characterize the binding interaction of aptamers and METTL3/14 complex at a single molecular level with the interpretation of molecular docking atomic models. Based on the positive evidence of aptamers, we further explored their potency to inhibit the cellular activity of METTL3 and to elicit anticancer effects on human cancer cell lines. In conclusion, this study provides insights into how aptamers bind to the METTL3/14 complex and further suggests their potential as therapeutic agents for cancer treatment.

Keywords: DNA-aptamer, METTL3/14, m^6A , HS-AFM, Molecular docking, Cancer

O-03 Green bio-fabricated silver nanoparticles from fungal endophyte induces anti-proliferative and apoptotic activities against breast cancer and suppresses *in ovo* neovascularization

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Abstract: Fungal endophytes are effective producers of bioactive compounds based on which in the current report, aqueous extract of fungal endophyte *Penicillium oxalicum* associated with the leaf of *Amoora rohituka* plant has been used for the green synthesis of silver nanoparticles (POAgNPs) and their anti-proliferative and apoptosis-inducing potential has been focused. A sharp UV–visible spectra at 420 nm, crystalline nature as per XRD analysis, functional groups demonstrating fungal biomolecules as detected through FTIR spectra, and spherical-shaped POAgNPs with an average size of 17 nm were revealed by AFM, TEM, and FESEM. The study revealed that mycogenic silver nanoparticles exhibit significant anti-proliferative activity through reduction of cell viability in breast cancer cells MDA-MB-231 and MCF-7 in a dose-dependent manner. Moreover, enhanced LDH release indicated a damaged plasma membrane and increased production of nitric oxide showing disruption of oxidative balance and apoptosis-mediated cell death. The synthesized green nanoparticles showed biocompatibility as evidenced through hemolysis assay. The anticancer potential of POAgNPs has been shown through inhibition of wound closure, apoptosis-specific modulations of nuclear morphology and differential gene expression related to apoptosis, tumor suppression and cell-cycle arrest. Moreover, an increased level of active form of Caspase-3 in treated breast cancer cells was also reported. Moreover, the anti-angiogenic activity of POAgNPs was also observed against *in ovo* model and acute toxicity study showed least toxic effects of POAgNPs in animal model. The study shows anti-breast cancer activity of fungal endophyte-derived silver nanoparticles and further exploration is intended to develop an underlying apoptosis-related signaling cascade and mechanistic pathway to explore nanodrugs in therapeutic applications.

Keywords: *Fungal endophytes, POAgNPs, Breast cancer, XRD, FESEM, Anti-angiogenic*

O-04 Effect of Glu78 on the transport of Cation-Protons across the cell membrane by *Ec-NhaA*

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Abstract: In both prokaryotic and eukaryotic cells, Na⁺/H⁺ antiporters help to exchange Na⁺ for H⁺ across the cytoplasmic membrane. They are necessary for the preservation of volume, pH, and Na⁺ homeostasis, all of which are essential for a variety of metabolic processes and cellular viability. These antiporters are therefore thought to be appealing therapeutic targets for humans. The prototype of the cation-proton antiporters (CPAs) family, which transports 2H⁺ and 1Na⁺ (or Li⁺) in opposing directions, is the 2Na⁺/H⁺ antiporter found in *Escherichia coli*, *Ec-NhaA*. The characteristic NhaA structural fold is produced by the crossing of two transmembrane segments (TMs) IV and XI in the middle of the membrane. This fold provides a delicate electrostatically balanced environment that is ideal for the binding of Na⁺/H⁺. Mutagenesis studies on *Ec-NhaA* have previously suggested that the Asp164, Asp163, and Asp133 residues are crucial components for Na⁺/Li⁺ binding and are predicted with significant role in function and structure. Nevertheless, the process and locations of the two protons' binding are still unclear and up for debate, even though they may be crucial for maintaining pH balance. In this work, we have examined the role of Glu78 in *Ec-NhaA*-mediated pH regulation within the cells. Despite the fact that we have produced a number of mutants, E78C has demonstrated a significant impact on NhaA stoichiometry and displayed comparable phenotype expression with WT. One lithium ion interaction with NhaA has been observed to cause the binding of about five protons, according to the ITC experiment. In comparison to WT *Ec-NhaA*, the phenotypic study on selective media revealed a considerable expression. This demonstrates the role that Glu78 plays in moving H⁺ across the membrane, as a single mutation by replacing the Glu with amino acid Cys at position 78 drastically changes the amount of H⁺. Moreover, this point mutation maintains the activity of the E78C variant of NhaA.

Keywords: *Ec-NhaA*, ion transport, amino acids, mutagenesis, protons

O-05 Antioxidant potential assessment of biosynthesized AgNPs and characterization of hepatoprotective phytoconstituents from *Vitis vinifera* extract using LC-MS/MS

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Abstract: Liver disorder is the 5th common cause of death worldwide. Oxidative stress and inflammation are the core mechanisms behind the cause of liver damage induced by drugs. *Vitis vinifera* (Black grapes) is widely cultivated for its potential pharmacological properties. Present research revealed the potent anti-oxidant and antibacterial activity of *Vitis vinifera* crude extract and its biosynthesized AgNPs against all tested strains. FTIR, SEM, and XRD analysis confirmed the stabilization of biosynthesized AgNPs with an average crystalline size (D) of 20.09 nm. Further, LC-MS/MS analysis extracted 38 phytoconstituents in the form of phenolics, flavonoids, and glycosides i.e. Resveratrol, trans- ϵ -Viniferin, Quercitin, Naringenin etc. These therapeutic phytoconstituents have potent hepatoprotective potential and pharmacokinetic importance. These findings suggested that *Vitis vinifera* crude extract as well as its biosynthesized AgNPs could be further investigated for *In vitro* and *In vivo* animal model. Moreover, these characteristic polyphenols should be isolated from *Vitis vinifera* fruit extract to carry out biosynthesis of AgNPs and used for the formulation of hepatoprotective drugs in pharmaceutical industry.

Keywords: Ag-nano particles; *Vitis vinifera*; hepatoprotective

O-06 Exploration and identification of the NPR1 gene mediated plant defense response mechanism in Chili against begomovirus Infection

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Abstract: Chili pepper productivity is severely affected by viral diseases in Indian subcontinent and for the diseases control in eco-friendly way, it is essential to understand the molecular mechanisms of viral resistance in chili pepper. NONEXPRESSOR OF PATHOGENESIS-RELATED GENES 1 (NPR1) genes are known to provide broad-spectrum resistance to various phytopathogens by activating the systemic acquired resistance (SAR) mechanism. Understanding NPR1 gene expression during begomovirus infection and its correlation with different biochemical and physiological parameters is crucial for improving chili pepper viral resistance. However, due to limited information on chili *CaNPR* genes and their role in biotic stress, their utilization in biotic stress-resistant genetic breeding is constrained. Genome mining identify 5 *CaNPR* genes in chili, using bioinformatics approaches. Promoter regions of *CaNPR* genes contained biotic stress-related cis-elements, signifying their involvement in biotic stress responses. Moreover, these gene promoters included components related to light, development, and hormone responsiveness, suggesting their roles in plant hormone responses and development. MicroRNAs played a vital role in regulating these five *CaNPR* genes, highlighting their significance in chili gene regulation. Inoculation with the cotton leaf curl Khokhran virus adversely affected chili plant growth, resulting in stunted development, fibrous roots, and visible virus symptoms. This also led to decreased chlorophyll and carotenoid levels but increased phenolic compounds, flavonoids, and antioxidant enzyme activity in virus-infected leaves. The q-rtPCR analysis of two local chili varieties, one susceptible (V1) and the other resistant (V2) to begomoviruses, indicated that *CaNPR1* likely provides extended resistance and plays a role in chili plant defense mechanisms, while the remaining genes are activated during the early stages of infection. These findings shed light on the function of chili's *CaNPR* in biotic stress responses and identify potential genes for biotic stress-resistant breeding. However, further research, including gene cloning and functional analysis, is needed to confirm these genes' roles in various physiological and biological processes. This in-silico analysis enhances our genome-wide understanding of chili *CaNPR* genes response during begomovirus infection.

Keywords: *NPR1, Geminivirus, Bigomovirus, chili pepper, Biotic stress, Virus titer, qPCR*

O-07 Isolation and screening of hydrocarbon degrading bacterial isolated from oil contaminated sites

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Abstract: Petroleum hydrocarbons are priority pollutants, which are recalcitrant in nature and are found to be involved in causing major environmental pollution of water and soil. Biotechnology can be used to assess the well-being of ecosystem, transform pollutants into benign substances, generate biodegradable materials from renewable sources and develop environmentally safe manufacturing and disposal processes. Environmental biotechnology employs the application of genetic engineering to improve efficiency and cost, which are key factors in the widespread exploitation of microorganisms to reduce the environmental burden of toxic substances in the future. The term bioremediation refers to the removal of these toxins from the environment using a microorganism to prevent environmental pollution. Petroleum and its products have harmful effects on the environment but its bioremediation is possible by the action of certain bacterial strains of the genus *Pseudomonas*, *Acinetobacter*, *Agrobacterium* and *Aeromonas*. In the present work, we have collected soil samples from various petroleum hydrocarbon contaminant sites and isolated the diverse species of bacteria. They were characterised and identified on the basis of staining and biochemical analysis like gram staining, IMVIC test, EMB agar test, urease production test, starch hydrolysis test etc. Identified strains of Gram-positive and negative bacteria, both were used to standardize the percentage degradation of petroleum. This analysis may assist in an understanding of microbial communities of pollutant sites and their response to the environment and pollutants. Further, by exploring the intricacies in the genetics of microbes, we can increase their ability to degrade pollutants.

Keyword: petroleum, hydrocarbon, bioremediation, microbes, pollutants

O-08 Single fluorescence-based FLIM indicator for observing changes in GTP/GDP ratio in cancer cells

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Abstract: Fluorescence imaging has revolutionized our understanding of biological systems, enabling the visualization of biomolecular structures and dynamics in complex systems. Genetically encoded fluorescent biosensors emerged as potential tools for monitoring biological events in living cells. Traditional fluorescence intensity-based biosensors detect their target analytes based on changes in their fluorescence intensity. However, these biosensors face challenges in quantitative analysis because they are dependent on expression level, excitation power, and photobleaching. On the other hand, fluorescence lifetime biosensors coupling with fluorescence lifetime imaging microscopy (FLIM) offer a more quantitative imaging approach. By measuring fluorescence lifetime rather than intensity, FLIM biosensors overcome the issues of changes in expression level, excitation power, and photobleaching, making them a robust and reliable measurement. The changes in the guanosine triphosphate/guanosine diphosphate (GTP/GDP) ratio are involved in various cellular activities. Activation of G-proteins via GDP/GTP exchange leads to interaction with downstream effectors and signaling pathway activation, while GTP hydrolysis to GDP results in G-protein inactivation. Therefore, changes in the GTP/GDP ratio would indicate the rate of G-protein activation, influencing various biological processes. Here, we report a genetically encoded fluorescence lifetime biosensor, termed FLIM-GTP/GDP, for precise quantitative imaging of the intracellular GTP/GDP ratio. We constructed FLIM-GTP/GDP by fusing a circularly permuted enhanced yellow fluorescent protein (cpEYFP) with a GTP/GDP-binding domain through peptide linkers. We randomized the linkers and screened for the best candidate using a 96-well plate screening method. Through screening more than 3000 mutants, we found the best one with a change of 0.7 ns between GTP-bound and GDP-bound states. FLIM-GTP/GDP showed a response to the GTP/GDP ratio within a physiological range of 0.1 to 10, regardless of changes in the total concentrations of GTP and GDP. We validated the working performance of FLIM-GTP/GDP in HeLa cells with the treatment of a glycolysis inhibitor and observed a change in the GTP/GDP ratio. We plan to apply FLIM-GTP/GDP to quantify and compare the GTP/GDP ratio in both normal and cancer cells to get deeper into the influence of the GTP/GDP ratio changes. FLIM GTP/GDP would be a potential tool for investigating the role of GTP and GDP metabolism and related biological functions.

Keywords: *GTP, FLIM, biosensors, fluorescent proteins*

O-09 Green synthesis, optimization, characterization and exploring the impact of biogenic zinc oxide nanoparticles derived from *Lantana camara* L. leaf extract on alleviating heat stress in wheat

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Abstract: Wheat faces increasing susceptibility to heat stress as a consequence of climate change, resulting in a significant annual reduction in global wheat yield. Nanotechnology emerges as a promising avenue, poised to revolutionize agriculture from seed treatment to post-harvest preservation. In this investigation, ZnO-NPs were synthesized using a sustainable approach employing *Lantana camara* leaf extract. The optimal synthesis parameters included zinc nitrate heptahydrate as a precursor, pH 7, a temperature of 40°C for 4 hours, and stabilization with 2 molar sodium hydroxide. Characterization utilizing contemporary analytical methods confirmed the crystalline nature of ZnO-NPs, with an average size of 9.6 nm according to XRD analysis. TEM and SEM imagery depicted rod-shaped nanoparticles, ranging from 9.6 nm to 25.5 nm. UV-VIS spectroscopy revealed notable absorption at 360 nm, characteristic of ZnO-NPs. FTIR analysis unveiled various functional groups, including alkenes, nitro compounds, and aliphatic ethers, on the nanoparticle surface. The current research also assessed the impact of biogenic ZnO-NPs on growth, morphology, biochemical properties, and molecular traits across four wheat genotypes. Application of ZnO-NPs, particularly at a concentration of 100 ppm, significantly enhanced multiple seed growth parameters. Genetic scrutiny uncovered substantial diversity among wheat genotypes under both standard and heat-stress conditions. Heritability and genetic advancement estimates pinpointed spike length and grain yield as promising traits for breeding programs. Path analysis elucidated the direct and indirect influences of traits on grain yield, emphasizing the importance of biomass, effective tillers per plant, and spike length. Physiological and biochemical responses demonstrated that ZnO-NPs ameliorated the detrimental effects of heat stress on chlorophyll content, relative water content, and cellular membrane stability. Concurrently, ZnO-NPs augmented proline, catalase, peroxidase, and superoxide dismutase activities. Examination of heat shock protein gene expression (HSP17, HSP23, and HSP70) in heat-tolerant and heat-sensitive genotypes revealed distinct responses, with HSP17 exhibiting the highest expression in PBW226 under stress conditions. In summary, this study underscores the potential of biogenic ZnO-NPs to enhance wheat resilience against climate change, highlighting the pivotal role of nanotechnology in modern agriculture and its contribution to global food security.

Keywords: Zinc oxide nanoparticles, wheat, heat stress, HSP, seed priming and gene expression

O-10 The oligomerization and neutralization capabilities of alpha-hemolysin (Hla) toxin from *Staphylococcus aureus* by mutant Hla proteins

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Abstract: *Staphylococcus aureus* is one of six highly virulent and antibiotic-resistant bacterial pathogens. Alpha-hemolysin (Hla) secreted from *S. aureus* binds to the cell surface, forms transmembrane pores, and induces cell lysis. Hla mutants such as HlaH35A, HlaH35L, and HlaH35L/H48L, have been shown to lack hemolytic activity and present promising antigen sources for vaccine development against *S. aureus*. The His35 site is critical in the oligomerization process of Hla during transmembrane pore formation, leading to cell lysis. This study employed high-speed atomic force microscopy (HS-AFM) to image the structures of HlaH35A, HlaH35L, and HlaH35L/H48L proteins on POPC/Chol lipid membranes. Single-site His35 mutations (HlaH35A, HlaH35L) allowed oligomerized structures to be observed, whereas the double mutants HlaH35L/H48L resulted in the protein remaining monomeric. These findings confirm that the region between His35 and His48 is crucial for protomer-protomer interactions essential for oligomerization and pore formation. To evaluate the ability to neutralize the Hla hemolytic toxin on rabbit RBCs by Hla mutants, we mixed Hla with the HlaH35A, HlaH35L, and HlaH35L/H48L at ratios of 10:1 and 5:1 (w:w). Hemolytic activity of Hla was significantly reduced using HlaH35A and HlaH35L at a 5:1 (w:w) ratio. Thus, HlaH35A and HlaH35L are promising candidates for developing supportive treatments for *S. aureus* infections.

Keywords: HS-AFM, alpha-hemolysin, *Staphylococcus aureus*, HlaH35A, HlaH35L, HlaH35LH48L

O-11 Unlocking the enhanced Antimicrobial and Anti-biofilm Potential of Microbial Metabolites: A Nanoformulation Approach

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Abstract: Antibiotic resistance among a growing spectrum of pathogens has given rise to a global health crisis. To address this, a potential avenue is being explored which includes the secondary metabolites (SMs) produced by the Actinobacteria. Actinobacteria are known to produce widespread SMs possessing diverse therapeutic properties such as anti-bacterial, anti-fungal, anti-oxidant, anti-biofilm, anti-diabetic, anti-cancer, etc leveraging them as significant prospects for pharmaceutical and healthcare industries. However, their practical implementation in drug development is limited due to their low solubility, low bioavailability, and high cytotoxicity. To address this, researchers have turned towards nanotechnology. On similar grounds, in this work, we have successfully created nanosuspension of the SMs (N-SM), which significantly increased their surface area compared to their volume. This boost in surface area allowed the N-SM to interact with more cells and potentially enhance their therapeutic effects. In this study, one-pot synthesis of N-SM was done in which SMs were combined with a biocompatible polymer resulting in the formation of a uniform sized nanoparticulate suspension. The resulting nanosuspension was then characterized with the help of different bioanalytical techniques comprising UV-visible spectrophotometry, Transmission Electron Microscopy (TEM), Fourier-Transform Infrared Spectroscopy (FTIR), Scanning Electron Microscopy (SEM), and Dynamic Light Scattering (DLS). The antimicrobial potency of the nanosuspension was evaluated by performing a zone-inhibition assay and determining of minimum inhibitory concentration against WHO-listed high-priority pathogens. The results demonstrated escalated antimicrobial efficacy of the nanosuspension in comparison to the SMs. Furthermore, the nanosuspension displayed enhanced solubility in aqueous medium which is an essential factor for the development of the drug, and increased anti-biofilm activity against reference strains which was confirmed using SEM. This study underscores the potential of N-SMs for their further development as novel pharmaceutical agents. These findings highlight the significance of exploring SMs produced by Actinobacteria and its integration with nanotechnology for therapeutic effectiveness. In conclusion, this approach has the potential to not only revolutionize drug development but also pave the way for an entirely new antimicrobial agent.

Keywords: *Actinobacteria, Secondary Metabolites, Nanosuspension, Antimicrobial, Antibiofilm*

O-12 High-efficiency Sperm Selection by Microchip Integrated of Electrospun Membrane

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Abstract: Sperm washing is a very important step in recent assisted reproductive methods. In this research, we study the sperm selection efficiency of an automatic filtering device using microfluidic technology. The microfluidic device consists of two PMMA plates to fix the electrospinning membrane in the middle to form 2 chambers. Sperm is loaded into the lower chamber; healthy sperm will follow the paths on the membrane to the upper washing chamber. The sample after filtration is evaluated for semen analysis before, after selection and 24 hours after selection. The selection process using Chip uses 1 mL of semen and 1 mL of storage medium. After 45 minutes, the semen suspension is collected, the quality after selection is evaluated, the results are recorded and the recovery efficiency is calculated. Finally, the sample after selection is placed in a 37°C incubator, the quality is evaluated, and the sperm endurance index is calculated after 24 hours of selection. The results of sperm selection using Chip had a recovery efficiency of progressively motile sperm of $24.15 \pm 12.56\%$. All white blood cells were removed from the sperm sample. The sperm quality assessment indexes increased after selection. After selection, the rate of motility and progressive motility were $89.08 \pm 18.09\%$ and $83.56 \pm 20.96\%$, respectively. The survival rate of sperm after selection was $93 \pm 14.89\%$. The rate of normal-shaped sperm in the sample after selection was $2.24 \pm 1.50\%$. The vitality index of sperm after 24 hours of selection was $68.76 \pm 24.93\%$. The motility index of sperm after 24 hours of selection was $60.63 \pm 25.63\%$. The research results show that the sperm selection efficiency of this Chip overcomes the limitations of the volume and selection time of previously published microfluidic devices. The sperm selection efficiency using the Chip is not inferior to the current popular methods such as the swim-up method (SU) and the discontinuous concentration gradient method (DGC). The research results are the premise for continuing to conduct further in-depth studies.

Keywords: *Sperm, Infertility, Microchip, Membrane, Microfluidic*

O-13 Synergistic Activation of p53 in Cancer Cells Using Zinc Oxide Nanoparticles: A Promising Approach for Cancer Therapy

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Abstract: Nanomedicine is currently vital for different disease therapeutics. Thus, we have synthesized zinc oxide nanoparticles from *Prunus nepalensis* and studied effect of Zinc Oxide nanoparticles (PNZnONPs) on the inhibition effect of breast cancer cell line (MCF7 and MCF10A). UV-Vis, SEM and XRD analytical methods were used for nanoparticles characterization. MCF10A and MCF-7 cells were treated with six different doses of PNZnONPs (5, 10, 20, 40, 50 and 100 µg/mL) for cell viability study by MTT assay. Moreover, two doses (40µg/mL and 100µg/mL) were used for the QRT-PCR and 100µg/mL used for western blotting studies to know the level of mRNA gene and protein expression respectively. Furthermore, molecular docking studies of revealed protein-ligand interaction significantly effective in inhibiting proliferation against breast cancer cells. Both the mRNA and protein levels of the tumour suppressor gene p53 and the apoptotic gene Bax were upregulated in PNZnONPs-treated MCF7 cells. PNZnONPs stimulated caspase-3 enzyme activity and DNA fragmentation in MCF7 cells, thus, has shown potential significant activity against cancer cell proliferation.

O-14 Novel Enzyme- Assisted Cellulose Nanofibre (CNF) Synthesis and its Application in CR Dye Adsorption Using RSM Optimization

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Abstract: The world is confronting urgent water crises due to the rapid depletion of available freshwater resources due to dye contamination. Disruption in environmental balance and poses significant risks to human health, as most dyes are toxic, non-biodegradable, and carcinogenic. For this use of some biodegradable nanomaterials as adsorbents in water purification has garnered significant attention due to their high specific surface area, high mechanical strength, chemical stability, etc. In the present work, Cellulose nanofibers (CNF) was synthesized using novel thermostable enzyme via enzymatic hydrolysis from agricultural waste sugarcane bagasse (SB). The prepared CNFs was characterized using field emission-scanning electron microscope (FESEM), scanning transmission electron microscope (STEM), Fourier transform infrared spectroscopy (FTIR), Brunauer-Emmett-Teller (BET), and zeta potential. The efficiency of CNFs for dye adsorption was evaluated using Congo Red (CR) dye from the aqueous solution. Initially, the reaction parameters were optimised using a response surface methodology (RSM). CNFs nanoadsorbent possess efficient adsorption efficiency towards CR dye with maximum removal percentage with process optimization of five variables (nanoadsorbent dose, initial dye concentration, pH, contact time, temperature with significant R^2 and $R^2_{(adj)}$ value. For the CR dye, the adsorption kinetics was described by pseudo-second-order model and the Langmuir isotherm was found to be in best fitted with R^2 value. According to the thermodynamic analysis, the adsorption process is endothermic and spontaneous. Hence, CNFs behaves as an efficient adsorbent in the removal of anionic dye (CR dye) from wastewater treatments.

Keywords: *cellulose nanofiber, response surface methodology, adsorption, dye, equilibrium*

O-15 Metabarcoding of fish species in mangrove nursery grounds using eDNA (environmental DNA) as a tool for conservation and fish stock assessment

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Abstract: Mangrove forests are critical ecosystems that provide essential services, including serving as nursery grounds for various marine species. However, these ecosystems are under threat due to overfishing, habitat destruction, pollution, and climate change. This study utilizes environmental DNA (eDNA) metabarcoding as a non-invasive tool to identify fish species in mangrove nursery grounds in Mindanao, Philippines. eDNA metabarcoding allows species detection by analyzing genetic material found in environmental samples, offering a cost-effective and highly sensitive method for fish species detection. Seawater samples were collected from selected mangrove nurseries, and the extracted eDNA was analyzed using high-throughput next-generation sequencing (NGS) techniques. Sampling sites were: South Cotabato, Surigao del Norte, Misamis Oriental, and Tawi-Tawi. It recorded 29 species belonging to 20 families. Notable species were *Zenarchopterus dunckeri* (Zenarchopteridae), a rare fish in the aquarium hobby, *Hippocampus comes* (Syngnathidae), the tiger-tail seahorse with conservation status of vulnerable by IUCN, *Sardinops melanostictus* (Clupeidae), being of high commercial value, *Siganus corallinus* (Siganidae), noted for food and aquarium trade and *Gymnothorax flavimarginatus* (Muraenidae), plays an important role in the food chain as a natural predator to the lionfish (an invasive species). Tawi-Tawi Island was considered the most diverse site, recording species from 11 families. The results highlight the critical role of mangrove nurseries in supporting diverse fish populations and underscore the effectiveness of eDNA metabarcoding in providing a comprehensive inventory of species. These findings are essential for informing conservation efforts and ensuring the sustainable management of these vital ecosystems.

Keywords: eDNA, mangrove, metabarcoding, NGS

POSTER PRESENTATION

PP-01 Synthesis of ceftriaxone loaded-gold nanoparticles against pathogenic bacteria

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Abstract: Pathogenic bacteria are harmful organisms that cause infections and contagious diseases and result in many serious complications. For a long time, pathogenic bacteria pose a threat to human health and pose significant medical concerns. Thanks to the development of antibiotics, many infections have been prevented and the number of patient deaths has been reduced. However, overuse of antibiotics has also led to the resistance of antibiotics and multidrugs in many bacterial strains. The discovery of new drugs cannot keep up with the change in drug-resistant bacterial strains, leading to difficulties in treatment. Many methods have been proposed to increase the effectiveness of drugs as well as support to destruction of pathogens. One of the most promising strategies to enhance the efficacy of antibiotics is to load them onto nano-delivery materials. Among these nano-delivery materials, gold nanoparticles (AuNPs) are a potential candidate due to their excellent properties such as photothermal effect and biocompatibility. In this report, we present a method for manufacturing gold nanoparticles loading with ceftriaxone molecules - a new third-generation cephalosporin with excellent activity against many Gram-negative Gram-positive bacteria. Green AuNPs were electrochemically synthesized and loaded with ceftriaxone molecules by the electrostatic force. The loading and releasing capacity of AuNPs with ceftriaxone molecules has been evaluated via UV-vis spectroscopy. The morphology of AuNPs and ceftriaxone loaded-AuNPs has been investigated using transmission electron microscopy. The antibacterial activity of ceftriaxone-loaded AuNPs has been studied using minimum inhibitory concentration (MIC) combined with the photothermal effect. The results showed that the complex of ceftriaxone-loaded AuNPs has the potential for the development of nano-delivery materials to enhance the treatment of bacterial pathogens using the photothermal effect.

Keywords: ceftriaxone, AuNP, antibacterial activity, photothermal effect

PP-02 The antibacterial activity of the emodin/chitosan combination formulation against drug-resistant bacteria

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Abstract: The low water solubility of emodin as well as most anthraquinone compounds limits the pharmacological properties of the drug. In this study, emodin/chitosan (EMD/CS) formulation was prepared by a bottom-up method with precipitation and sonication steps to enhance the solubility of emodin. Emodin crystals were precipitated in the presence of chitosan, which was ionically crosslinked at the same time, then this suspension was sonicated using a probe sonication for improving the dispersibility and stability of the formulation. As a result, the formulated EMD/CS particles had a rectangle shape attracted by multiple needle-shaped crystal bars with an average particle size of 342 nm. The antibacterial activity of EMD/CS against representative Gram-positive (MRSA) and Gram-negative (*Escherichia coli* O157:H7) bacterial strains was significantly higher than that of emodin or chitosan. The emodin (0.4 mg/mL) and chitosan (7.2 mg/mL) formulation could completely kill MRSA, while the emodin (0.5 mg/mL) and chitosan (9.0 mg/mL) formulation could significantly inhibit the proliferation of *E.coli* O157:H7. The interaction of EMD/CS particles on the bacterial cells led to membrane damage and cytoplasm leakage, which induced bacterial cell death. It was observed that the density of EMD/CS particles latching on MRSA cells was notably higher than *E. coli* O157:H7 cells. The enhanced solubility, stability, and antibacterial activity of EMD/CS formulation suggest that it may be beneficial in the treatment of infectious diseases, such as gastrointestinal tract infections.

Keywords: emodin, chitosan, nanoparticles, antibacterial, solubility

PP-03 An simultaneous electroencephalography and eye-tracking dataset of ALS patients and healthy individuals using a human-computer interface system controlled by eye gaze

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Abstract: This research presents a dataset consisting of electroencephalogram (EEG) and eye tracking (ET) data from 170 healthy individuals and six patients in a locked-in state (LIS) due to amyotrophic lateral sclerosis (ALS). The ALS patients exhibited varying degrees of disease progression, ranging from being partially mobile or able to speak but significantly weakened by the disease, to complete paralysis and loss of speech. Despite this, the ALS patients still had good eye function and could use a virtual keyboard to communicate. The dataset for the healthy participants was gathered once in a laboratory setting, whereas the ALS patients' data was collected multiple times at their homes. The data collection process consisted of nine recording sessions per participant, each corresponding to a common human action or demand. This dataset can serve as a benchmark for studying motor imagination, investigating ALS, exploring motor cortex function, improving spelling systems with BCI-based recommendation engines, and monitoring motor impairment progress in patients undergoing rehabilitation.

Keywords: *electroencephalogram (EEG), eye tracking (ET), amyotrophic lateral sclerosis (ALS), dataset, brain-computer interfacing (BCI)*

PP-04 Study on the drug release and shape memory effect of multifunctional triple-layer composite membranes based on electrospun poly (ϵ -caprolactone)

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Abstract: This study developed a shape-memory polymer membrane for controlled drug release, providing multifunctional materials for biomedical applications. This composite membrane was composed of triple layers: The bottom and top layers were the thin electrospun polycaprolactone (PCL) fiber mat containing graphene oxide (GO) and benzophenone (BP) components, in which BP was the initiator used to cross-link PCL molecules under UV light to enhance the shape memory effect of the PCL/BP/GO membrane. The middle layer is a berberine (BBR) loaded PCL fiber mat; it is supplemented with GO and polyethylene glycol (PEG) components with the aim of significantly enhancing hydrophilicity for good BBR release in the composite membrane. The chemical characteristics, morphology, and thermal stability of each monolayer membrane were studied using Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), and differential scanning calorimetry (DSC), respectively. The results showed that the triple-layer composite membranes (PB/PPBe/PB) exhibited excellent shape-memory performance under temperature actuation at 55 °C with the fixation ratio (Rf) and the recovery ratio (Rr) as high as over 97% and 70%, respectively. Further, encapsulated BBR can be released from the PB/PPBe/PB membrane in a controlled manner, owing to the thermo-sensitive shape memory effect. The study indicated the BBR release was more sustained when the drug was encapsulated inside the triple layers PB/PPBe/PB membrane, besides this membrane exhibits superior antibacterial ability due to the role of the BBR and BP components. The study is expected to provide a new multifunctional shape-memory material that can control drug release, broadening the application area of shape memory material in biomedical fields.

Keywords: *Electrospinning, crosslinking, shape memory materials, drug release, poly(ϵ -caprolactone)*

PP-05 Antibacterial and fruit preservative ability of nano Chitosan/Zn complex

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Abstract: This study reports the fabricated methods, the characterizations of materials, antibacterial activity and preservative application of nano chitosan/zinc complexes (CS/Zn). CS/Zn complexes were prepared by mixing chitosan nanoparticles solution (CS NPs) fabricated by ionic gelation method and zinc oxide nanoparticles (ZnO NPs) solution greenly synthesized by electrochemical method. The SEM pictures, XRD and FTIR analysis revealed that CS NPs linked with Zn²⁺ ions in solution to form CS/Zn complex. This complex had stronger antibacterial activity in comparison to CS NPs and ZnO NPs only. Namely, the complex killed E. coli at a concentration of two-fold dilution (corresponding 1.2 mg/mL of CS NPs and 10.17 µg/mL of Zn²⁺) whereas CS NPs concentration was 2.4 mg/mL. Moreover, the coating with CS/Zn complex prolonged the shelf life of strawberries to 5 days in room temperature instead of 2 days in uncoated samples. Besides, the weight loss and rate of rotting were also evaluated during storage. In conclusion, the CS/Zn complex performed its advantages and potential applications in post-harvest preservation technology.

Keywords: *Strawberry preservation, chitosan nanoparticles, ZnO nanoparticles, antibacterial activity, edible coating*

PP-06 Toward aptamer-based biosensor for cross-species detection of botulinum neurotoxin: binding mechanism from a comprehensive computational investigation

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Abstract: Botulism is a potentially fatal illness caused by toxin produced by a bacteria called *Clostridium botulinum* found in food. The treatment of this illness requires very expensive antitoxin drugs. Therefore, there is a strong need for the development of sensitive biosensors for early detection of the toxin in food production. These bacteria produce a protein called Botulinum neurotoxin (BoNT). In this work, by using comprehensive atomistic computer modeling and simulation, we investigate aptamers that binds BoNT protein of serotypes A, B and C for use in biosensors for cross-species detection. Known aptamers targeting BoNT/A and BoNT/C are investigated in this work to understand whether they can cross bind to other serotypes. In this way, one can compare their structural and interaction pictures, identify similarities and differences to understand the underlying physical mechanism. Our results stress the importance of structural relaxation of the aptamers that standard docking procedures cannot capture. During molecular dynamics, most of the aptamer structural relaxation correlates with its binding to the protein. Among the aptamer chosen, we find two aptamers A4 and A5 that binds equally strong among all three serotypes. C5 binds equally strongly to its designated target of serotype C, but it binds other serotypes with much lesser strength. These best aptamers for BoNT are all ssDNA aptamers and share a common feature of a DNA double-helix of 5-6 nucleotide base pairs. For all aptamers investigated, there are two binding sites for an aptamer on the BoNT, which are located on opposite sides of the protein. This supports the experimental setup of a sandwich array to allow aptamers to bind to both binding sites for optimal sensitivities. Our computational results provide molecular mechanism of binding, support current experiments, and assist in further optimization and design of new aptamers for these botulinum neurotoxin proteins.

PP-07 Green Synthesis and Characterization of Piper nigrum-Mediated Copper Nanoparticles with Enhanced Bioactivities

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Abstract: This study explores the green synthesis of copper nanoparticles (CuNPs) using black pepper (*Piper nigrum*) extract as a reducing and stabilizing agent. This eco-friendly approach offers advantages comprising of non-toxicity and cost-efficiency compared to traditional methods. X-ray diffraction (XRD), Scanning Electron Microscopy (SEM), and Fourier Transform Infrared Spectroscopy (FTIR) confirmed the successful synthesis of stable PN-CuNPs. The synthesized PN-CuNPs exhibited enhanced bioactivities compared to individual components (pepper extract and copper nanoparticles). They demonstrated that PN-CuNPs displayed a concentration-dependent enhancement in antioxidant property (DPPH and ABTS radical scavenging activity) compared to the pepper extract alone. Furthermore, PN-CuNPs showed the inhibition zone against *Staphylococcus aureus* was larger than that of *Escherichia coli*. Additionally, their minimum inhibitory concentration (MIC) and minimum bactericidal concentration (MBC) values were lower than those of the extract and CuNPs alone. These results suggest a potential synergistic effect between the black pepper extract biomolecules and CuNPs, leading to improved bioactivities. This work highlights the potential of black pepper derived CuNPs for developing multifunctional therapeutic agents with superior properties. Additionally, in vivo studies are crucial to assess the safety and efficacy of these nanoparticles for potential therapeutic applications.

Keywords: *Piper nigrum*, Green-synthesis, copper nanoparticles, antibacterial activity, antioxidant activity

PP-08 Green synthesis of silver nanoparticle using fermented passion fruit peel

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Abstract: The toxicity and environment impact of silver nanoparticles (AgNP) synthesised by conventional method is a major concern. Therefore, this research focuses on the environmentally friendly synthesis of AgNP using fermented passion fruit peel extract, with a comprehensive analysis of their physical properties, biocompatibilities, and biological activities. Solid-state fermentation had shown to significantly boost levels of polyphenols in the extract, which are the major agents responsible for reducing and stabilizing biosynthesized AgNP. The AgNP synthesis product using unfermented (AgNP-U) and fermented (AgNP-F) passion fruit peel extract was compared in term of their synthesis conditions, physical and biological properties. The synthesis conditions for AgNP-U and AgNP-F were systematically investigated considering three crucial parameters: pH value, extract concentration, and AgNO₃ concentration. Conditions for AgNP-F and AgNP-U for achieving the smallest size and highest yield of AgNP were relatively the same and determined as 15 mg/mL concentration of the extract with 10 mM of AgNO₃ at pH 9. At this condition, AgNP-F, compared to AgNP-U, exhibited larger average particle sizes and possessed higher intensity with lower polydispersity index. In terms of biological activities, AgNP-F exhibited higher antioxidant and antibacterial activities. Furthermore, AgNP-F displayed greater stability in size distribution and antibacterial activities compared to AgNP-U. This research highlights the potential of solid-state fermented passion fruit peel extract for green synthesis of AgNP with enhanced biological activities and stability, paving the way for sustainable and efficient nanoparticle production.

Keywords: *green synthesis, silver nanoparticle, plant extract, solid-state fermentation, antioxidant activities, antimicrobial activities*

PP-09 Immuno-PCR assay using antibody conjugated microbeads for detection of White spot syndrome virus

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Abstract: White spot disease caused by white spot syndrome virus (WSSV) is a common, contagious, lethal viral disease in shrimp. The presence of WSSV in most cases is only diagnosed after the symptoms become visible, resulting in a huge loss to the aquaculture industry. Therefore, in this work, we developed a quick screening method to identify and minimize the spreading of WSSV in pond water before cultivation. Using EDC/NHS crosslinking, an antibody that binds specifically to the envelop protein VP28 of WSSV was conjugated with amino-functionalized silica (SiO₂-NH₂) beads. The conjugated beads were confirmed by the dot blotting technique. Thenceforth, these beads were incubated with virus samples for approximately 1.5 hours and were heated afterward as the supernatant was used for the PCR. The results showed that the antibodies successfully formed amide bonds with the amino group on the SiO₂-NH₂ beads' surface. The presence of WSSV in the sample was confirmed by using a specific primer pair and a probe targeting a 200-bp fragment combined with PCR/gel electrophoresis and real-time PCR. The limit of detection was determined as low as 10¹ copies of the synthetic plasmid containing the target amplicon. Furthermore, we will carry on developing and optimizing the procedure of this method with spiked water samples.

Keywords: *white spot syndrome virus, EDC/NHS crosslinking, amino-functionalized silica bead, real-time PCR*

PP-10 Investigation of the antibacterial activity of green silver nanoparticles and silver ions against Extended-Spectrum β -Lactamase-Producing *Escherichia coli* strains

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Abstract: The antibacterial activity of silver nanoparticles (AgNPs) and silver ions have been reported in many articles. However, their antibacterial effect depends on the synthetic approaches of AgNPs as well as the bacterial strains used for evaluation. This study was conducted to demonstrate the antibacterial effect of green AgNPs prepared by the electrochemical method in comparison with that of silver ions. Bacterial tests of Kirby – Bauer agar disk diffusion method and minimum inhibitory concentration (MIC) were performed on 10 extended-spectrum β -Lactamase-Producing *Escherichia coli* (ESBL-producing *E.coli*) strains (antibiotic-resistant Gram-negative strains) isolated from different clinical samples. Results showed that the antibacterial effect of AgNPs against 7/10 ESBL-producing *E.coli* strains isolated from different clinical samples was better than that of ACCT *E.coli* strain, while the antibacterial effect of silver ions against ACCT *E.coli* was better than that of all ESBL-producing *E.coli* strains isolated from clinical samples. MIC of AgNPs against 8/10 ESBL-producing *E.coli* strains was 6.25 $\mu\text{g/mL}$, and 3.125 $\mu\text{g/mL}$ for 2/8 strains. Meanwhile, MIC of silver ions was 3.125 $\mu\text{g/mL}$ for 8/10 ESBL-producing *E.coli* strains, and 1.56 $\mu\text{g/mL}$ for 8/10 strains. This study showed the difference in the antibacterial effectiveness of both green AgNPs and silver ions against ESBL-producing *E.coli* strains isolated from different patient samples.

Keywords: AgNPs, silver ions, ESBL-producing *E.coli*, antibacterial effectiveness

PP-11 Biosensor as a future diagnostic approach for detection ESKAPE

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Abstract: ESKAPE is an acronym for a group of bacteria known for their ability to "escape" the effects of antibiotics. The ESKAPE pathogens include *Enterococcus faecium*, *Staphylococcus aureus*, *Klebsiella pneumoniae*, *Acinetobacter baumannii*, *Pseudomonas aeruginosa* and *Enterobacter* species. A biosensor for detecting ESKAPE pathogens would be a device that uses biological molecules to detect the presence of these bacteria in a sample. This could involve using specific antibodies or DNA probes designed to bind to the surface of the ESKAPE pathogens and produce a measurable signal, such as fluorescence or electrical current.

Due to the important role of graphene, biosensors based on graphene provide a rapid, efficient and low-cost diagnostic process for analytes. This review presents simple, inexpensive, portable and autonomous graphene-based devices for identifying pathogenic strains of ESKAPE. The proposed work shows the benefit of graphene modified with reduced graphene oxide-screen printed electrode. It will also show the development of graphene biosensors that are prepared with various techniques that will be support for detecting the ESKAPE. Besides, it compares the common techniques used for the diagnostic process of ESKAPE with that of graphene biosensors. This work provides a novel broach for the detection process of the ESKAPE. The biosensor could be used in clinical settings to quickly and accurately diagnose infections caused by ESKAPE pathogens, allowing for more targeted and effective treatment. It could also be used in environmental monitoring to detect the presence of these bacteria in water or other samples, helping to prevent the spread of antibiotic-resistant infections.

PP-12 Formulation and Evaluation of Nano-Curcumin Cream for Anti-microbial Activities

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Abstract: Curcumin, a compound known for its antioxidant, anti-inflammatory, and antimicrobial properties, was utilized to synthesize lipid-based nanoparticles. These nanoparticles were prepared by incorporating lecithin with pure curcumin. The characterization of the synthesized nanoparticles was performed using Zeta potential analysis, Field Emission Scanning Electron Microscopy (FE-SEM), and High-Resolution Transmission Electron Microscopy (HR-TEM). Preliminary results indicated that the curcumin nanoparticles exhibited promising antibacterial and antioxidant activities. However, the limited bioavailability of curcumin necessitates the use of nanoparticles to enhance its absorption. To address the handling difficulties of nanoparticles in typical environments, a nano cream formulation was developed, incorporating the nanoparticles for further testing. This nano cream was evaluated against bacterial cultures and demonstrated significant efficacy against *Escherichia coli*, *Enterococcus sp.*, *Proteus mirabilis*, and *Staphylococcus aureus*. These findings suggest that curcumin nanoparticles have substantial potential as antibacterial agents.

Keywords: Curcumin, Nanoparticles, FE-SEM, HR-TEM, Nano Cream, Nano Curcumin

PP-13 In silico prediction of Diagnostic biomarkers for Gall bladder cancers: A miRNA-based study.

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Abstract: Gallbladder cancer (GBC) is the most common type of carcinoma of the biliary tract characterized by poor prognosis. Survival chances of patients range from 4% to 60% due to delay in diagnosis of GBC resulting in diagnosis at an advanced stage and lack of effective treatment available. The identification of biomarkers at an early stage may assist in managing the GBC patient effectively which will improve the survival of the patients. miRNAs play vital role in tumorigenesis at the molecular level and affect the expression and functioning of their target genes making them potential biomarkers for cancer detection. In the present work, we analyse four miRNAs (hsa-miR-26a, hsa-miR-20a, hsa-miR-34a, and hsa-miR-21) which were observed to have a role in gallbladder cancer based on previous literatures. The target genes of these miRNAs were then collected using online miRNA databases i.e., miR Walk, miRTarBase, and miRDB, followed by identification of recurring differentially expressed genes (DEGs) among the four different miRNAs using FunRich. Further, STRING has shown the 135 nodes and 166 edges with a PPI Enrichment value of 0.00127 out of 135 DEGs. Cytoscape and Metascape were exploited to find out the Hub genes and to analyse their involvement in various other metabolic pathways respectively. We observed promising 10 hub genes (PTEN, CREB1, CDC42, MYC, CCND1, ESR1, SMAD4, XIAP, CSNK1A1, PPARGC1A), which can be proposed as novel biomarkers in the early detection of GBC leading to an efficient cure. We have to conduct the *in-vivo/ in-vitro* analysis of proposed miRNAs/ target genes to validate the results of this study.

Keywords: gall bladder, cancer, biomarkers, miRNA, diagnosis, hub genes

PP-14 Green Synthesis of Fluorescent Carbon quantum Dots Nanohybrids for Heavy Metal Detection

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Abstract: This study explores a green synthesis method for creating carbon dot-decorated silver heteronanocomposites (Ag@CQD HNCs) using oranges. Fluorescent carbon quantum dots (CQDs) are extracted from orange juice, while silver nanoparticles (Ag NPs) are synthesized from silver nitrate using orange peel extract as a sustainable reducing agent. The resulting Ag@CQD HNCs demonstrate significant interactions between their components, with a larger particle size (20-30 nm) compared to individual CQDs and a distinct visible light absorption peak at 390 nm. Both CQDs and Ag@CQD HNCs exhibit fluorescence, with the HNCs showing a shifted emission peak and photoluminescence (PL) quenching, indicating potential energy transfer between CQDs and Ag NPs. This eco-friendly synthesis not only supports sustainable nanomaterial production but also enables the creation of innovative sensors for heavy metal detection. The calibration curve for heavy metal detection shows a linear range of 100–160 nM, with a limit of detection (LOD) estimated to be between 1 and 5 nM. The unique optical properties and potential interactions between CQDs and Ag NPs underscore the need for further exploration of their applications in environmental monitoring.

Keywords: Carbon quantum dots, Surface alteration, Nanohybrids, Heavy Metal, Optical properties

PP-15 Surface ligand modified silver nanoparticles-based SERS sensing platform for ultrasensitive detection of the pesticide thiram in green tea leaves: roles of coating agents in sensing performance

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Abstract: Silver nanoparticles (AgNPs) have been regarded as a highly promising substrate for surface-enhanced Raman scattering (SERS) sensors. In this study, we focused on the electrochemical synthesis method by developing three kinds of AgNPs using three different electrolytes: citrate (e-Ag-C), oleic acid (e-Ag-O) and fish mint (*Houttuynia cordata* Thunb.) extract (e-Ag-bio). The as-prepared AgNPs were characterized and then employed as SERS substrates to detect the pesticide thiram. The obtained results show that e-Ag-O exhibits the best SERS performance. The effect of the coating agent was explained by chemical and electromagnetic enhancements (CM and EM). Although thiram could absorb onto e-Ag-C at the highest level, allowing its Raman signal to be best enhanced via the CM, the smallest interparticle distance of e-Ag-O could have resulted in the largest improvement in the EM. Using e-Ag-O to develop SERS-based sensors for thiram, we obtain the impressive detection limit of 1.04×10^{-10} M in standard samples and 10^{-9} M in tea leaves. The linear ranges are from 10^{-4} M to 10^{-7} M and from 10^{-7} M to 10^{-9} M, covering the maximum residue levels for plant commodities established by the United States Environment Protection Agency and European Food Safety Authority (2–13 ppm $\sim 7.7 \times 10^{-6}$ M to 5×10^{-5} M).

Keywords: SERS, silver nanoparticles, electrochemical synthesis, coating agent

PP-16 3D Solar Cell Based on NiSi_xNWs

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Abstract: Solar cells utilizing silicon nanowires have emerged as promising candidates for practical applications, offering the prospect of cost-effectiveness and heightened efficiency. Nonetheless, despite over two decades of development, challenges persist, notably in the realms of complex fabrication processes, leading to elevated costs, and connectivity issues, resulting in diminished efficiency. In this study, we propose a pioneering 3D solar cell architecture employing metal nickel silicide nanowires (NiSi_xNWs) in conjunction with p-i-n core-shell nanowires, boasting a streamlined fabrication process. Our devised structure attains an impressive efficiency of approximately 11.04%, accompanied by a photocurrent density of roughly 22.08 mA/cm². Furthermore, the open-circuit voltage (V_{oc}) is obtained at approximately 0.70 V, with a fill factor (FF) of around 72.03%. These findings underscore the considerable potential of our approach in realizing high-efficiency solar cells at a reduced cost, thereby fostering optimism for future advancements in the field.

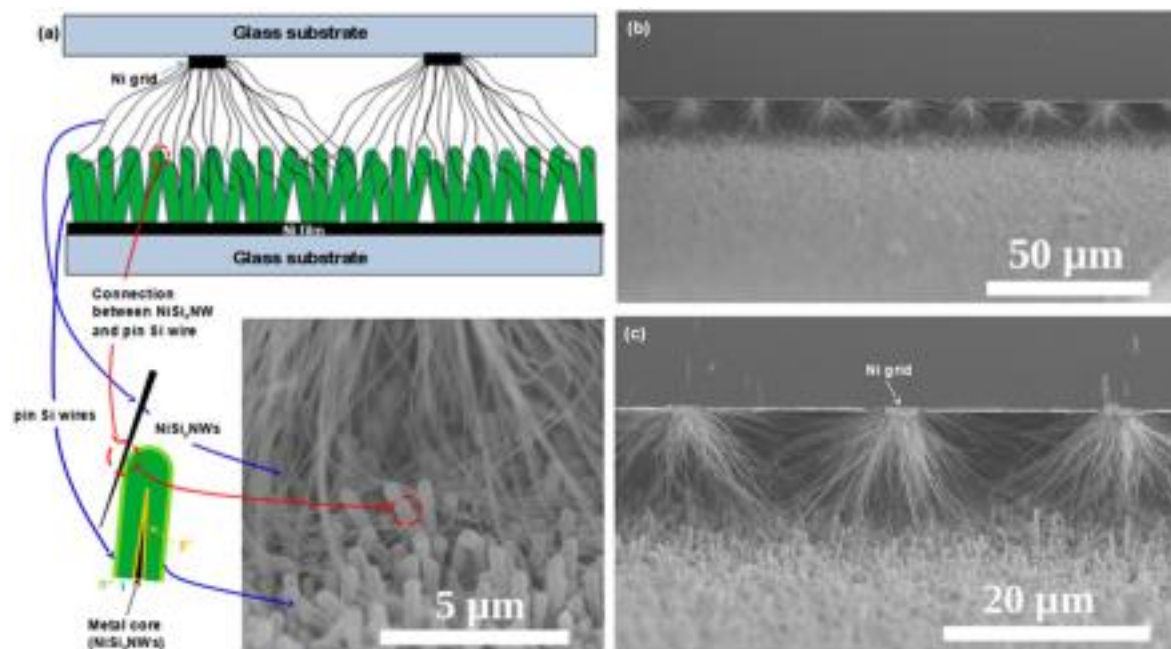


Figure 1. The 3D solar cell structure used in this work. NiSi_xNWs grow out from the top electrode and connect with p-i-n Si wires at the bottom. (a) Model of the 3D structure, the inset at the bottom part of panel shows an enlarged view of NiSi_xNWs contacting p-i-n Si wires; (b) A scanning electron microscope (SEM) view of a completed device; (c) An enlarged SEM view of the structure.

PP-17 Evaluating interactions between M-cell targeting peptide Co1 and C5aR receptor using molecular docking

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Abstract: Prevention of gastrointestinal infections with oral vaccines is considered a more effective solution than injectable vaccines due to its ability to stimulate both mucosal and systemic immune responses. However, the development of oral vaccines faces various challenges, mainly due to the failure to induce an effective response. The Co1 peptide shows potential in targeting antigen to M cells, which are known as the "gateway of the gastrointestinal immune system" via the surface-expressed C5aR receptor. In this study, we applied bioinformatics tools such as peptide structure prediction, molecular docking, and dynamic simulation to analyze the details of the interaction between Co1 peptide and C5aR receptor. From the analysis of the docked complex, this study discovered amino acids that play an important role in the interaction between the Co1 peptide and the C5aR including S1, H3, Q4, R8, S9, P12; and surprisingly, R8 contributed the most to total binding free energy of peptide-receptor complex. With the obtained results, the Co1 peptide has potential to improve the ability to target M cells, supporting the development of oral vaccines.

Keywords: Oral vaccine, Co1, C5aR, structure modeling, molecular docking, molecular dynamics simulation, binding free energy

PP-18 Investigating the binding of Morphine and TRV130 agonists to the stability of μ -opioid receptor

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Abstract: Opioid agonists expressing analgesia are usually followed by adverse reactions such as heart failure, respiratory depression, constipation, etc. Agonist binding to μ -opioid receptors (μ OR) can activate two intracellular signaling pathways: (i) the G protein signal is responsible for alleviating pain; (ii) β -arrestin results in unwanted side effects. Here, we utilize recent advances in computational power and molecular dynamics (MD) simulations to analyze and evaluate the influences of unbiased (Morphine – M6G) and biased (TRV130) compounds of the G protein signal, on the structural stability and functions of the μ OR receptor. We have identified that M6G with hydroxyl groups, forms Hydrogen bond and electrostatic interactions with key residues in the catalytic site of the μ OR receptor, whereas TRV130 prefers binding by hydrophobic and van der Waals interaction types. The binding to M6G leads to the higher flexibility of the μ OR's TM VII which is known to activate the β -arrestin signal, while this TM VII is more stable in the TRV130- μ OR complex. Additionally, the allosteric pockets of the Sodium (Na^+) ion are different in these μ OR complexes. Taken together, these studies may provide new avenues for the design of biased opioids with appropriate efficacy.

Keywords: μ -opioid receptors, molecular dynamics (MD) simulations, Morphine – M6G, TRV130, Sodium (Na^+) ion

PP-19 Optical and Electrochemical Diagnosis Using an Epigenetic Biomarker for Breast Cancer

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Abstract: Breast cancer is the most common cancer among women, accounting for nearly one-third of all malignant tumors in women. In 2021, breast cancer caused 670,000 deaths worldwide, and in 157 out of 185 countries, breast cancer was the leading cause of cancer in women in 2021. However, between 0.5% and 1% of men were affected (WHO, 2023). In Brazil, an estimated 59.7 thousand new cases will be recorded for the year 2021-2023 (INCA, 2022). It is a condition characterized by the uncontrolled growth of abnormal cells in breast tissue. These cancer cells can form a mass or tumor that can spread to other parts of the body. With the aim of promoting a rapid, simple, sensitive, selective, and economical diagnosis, we have proposed the development of an electrochemical genosensor and a colorimetric kit based on gold nanoparticles for breast cancer. Thus, DNA probes complementary to microRNAs were selected using bioinformatics techniques, and microRNA samples will be enriched with blood plasma from healthy patients. Samples from healthy and sick patients, obtained from the cancer hospital of the Federal University of Uberlândia, will be used in the electrochemical and optical biosensor. For the construction of the electrochemical biosensor, printed electrodes will be constructed using a PVC sheet and a vinyl adhesive as a substrate produced in the laboratory. The structural and morphological characterization of the obtained nanomaterials, to date, is carried out by spectrophotometry, transmission electron microscopy, scanning electron microscopy, and atomic force microscopy. For the realization of the colorimetric and optical kit, the synthesis of gold nanoparticles was carried out according to the Turkevich Frens method, by reducing tetrachloroauric acid with citrate under heating (100°C). Then, the characterization was carried out by transmission electron microscopy (TEM). The specific probe will be anchored to the surface of the printed electrodes (electrochemical biosensor) and gold nanoparticles (optical kit) through a nanoparticle functionalization strategy with cysteamine, aiming to promote the orientation and binding of the DNA probe to the surface. Spectrophotometric analyses and TEM were performed to prove the anchoring of the probe biomolecule. The detection of microRNA molecules will be obtained by electrochemical techniques and by aggregation of nanoparticles in the presence of the analyte of interest. All experiments are performed in quintuplicate and numerical results are presented as arithmetic mean $\pm$ standard deviation.

To date, it has been possible to synthesize gold nanoparticles, anchor the synthetic DNA probe onto NpsGold, detect the complementary target, and perform atomic force and scanning microscopy of these electrodes.

Keywords: breast cancer, microRNA, colorimetric biosensors, biosensors, gold nanoparticles.

PP-20 In silico prediction of novel peptide derived from *Brucella abortus* Hsp60 targeting M cells

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Abstract: Gastrointestinal tract infections manifest in both developed and developing nations. The administration of oral vaccines has the potential to effectively prevent illnesses transmitted through the oral route by enhancing both humoral and mucosal immunity. Indeed, the development of oral vaccinations has been hindered by several constraints in effectively eliciting a sufficient immune response. A currently explored approach involves the use of guide molecules that combine with vaccination antigens to specifically target M cells, which are regarded as the primary source of mucosal immunity on the surface of the intestinal epithelium. However, guide molecules with a big and bulky structure can have adverse impacts in the creation of recombinant vaccines. The present work primarily investigated *Brucella abortus* Hsp60, which serves as a ligand for the cellular prion protein found on maturing M cells. A highly reliable 3D structure of Hsp60 was generated using a homology modeling technique based on the GroEL template. Through molecular docking, we have discovered two new peptides originated from *Brucella abortus* Hsp60. Among them, PEP1 exhibited the highest binding capacity, with a predicted affinity HG of -9.5 kcal/mol. The results indicated that the calculated peptide had a strong binding affinity with the receptor, and the complex remained stable throughout the 100 nanosecond simulations. Therefore, this discovery established the foundation for subsequent scientific investigations in the advancement of oral vaccines.

Keywords: Cellular prion protein, Hsp60, Molecular docking, Molecular dynamics simulations, Structural bioinformatics, Oral vaccine

PP-21 Fabrication neem oil nanoemulsion and evaluation antifungal activity against *Pyricularia orizae*

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Abstract: Biopesticides are considered to be safe, target specific, biodegradable and eco-friendly. Neem oil can function as antifungal agents and a safe usage in agriculture. However, neem oil is unstable and hydrophobic, which limits its use. This study aimed to optimize composition preparation neem oil nanoemulsion by using method low energy followed by its characterization and determination for antifungal effectiveness of nano-emulsion against *Pyricularia orizae*. In two methods fabrications, we selected phase inversion composition (PIC) method to optimum components nano-emulsion. The result showed selected formulation with optimum components' concentration was 10% of neem oil, 10% of Tween 80, 10% SLES and 70% of distilled water. The particle size, polydispersity index, zeta potential and viscosity of nanoemulsion were 158.1 nm, 0.148 and -27.43 mV, 17.64 cP, respectively. Nanoemulsions was still homogeneous and unchanged after centrifuging at 5,000 rpm for 5 min and were more stable when kept at room temperature after two months storage. Furthermore, in vitro nanoemulsion showed good antifungal activity and the inhibition efficiency of nano-emulsion was above 80% against *Pyricularia orizae* at the concentration from 312.15 ppm to 10,000 ppm after 12 days storage. This study suggests that the prepared nanoemulsion could be a potential candidate for use as an alternation for synthetic fungicides.

Keywords: antifungal, droplet size, *Pyricularia orizae*, phase inversion composition (PIC), neem oil, nanoemulsion

PP-22 Innovative Fluorescence-Based Sensing of Cadmium Ions and Detection of Latent Fingerprints Using CQD@Au Nanocomposites

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Abstract: In this study, we present the synthesis of novel carbon quantum dot-gold nanoparticle (CQD@Au) nanocomposites using eco-friendly green precursors and a plasma-assisted method. In these nanocomposites, carbon quantum dots (C-dots) function as the donors, while gold nanoparticles (Au NPs) serve as the acceptors in a fluorescence resonance energy transfer (FRET) process, leading to the quenching of C-dot fluorescence. The addition of cadmium ions (Cd^{2+}) reverses this fluorescence quenching through the oxidation of Au NPs by Cd^{2+} , establishing an efficient on-off switching mechanism. This "turn-on" fluorescence response exhibits a detection as low as 3 μM , demonstrating its high sensitivity for Cd^{2+} ion detection. Furthermore, the CQD@Au nanocomposites are successfully applied in the visualization of latent fingerprints. When exposed to ultraviolet light, the enhanced fluorescence significantly improves contrast and detail in fingerprint residues on various surfaces, allowing for clear imaging. The use of green precursors and a plasma-assisted synthesis method underscores the sustainability of this approach. Overall, the CQD@Au nanocomposites provide a versatile, rapid, and eco-friendly platform for both environmental monitoring and forensic applications.

Keywords: Carbon Quantum Dots, Gold Nanoparticles, FRET, Latent Fingerprint, Plasma

PP-23 Enabling Fast-Charging and High Specific Capacity of Li-ion Batteries with Nitrogen-doped Bilayer Graphdiyne: A First-Principles Study

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Abstract: Carbon-based materials are the most important anode materials for Lithium-ion batteries (LIBs). To improve the electrochemical performance of LIBs for high energy density and fast charging, advanced carbon allotropes are in the research focus. Graphdiyne (GDY) is a new carbon allotrope consisting of sp - and sp^2 - hybridized carbon that could perform unique and fascinating properties compared to the others. In this study, we applied the density functional theory to investigate the most stable structures and electronic properties of monolayer, bilayer AB AB($\beta_x = 1 \div 2$)-stacking graphdiyne and Nitrogen-doped bilayer, namely GDY, AB(β_1), AB(β_2) and N - BDGY. The structures GDY, AB(β_1), and N - AB(β_1) were the most stable structures of GDY materials and represent for GDY single, BDGY (Bilayer GDY), and N - BDGY (N - doped Bilayer GDY), respectively. Electronic analysis show that BDGY and N - BDGY is antiferromagnetic semiconductors with an energy gap of 0.429 eV and 0.226 eV, respectively, which are lower than that of GDY (0.550 eV). The BDGY and N - BDGY exhibit promising characteristics in Li-ion adsorption and intercalation, with the specific capacity improving from 744 mAh.g⁻¹ in the monolayer GDY to 807 mAh.g⁻¹ in the bilayer, with the average Open Circuit Voltage (OCV) is 0.48 V and 0.76 V, respectively. However, N-doping in BDGY does not effect the capacity through a bilayer structure, it increase the OCV to 0.82 V and enhances the structural stability during Lithiation process, with a volume expansion of 1.90%, which is lower than that of BDGY (2.14%) and Graphite (10%) during maximum Li-ion intercalation. Since, BDGY and N - BDGY structures provide higher Li-ion specific capacity compared to single-layer GDY and another carbon-based material, these materials are potential candidates for LIBs anode.

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PP-24 *In Silico* Interactions Analysis of Claudin-4 Receptor and CPE17 Peptide that Precisely Target Antigens to M Cells

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Abstract: In comparison to injectable vaccines, oral vaccines have been currently emerging as a potential alternative for the prevention of gastrointestinal infectious diseases. In order to improve immunostimulation in the intestinal mucosa, vaccine antigens must be delivered to M cells through ligand-receptor interactions on the cell surface. It was discovered that the 17-amino acid C-terminus of the *Clostridium perfringens* enterotoxin (CPE17) exhibits the binding ability to the Claudin-4 receptor (CLDN4) on M cells and shows no cytotoxicity. For the purpose of expanding the library of CPE-derived M cell-targeting peptides, in this study, we integrated bioinformatics tools such as structure modeling, molecular docking, and molecular dynamic simulations (MDs) to identify the crucial residues involved in the interaction between the CPE17 and CLDN4 receptor. The 3D structures of POPC membrane-embedded CLDN4 and CPE17 were successfully constructed with high confidence. Docking and MDs results demonstrated that the peptide-CLDN4 stability was maintained during 100 ns period; it also revealed that five residues N1, Y10, S11, I12, and Q15 positively contributed to the interaction of CPE17 and ECL2 region of CLDN4. These findings were the foundation for designing peptides with higher affinity to CLDN4 for oral vaccine development.

Keywords: Claudin-4, CPE17, Molecular docking, Molecular dynamics simulation, Bioinformatics, Oral vaccine.

PP-25 Functionalized gold nanostructures through *Caesalpinia minax* Hance extract for detecting lead ions in aqueous solution

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Abstract: In this study, gold nanoparticles (GNPs) were produced in the aqueous extract of *Caesalpinia minax* Hance (*C. minax* Hance), serving as an effective stabilizer and reducing agent through the green synthesis approach. The optimal conditions for GNPs synthesis included *Caesalpinia minax* Hance extract to HAuCl₄ ratio of 0.26 (v/v), HAuCl₄ concentration of 1.3 mM, temperature of 42 °C for 38 min, and pH 7. The structural, and morphological properties of the synthesized GNPs were characterized using Fourier-transform infrared spectroscopy (FT-IR), field-emission scanning electron microscopy (SEM), and transmission electron microscopy (TEM). TEM analysis revealed that the GNP nanoparticles exhibited a spherical shape with an average particle size ranging from 10 to 12 nm. The detection of Pb²⁺ in the solution was performed using a colorimetric assay, which identified the color shift of gallic acidcapped gold nanoparticles (GA-GNPs) and Pb²⁺ aggregates, with a detection limit of 0.024 mg/L, a recovery rate of 99-101%, and high selectivity for Pb²⁺ in the presence of other interfering metal ions. Additionally, GA-GNPs demonstrated catalytic degradation potential for methylene blue, methylene red, and crystal violet dyes, achieving removal rates of 98% after 120 minutes, 99% after 30 minutes, and 94% after 60 minutes at a concentration of 100 mg/L, respectively. Furthermore, GA-GNPs at concentrations ranging from 10% to 40% exhibited inhibitory effects against *Aspergillus* spp. fungi, contributing to the control of green mold disease on soybean seeds, and enhancing the germination rates.

Keywords: *Aspergillus* spp., biosensor, lead ions, gold nanoparticles, dyes

PP-26 Evaluation of the Cytotoxicity and Cancerous Tumor Inhibition Ability of the M1 Extract Derived from Mushrooms of *Ganoderma lucidum* and *Cordyceps militaris*

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Abstract: Nowadays, cancer has become a significant societal problem. It is the second leading cause of death worldwide, and this number is on the rise. Given this situation, the development of natural cancer-supporting therapies is increasingly being prioritized. The M1 extract, derived from mushrooms of *Ganoderma lucidum* and *Cordyceps militaris*, consists of valuable medicinal ingredients known for their potential to combat serious diseases and promote health, as supplied by the research team at the Institute of Agricultural Engineering and Post-Harvest Technology. We conducted an in vitro toxicity evaluation of the M1 extract on two cancer cell lines of H358 and Sarcoma-180, as well as on the healthy cell line HEK293. Additionally, we assessed the tumor growth inhibition in an in vivo mouse model induced by Sarcoma-180 cells and the peripheral blood indices of mice administered with the M1 extract. The toxicity results after 48 hours revealed that the M1 extract exhibited cytotoxicity against the two cancer cell lines H358 and Sarcoma-180, with IC₅₀ values of 199.8 µg/mL and 97.7 µg/mL, respectively. Notably, the M1 extract demonstrated low toxicity in the healthy HEK293 cell line, with an IC₅₀ of 377 µg/mL. Furthermore, the M1 extract inhibited cancerous tumor growth by up to 28.2% and did not negatively affect the peripheral blood indices of the mice.

Keywords: Cancer, M1 preparation, H358; Sarcoma-180, HEK293; IC₅₀, tumor

PP-27 Extending the release of metformin hydrochloride using atomic layer deposition of SiO₂ thin films at room temperature

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Abstract: Metformin, a widely-use antidiabetic agent, has a short half-life and a high water solubility. Therefore, in the clinical context, the medication is often prescribed twice daily, which leads to certain obstacles to treatment adherence and risk of adverse effects due to the fluctuation of drug concentration in the body. In this study, atomic layer deposition (ALD) was employed in order to modify characteristics of metformin hydrochloride powder. The technique was performed at the room temperature, using a home-built fluidized bed reactor, with silicon tetrachloride and distilled water as precursor and coreactant, respectively. By sequential introduction of precursor and co-reactant to the reacting chamber, a coating layer on the surface of metformin hydrochloride powder was generated. While the XPS result revealed that SiO₂ was the major constituents of the coating layers, Fourier-transform infrared spectroscopy (FTIR) and X-ray diffraction (XRD) experiments confirmed no change in the structure of the initial material, which is predicted to maintain its pharmacological effects. In addition, as the number of ALD cycles increased, the thicker coating layer was obtained, and this contributed to a remarkably delayed *in vitro* release. Specifically, applying 50 ALD cycles slowed down the release rate by 3.2 times, whereas the value was increased to 8.7 times with 100 ALD cycles. This result opens up the potential for creating an extend-release dosage form for metformin hydrochloride, in which its release rate can be controlled by adjusting the thickness of coating layer.

PP-28 Hydrothermally Synthesized Rice Straw Carbon Dots for Simultaneous Electrochemical Detection of Ractopamine and Clenbuterol

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Abstract: This study presents the synthesis of carbon dots from rice straw (RSCD) using a hydrothermal method for the simultaneous electrochemical detection of ractopamine (RTP) and clenbuterol (CLB). The RSCD's properties were characterized using XRD, FTIR, Raman spectroscopy, TEM, UV-Vis photoluminescence, and EDX mapping. When modified onto a glassy carbon electrode (RSCD/GCE), the RSCD displayed enhanced electrochemical activity in cyclic voltammetry (CV) and differential pulse voltammetry (DPV) compared to a bare electrode. Distinct oxidation peaks for RTP (+0.88 V) and CLB (+1.88 V) were observed, indicating high selectivity. The method covered a linear detection range from 0.1 μM to 92 μM with detection limits of 0.09 μM for RTP and 0.03 μM for CLB. Interference tests revealed minimal impact from common ions and organic substances. Additionally, the RSCD/GCE exhibited good repeatability, reproducibility, and stability over one week. This work demonstrates the potential of RSCD/GCE for reliable, sensitive detection of β -agonist residues, contributing to food safety monitoring.

Keywords: Carbon dots, electrochemical detection, ractopamine, clenbuterol, rice straw

PP-29 Assessing the Incidence of the Hepatitis E virus Shellfish

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Abstract: Hepatitis E virus (HEV) is a non-enveloped single stranded RNA virus that causes acute viral infection in most Asian and African nations. HEV mostly transmits through fecal oral pathways, occurring in both human and animal feces. Furthermore, the presence of this virus is also contained in contaminated water that potentially affect another surrounding stream by sewage elimination from piggery. Shellfish, especially crustaceans, work as vectors to carry the viral transmission to humans through contaminated water supplement. In this study, 120 shellfish samples were collected in various local markets including 20 tiger prawns (*Macrobrachium rosenbergii*), 50 giant river prawns (*Penaeus monodon*), and 50 mussels (*Mytilus edulis*). Nested PCR targeting ORF1 was performed to screen for the presence of HEV in the collected samples. Resultedly, none of the samples (0/120) was positive with HEV. In conclusion, HEV was not detected in the local shellfish using nested PCR targeting ORF-1.

Keywords: Genotype 3; Hepatitis E virus; Nested PCR; Shellfish

PP-30 Investigating the structural features of SARS-CoV-2 Mpro binding site bound covalent and non-covalent ligands at physiological temperature

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Abstract: The laws of physics are an indispensable basis for the development of science and technology fields, especially interdisciplinary fields such as biomedical physics, drug design, and health sciences. In this research, by applying the laws of physics and the power of computers, we investigate the structural characteristics of the binding site when binding to the ligands with and without a covalent bond in the SARS-CoV-2 Mpro receptor – a main protein that plays an important role in the replication and transcription of the SARS-CoV-2 virus causing the global COVID-19 pandemic, using the Molecular Dynamics (MD) simulation at physiological temperature (at 310K), and compare with their X-ray experimental structure (at 273K). We found that conformations of both the Mpro proteins and the ligand are stable during 500ns of the simulation time. In the SARS-CoV-2 Mpro complex with a covalently bound ligand (ACR), the H41's side chain is flipped compared to the experimental structure (at 273K), forming a strong Hbond with a catalytic water molecule, and keeps the cyclohexyl ring of the ligand stable by π - π stacking interaction. In contrast, in the SARS-CoV-2 Mpro complex with a non-covalently bound ligand (ANR), the Hbond between H41 and the catalytic water is not found, leading to conformations of H41 and the attached ligand are more flexible during the simulation. Therefore, through molecular dynamics simulations at physiological conditions (310K), the catalytic water molecule plays an important role in stabilizing the catalytic structure and combining with the catalytic-dyad H41-C145 to carry out the main functions of the Mpro receptors. These results form important basis for studying candidate drugs against SARS-CoV 2.

Keywords: SARS-CoV-2 Mpro receptor, Molecular Dynamics (MD) simulation, covalent ligand, physiological conditions

PP-31 Application of Molecular Markers in Studying the Genetic Diversity of Several Common Carp Strains in Vietnam

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Abstract: In this study, genetic diversity, population structure, and phylogenetics of seven common carp strains including Vietnamese white carp (VN), breeding carp V1 (V1), Hungarian scaly carp (HV), Indonesia goldfish (IN), Hungarian scaly carp Tata (TAT), Hungarian scaly carp Szarvas (SZA) and Czech Republic carp (SE) that were studied and based on COI and D-loop sequences analysis. Results showed that VN and V1 were the highest genetic diversity populations while HV, TAT, SZA, SE, and IN had low genetic diversity in COI and D-loop genes. This study identified a total of 53 haplotypes and all haplotype sequences were deposited in the GenBank database, accession numbers MW450991-MW451003 (for COI gene) and MW463062-MW463101 (for D-loop gene). In terms of genetic differentiation, the most notable was the genetic difference in the COI gene between SE and all other populations, specifically, between SE and HV, Se and SZA (both had $F_{st} = 1$), this suggests that there was no genetic sharing between these populations based on studied genes. All populations had a clear population structure due to the significant contribution of the genetic differences among populations based on COI AMOVA analysis. Phylogenetics indicated a long genetic relationship between SE and other remaining populations (for the COI gene) and a close genetic relationship between seven studied populations (for the D-loop gene). Our research contributed to creating a database of references and supporting studies that need information on genetic resources of some common carp populations in Vietnam as well as serving for breeding and conserving genetic resources.

Keywords: COI, D-loop, common carp, genetic diversity, haplotype

PP-32 Modification of biodegradable organosilica nanoparticles with polyethylene glycol to enhance anticancer drug loading and control release

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Abstract: Thanks to the difference between tumor and normal cells, the surface of nanoparticles can be modified to adjust the loading capacity and their release. In this work, we modified the surface of phenylene-containing tetrasulfide-based biodegradable periodic mesoporous organosilica nanoparticles (P4S) with a biocompatible and hydrophilic polyethylene glycol (PEG). The physicochemical analysis demonstrated the successful modification with PEG. Camptothecin (CPT) was chosen to be loaded onto the PEG-modified P4S. HPLC analysis results revealed a higher CPT loading in the PEG-modified sample than the non-modified one. Furthermore, drug release assessments demonstrated the pH-responsive properties of P4S nanoparticles upon PEG functionalization, leading to increased drug release at low pH and enhanced cellular uptake potential. Notably, the cytotoxicity of CPT against HepG2 cancer cells was significantly improved when loaded into P4S-PEG nanoparticles. These findings reveal the efficacy of PEG surface modification in augmenting the activity of CPT, indicating promising prospects for clinical applications.

Keywords: *Nanomaterials, PEG, organosilica, biodegradable, drug delivery*

PP-33 Evaluation of *In Vivo* Toxicity and Immunomodulatory Potential of M1 Extract from *Ganoderma lucidum* and *Cordyceps militaris* Cultivated in Vietnam

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Abstract: The trend of combining herbal medicines is gaining attention for their safety and benefits, expected to create synergy among bioactive compounds that enhances immunity and supports disease treatment. The M1 product, extracted from *Ganoderma lucidum* and *Cordyceps militaris* by a research team at the Vietnam Institute of Agricultural Engineering and Post-Harvest Technology, has undergone preliminary acute toxicity evaluation via oral administration in Swiss mice. Results indicated that M1, at doses of 2000–10,000 mg/kg, did not exhibit acute toxicity. the research team proceeded to evaluate the subacute toxicity and the immunomodulatory potential of M1 in an *in vivo* model. Administration of M1 at 2000 mg/kg/day for 30 days did not adversely affect peripheral blood parameters, and no abnormalities were observed in histopathological images of the liver, kidneys, and spleen, or in the general condition of the mice. Additionally, Real-time PCR and ELISA results showed that M1 inhibited mRNA expression of pro-inflammatory cytokines TNF- α , IL-1 β , and IL-6, with reductions of 49%, 69.5%, and 84% ($p < 0.05$, $n = 3$), along with a 43.6% decrease in serum TNF- α protein levels. These findings lay the groundwork for further studies on the anti-tumor efficacy of M1, highlighting its potential for developing supportive therapies for cancer patients.

Keywords: M1 product, *in vivo*, acute toxicity, subacute toxicity, pro-inflammatory cytokine

PP-34 Investigation of Luminescent Magnetic PDMS Microspheres Encapsulating NiFe₂O₄ and Rhodamine B for the Detection of White Spot Syndrome Virus

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Abstract: The PDMS microspheres encapsulating NiFe₂O₄ and Rhodamine B (denoted as PDMS/NiFe₂O₄-RhB) were synthesized using a microfluidic technique, yielding microspheres with an average diameter of 78.21 μm. These microspheres exhibit both magnetic and luminescent characteristics, rendering them suitable candidates for dual-mode detection systems that incorporate magnetic separation and optical signaling. Quantitative analysis of the fluorescence intensity, performed using a fluorescence microscope, indicated a linear correlation with the size of the particles. Following functionalization with amine groups and antibodies specific to the White Spot Syndrome Virus (WSSV), a notable decrease in fluorescence intensity was observed, suggesting effective binding. The specific detection capability of these microspheres for WSSV was further assessed utilizing the Immuno-Dotblot method. This report elucidates the potential application of the optical properties exhibited by these microspheres as a signaling mechanism for the detection of WSSV.

Keywords: Biosensor, White Spot Syndrome Virus, Magneto-fluorescent, PDMS spheres, Microfluidic method.

PP-35 Evaluating Loblolly Pine Bioenergy Development Potential Using AHP Integrated Weighted Overlay and Network Optimization in Virginia, USA

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Abstract: With ever fluctuating fossil fuel prices, bioenergy is an essential piece of the United States' (US) energy portfolio. However, questions surrounding bioenergy sourcing and adoption at the producer level remain persistent challenges, hampering proliferation in areas where it is not already available. To establish new industries, individual regions must be evaluated for various bioenergy feedstocks and incorporate elements for environmental, societal, and economic growth. In this study, we assess the overall potential for loblolly pine (*Pinus taeda*) in Virginia, US for domestic bioenergy by utilizing stakeholder preferences for site selection and potential biomass yield from a regional growth and yield model. Our results show that bioenergy in the state requires widespread planting of loblolly pine to provide sufficient feedstock for bioenergy development and that additional studies on the moisture content of pine across the region should be deployed to accurately map the expected quality of feedstock. A secondary result shows that additional outreach to landowners will be necessary due to narrower land quality preferences compared to other stakeholder groups, though these narrower preferences do lead to overall higher yields and space efficiency. Our analysis provides justification to increase plantings of loblolly pine to supplement the local forest industry and increase bioenergy in Virginia. However, differences between stakeholder groups constitute a major roadblock to establishment in this region and others like it.

Keywords: *Loblolly pine, Pinus taeda, Timber Waste, CHP, AHP, GIS, Network Analysis, Allocation Location*

PP-36 Effects of ABS (Acrylonitrile Butadiene Styrene) 3D printing plastic on Embryonic Development in a Model of Zebrafish (*Danio rerio*)

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Abstract: Acrylonitrile Butadiene Styrene (ABS) plastic, produced via 3D printing using digital light processing (DLP-ABS) technology, is extensively utilized in various applications. However, there exists a significant gap in research pertaining to the environmental implications of discarded DLP-ABS plastic waste. This investigation aims to assess the toxicity of leachates from DLP-ABS plastic products, referred to as release-ABS, focusing on its embryotoxic effects on zebrafish lines AB and Tg(fli1:EGFP). The concentration of release-ABS was quantified utilizing thermogravimetric analysis (TGA). Toxicological assessments revealed lethal concentration (LC50) at 6.16 µg/mL and effective concentration (EC50) at 5.079 µg/mL, with observed morphological anomalies including hemorrhage, darkened yolk, pericardial edema, hypopigmentation, and tail deformities. Vasculogenic assessment of transgenic larvae indicated that release-ABS adversely affects angiogenesis through the bone morphogenetic protein (BMP) signaling pathway. Furthermore, release-ABS concentrations reached 445 µg/mL after 96 hours of exposure, demonstrating lethality to all embryos. This study highlights the potential environmental risks associated with DLP-ABS plastic waste, emphasizing the urgent need for stringent waste management strategies.

Keywords: Zebrafish, Toxicity, 3D printing, Acrylonitrile Butadiene Styrene, polymer waste.

PP-37 Optimization of the Poloxamer 407-conjugated Gelatin to Synthesize pH sensitive Nanocarriers for Controlled Paclitaxel Delivery

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Abstract: Chemotherapy is one of the most prevalent and efficacious treatments for a wide variety of cancers; however, chemotherapeutic agents have clinically limited applications due to their low water solubility and risk of side effects. Nanomedicine can help to easily deliver hydrophobic and hydrophilic agents for cancer treatment. Here, we describe a nanocarrier system that enables the sustainable and controllable release of hydrophobic anticancer drugs, Paclitaxel, based on poloxamer 407-conjugated gelatin (GeP) copolymers. The particle size, zeta potential, morphology, and thermal stability of the nanogels were characterized. The successful synthesis of nanogels was confirmed by analyzing their chemical components. Among the GePs at different amounts of poloxamer 407, a ratio of gelatin and poloxamer (Ge:P) at 1:15 for preparation resulted in the nanogels being positive in charge, spherical in shape, and 97.84 ± 2.94 nm in hydrodynamic diameter (Dh), with optimal drug-carrying efficacy. The in vitro drug release from nanogels was accelerated in the tumor microenvironment at pH 5.5 in comparison to pH 7.4, and the drug release kinetics from nanogels were due to Fickian diffusion. Finally, the cytotoxicity assays indicated that GePs were biocompatible nanocarriers without toxicity on both normal (VERO) and breast cancer cell (MCF-7) lines, which could improve the pharmacokinetics and pharmacodynamics of paclitaxel. Overall, these results revealed an optimal ratio (1:15) of Ge:P for the synthesis of pH-responsive hybrid nanogels for sufficient paclitaxel releasement to kill MCF-7 for effective cancer treatment.

Keywords: Nanogels, Gelatin, Poloxamer, pH-responsive release, Paclitaxel, Drug delivery.

PP-38 Research and fabrication of nano-particle-incorporated coating films for preserving Dak Lak avocado

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Abstract: In recent years, Vietnamese fruits have seen significant development in terms of production quantity and diversity of types, highly appreciated by most markets. However, due to the perishable nature of tropical fruits caused by natural factors like bacteria, mold, and viruses, long-distance transportation poses a major challenge. Therefore, the development of sustainable fruit and food preservation technologies has attracted considerable attention from economies worldwide. Avocado recognized by the Guinness World Records for its nutritional richness, holds high utilization and economic value. Nonetheless, with its short ripening period of around 7 days, transportation costs increase when exporting to distant markets. In this study, we have developed advanced bio-polymer coatings to extend the ripening time of avocados, thereby reducing the cost escalation during transportation. These bio-polymer coatings are based on the combination of advanced nano-materials such as nano ZnO, and nano Ag, with bio-polymers like Alginate and CMC. Research results indicate that the coating extends the ripening period from 7 days to 35 days, minimizing damage and preserving high nutritional value throughout storage, unlocking the export potential for Dak Lak avocado.

Keywords: *Coating film, CMC, nano-materials*

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