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Gặp gỡ Việt Nam lần thứ 22



4th INTERNATIONAL CONFERENCE ON NANO LIFE SCIENCE: NANO BIOTECHNOLOGY, BIOPHYSICS, COMPUTATION (NanoBioCoM 2026)

ABSTRACT BOOK

September 15 – 18, 2026
ICISE Quy Nhon, Vietnam

SPONSORS/ORGANIZERS

NanoBioCoM2026 is organized and supported by Rencontres du Vietnam, International Centre for Interdisciplinary Science and Education (ICISE), Vietnam; Vietnamese Biophysical Society (VBS), International Union of Pure and Applied Biophysics (IUPAB), Nano Life Science Institute, Kanazawa University, Japan



Welcome Message from the Organizing Committee of NanoBioCoM2026

Dear Esteemed Colleagues, Distinguished Guests, and Participants,

On behalf of the Organizing Committee, it is our privilege to extend our warm welcome to the XXIInd Rencontres du Vietnam: The 4th International Conference on Nano Life Science: Nano Biotechnology, Biophysics, and Computation (NanoBioCoM2026), held at the International Centre for Interdisciplinary Science and Education (ICISE) in Quy Nhon, Vietnam, from September 15–18, 2026.

NanoBioCoM2026 serves as a premier international platform bringing together leading researchers, academicians, and industry pioneers at the forefront of nanobiotechnology, biophysics, and computation in life science. As these converging disciplines continue to redefine the boundaries of molecular life sciences and advanced material design, this conference offers a dedicated forum to share groundbreaking discoveries, discuss paradigm-shifting methodologies, and address global scientific challenges.

Building upon the success of previous editions, our 2026 program features a comprehensive scientific agenda, including plenary, keynote and invited lectures by internationally renowned scholars, thematic oral sessions, interactive poster presentations, and strategic panel discussions focused on international research collaborations and educational advancement.

NanoBioCoM2026 holds a vital mission to empower the rapidly growing local biophysics and nanobioscience community in Vietnam. By facilitating direct engagement with the global scientific community, the conference serves as a catalyst for cross-border knowledge exchange, joint research initiatives, and long-term academic partnerships.

We invite you to actively participate in these enriching scientific discussions, expand your professional networks, and explore novel research synergies. We are confident that the inspiring academic atmosphere of ICISE, set against the coastal beauty of Quy Nhon, will provide an exceptional backdrop for a memorable and impactful conference.

Thank you for your valuable contribution to the success of NanoBioCoM2026.

Warmest regards,

The Organizing Committee

NanoBioCoM2026

Quy Nhon, Vietnam | September 15-18, 2026

Tran Quang Huy Chairman  	Ngo Xuan Kien Chairman  	Tran Thi Thu Hanh Co-Chairman  	Nguyen Bao Quoc Co-Chairman  
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Preface

Over recent years, rapid advancements in artificial intelligence and novel computational-experimental paradigms have fundamentally reshaped the landscape of scientific discovery. The 4th International Conference on Nano Life Science: Nano Biotechnology, Biophysics, and Computation (NanoBioCoM2026) was convened to address these transformative changes, focusing on the core of biophysics - the interdisciplinary frontier where physical laws and biological systems converge to elucidate the mechanistic underpinnings of life. A central challenge driving this year's symposium is bridging the spatio-temporal gap between single-molecule measurements and ensemble-level observations, a crucial step toward pushing the boundaries of nano life science.

Hosted at the International Centre for Interdisciplinary Science and Education (ICISE) in Quy Nhon, Gia Lai province, Vietnam, NanoBioCoM2026 represents our most globally diverse gathering to date. The conference brought together distinguished researchers and emerging scholars representing 13 countries and territories - including Vietnam, Japan, France, Russia, Germany, the United Kingdom, Australia, Kazakhstan, Taiwan, Canada, Thailand, and the United States. Out of numerous submissions, the scientific committee curated a high-impact program comprising 52 plenary, keynote, invited, and oral presentations, alongside 35 interactive poster sessions. This rich diversity of perspectives serves as the cornerstone of our academic dialogue.

At its core, NanoBioCoM2026 aims to integrate experimental breakthroughs with advanced computational frameworks - ranging from atomistic molecular dynamics simulations to machine-learning-driven predictive models - to solve fundamental problems in molecular biology and materials science. For Vietnam, a nation rapidly advancing its research capabilities, this symposium acts as a vital catalyst connecting dynamic local talent with global leaders to foster collaborative initiatives in nanomedicine, biosensing, and computational biology.

We extend our profound gratitude to Prof. Jean Tran Thanh Van, President of Rencontres du Vietnam, and Prof. Le Kim Ngoc for their unwavering leadership and visionary support. We are especially indebted to the Vietnamese Biophysical Society (VBS) for co-organizing the event, the WPI Nano Life Science Institute (NanoLSI) at Kanazawa University for their generous grant supporting, reinforcing our commitment to an inclusive scientific community. Furthermore, we express our sincere appreciation to the International Union of Pure and Applied Biophysics (IUPAB) and WEMBLEY Medical for their invaluable sponsorship and dedicated support of this conference. Finally, we convey our heartfelt thanks to all authors, session chairs, reviewers, and supporting institutions whose collective efforts made this event possible. We look forward to NanoBioCoM continuing its trajectory as a premier international platform for collaborative science.

The Organizing Committee

NanoBioCoM2026

Quy Nhon, Vietnam

September 15–18, 2026

SPONSORS



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VÀ NHIỀU SẢN PHẨM PHỤ TRỢ KHÁC & OTHER PRODUCTS



TÌM HIỂU THÊM THÔNG TIN
SCAN FOR MORE INFORMATION



Lô I-10-7, Đường D7, Khu Công Nghệ Cao, P. Tăng Nhơn Phú, TP.HCM
Lot I-10-7, D7 Street, Saigon Hi-Tech Park, Tang Nhon Phu Ward, HCMC

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The NanoBioCoM2026 Program

DAY 1 Tuesday, September 15, 2026		
7:45 – 8:15	Moving to ICISE from Seagull Hotel by Shuttle Buses	
8:15 – 9:00	Registration	
9:00 – 9:45	Opening ceremony • Welcome speech by Prof. Jean Tran Thanh Van (ICISE) • Speech by a representative of the Department of Science and Technology of Gia Lai Province • Opening speech by the Chairman of NanoBioCoM2026 (Assoc. Prof. Tran Quang Huy) • Group photo	
9:45 – 10:00	Coffee break	
	PLENARY SESSION, HALL 1 Chairs: Assist. Prof. Kien Xuan Ngo and Prof. Arne Gennerich	
10:00 – 10:30	K-01: Ca ²⁺ signals during Enteropathogenic <i>E. coli</i> infection of epithelial cells	Prof. Guy Tran Van Nhieu University of Paris Saclay, France
10:30 – 11:00	K-02: Load-dependent assembly of multi-dynein complexes enhances force generation	Prof. Arne Gennerich Albert Einstein College of Medicine, USA
11:00 – 11:30	K-03: Approaches to the Implementation of Bio-Inspired Vascular Phantoms and Adaptive Biomechatronic Systems for an Anthropomorphic robot-simulator	Prof. Robert Nakibovich Khizbullin Kazan State Power Engineering University, Russia
11:30 – 12:00	K-04: Smart multi-functional nano-biosensors for food safety & environmental monitoring: from fabrication, sensing performance to on-site field-deployable applications	Prof. Anh Tuan Le Phenikaa University Nano Institute, Phenikaa University, Vietnam
12:00 – 13:30	Lunch	

	PLENARY SESSION, HALL 1 Chairs: Prof. Guy Tran Van Nhieu and Assoc. Prof. Nguyen Bao Quoc	
13:30 – 14:00	K-05: How peptide group solvation influences protein folding	Assoc. Prof. Trinh Xuan Hoang Institute of Physics, Vietnam Academy of Science and Technology, Vietnam
14:00 – 14:30	K-06: The actin cytoskeleton before eukaryotes	Prof. Robert Charles Robinson Okayama University, Japan and VISTEC, Thailand
14:30 – 15:00	K-07: Reconstitution of actin cytoskeletal dynamics	Dr. Makito Miyazaki RIKEN Center for Integrative Medical Sciences, Yokohama, Kanagawa, Japan
15:00 – 15:25	I-01: Application of a coarse-grained angular DNA model for evaluating genetic disorders	Prof. Stepan Dzhimak Kuban State University, Russia
15:25 – 15:55	Coffee break	
	PLENARY SESSION, HALL 1 Chair: Assoc. Prof. Trinh Xuan Hoang	
16:00 – 16:40	PL-01: Plasmonic and magnetic nanoparticles for biomedical applications	Prof. Nguyen Thi Kim Thanh University College London, and UCL Healthcare Biomagnetics and Nanomaterials Laboratory, UK
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (HALL 1) Chairs: Prof. Guo-En Chang and Assist. Prof. Tri Thanh Pham	Session 2: Biophysics and Computation (HALL 2, 2 nd floor) Chairs: Assoc. Prof. Tran Thi Thu Hanh and Dr. Quang Quan Nguyen
16:40 – 17:05	IN-02: Nanogold-Linked Waveguide Immunosorbent Assay Achieving Ultra-Sensitive and Rapid Biosensing Prof. Guo-En Chang National Yang Ming Chiao Tung University, Taiwan	IB-02: Calibrated Weighted Rank Aggregation: Learning Target-Adaptive Consensus from Heterogeneous Scoring Modalities in Virtual Screening Assoc. Prof. Ferdinand Molnár Nazarbayev University, Kazakhstan
17:05 – 17:30	IN-03: Quantitative imaging of calcium levels across subcellular organelles using multicolor fluorescence lifetime indicators Assist. Prof. Cong Quang Vu WPI-NanoLSI, Kanazawa University, Japan	IB-03: Computational simulation study of bio-hybrid materials for drug delivery: Fullerene-Chitosan-Fibroin Assoc. Prof. Tran Thi Thu Hanh Ho Chi Minh City University of Technology (HCMUT), VNU-HCM, Vietnam

17:30 – 17:55	IN-04: Plant extracts and natural delivery enhancers have synergistic benefits in inhibiting cancer cell proliferation Assist. Prof. Tri Thanh Pham Nazarbayev University, Kazakhstan	IB-04: Structural basis for alpha-actinin inhibition of cooperative cofilin binding to actin filaments Assist. Prof. Kien Xuan Ngo WPI-NanoLSI, Kanazawa University, Japan
17:55 – 18:15	O-01: Fabrication of PLGA and Chitosan Coated Hesperidin Nanoparticles (PCH-NPs) for the Evaluation of its Anticancer Potential Harshita Tiwari PhD student Institute of Medical Sciences, Banaras Hindu University, India	O-02: Geant4-DNA Simulation of Radiation-Induced DNA Damage in reduced-scale Human Fibroblast Cell model: Quantification of Strand Breaks and Oxidative Base Lesions Khuong Minh Tu PhD student Department of Radiation Science, University of Science and Technology, Korea
18:15 – 18:45	Moving to Seagull Hotel by shuttle buses, free excursion	
DAY 2 Wednesday, September 16, 2026		
8:15 – 9:00	Moving to ICISE from Seagull Hotel by Shuttle Buses, and hanging posters	
	PLENARY SESSION, HALL 1 Chairs: Prof. Hang Ta and Prof. Anh Tuan Le	
9:00 – 9:40	PL-02: Gear ratio of ATP synthase	Prof. Hiroyuki Noji Graduate School of Engineering, The University of Tokyo, Japan
9:40 – 10:10	K-08: Organ-on-chip: Microfluidic models for biomedical applications	Prof. Hang Ta Queensland Quantum and Advanced Technologies Research Institute, Griffith University, Australia
10:10 – 10:40	K-09: Exploring the epigenetic regulation through Fv-Catch	Prof. Yusuke Miyanari WPI-NanoLSI, Kanazawa University, Japan
10:40 – 11:00	Coffee break	
	PLENARY SESSION, HALL 1 Chairs: Prof. Mikihiro Shibata and Prof. Robert Nakibovich Khizbullin	
11:00 – 11:30	K-10: Introduction of nanomedicine delivery based on hybrid materials	Assoc. Prof. Dao Thi Ngoc Anh Graduate School of Integrated Science and Technology, Nagasaki University, Japan
11:30 – 12:00	K-11: Thermal cell engineering: measuring and manipulating heat in cells	Prof. Arai Satoshi WPI-NanoLSI, Kanazawa University, Japan

12:00 – 13:30	Lunch	
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (HALL 1) Chairs: Assist. Prof. Cong Quang Vu and Dr. Pham Thi Huong Quynh	Session 2: Biophysics and Computation (HALL 2, 2 nd floor) Chairs: Assoc. Prof. Ferdinand Molnár and Dr. Makito Miyazaki
13:30 – 13:50	O-03: Smart Near-IR Light-Controlled Drug Delivery Using SDF-1 α -Loaded Chitosan Nanoparticles Coated with Chlorin e6 Dr. Krishnamoorthy Ganesan Department of Chemistry, Indian Institute of Technology Guwahati (IITG), India	O-04: Generative AI for De Novo Design of DNA Origami Dr. Truong Quoc Chien School of Mechanical Engineering, Hanoi University of Science and Technology, Vietnam
13:50 – 14:10	O-05: Strategies for high-yield production of functional recombinant proteins/antibodies Dr. Pham Thi Huong Quynh WPI-Nano Life Science Institute, Kanazawa University, Japan	O-06: Carbon dots: From biophysical mechanisms to biomedical and sensing applications Dr. Nguyen Ba Hung Vietnam Military Medical University, Vietnam
14:10 – 14:35	IN-05: PEG-coated Au nanorods for simultaneous photothermal therapy and CT X-ray attenuation Assoc. Prof. Timur Atabaev Nazarbayev University, Kazakhstan	IB-05: Microtubule lattice tension regulates kinesin force generation Dr. Quang Quan Nguyen Department of Biochemistry and Gruss Lipper Biophotonics Center, Albert Einstein College of Medicine, Bronx, NY 10461, USA
14:35 – 15:00	IN-06: Thiolated Organosilica Nanoparticles for GSH-Activated Intracellular Delivery of Doxorubicin Dr. Balnur Zhaisanbayeva Nazarbayev University, Kazakhstan	IB-06: A simple method for classifying euchromatin and heterochromatin from Hi-C maps providing insights into genome organization Assist. Prof. Takashi Sumikama Graduate School of Biostudies, Kyoto University, Kyoto, Japan

15:00 – 15:25	IN-07: Nano–bio interfaces: Live-cell imaging of surface-functionalized organosilica nanoparticle interactions with cells Assist. Prof. Ellina Mun Nazarbayev University, Kazakhstan	IB-07: Cryo-EM Reveals a Molecular Switch in Late-Stage Maturation of the Human Mitochondrial Respirasome Dr Nguyen Minh Duc Faculty of Pharmacy, Phenikaa School of Medicine and Pharmacy, PhenikaaUniversity, Vietnam
15:25– 15:55	Coffee Break	
	PLENARY SESSION, HALL 1	
15:55 – 16:30	Flash Talk by the poster presenters: odd numbers	
16:30 – 18:00	Poster presentation	
18:00 – 21:30	Cocktails and Gala Dinner	
21:30	Moving to Seagull Hotel by shuttle buses	
DAY 3 Thursday, September 17, 2026		
8:30 – 9:00	Moving to ICISE from Seagull Hotel by Shuttle Buses	
	PLENARY SESSION, HALL 1 Chairs: Prof. Tran Van Hieu and Prof. Stepan Dzhimak	
9:00 – 9:30	K-12: Multiscale self-organization of CaMKII filmed by high-speed AFM	Prof. Mikihiro Shibata WPI-NanoLSI, Kanazawa University, Japan
9:30 – 10:00	K-13: Local bilayer perturbation promotes productive binding and processive hydrolysis by secreted phospholipase A2	Assoc. Prof. Ayumi Sumino Graduate School of Biostudies, Kyoto University, Kyoto, Japan
10:00 – 10:25	I-08: High-Speed Atomic Force Microscopy for Dynamic Nano Life Science: From Molecular Movies to Multimodal Measurements	Dr. Takashi Morii CEO, Research Institute of Biomolecule Metrology Co., Ltd. (RIBM)
10:25 – 10:50	I-09: From Traditional to Modern Platforms: The Evolution of Vietnam's Vaccine Manufacturing Landscape	Assoc. Prof. Nguyen Van Trang National Institute of Hygiene and Epidemiology, Hanoi, Vietnam
10:50 – 11:10	Coffee break	

	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (HALL 1) Chairs: Assoc. Prof. Dao Thi Ngoc Anh and Dr. Mussabek Gauhar	Session 2: Biophysics and Computation (HALL 2, 2 nd floor) Chairs: Dr. Trinh Duy Chi and Dr Nguyen Minh Duc
11:10 – 11:35	IN-10: Nano-sized materials shaping biomedical research Prof. Tran Van Hieu University of Science, Vietnam National University, Ho Chi Minh City, Vietnam	IB-10: Structural and Dynamic Insights into Asgard Tubulin Reveal the Evolution of Microtubules Dr. Tran Thuy Linh RIKEN Center for Integrative Medical Sciences, Kanagawa, Japan.
11:35 – 12:00	IN-11: Lipid-based nanocarriers for targeted drug delivery: applications and challenges Assoc. Prof. Tran Quang Huy Phenikaa University Nano Institute, Phenikaa University, Vietnam	IB-11: Differential growth controls organ curving: experimental and computational approaches Dr. Trinh Duy Chi Department of Life Sciences, University of Science and Technology of Hanoi, Vietnam
12:00 – 13:30	Lunch	
	PARALLEL SESSIONS	
	Session 1: Nano Biotechnology (HALL 1) Chairs: Dr. Krishnamoorthy Ganesan and Dr. Tran Thuy Linh	Session 2: Biophysics and Computation (HALL 2, 2 nd floor) Chairs: Dr. Nguyen Ba Hung and Dr. Tran Ngoc Trang
13:30 – 13:50	O-07: Nanobody Development for Detecting and Inhibiting Botulinum Toxin, Snake Venom Toxins, and the CD26 Lung Cancer Biomarker Dr. Le Thi Hong Nhung Faculty of Biology, VNU University of Science, VNU-Hanoi, Vietnam	O-08: Synergy between ADP and magnesium in the assembly of high molecular weight complexes of 2-cys peroxiredoxin Dr. Tran Ngoc Trang WPI-NanoLSI, Kanazawa University, Japan
13:50 – 14:10	O-09: Functional Carbon Dots: From Surface Engineering to Optical Sensing and Biomedical Applications Dr. Mussabek Gauhar Al-Farabi Kazakh National University, Kazakhstan	O-10: Ontological Validation of Non- Stationary Cardiac Electrodynamics via Pushdown Automata and Topological Invariants in Ultra-Lightweight Edge Architectures Dr. Nguyen Anh Vu University of Medicine and Pharmacy at Ho Chi Minh City, Vietnam

14:10 – 14:30	O-11: Mucoadhesive, antioxidant, and lubricant catechol-functionalized poly(phosphobetaine) as biomaterial nanotherapeutics for treating ocular dryness Dr. Bui Hoang Linh Phenikaa School of Engineering, Phenikaa University, Hanoi, Vietnam	O-12: Distinct Effects of Mechanical Pressure and HepG2 Paracrine Signaling on Hepatic Stellate Cell Activation Dr. Trinh Van-Le Vietnam National University, Ho Chi Minh City, Viet Nam
14:30 – 14:50	O-13: Berberine susceptibility depends on bacterial cell shape rather than Gram type or cell wall architecture Malika Toleubekova PhD student Nazarbayev University, Kazakhstan	O-14: Cation-Substituted Zinc Cobaltite Spinels for Enhanced Electrochemical Sensing Performance of Small Molecules: A Combined DFT and Experimental Study Dr. Ngo Xuan Dinh Phenikaa University Nano Institute, Phenikaa University, Vietnam
14:50 – 15:10	O-15: Investigating lipid sensitivity of ToxA and ToxB toxins causing Acute Hepatopancreatic Necrosis Disease in shrimp using High-speed Atomic Force Microscopy Bui Nguyen Tram Anh Graduate student University of Science, VNU-Ho Chi Minh City, Vietnam	O-16: Computational Investigation of Curcumin/ β -Cyclodextrin Drug Delivery Systems for Potential Cancer Therapy Applications Nguyen Ngoc Thuy Vy Graduate student Ho Chi Minh City University of Technology (HCMUT), VNU-Ho Chi Minh City, Vietnam
15:10 – 15:30	O-17: Within-host evolution of <i>Pseudomonas aeruginosa</i> during antibiotic therapy in fatal ICU infections Vu Dieu Thu PhD student International University, VNUHCM, Ho Chi Minh City, Vietnam	O-18: Topography-Aware Adaptation of Vision Foundation Models for AFM Nguyen Tran Vinh Thuyen Graduate student University of Science, VNU- Ho Chi Minh City, Vietnam
15:30 – 16:00	Coffee Break	
	PLENARY SESSION, HALL 1 Chairs: Assoc. Prof. Tran Quang Huy and Assist. Prof. Kien Xuan Ngo	
16:00 – 16:30	Flash Talk by the poster presenters: even numbers	
16:30 – 18:00	Poster presentation and networking	
18:00–18:30	Moving to Seagull Hotel by Shuttle Buses	
DAY 4 Friday, September 18, 2026 (Mixing session, Hall 1)		
8:30–9:00	Moving to ICISE from Seagull Hotel by Shuttle Buses	

9:00–9:20	<i>The 2nd Vietnamese Biophysical Society (VBS) Annual Meeting:</i> - Opening and keynote remark from VBS president
9:20–9:50	<i>VBS 2026 activities:</i> - Overview of VBS membership - International collaboration, IUPAB activities, publication, conference, award
9:50–10:30	<i>VBS Scientific excellence awards 2026:</i> The winners of the 2026 Outstanding Young Researcher Award and Outstanding Student Award in Biophysics.
10:30–11:20	<i>Award lectures:</i> - 30 min lecture for young researcher award - 20 min lecture for outstanding student award
11:20–12:00	<i>VBS2027:</i> - Priorities & Action Plans
12:00–12:30	Delivering the sponsorship certificate and best poster prize Closing ceremony
12:30–14:00	Lunch
14:00–14:30	Moving to Seagull Hotel by Shuttle Buses
19:00	Dinner and networking (All participants are welcome to join on a cost-sharing basis)

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PLENARY LECTURES

PL-01 Plasmonic and Magnetic Nanoparticles for Biomedical Applications

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Abstract: The development of new chemical methods for the next generation of nanoparticles with very high magnetic moment, fine tuning Au nanorods and novel hybrid and multifunctional nanostructure is presented. Detailed mechanistic studies of their formation by sophisticated and advanced analysis of the nanostructure allows tuning of the physical properties at the nanoscale; these can subsequently be exploited for diagnosis and treatment of various diseases. The studies are conducted to provide insight for future material design approaches. It will also help to identify the critical process parameters that can be manipulated in order to obtain the suitable physical properties for the intended applications such as small iron oxide nanoparticles for T1 MRI contrast agent, magnetic hyperthermia cancer treatment, lateral flow tests for detection of infectious diseases and magnetoelectric nanoparticles for neurological diseases.

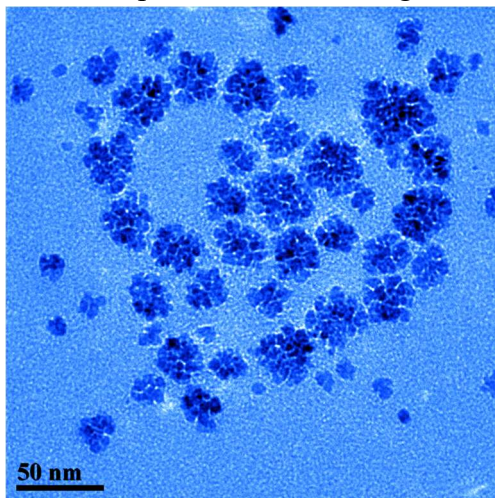


Figure 1. A TEM image of Nanoflowers at 40 k times magnification with outstanding heating efficiencies (ILP of $8.4 \text{ nH m}^2/\text{kg}_{\text{Fe}}$ or $\text{SAR} = 2426 \pm 76 \text{ W/g}_{\text{Fe}}$) measured at a frequency of 488 kHz and a field strength of 25 kA m^{-1} [1, 2].

Reference

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- ^{2.} See more publications here: <https://ntk-thanh.co.uk/publications/>

PL-02 Gear ratio of ATP synthase

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Abstract: ATP synthase is a rotary molecular machine composed of two coupled motors, F_1 and F_o . F_1 motor catalyzes ATP synthesis and hydrolysis, with three ATP molecules synthesized or hydrolyzed per full rotation, whereas F_o motor is driven by proton flow down the proton-motive force and translocates a number of protons per rotation determined by the number of proton-binding c -subunits in its c -ring. Thus, when the two motors are mechanically coupled, the H^+/ATP ratio is determined by the ratio between their rotational reaction stoichiometries. We refer to this coupling stoichiometry as the “**gear ratio**” of ATP synthase. This gear ratio is a critical parameter in cellular bioenergetics because it determines the stoichiometry of energy conversion between the proton-motive force and ATP synthesis. The c -ring stoichiometry varies substantially among organisms, from 8 in mammalian mitochondrial ATP synthase to typically 9–12 in many microorganisms and 12–14 in photosynthetic organisms.

We previously explored whether this gear ratio could be altered by engineering the architecture of ATP synthase. In the canonical F-type ATP synthase, the rotary catalytic machinery is supported by a single peripheral stalk. By artificially increasing the number of peripheral stalks together with the ion-conducting subunit a , we successfully constructed ATP synthases with substantially increased H^+/ATP ratios, demonstrating that the gear ratio of this molecular machine is tunable by structural engineering.

This success in engineering prompted us to further explore alternative architectures of ATP synthase. In doing so, we identified several naturally occurring ATP synthases with unusual gene organizations strikingly similar to those used in our engineered multi-stalk enzymes. Structural and biochemical analyses revealed that these ATP synthases indeed possess multiple peripheral stalks. Thus, an architectural strategy that we had initially developed artificially turned out to have already been explored in nature.

These findings substantially broaden the conventional view of ATP synthase architecture. In addition to the familiar canonical enzyme with a single peripheral stalk, naturally occurring ATP synthases exhibit considerable structural diversity that can alter their energetic coupling and gear ratio. In this presentation, I will describe our engineering approach, the discovery and characterization of naturally occurring multi-stalk ATP synthases, and discuss the physiological and evolutionary implications of diversification in the gear ratio of ATP synthase.

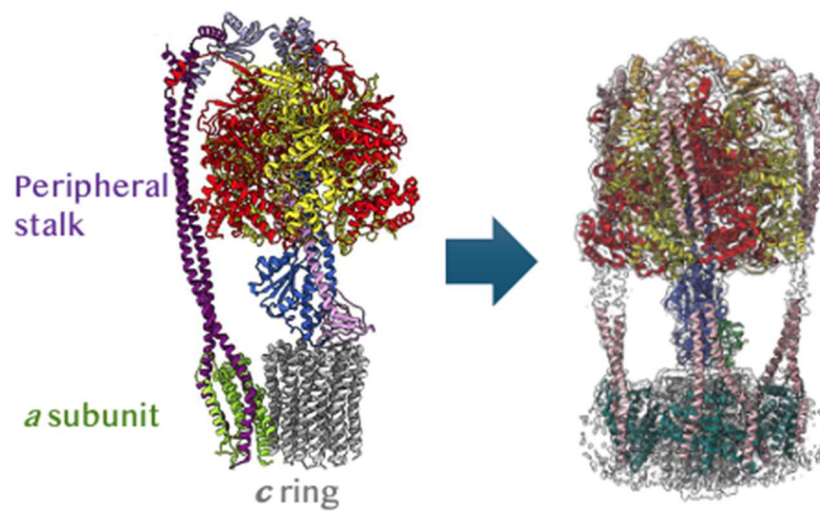


Figure. Engineered ATP synthase with triple peripheral stalks.

Reference

1. Ueno H, Yasuda K, Hamaguchi-Suzuki N, et al. Engineering of ATP synthase for enhancement of proton-to-ATP ratio. *Nature Communications*. 2025;16:5410.

KEYNOTE LECTURES

K-01 Ca^{2+} signals during Enteropathogenic *E. coli* infection of epithelial cells

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Abstract: Enteropathogenic *Escherichia coli* (EPEC) is a major bacterial enteropathogen causing infectious diarrhea among children in developing countries. EPEC infection is associated with inflammation and disruption of the intestinal epithelium integrity through the action of bacterial effectors injected via a type III secretion system (T3SS). Previous works showed that EPEC triggers cytosolic Ca^{2+} increase associated with the death of infected cells. However, the mechanisms underlying this Ca^{2+} -increase, as well as the bacterial effectors involved remain unclear. In this study, we investigated in more details the role of the T3SS translocon in EPEC-induced Ca^{2+} signals at the onset of epithelial cell infection. We found that EPEC induced isolated Ca^{2+} responses triggered by extracellular ATP, likely released via the T3SS pore-forming translocon. These EPEC-induced Ca^{2+} responses showed varying amplitudes and occurred in only a minority of infected cells, suggesting a negative regulation of the T3SS translocon. Consistently, an EPEC mutant strain deficient for EspC, a bacterial secreted protease that negatively regulates the T3SS translocon, elicited a sharp increase in the frequency of Ca^{2+} -responding cells. In addition, we discovered that these Ca^{2+} -responses were preceded by atypical very fast and small global responses with durations of less than 10 seconds and an amplitude not exceeding 5 % of the maximal response. We could detect these small and fast Ca^{2+} responses over extended periods during the first hours of bacterial challenge, in the absence of larger and more classical Ca^{2+} responses. While sharing an amplitude and duration similar to so-called “puff responses”, these EPEC-induced responses did not involve a localized subcellular region, and appeared to result from the coordinated activation of elementary clusters throughout the cell. We hypothesized that this yet unreported Ca^{2+} response pattern was due to Ca^{2+} release associated with low inositol 1,4,5-trisphosphate (IP3) levels, barely sufficient to activate elementary IP3 receptor clusters. In line with this, we observed a similar pattern when cells were stimulated with low ATP concentrations. Computational simulations of a model of Ca^{2+} puffs supported the role of low levels of IP3 in the elicitation of these coordinated puffs. The model predicts that the observed EPEC-induced Ca^{2+} signals result from the synchronised opening of small IP3R clusters that slightly communicate via Ca^{2+} . Our results highlight a major role for ATP release by the T3SS translocon in EPEC-induced Ca^{2+} responses and reveal an original pattern of short and fast Ca^{2+} responses triggered by low ATP concentrations.

Keywords: EPEC, Ca^{2+} signaling, extracellular ATP, NF-kappaB, inflammation

K-02 Load-dependent assembly of multi-dynein complexes enhances force generation

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Abstract: Cytoplasmic dynein drives long-distance transport along microtubules, but how a single motor complex adapts to the mechanical loads it encounters in cells has remained an open question. I will present our discovery that the dynein-dynactin-BicD2 (DDB) complex is not a fixed machine but a load-responsive assembly that changes composition under force. Using optical trapping, multi-color single-molecule fluorescence, and structural approaches, we show that DDB recruits a third dynein under mechanical tension through an auxiliary BicD2 adaptor, forming a tri-dynein complex that nearly doubles the force output of the two-dynein state. This recruitment is gated by Lis1, which prevents force-limiting autoinhibited conformations and increases load-bearing capacity. Our findings establish a new principle in motor biology: that a cytoskeletal motor adapts to load by dynamically changing its stoichiometry, the first such demonstration for any motor protein. These results reframe intracellular transport as an emergent, mechanosensitive process in which motor number, not just motor properties, is tuned to match mechanical demand.

Keywords: *dynein, dynactin, cargo adaptors, KIF5B*

K-03 Approaches to the Implementation of Bio-Inspired Vascular Phantoms and Adaptive Biomechatronic Systems for an Anthropomorphic robot-simulator

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Abstract: The development of highly realistic medical simulators is driven by the necessity to practice complex diagnostic and surgical procedures under conditions as close to clinical practice as possible. Traditional silicone phantoms fail to accurately reproduce the biomechanical properties of living tissues and provide reliable tactile feedback, while creating a fully functional bio-inspired anthropomorphic simulator robot remains an unsolved global challenge. This paper proposes comprehensive scientific and technical solutions to two key problems: non-invasive evaluation of the vascular bed with the selection of biomimetic materials, and the creation of an adequate dynamic model of neonatal motor function.

For non-invasive monitoring of vascular elasticity and hydrodynamic parameters, methods of laser photoplethysmography, pulse oximetry, and pulse transit time (PTT) measurement were applied. The mathematical framework includes the Voigt viscoelastic model, relating volumetric changes to pressure, and the laws of geometrical optics (Beer–Lambert law, refraction, and scattering at biological media interfaces). By adapting the circuit principles of optoelectronic liquid level measurement systems, the theoretical foundations of precision measurement complexes tracking media interface dynamics were developed. Analysis of elastomers revealed a mismatch between commercial materials and native arteries in hydrodynamic and opto-tactile properties, substantiating the need for synthesizing biomimetic polymers for vascular phantoms of simulator robots. A scientifically grounded biomechatronic platform for a neonatal simulator was developed, combining stochastic harmonic synthesis with a microcontroller-based feedback control system.

The study demonstrated the effectiveness of mitigating the impact of actuator mechanical characteristics through 1/f noise generation and dynamic motion profiling. These results lay the groundwork for mass production of high-precision medical simulators and the development of international standards for biomimetic modeling. During the study, the critical task of quantitatively assessing the movement realism of the medical simulator robot was addressed. A methodology based on parametric analysis of limb kinematics was developed and tested. Comparative analysis showed that simulated movement had significantly narrower spectral width and lower trajectory complexity compared to reference samples. These shortcomings are attributed to the structural simplicity of the prototype. Thus, the study highlights the necessity of developing more complex kinematic designs and control algorithms to achieve a high level of movement realism in neonatal medical simulators. The developed approaches can serve as tools for further refinement of medical simulation systems.

Keywords: *Medical simulators, bio-inspired robotics, vascular phantoms, biomimetic materials, neonatal motor function, photoplethysmography, pulse transit time, biomechatronics.*

K-04 Smart Multi-Functional Nano-Biosensors for Food Safety & Environmental Monitoring: From Fabrication, Sensing Performances to On-Site Field-Deployable Applications

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Abstract: Our proposed talk aims to present about recent advances in the smart rapid alert system (SRAS) platforms for field-deployable applications in food control and environmental monitoring. We will provide novel design and operation of two smart sensing platforms based on advanced nanomaterials employed electrochemical and surface-enhanced Raman scattering sensors. The results obtained of sensing responses of these multi-functional nanosensors towards food control and environmental monitoring will be analyzed & discussed. The sensing mechanisms and enhanced detection performances (sensitivity, reliability, selectivity) of these sensing platforms are presented in combination with deep analysis of density functional theory (DFT) & electromagnetic (EM) simulations as well as machine learning (ML) classification algorithm models. Furthermore, the on site field-deployable applicability of these sensing technology platforms will be validated with real samples, i.e., rapid screening for heavy metal ions and pesticides in fruit and vegetable samples with some farms; or rapid detection of volatile organic compounds such as styrene in industrial chemicals manufacturing factories. Finally, the challenges and opportunities of these SRAS platforms for the future in technology transfer and/or commercialization are discussed.

Keywords: *Smart Rapid Alert System (SRAS), Nano-Biosensors; Electrochemical Nanosensors, SERS Nanosensors, Food Control, Environmental Monitoring*

K-05 How peptide group solvation influences protein folding

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Abstract: The aqueous solvent profoundly influences protein folding, yet its effects are relatively poorly understood. In this talk, I will review theoretical and computational approaches to address protein solvation and present our recent study of protein folding using a lattice model that incorporates solvation of the peptide backbone. This study shows that a negative solvation energy, indicating an attraction between a fully exposed amino acid residue and the solvent, substantially enhances folding cooperativity and the correlation between folding rates and the relative contact order (RCO). It is suggested that solvation of peptide groups is a key factor contributing to the extraordinary folding cooperativity and the topology-folding rate dependence observed in two-state proteins.

Keywords: *Protein folding, folding cooperativity, folding rates, native state topology, lattice model, Monte Carlo simulation*

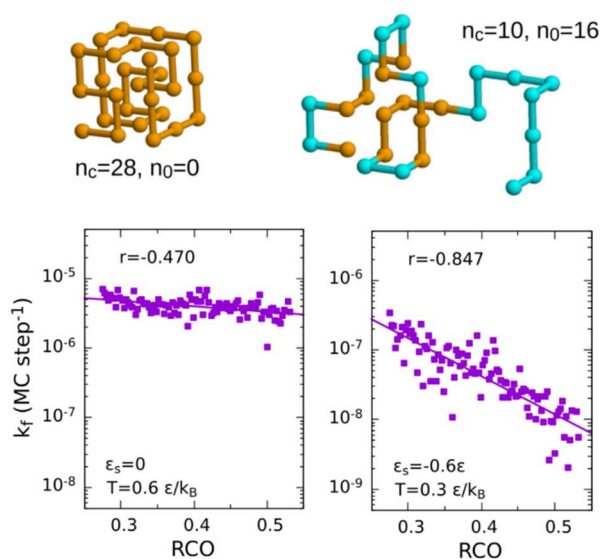


Figure: (Top) Examples of protein conformations in a lattice model with solvation. (Bottom) Dependence of the folding rate on the relative contact order (RCO) of lattice proteins in the models without solvation (left) and with solvation (right).

K-06 The actin cytoskeleton before eukaryotes

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Life on our planet can be divided into two classes of organisms. Firstly, prokaryotes, which are generally microscopic single cellular life forms that comprise bacteria and archaea. Secondly, eukaryotes, which account for most of the living things that can be observed by the naked eye, including plants and animals. The origin of the eukaryotic cell is one of the greatest mysteries in modern biology. DNA sequencing of environmental samples identified a new group of archaea that possess genes that appear to have similarity to distinctive eukaryotic genes. These organisms have been collectively named, Asgard archaea, after the home of the Gods in Norse mythology. Our laboratory has been exploring the properties of some of the protein machines that exist in Asgard archaea and has compared them to the more sophisticated eukaryotic versions. We have focused on the putative cytoskeletal proteins from Asgard archaea, which act as force generating systems in eukaryotes. We have shown that Asgard archaea possess an ancient, regulated actin system, which is likely to integrate force into membrane remodeling processes through directed actin polymerization. These insights into the evolution of the actin cytoskeleton have implications for the potential archaea-to-eukaryotic transition. Asgard archaea offer an intriguing window into the pre-eukaryotic world.

K-07 Reconstitution of actin cytoskeletal dynamics

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Abstract: The actin cytoskeleton plays pivotal roles in regulating key cellular functions, including cell division, motility, and polarity establishment. Decades of ultrastructural and molecular biological studies have elucidated the nanoscale organization, molecular components, and signaling pathways that govern actin cytoskeleton dynamics. However, a major question remains: how do nanometer-scale molecules self-organize into cell-scale structures that generate coordinated biological functions? To address this question, we adopt a bottom-up in vitro reconstitution approach. By reconstructing active actin cytoskeletons inside cell-sized vesicles or on lipid bilayer membranes using purified proteins or cell extracts, we seek to uncover the physical principles governing cytoskeletal self-organization and cell morphogenesis. These minimal cell models allow us to systematically identify the conditions under which cell-scale cytoskeletal structures and functions resembling those of living cells emerge from molecular self-organization. I will present our recent findings on the physical mechanisms regulating cellular mechanics and morphogenesis, followed by a discussion of future research directions.

Keywords: *Cell motility, Cell division, Cell morphogenesis, Artificial Cell, Optogenetics, Self-organization*

K-08 Organ-on-Chip: Microfluidic Models for Biomedical Applications

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Abstract: Atherosclerosis is an inflammatory disorder of blood vessels that is a major cause of death worldwide. Atherothrombosis, an atherosclerotic plaque disruption condition with superimposed thrombosis, is the underlying cause of cardiovascular episodes. Monocyte recruitment and transmigration are crucial in atherosclerotic plaque development. The multi-disease complexities aggravate the situation and continue to be a constant concern for understanding atherosclerosis plaque development. We have developed 3D models mimicking the development of atherosclerosis and thrombosis under static conditions in 96-well plates and under flow conditions in dual-channel microfluidic devices. We have demonstrated that these models could be employed to study disease development, to test efficacy of drugs and nanomedicine, and to evaluate thrombosis risk and treatment strategies. Furthermore, we developed a gut-on-a-chip model based on a five-channel microfluidic device to investigate gut–heart interactions and their role in inflammatory diseases, including their potential contribution to the early development of atherosclerosis.

K-09 Exploring the epigenetic regulation through Fv-Catch

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Abstract: Chromatin is organized in a non-random fashion within 3D nuclear space. During developmental processes, the nuclear architecture is dramatically reconstructed, resulting in the establishment of cell-type specific nuclear organization. Defects in the structural components of the nucleus are responsible for developmental aberrations and several human diseases. Remodelling of the nuclear architecture and epigenetic information leads to spatial arrangement of genes, which could affect genome functions including gene expression. We aim to reveal the role of chromatin dynamics in cell lineage-allocation by deciphering the molecular mechanisms underlying the remodelling of nuclear organization and their effects on developmental gene expression, using mouse early embryos and embryonic stem (ES) cells as model systems. I will present our recent studies to show you how we tackle our questions.

Keywords: *Epigenetics, recombinant antibody*

K-10 Introduction of Nanomedicine Delivery Based on Hybrid Materials

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Abstract: For the last few decades, drug delivery research and practice have been intensively involving nanotechnology to advance the creation of multifunctional drug carriers, and often employed in combination cancer therapy, in which it can accomplish targeting a tumor, delivering therapeutic molecules, imaging and monitoring drug response. Many models were built and tested; still the challenge is at the choice of the appropriate materials and the facilitation of carrier preparation to achieve both safety and efficacy. Reflecting such needs, silk protein was chosen to provide a biodegradable and biocompatible matrix for dispersing noble metallic nanoparticles, as a modifier, and drug molecules, as a therapeutic agent. Such systems with controllable structures and compositions can be an advanced type of drug carriers and further contribute to the improvement of cancer therapy.

In our research, silk nanoparticles (NPs) were obtained in uniform morphology, with the size can be tuned from 10 to 100 nm. The surface charges of as-synthesized silk nanoparticles can be either negative or positive, depending on the characteristics of the dope solution, bringing out the possibility of loading different types of drugs. The obtained silk NPs showed good drug uptakes, adequate stability in aqueous and almost no toxicity at cellular level. When gold NPs, the first tested model for noble metals, is incorporated into a silk matrix, the obtained hybrid structure showed assemble properties to those mentioned above. Moreover, gold/silk NPs also show dual pH- and photothermal-responsive drug release behavior. This presentation focuses on our recent results in the establishment of multifunctional Au/silk NPs for delivery, imaging and targeting in cancer treatment, while further investigation is needed on controlling the composition and surface properties of Au/silk NPs.

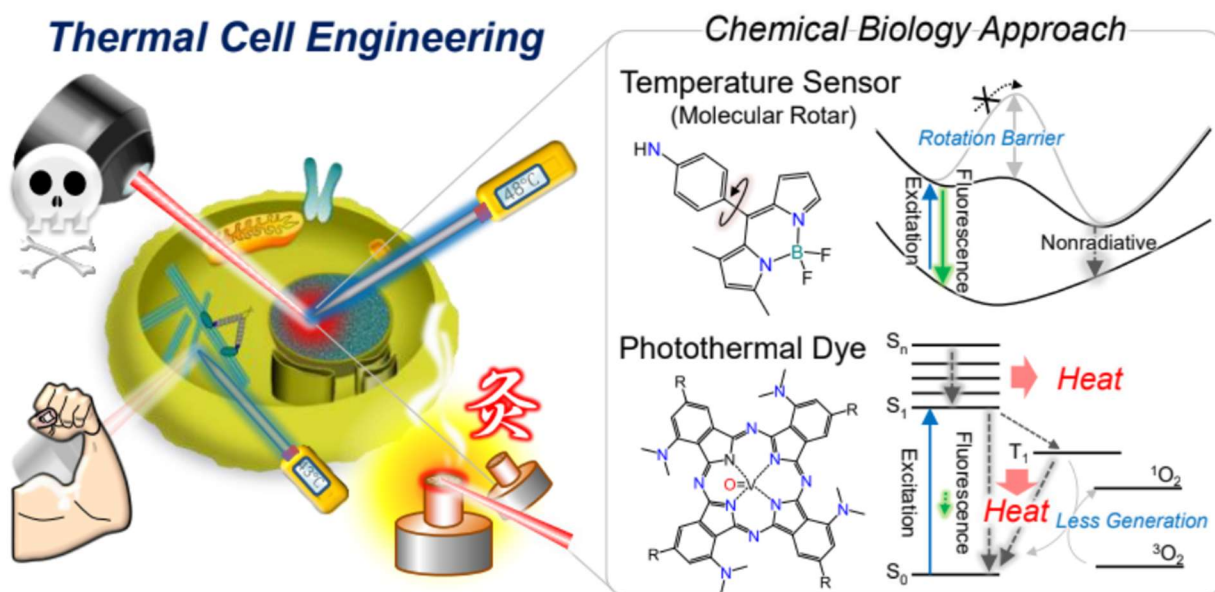
Keywords: *noble metal, drug delivery, cancer therapy*

K-11 Thermal Cell Engineering: Measuring and Manipulating Heat in Cells

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Abstract: Temperature is a fundamental physicochemical parameter that governs various cellular processes. Understanding and controlling their behavior requires technologies capable of measuring and manipulating temperature at the nano- and microscale. We have developed functional dyes whose fluorescence lifetime responds strongly to temperature and applied them to quantitative thermometry in organelles, including mitochondria and the endoplasmic reticulum. This talk will highlight thermogenic cells, such as brown adipocytes and skeletal muscle cells. We have also developed photothermal dyes that generate localized intracellular heat upon near-infrared irradiation. By targeting these dyes to specific subcellular regions, heat can be delivered locally without heating the entire cell or surrounding medium. Using this approach, we found that the behavior of heat shock factor 1 (HSF1) depends on the spatial pattern of heat input. We are further investigating the cellular changes that occur following the formation of nuclear HSF1 foci. Together, these manipulation technologies constitute an emerging framework that we term “thermal cell engineering.”



Keywords: Fluorescence Lifetime Imaging, Thermodynamic Cell Engineering, Functional Dyes

K-12 Multiscale self-organization of CaMKII filmed by high-speed AFM

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Abstract: CaMKII is among the most abundant proteins at excitatory postsynapses and is central to long-term potentiation. Two structural questions about the ring structure of its dodecameric holoenzyme remain open: how individual subunits behave within a single ring, and how holoenzymes interact with one another in the crowded interior of a dendritic spine. High-speed atomic force microscopy can address both, capturing single proteins in solution at nanometer resolution and in real time. We first examined α/β heterododecamers assembled at the 3:1 forebrain ratio. Individual subunits could be identified from the mobility of their kinase domains, revealing that β subunits occupy adjacent positions within the ring rather than being randomly distributed. Upon $\text{Ca}^{2+}/\text{CaM}$ binding, these neighbouring β subunits formed long-lived kinase-domain complexes that lowered kinase activity while prolonging the activated conformation [1]. At densities approaching those reported for the postsynaptic density, holoenzymes further self-organize into chain-like clusters through kinase-domain contacts, expanding upon activation, whereas a variant linked to intellectual disability clustered extensively even in the basal state [2]. Together, these results show how CaMKII organizes itself, from single subunits to assemblies of several hundred nanometers. [1] Matsushima, K. *et al. Nat. Commun.* **16**, 10603 (2025). [2] Suzuki, T. *et al. Sci. Adv.* (2026), in press.

Keywords: high-speed AFM, CaMKII, single-molecule imaging, self-assembly, synaptic plasticity

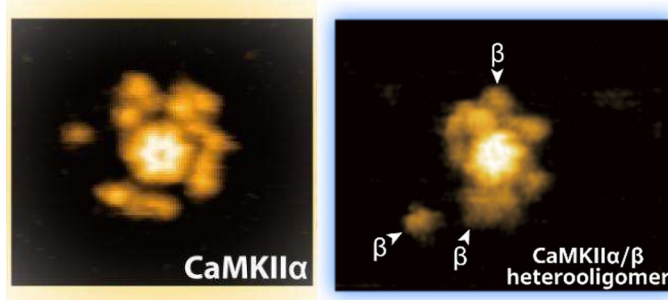


Figure: High-speed atomic force microscopy images of CaMKIIα homooligomers (left) and CaMKIIα/β heterooligomers (right). These images were taken at 3.3 frames/second.

K-13 Local bilayer perturbation promotes productive binding and processive hydrolysis by secreted phospholipase A2

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Abstract: Secreted phospholipase A2 (sPLA2) enzymes hydrolyze phospholipids at membrane interfaces and mediate diverse biological processes. However, how these soluble enzymes select productive regions of lipid bilayers and sustain catalysis remains unclear. Here, we show that local bilayer perturbation, characterized by expanded lipid headgroup spacing, enables sPLA2 binding and processive hydrolysis. Using high-speed atomic force microscopy (HS-AFM), we observed concentration-dependent degradation of supported lipid bilayers. Hydrolysis initiated primarily from membrane edges and showed an apparent nanomolar affinity for edge-associated hydrolysis. In contrast, molecular dynamics (MD) simulations showed that sPLA2 did not stably associate with intact planar bilayers even under high effective enzyme concentrations, whereas nearly all sPLA2 molecules stably bound to membrane edges within 2 μ s. We further found that melittin, a membrane-perturbing amphipathic peptide, enabled hydrolysis from planar bilayer regions without changing the hydrolysis rate at pre-existing edges. This result indicates that bilayer perturbation promotes productive sPLA2 binding rather than accelerating the catalytic cycle itself. MD simulations also showed that edge-bound sPLA2 can recruit phospholipids into the active site without forced substrate insertion. Quantitative analysis of HS-AFM movies allowed us to estimate that each bound sPLA2 molecule hydrolyzes approximately 40 phospholipids per binding event. Together, these findings suggest that sPLA2 exploits locally perturbed membrane states as high-affinity productive reaction sites. Local bilayer perturbation may therefore serve as a physiological cue for sPLA2 activation at curved, remodeled, damaged, or protein-perturbed biological membranes.

Keywords: Phospholipase, Lipid bilayer, Melittin, High-speed atomic force microscopy, Molecular dynamics simulation

INVITED TALKS

I-01 Application of a Coarse-Grained Angular DNA Model for Evaluating Genetic Disorders

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Abstract: Torsional and tensile stresses, as well as local bends in the DNA structure, can serve as signals for triggering various cellular processes, including transcription, DNA repair, and chromatin remodeling. At the same time, DNA bends can influence the rate and pattern of mutagenesis in the genome, thereby affecting gene expression and the accessibility of DNA to enzymes. Open states arising from mechanical stresses in DNA play an important role in transcription and replication, as well as in DNA–protein recognition during nucleic acid repair.

The angular model of the DNA molecule is based on an analogy between the double-stranded DNA molecule and a mechanical system consisting of two chains of coupled pendulums. It is described by a system of ordinary differential equations for the angular deviations of the pendulums. This system is solved numerically.

Furthermore, the angular model allows calculation of the sites of mechanical energy localization in the DNA molecule under external perturbation, thereby enabling prediction of the nucleation sites of open states.

Further development of the model has made it possible to link the dynamics of open states to alterations in the ATXN2 gene, which is responsible for several neurodegenerative diseases. It has been shown that additional open-state zones of various sizes can form in the expanded CAG-repeat region. The frequency of occurrence of large additional zones increases with CAG-tract expansion. It was found that the inverse of this frequency correlates with the dependence of the mean age of disease onset.

It has been shown that, in the range of weak torsional perturbations, additional bends appear in the ATXN2 gene within the expanded CAG-tract region. Thus, the expanded CAG-tract region constitutes a "hot spot" in which effects distinct from those in the normal gene are observed under external perturbation.

The dynamics of collective conformational changes in the APOE and COL4A1 genes under an external torsional moment have been investigated. It was found that even weak torsional perturbation leads to the formation of regions with similar collective states and bends. Calculations revealed a clear dependence of the formation of these states on both the magnitude of the external perturbation and the nucleotide sequence.

The dynamics of collective conformational rearrangements in the IL1RN gene (encoding the interleukin-1 receptor antagonist (IL-1Ra), a key anti-inflammatory protein) under an external

torsional moment have been studied. It was shown that torsional perturbation with small values of the twisting moment applied to the gene containing a mutation (an extra segment of 86 nucleotides) leads to the formation of bend regions distinct from those in the normal gene.

Mutations in the APP gene lead to the development of Alzheimer's disease. It was found that single-nucleotide mutations (London and Florida) affect neither the conformational pattern of the DNA segment nor the formation and dynamics of open-state zones. The double-nucleotide Swedish mutation of the APP gene influences the propensity of the mutated DNA region to form open states; in particular, in APP^{swe}, the characteristic nucleation zones for open states to the right of the mutated nucleotide site are absent.

Funding: The work was supported by the Ministry of Science and Higher Education of the Russian Federation for conducting scientific research jointly with Cuban organizations (Agreement No. 075-15-2025-283 dated 04/28/2025).

Keywords: *Coarse-grained DNA mathematical model, IL1RN gene, APP gene, ATXN2, APOE and COL4A1 genes, open states of DNA, trinucleotide repeat diseases, gene bends*

IN-02 Nanogold-Linked Waveguide Immunosorbent Assay Achieving Ultra-Sensitive and Rapid Biosensing

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Abstract: We demonstrate a cost-effective waveguide-enhanced nanogold-linked immunosorbent assay (WENLISA) based on nanoplasmonic waveguide biosensors for the rapid and sensitive detection of procalcitonin (PCT), a sepsis-related inflammatory biomarker. The WENLISA biosensor comprises a suspended glass planar WG on a glass substrate integrated with a microfluidic channel fabricated using simple, cost-effective, and vacuumless processes.²⁶ In addition, to enhance the LOD to meet the clinical requirements for PCT detection, we introduced a new sensing strategy using gold nanoparticles (AuNPs) with a unique sandwich architecture. The AuNPs not only significantly modify the distribution of the evanescent wave of the guided mode within the WG but also induce strong resonance of AuNP plasmon modes to significantly enhance absorption near the PCT biomarker. Consequently, the concentration of the biomarker to be detected can be converted to the transmitted light intensity of the WG, which is modulated by the absorption of evanescent waves to achieve ultrasensitive and rapid PCT detection. The biosensing experiments revealed excellent PCT sensing performance with a record-low LOD of 48.7 fg/mL (3.74 fM), low nonspecific adsorption, and a short detection time of ~8 min. Most importantly, we successfully verified the capability of WENLISA to accurately detect and quantify PCT levels in clinical samples by testing blood samples from both healthy individuals and patients with sepsis.

Keywords: *Photonic Crystal, Gold nanoparticle, Reflection, Localized Surface Plasmon Resonance, Digital-Resolution Biosensing.*

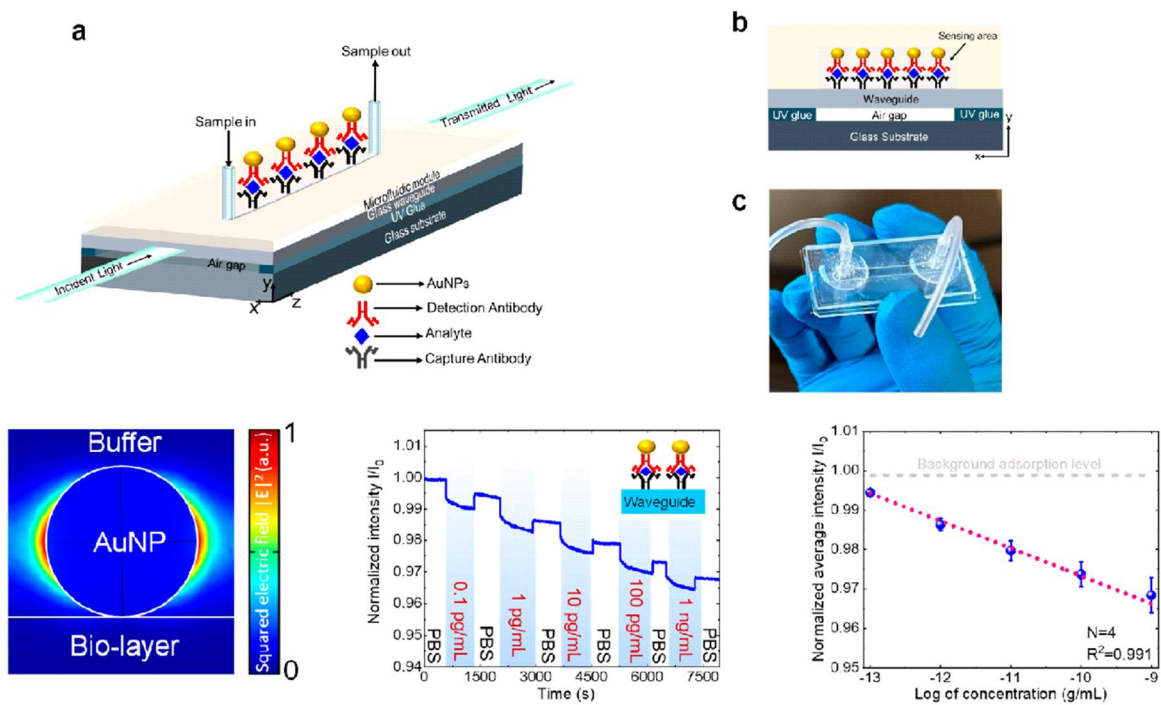


Figure: (a) 3D schematic diagram and (b) cross-section of the proposed WENLISA biosensor. (c) Optical image of the fabricated sensor. (d) Simulated squared electric field distribution of AuNP at $\lambda = 521.5$ nm. (e) Real-time responses for serial sample injections at different PCT concentrations. (f) Calibration curve for normalized intensity as a function of PCT concentration. T

IB-02 Calibrated Weighted Rank Aggregation: Learning Target-Adaptive Consensus from Heterogeneous Scoring Modalities in Virtual Screening

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Abstract: Virtual screening must prioritize a handful of compounds from very large libraries, yet the many available scoring methods disagree, use incompatible scales, and even point in opposite directions, so the common equal-weight consensus leaves performance on the table. I will present Calibrated Weighted Rank Aggregation (CWRA), a data-driven framework that direction-corrects and normalizes eleven heterogeneous modalities, spanning machine-learning affinity predictors, structure-based scoring, and ligand similarity, then learns nonnegative fusion weights from known actives by optimizing an early-recognition objective. On de novo generated libraries for the vitamin D receptor, CWRA more than doubles very-early enrichment over equal-weight fusion and outperforms the strongest single predictor, with target-specific recalibration reproducing these gains on the mechanistically distinct GABA-A receptor. I will discuss the method, its benchmarking, and what the learned weights reveal about complementarity among physical and learned scoring signals.

Keywords: *Drug discovery, Generative AI, Virtual screening, Consensus scoring*

IN-03 Quantitative imaging of calcium levels across subcellular organelles using multicolor fluorescence lifetime indicators

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Abstract: Real-time quantification of the second messenger calcium ion (Ca^{2+}) is essential for understanding its roles in cellular signaling. Genetically encoded fluorescence lifetime-based calcium indicators enable robust and quantitative imaging of Ca^{2+} using fluorescence lifetime imaging microscopy (FLIM). However, currently available FLIM-based Ca^{2+} indicators are largely limited to measurements in the cytosol. Ca^{2+} concentrations span several orders of magnitude across subcellular compartments, ranging from 10^{-8} – 10^{-7} M in the cytosol, 10^{-7} – 10^{-6} M in mitochondria, 10^{-5} – 10^{-3} M in endoplasmic reticulum (ER), and 10^{-3} – 10^{-2} M in the extracellular space. FLIM-based Ca^{2+} indicators spanning nanomolar-to-millimolar concentrations across subcellular compartments are needed. Here, we introduce a family of green, red, and cyan FLIM-based Ca^{2+} indicators (FLIM-Ca-G/R/C) for quantitative measurement of Ca^{2+} across multiple subcellular compartments, including the cytosol, mitochondria, ER, and extracellular space. Using FLIM-Ca-G/R/C, we measured consistent Ca^{2+} levels in the cytosol, mitochondria, and ER of HeLa cells across spectrally distinct variants. We further demonstrated multiplexed imaging of Ca^{2+} dynamics in the cytosol, mitochondria, and ER within single cells in response to different drug stimulations. Finally, we achieved simultaneous multiplex FLIM imaging of Ca^{2+} , ATP, and lactate using different color fluorescence lifetime-based indicators. **Keywords:** Ca^{2+} , genetically encoded Ca^{2+} indicators, FLIM, multiplex imaging

IB-03 Computational simulation study of bio-hybrid materials for drug delivery: Fullerene-Chitosan-Fibroin

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Abstract: In the context of drug delivery systems (DDS) playing an increasingly crucial role in modern biomedicine, the development of biohybrid materials capable of effectively combining structural stability, biocompatibility, and controlled drug loading and release is becoming a widely pursued research direction. Stemming from this need, this study focuses on the design and investigation of a Fullerene–Chitosan–Fibroin (FCF) biohybrid material system for DDS applications, with curcumin selected as the model drug, through multi-scale computational simulation methods. The core objective of the study is to build a comprehensive computational modeling framework to elucidate the interaction mechanisms at the atomic level, while evaluating the structural stability and the encapsulation and release capabilities of the FCF system under physiological pH conditions.

Keywords: *Drug delivery, biohybride, fullerene, in silico, chitosan, fibroin, simulation, pH conditions.*

IN-04 Plant extracts and natural delivery enhancers have synergistic benefits in inhibiting cancer cell proliferation

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Abstract: In traditional Chinese and Ayurvedic medicine, plant compound extracts like curcumin and berberine have been utilized to treat infections and digestive problems. These substances have demonstrated strong antibacterial properties and the ability to fight cancer by inhibiting the proliferation of tumor cells and triggering program cell death. Our preliminary screening appears to indicate that berberine is only efficient at inhibiting most cocci bacteria and is less effective against bacilli. Partial inhibition of bacilli is comparable with previously documented berberine-induced cell elongation, as elongating cells continue to gain optical density. However, cocci rely on the divisome machinery for nearly all peptidoglycan synthesis. Cell viability experiments utilizing the Presto Blue assay show that berberine and the delivery enhancer work synergistically to prevent cancer cell proliferation. Our findings indicate that co-administration of plant extracts with a delivery enhancer can boost their efficacy in preventing cancer cell proliferation. Our findings highlight the potential of delivery enhancers in assisting plant extracts in fighting cancer more effectively.

IB-04 Structural basis for alpha-actinin inhibition of cooperative cofilin binding to actin filaments

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Abstract: Actin is a conserved cytoskeletal protein essential for morphogenesis, motility, and division. Its versatility arises from filament assembly and regulation by actin binding proteins. Among these, alpha-actinin organizes filaments into bipolar or unipolar networks, whereas cofilin binds preferentially to ADP-actin regions and forms clusters to shorten the half helical pitch (HHP). Here, we investigated the molecular mechanism of how alpha-actinin alters filament and protomer conformations and influences cofilin binding. Using all-atom molecular dynamics simulations, principal component analysis, and high-speed atomic force microscopy, we show that alpha-actinin crosslinking stabilizes actin filaments in the canonical helical state, thereby preventing the cofilin-induced helical shortening required for cooperative filament decoration. Stabilization occurs without significant changes in protomer twist and rise and subdomain geometry and maintains a flattened protomer conformation that restricts twisting needed for cofilin cooperative binding. By contrast, the isolated alpha-actinin-1 actin binding domain mutant (ABD-E235K), comprising two calponin homology domains (CH1-CH2), transiently binds to actin filaments and induces local transitions from the canonical double-helical filament to the single- and parallel-helical protofilament states, weakly affecting cofilin binding and cluster formation through a distinct structural and binding mechanism. Together, these findings reveal a mechanistically distinct function of full-length alpha-actinin and its isolated ABD and support a stepwise mechanism in which cooperative cofilin binding to double-helical actin filaments requires initial binding to actin regions with shortened HHP, followed by protomer twisting and further helical shortening. By stabilizing the canonical filament architecture or perturbing filament organization, alpha-actinin suppresses these structural transitions and thereby perturbs cofilin cooperativity.

Keywords: *Alpha-actinin, calponin homology domain, actin, cofilin, myosin II, unipolar and bipolar models, HS-AFM, all-atom MD simulations, PCA.*

IN-05 PEG-coated Au nanorods for simultaneous photothermal therapy and CT X-ray attenuation

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Abstract: Gold nanorods (Au NRs) combine strong near-infrared (NIR) photothermal conversion with high X-ray attenuation, making them attractive candidates for cancer theranostic applications. In this study, PEG-coated Au NRs (PEG-Au NRs) were synthesized using a wet-chemical method and evaluated as potential agents for photothermal therapy and computed tomography (CT) imaging. The PEG-Au NRs (Figure 1) exhibited a pronounced plasmonic absorption band centered at approximately 800 nm, and irradiation with an 808 nm LED lamp rapidly increased their temperature from room temperature to approximately 60 °C within 5 min. Furthermore, CT measurements demonstrated that PEG-Au NRs produced approximately 2.6-fold higher X-ray attenuation than the commercially available iodinated contrast agent iopromide. In vitro experiments using normal CCD 841 and cancerous SW480 cell lines under dark conditions and 808 nm LED illumination demonstrated that PEG-Au NRs exhibit efficient photothermal activity and can effectively induce cancer cell killing upon NIR irradiation. These findings highlight the potential of PEG-Au NRs as dual-functional nanomaterials for NIR-triggered photothermal therapy and localized CT imaging.

Keywords: *Gold nanorods, PEG coating, photothermal agent, cytotoxicity, cancer cells deactivation*

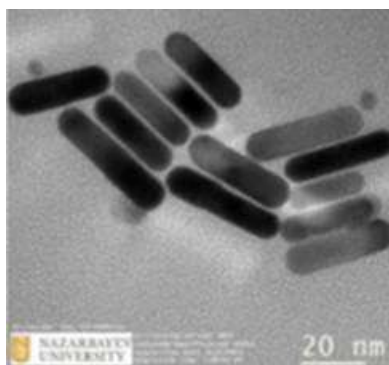


Figure 1: TEM image of PEG-Au NRs

IB-05 Microtubule lattice tension regulates kinesin force generation

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Abstract: Microtubule-based kinesin motors drive intracellular transport and mitotic spindle organization by converting chemical energy into mechanical work. Although kinesins are often treated as autonomous force-generating machines, whether their activity is influenced by the mechanical state of the microtubule track has remained unclear. Here we show that tension within the microtubule lattice itself regulates kinesin force production. By systematically decoupling vertical loading, microtubule attachment constraints, lattice spacing, and axial tension, we find that vertical forces primarily affect stalling kinetics, whereas axial lattice tension suppresses kinesin force generation. Weakly constrained microtubules support higher force output by both KIF1A and KIF5B, whereas rigid attachment or axial loading reduces motor performance. Measurements of motor binding kinetics further reveal that increasing lattice tension weakens kinesin–microtubule affinity over a finite force range. Together, these findings identify the microtubule lattice as an active mechanical regulator of motor function and reveal that the mechanical state of the microtubule track is a major determinant of kinesin force production.

Keywords: *microtubule lattice tension, kinesin, KIF1A, KIF5B*

IN-06 Thiolated Organosilica Nanoparticles for GSH-Activated Intracellular Delivery of Doxorubicin

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Abstract: Nanomedicine offers a powerful strategy to enhance therapeutic efficacy through selective drug delivery and reduced systemic toxicity compared to conventional chemotherapy. In this study, we developed a redox-responsive thiolated organosilica nanoparticle (Si NP–SH) platform for glutathione (GSH)-triggered drug release in tumour-like intracellular environments. Doxorubicin (DOX), a clinically established fluorescent chemotherapeutic agent, was selected as a model drug for conjugation studies. DOX was conjugated to SiNP–SH through a cleavable disulfide bridge, aiming to achieve stable bonding under extracellular conditions and accelerated release under elevated intracellular GSH concentrations typical of tumour cells. The resulting DOX–nanoparticle conjugates were successfully synthesised and characterised to confirm surface functionalisation and redox-responsive behaviour. Drug release experiments demonstrated enhanced DOX release under reducing conditions, supporting the mechanism of disulfide bond cleavage by GSH. In vitro viability studies on tumor cells demonstrated that released DOX retained potent cytotoxic activity.

Overall, these findings highlight the potential of thiolated organosilica nanoparticles as biofunctional and therapeutic nanomaterials for intracellular, tumour-selective drug delivery, offering a promising strategy to improve the efficacy and safety profile of anticancer therapies.

Keywords: *organosilica, thiolated nanoparticles, doxorubicin, glutathione, redox-responsive release*

IB-06 A simple method for classifying euchromatin and heterochromatin from Hi-C maps providing insights into genome organization

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Abstract: I will briefly present our recent progress in collaborative research combining simulations and modeling with atomic force microscopy (AFM) measurements. Then, I will focus on a simple approach to discriminate between euchromatin and heterochromatin based on Hi-C maps. Hi-C is a technique to map contact frequencies between pairs of loci in chromosomes. Plaid patterns in Hi-C are related to heterochromatin (B compartment) and euchromatin (A compartment) regions. The conventional classification procedure of A/B-compartment using principal component analysis (PCA) has appeared to work well; however, it is complicated to intuitively understand why it works and so it does not give any insights into the structural information of A/B compartments. We proposed a new intuitive metric called scaled contact frequency (SCF), which is the summation of columns of Hi-C in a chromosome normalized by the average of the averaged summation of columns in whole chromosomes. Notably, SCF gave clear insights into chromatin organization, which was not obtained by the previous classification based on PCA: euchromatin is the region in more contact than average, while heterochromatin is less. To validate SCF, we estimated the ratio of euchromatin using H3K36me3 histone mark and compared it with those obtained by PCA and SCF. The correlation coefficients between the euchromatin ratios estimated by H3K36me3 histone mark and PCA were almost 0, while those between H3K36me3 and SCF were close to 0.8. Thus, the conventional analysis seemingly works well, but is not accurate enough to be used for estimating the euchromatin ratio. Therefore, a new metric, SCF, is better to estimate euchromatin regions and provides a comprehensive insight into euchromatin organization.

Keywords: *Hi-C, principal component analysis, scaled contact frequency*

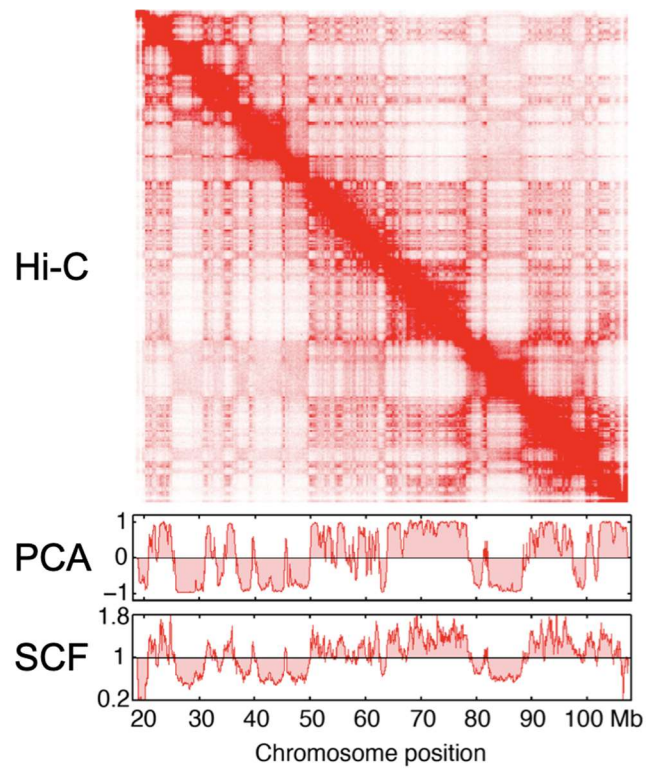


Figure: *Hi-C map, and eigenvector analyzed by PCA and SCF values.*

IN-07 Nano–Bio Interfaces: Live-Cell Imaging of Surface-Functionalized Organosilica Nanoparticle Interactions with Cells

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Abstract: Over the past few decades, nanoparticles have been attracting significant attention from researchers in chemical, biomedical and pharmaceutical sciences, due to their unique physicochemical properties. While significant progress has been made on synthetic methodologies of nanoparticles, investigation of their mechanical properties, composition and functionality, their biological behaviors and theranostic performances remain at the preliminary level and poorly investigated. As a consequence, the current focus in the development of nanoparticles has been shifted from synthetic methodologies to studying the downstream of their applications in vivo favoring medical advances, including microscopic characteristics, as very little is known in this front. Understanding how nanoparticle surface chemistry governs cellular interactions is critical for the rational design of nanomedicines.

Our work focuses on developing functionalized organosilica nanoparticles (thiolated, PEGylated, functionalized with cell-penetrating and tumor-targeting peptides) and generating valuable datasets using multidisciplinary approach integrating chemistry, materials science, biology, biophysics and biomedical engineering towards comprehensive analysis and understanding of the interaction of modified organosilica nanoparticles with biological systems. We present a systematic investigation of organosilica nanoparticles bearing distinct surface functionalities and their interactions with living cells, monitored in real time using live-cell imaging. This was persuaded through measuring the biophysical and biomechanical parameters of normal and cancer cells for analysis and characterization of the behavior of both cell types in response to application of organosilica nanoparticles. Also, the *Drosophila* neural stem cells or neuroblasts, the precursors of the fly's central nervous system, were used as an excellent model for addressing the effect of various compounds on biophysical and biomechanical properties of the cell.

By correlating surface chemistry with biophysical and biomechanical properties of the cell, this approach provides direct visual and quantitative insights into nano–bio interfaces that are inaccessible through endpoint assays. Live-cell imaging emerges as a powerful tool for elucidating structure–interaction relationships, enabling a more mechanistic understanding of how surface functionalization modulates nanoparticle behavior at the cellular level.

Keywords: *organosilica, nanoparticles, live-cell imaging, surface functionalization.*

IB-07 Cryo-EM Reveals a Molecular Switch in Late-Stage Maturation of the Human Mitochondrial Respirasome

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Abstract: Mitochondria produce most of the energy required by human cells through nanoscale protein machines embedded in their inner membranes. Several of these machines associate to form a larger structure known as the respirasome, which transfers electrons, pumps protons, and supports ATP production. Although the architecture of the respirasome is increasingly well understood, how its assembly is completed has remained unclear. Here, we combined cryo-electron microscopy and biochemical experiments to visualize late stages in the assembly of the human respirasome. Our structures captured several molecular states of complex IV, the component that transfers electrons to oxygen. These states reveal a sequential exchange between two small proteins, HIGD2A and NDUF4A. HIGD2A first occupies a binding site in complex IV and maintains the protein machine in an assembly-ready state. NDUF4A subsequently enters the same region, displaces HIGD2A, and completes the maturation of complex IV within the respirasome. This work illustrates how cryo-electron microscopy and computational classification can reconstruct a dynamic biological assembly pathway from a heterogeneous population of molecular particles. The findings provide a mechanistic framework for understanding how human respiratory nanomachines are assembled and how failures in their final maturation may contribute to mitochondrial disease.

Keywords: Cryo-EM, Mitochondria, Respirasome, Supercomplex, Assembly factor.

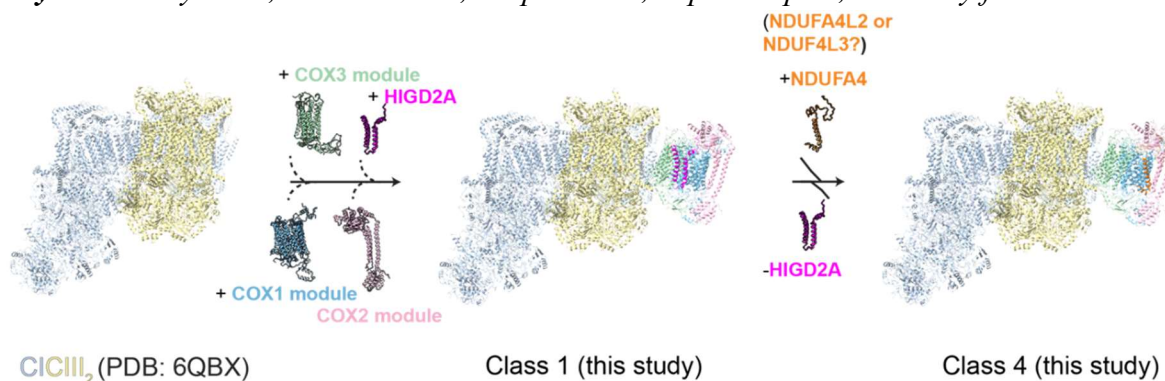


Figure: Proposed model for the assembly of CIV within the respirasome $CI + CIII_2 + CIV$, based on the existing models and this study. CI and CIII are shown as light steel blue and yellow, respectively. Multiple intermediate steps might exist between the $CI + CIII_2$ state and the class 1 (this study) state. The order of assembly of the COX modules into $CI + CIII_2$ has not been elucidated yet. The proteins from COX1, COX2, and COX3 modules are shown as light blue, light pink, and green, respectively. The HIGD2A and NDUF4A (or alternatively NDUF4A4L2 or NDUF4A4L3) are shown as magenta and orange.

I-08 High-Speed Atomic Force Microscopy for Dynamic Nano Life Science: From Molecular Movies to Multimodal Measurements

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Abstract:

Background: Many biomolecular events, such as conformational changes and motor stepping, occur on millisecond-to-second time scales. Conventional atomic force microscopy (AFM) provides nanometer-scale topography in liquid, but its slow imaging speed precludes direct observation of rapid biomolecular events. High-speed AFM (HS-AFM) overcomes this limitation, enabling real-time visualization of molecular structure and dynamics under near-physiological conditions.

Methods: HS-AFM combines small cantilevers with high resonance frequencies and low spring constants, fast amplitude detection, high-speed feedback control, and high-bandwidth scanners with resonance suppression to achieve rapid, minimally invasive imaging. Both sample-scanning and probe-scanning configurations have been developed; the latter also permits integration with inverted optical microscopy and imaging of larger specimens such as cells.

Results: HS-AFM has directly visualized dynamic molecular processes inaccessible to static structural or ensemble-averaged measurements, including motor-protein motion, DNA replication, protein–DNA interactions, and conformational changes of CRISPR-Cas9. Recent developments further expand its capabilities: Only Trace Imaging (OTI) reduces the non-imaging retrace time, allowing higher frame rates with low sample disturbance; high-speed in-line force mapping correlates topography with force–indentation measurements in space and time; and integration with fluorescence microscopy is extending HS-AFM toward multimodal measurements in which molecular identity, morphology, dynamics, and mechanics can be examined within a single framework.

Conclusion: HS-AFM has evolved from a specialized imaging technique into a versatile platform for dynamic nano life science. By observing molecular events in real time and integrating structural, mechanical, and optical information, it bridges single-molecule observations and ensemble-level biophysical understanding, opening new opportunities for studying dynamic biological processes from individual biomolecules to living cells.

Keywords: *high-speed atomic force microscopy; biomolecular dynamics; single-molecule imaging; force mapping; multimodal microscopy*

I-09 From Traditional to Modern Platforms: The Evolution of Vietnam's Vaccine Manufacturing Landscape

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Abstract: Over the past 50 years, Vietnam has emerged as one of the few developing nations to establish strong capabilities in human vaccine production. Local vaccines developed through traditional attenuation and inactivation methods have been successfully integrated into the Expanded Program on Immunization (EPI), saving millions of lives. However, a lack of local capacity for next-generation platforms (such as protein- and nucleic acid-based vaccines) leaves the country heavily reliant on costly imports, highlighting the urgent need to transition toward modern technologies to address unculturable or high-consequence pathogens. In this presentation, we demonstrate the feasibility of localized Virus-Like Particle (VLP) vaccine production using HPV and Norovirus as models. Additionally, we highlight the critical technical and infrastructural hurdles local manufacturers must overcome to successfully transition to modern biomanufacturing. Overcoming these challenges will be key to expanding Vietnam's vaccine portfolio, ensuring national health security, and facilitating affordable access to next-generation vaccines.

IN-10 Nano-sized materials shaping biomedical research

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Abstract: Nanotechnology is increasingly transforming biomedical research by providing versatile platforms for disease diagnosis, therapeutic delivery, and targeted antigen uptake. In this work, we highlight three complementary applications of nano-sized materials and nanoscale bioengineering strategies spanning biosensing, regenerative medicine, and mucosal vaccine development.

For rapid viral detection, we developed a physiologically compatible surface-enhanced Raman scattering (SERS) platform based on gold nanostars (AuNSs) functionalized with a bifunctional fusion protein. The gold-binding protein Mp, identified from *Escherichia coli* BL21(DE3) by nanoLC–MS/MS-based proteomic screening, was fused to the Fc-binding domain of Protein A (ProAx1). The resulting Mp-ProAx1 protein enabled stable AuNS binding under physiological conditions and oriented immobilization of anti-Enterovirus 71 (EV71) antibodies. The functionalized AuNSs generated a concentration-dependent SERS response, with Raman intensity at 915 cm⁻¹ decreasing proportionally over 10¹–10⁶ TCID₅₀/mL ($R^2 = 0.997$), demonstrating the potential of plasmonic nanomaterials for sensitive viral detection.

For therapeutic applications, carboxymethyl cellulose (CMC) nanoparticles were developed as nanocarriers to stabilize fibroblast growth factor 2 (FGF-2), an important mediator of wound healing. The spherical nanoparticles had an average diameter of approximately 86 nm and showed no cytotoxicity toward NIH/3T3 cells. FGF-2 encapsulation exceeded 90%, while the nanoparticles protected FGF-2 from proteolytic degradation, maintained its biological activity, and provided sustained release. In a mouse burn model, CMC nanoparticles enhanced wound closure, granulation tissue formation, re-epithelialization, and angiogenesis compared with free FGF-2 and control nanoparticles.

Beyond nanoscale materials, molecular engineering at the peptide level offers opportunities for targeted delivery across biological barriers. Using structure-guided computational docking, we identified PEP1, a novel PrPC-binding peptide derived from *Brucella abortus* Hsp60. When fused to a model protein, PEP1 promoted receptor-mediated targeting to intestinal M-cell-associated regions and enhanced mucosal IgA and systemic IgG responses compared with an untargeted protein.

Collectively, these studies demonstrate how nano-sized materials and nanoscale biomolecular engineering can address major challenges in biomedical research, from sensitive pathogen detection and stabilization of therapeutic proteins to receptor-mediated antigen delivery. The integration of nanomaterials, recombinant proteins, and rationally designed peptides provides a versatile foundation for developing next-generation diagnostic, therapeutic, and vaccine technologies.

Keywords: EV-71, SERS, AFM, burn, FGF-2, carboxymethyl cellulose, mucosal vaccine, Hsp60, M cells, molecular docking, molecular dynamics

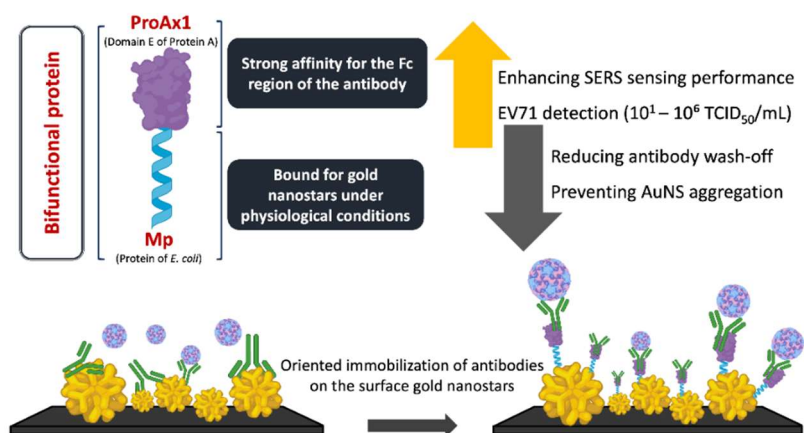


Figure: Schematic illustration of the oriented immobilization of anti-EV71 antibodies on gold nanostars (AuNSs) via the bifunctional Mp-proAx1 fusion protein for SERS-based EV71 detection

IB-10 Structural and Dynamic Insights into Asgard Tubulin Reveal the Evolution of Microtubules

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Abstract: Investigating the potential origins of the eukaryotic cell and the emergence of its cellular functions is important for predicting the characteristics of organisms that participated in eukaryogenesis. To trace cytoskeletal evolution, we studied tubulin-like proteins from Asgard archaea. We first reported the structure and dynamics of Odinararchaeota tubulin (OdinTubulin), which forms protomers and protofilaments similar to eukaryotic microtubules yet assembles into ring systems resembling prokaryotic FtsZ, suggesting an intermediate evolutionary stage. A recent study showed that Candidatus Lokiarchaeum ossiferum encodes α/β -tubulin homologs assembling into five-protofilament microtubules, with cellular dimensions aligning with estimates of the last eukaryotic common ancestor (LECA). To address how tubulin architecture adapts to different contexts, we identified and characterized a Heimdallarchaeales tubulin system. Heim α/β tubulin forms heterodimers, undergoes GTP-dependent polymerization, and assembles into four-protofilament microtubules with dynamic instability and membrane-deforming forces. Despite fewer protofilaments, Heim tubules share key eukaryotic features but exhibit lower stiffness. Thus, reduced protofilament numbers may benefit small cells, whereas increased mechanical load, cell size, and flagellar motility likely drove evolution of higher protofilament numbers during eukaryogenesis.

Keywords: *Asgard Archaea, Microtubule and Eukaryogenesis*

IN-11 Lipid-based nanocarriers for targeted drug delivery: applications and challenges

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Abstract: Lipid-based nanocarriers represent a convergence of nanotechnology, biotechnology, and biophysics, enabling therapeutic agents to cross biological barriers with improved spatial and temporal control. Building on our recent studies and on advanced nanocarrier-mediated delivery, bioactive nanoformulations, electron-microscopic imaging, and nano–bio interactions, this presentation discusses liposomes, solid lipid nanoparticles, nanostructured lipid carriers, and ionizable lipid nanoparticles as versatile platforms for targeted therapy. Their nanoscale dimensions, biocompatibility, tunable interfaces, and ability to encapsulate hydrophilic and hydrophobic drugs, proteins, and nucleic acids can improve solubility and stability, prolong circulation, enhance cellular uptake, and reduce off-target toxicity. Applications increasingly encompass anticancer and antimicrobial therapies, natural bioactive compounds, vaccines, RNA therapeutics, and precision medicine.

From a biophysical perspective, therapeutic performance is governed not only by chemical composition but also by lipid self-assembly, particle size and morphology, membrane fluidity, surface charge, interfacial interactions, protein-corona formation, cellular uptake, endosomal escape, and stimulus-responsive payload release. These structure–property–function relationships illustrate the central meaning of nanobiotechnology: engineering nanoscale materials to interact predictably with complex biological systems and generate clinically useful functions. Nevertheless, translation remains constrained by colloidal instability, limited tissue penetration, heterogeneous biological barriers, rapid immune clearance, insufficient endosomal escape, lipid-associated toxicity, batch variability, scale-up difficulties, and evolving regulatory requirements. Future progress will therefore depend on mechanism-guided lipid design, advanced physicochemical characterization, physiologically relevant biological models, and reproducible manufacturing. Integrating nanobiotechnology with quantitative biophysics may ultimately transform lipid nanocarriers from empirical formulations into programmable delivery systems for safer and more personalized therapy.

Keywords: *lipid nanocarriers; targeted drug delivery; nanobiotechnology; biophysics; nano–bio interactions; precision medicine.*

IB-11 Differential growth controls organ curving: experimental and computational approaches

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Abstract: Organ curving is a fundamental property of many plant organs, and is thought to arise from differential growth between distinct regions. However, the precise relationship between regional growth behaviours and the degree of curving remains poorly characterised. Here, we used the *Arabidopsis thaliana* sepal to investigate how differential growth controls organ curving, especially the differential growth rate between the sepal tip and sepal body. We examined the sepal of the wild-type (WT) and of a gain-of-function mutant which has significantly more curved sepals. Individual cell growth rate was quantified from confocal time-series images using the software MorphoGraphX. We then correlated the differential growth rate between the sepal tip and sepal body of each sepal and its curving, and found that there is a significant correlation between differential growth between regions and the degree of curving. We also performed computational modelling to test more complex growth scenarios. Modelling confirmed that differential growth between the tip and the body drives tip curving, and further showed that the margin substantially amplifies curving beyond what differential growth alone produces. Increasing the number of growth zones in the model recapitulates more faithfully the actual shape of the sepal seen in the plant. These findings suggest that organ curving is governed by a combination of regional differential growth and margin behaviours, pointing to the margin as a priority target for future in planta experiments.

Keywords: *Arabidopsis thaliana*, computational modelling, differential growth, morphogenesis, organ curving

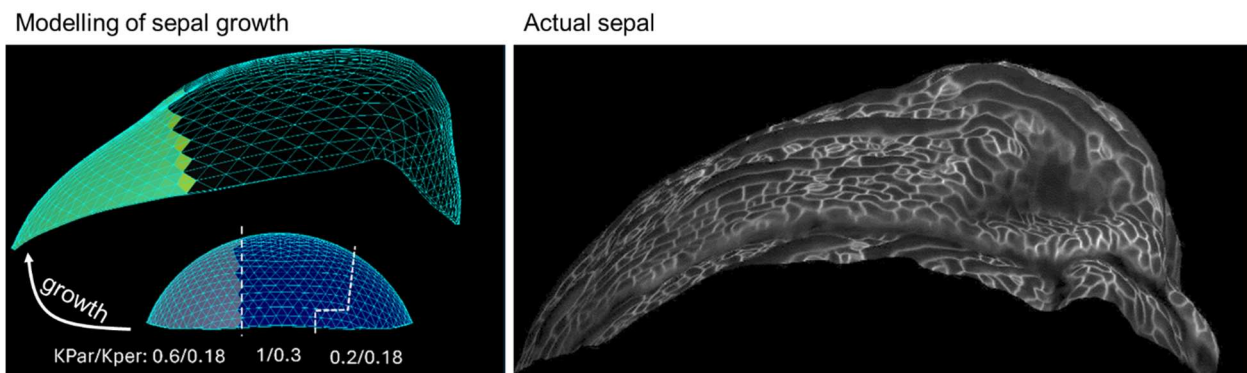


Figure: Computational modelling of sepal growth with three different zones having different growth behaviours recapitulates the actual sepal observed in *Arabidopsis* plants.

ORAL PRESENTATIONS

O-01 Fabrication of PLGA and Chitosan Coated Hesperidin Nanoparticles (PCH-NPs) for the Evaluation of its Anticancer Potential

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Breast cancer is the most common form of cancer diagnosed in women worldwide. Hesperidin, a naturally occurring flavonoid, possesses significant anticancer, antioxidant, and anti-inflammatory properties; however, its poor aqueous solubility and limited bioavailability restrict its clinical application. The present study focuses on the synthesis and evaluation of poly(lactic-co-glycolic acid) (PLGA) and chitosan-coated hesperidin nanoparticles (PCH-NPs) for enhanced anticancer activity against breast cancer cells. The nanoparticles were synthesized using separately prepared aqueous and organic phases followed by emulsification and nanoparticle formation. The spectroscopic characterization including FTIR, Raman and NMR spectroscopy revealed presence of certain functional groups, vibrational attributes and chemical structure respectively. The microscopic characterizations including TEM and FE-SEM revealed the 2D and 3D morphology of the synthesized nanoparticles. The anticancer activity of the developed nanoparticles was evaluated against breast cancer cell lines using cell viability assay which revealed dose dependent cytotoxicity of PCH-NPs against MCF-7 and MDA-MB-231 cells. Hemolysis assay was also performed for the evaluation of hemotoxicity which confirmed minimal red blood cell damage up to 1000 µg/mL, supporting a favourable safety profile. High content analysis and cell electrical impedance measurement studies further supported cytotoxic potential of the PCH-NPs. *In vitro* biochemical assays indicated enhanced glucose uptake and reduced cell proliferation in treated cells. Differential gene expression analysis by qRT-PCR and quantification of protein through sandwich ELISA conclusively displayed cytotoxic potential at molecular level. Furthermore, our work aims to evaluate *in vivo* toxicity and anticancer potential of PCH-NPs in rat models to strengthen our data. Conclusively, our work demonstrates the development of PCH-NPs as a potent biocompatible and cytotoxic agent against breast cancer.

Keywords: *Hesperidin, Breast Cancer, Nanoparticles, Anticancer, PCH-NPs*

O-02 Geant4-DNA Simulation of Radiation-Induced DNA Damage in reduced-scale Human Fibroblast Cell model

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Background: Ionizing radiation interacts with cellular DNA both directly and through the generation of reactive oxygen species (ROS), producing a spectrum of lesions including strand breaks and oxidative base damage. Among the most biologically significant oxidative lesions are 8-oxo-7,8-dihydroguanine (8-oxo-G) and thymine glycol (Tg), which, when occurring in close proximity to strand breaks or other lesions, form clustered DNA damage sites. These clustered lesions are particularly challenging for cellular repair machinery and are implicated in genomic instability and mutagenesis. Computational modeling via Monte Carlo simulation provides a powerful framework to quantify such damage at the nanoscale, enabling mechanistic insight that is difficult to obtain experimentally.

Methods: We used Geant4-DNA, a biologically oriented extension of the Geant4 Monte Carlo toolkit, to simulate radiation-induced DNA damage in a geometrical model of a human fibroblast cell nucleus. To balance computational feasibility with biological relevance, we downscaled the full 6.5 Gbp cell nucleus to 13.2 Mbp and 7.2 Mbp models by reducing the dimensional ratio while preserving the base-pair linear density. Strand break induction was tracked using the standard Geant4-DNA damage scoring framework. We recorded ROS-DNA base interaction events and implemented a post-processing algorithm to classify each hit as an 8-oxo-G or Tg lesion. This classification is based on the cite-specific hit probability from existing experimental and simulation data. The resulting lesion maps were then analyzed to characterize the spatial distribution and clustering properties of mixed damage sites containing both strand breaks and base lesions.

Results: Simulations reproduced strand break yields consistent with published Geant4-DNA benchmarks. Non-DSB lesions dominated across all radiation types (92–98% of total damage), with DSB yields rising and SSB frequencies declining at higher LET. Despite differences in genomic content, our results aligned closely with experimental damage yields. For Co-60 γ irradiation, simulated 8-oxodG yields fell within the experimentally reported range. Predicted Tg/DSB ratios were consistent with Nth-sensitive lesion data, supporting the biological validity of the model. Non-DSB clustered lesions were the most abundant cluster type (non-DSB/DSB ratios of 4.5–14).

Conclusion: This work establishes a computational pipeline for simulating the full spectrum of radiation-induced DNA damage, focusing on oxidative base lesions, within a scaled-down human fibroblast cell geometry. By integrating stochastic ROS-base interaction modeling into the Geant4-DNA framework, we move beyond conventional strand break dosimetry toward a more complete

damage characterization. The cluster damage profiles produced here constitute the essential input for a mechanistic BER simulation.

Keywords: *Geant4-DNA, Monte Carlo simulation, oxidative base damage, 8-oxo-G, thymine glycol, clustered DNA damage*

O-03 Smart Near-IR Light-Controlled Drug Delivery Using SDF-1 α -Loaded Chitosan Nanoparticles Coated with Chlorin e6

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Abstract:

In this talk, I focus the development of a novel near-infrared (NIR) light-responsive drug delivery system based on chitosan nanoparticles (CNs) loaded with stromal-cell-derived factor-1 α (SDF-1 α) and coated with the photosensitizer chlorin e6 (Ce6). These Ce6-CN-SDF-1 α nanoparticles were synthesized via ionotropic gelation and exhibit controlled, on-demand release behavior under 660 nm NIR light irradiation, mediated by photoinduced singlet oxygen generation. The nanoparticles, with sizes ranging from 90–135 nm and negative surface charge, demonstrate high biocompatibility and non-cytotoxicity in human fibroblast cell lines. The design enables precise, light-triggered release of bioactive SDF-1 α , holding significant potential for regenerative medicine and targeted therapies. Here, I discuss the synthesis, characterization, release kinetics, photodynamic properties, and biomedical implications of this smart nanocarrier system.

Keywords: Photostability, Photodegradation, Singlet oxygen, Photodynamic effect, Biocompatibility.

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O-04 Generative AI for De Novo Design of DNA Origami

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Abstract: DNA origami provides a powerful way to build nanoscale structures, but designing complex free-form geometries is still difficult because current workflows rely heavily on predefined rules and limited structural data. In this work, we developed Generative SNUPI, a diffusion-based framework for the de novo design of DNA origami structures. The model was trained using equilibrium conformations of 450 wireframe designs. Starting from a user-defined line geometry, the framework generates base-pair-level structures and then completes scaffold routing, staple assignment, and simulation-based evaluation. It was used to create more than 100 two- and three-dimensional designs, including auxetic structures, reconfigurable geometries, and modular assemblies. Several designs were further validated experimentally using gel electrophoresis and atomic force microscopy. The results show that combining generative modelling with physics-based simulation can simplify the design process and broaden the range of DNA origami structures that can be explored.

Keywords: DNA origami; generative design; diffusion model; multiscale simulation; reconfigurable nanostructures

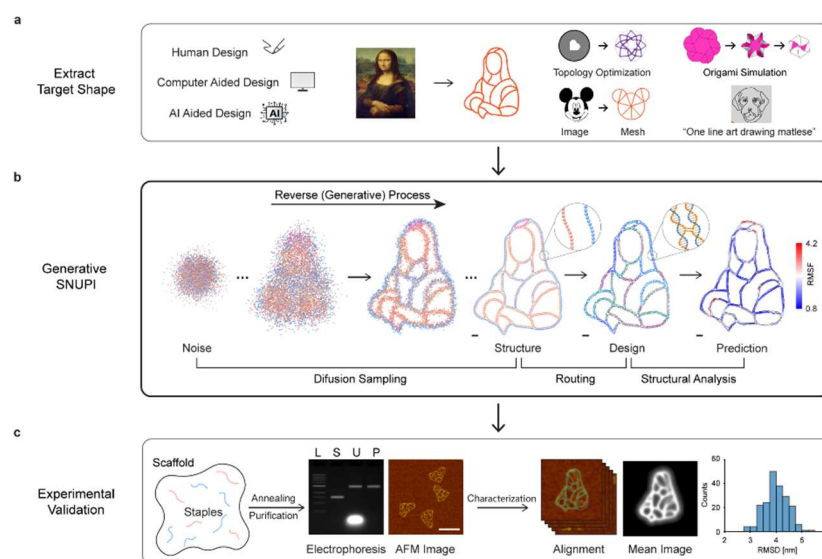


Figure: Overview of Generative SNUPI design framework

O-05 Strategies for high-yield production of functional recombinant proteins/antibodies

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Abstract: High-yield production of functional recombinant proteins is essential for biological research and biotechnology, yet many disulfide bond-containing proteins remain difficult to express in *Escherichia coli* because its reducing cytoplasmic environment limits proper protein folding. In addition, large-scale preparation of recombinant proteins and antibodies is often labor-intensive and time-consuming. Here, we developed streamlined strategies for the efficient production of functional recombinant proteins and antibodies.

As a first example, we established a scalable production platform for recombinant proaerolysin, a pore-forming toxin used for PIGA-based negative selection in genome editing and nanopore applications. Because proaerolysin requires two disulfide bonds for proper folding, expression in conventional *E. coli* BL21(DE3) is inefficient. By employing the engineered *E. coli* SHuffle strain, which provides an oxidative cytoplasmic environment that promotes disulfide bond formation, together with sequential immobilized metal affinity chromatography (IMAC) and size-exclusion chromatography (SEC), we obtained approximately 3 mg of soluble proaerolysin at 99.3% purity from a 50 mL bacterial culture. The purified protein exhibited biological activity in mouse embryonic stem cells comparable to previously reported preparations, providing a practical and cost-effective resource for research.

As a second example, we optimized the production of recombinant Fv-clasp antibodies (~40 kDa), which were expressed as inclusion bodies and subsequently refolded *in vitro* to form the correct disulfide bonds between the heavy chain (HC) and light chain (LC). We enhance HC/LC expression by optimizing mRNA secondary structure to reduce the opening energy around the translation initiation site, resulting in several-fold higher expression in *E. coli*. Besides, to facilitate purification of correctly assembled antibodies, the HC and LC were engineered with SpyTag and His-tag, respectively, enabling an automated AKTA workflow combining sequential affinity chromatography and SEC. Consequently, purification time is reduced from 2-3 days to four hours. Using this platform, we generated approximately 40 recombinant antibodies targeting peptide tags and histone modifications. Most antibodies demonstrated high specificity and affinity in Western blotting, immunostaining, ELISA, peptide array, and SNAP-ChIP assays. Furthermore, these small recombinant antibodies outperformed conventional IgG antibodies (~150 kDa) in CUT&RUN and CUT&Tag by improving target accessibility, reproducibility, and resolution in densely packed chromatin. Together, these scalable production strategies provide valuable resources for preparative chromatin studies, super-resolution imaging, and other advanced molecular biology applications.

Keywords: recombinant protein production; proaerolysin; recombinant antibodies; Fv-clasp antibody; disulfide-bonded proteins; automated purification

O-06 Carbon Dots: From biophysical mechanisms to biomedical and sensing applications

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Abstract: Carbon dots (CDs) are emerging zero-dimensional carbon nanomaterials with distinctive photoluminescence, abundant surface functional groups, and readily tunable optical properties, enabling their integration into diverse biomedical and sensing platforms. Here, the biophysical basis of CD photoluminescence and their biomedical applications in bioimaging, molecular diagnosis, photothermal therapy, and photodynamic therapy will be highlighted. Their capacity to translate interactions with biological targets into optical signals provides a foundation for multifunctional platforms that combine imaging, sensing, and therapeutic functions. Our research from the Department of Physics - Biophysics at Vietnam Military Medical University on the development of CD-based optical sensing systems is also presented, with a focus on multicolor and dual-emission CDs for analyte detection. These materials have been applied to tetracycline detection and ion sensing, before being translated into polymer-supported CD films for portable, on-site analysis. We further explore smartphone-integrated sensing as a route towards accessible and digitally assisted optical detection. Together, this talk provides an overview of the development of CDs in biomedicine and highlights their potential to inspire new applications of CDs and their derivatives across diverse scientific and technological fields.

Keywords: *carbon dots, biomedical applications, CD films, dual-emission CDs, Department of Physics - Biophysics.*

O-07 Nanobody Development for Detecting and Inhibiting Botulinum Toxin, Snake Venom Toxins, and the CD26 Lung Cancer Biomarker

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Abstract: Nanobodies, also known as single-domain antibodies, have emerged as promising tools for diagnostic and therapeutic applications because of their small size, high stability, strong binding affinity, and ease of recombinant production. In our laboratory, we focus on developing nanobody-based strategies for detecting biological toxins, particularly botulinum neurotoxins and snake venom toxins, as well as CD26, a potential biomarker for lung cancer. We have successfully synthesized several nanobodies targeting botulinum neurotoxin serotypes A and B and phospholipase A₂ (PLA₂) toxins found in snake venom. These nanobodies have been applied in enrichment, immunoassays and biochip-based systems for rapid, on-site detection. We are also developing nanobodies targeting CD26 in lung adenocarcinoma. We aim to detect cancer biomarkers using fluorescently labeled nanobodies. Nanobodies with toxin neutralizing or inhibitory activity may also have potential therapeutic applications. Overall, our research highlights the potential of nanobodies as versatile tools for both detection and treatment.

Keywords: *Nanobody, single domain antibody, detection, treatment, botulinum toxin, PLA₂, CD26, lung can*

O-08 Synergy Between ADP and Magnesium in the Assembly of High Molecular Weight Complexes of 2-Cys Peroxiredoxin

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Abstract: 2-Cys peroxiredoxin 2 (Prx2) is a thiol-dependent antioxidant enzyme that undergoes redox-driven structural transitions, yet the role of nucleotides and cations in its higher-order organization remains unclear. In this study, we investigated how ADP and Mg^{2+} cooperatively regulate Prx2 oligomerization under lipid-induced conditions. Chromatographic fluorescence analysis revealed that Mg-ADP binds selectively to the Prx2WT-PS oligomeric assembly, whereas the P44A/S76A mutant failed to retain Mg-ADP, highlighting residues essential for nucleotide-competent architecture. High-speed atomic force microscopy (HS-AFM) further showed that the mutant adopts a more compact geometry than WT, consistent with its inability to support nucleotide association. Functionally, ADP destabilized WT oligomers, while Mg^{2+} induced non-selective disassembly. Notably, under Mg-ADP conditions, both WT and mutant formed high molecular weight (HMW) assemblies, but only WT exhibited a distinct maturation trajectory. Together, these findings identify a synergistic contribution of ADP and Mg^{2+} to Prx2 assembly and reveal structural features required for nucleotide-responsive HMW states, providing new insight into the regulation of Prx2 in redox biology.

Keywords: peroxiredoxins, oxidative stress, ADP, negatively charged lipid, high-molecular-weight complex, HS-AFM.

O-09 Functional Carbon Dots: From Surface Engineering to Optical Sensing and Biomedical Applications

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Abstract: Carbon dots (CDs) are an emerging class of fluorescent nanomaterials attracting considerable attention because of their tunable optical properties, low toxicity, and simple synthesis. In this work, we summarize our recent studies on the synthesis, structural characterization, and functionalization of carbon dots for sensing and biomedical applications. The influence of surface functional groups, particle size, and heteroatom doping on the optical properties of CDs was investigated using complementary spectroscopic and microscopic techniques. The developed nanomaterials demonstrated tunable photoluminescence and promising performance for optical sensing, fluorescence thermometry, and bioimaging. The obtained results reveal clear relationships between the structural characteristics of carbon dots and their photophysical behavior, providing effective approaches for tailoring their properties toward specific applications. These findings contribute to the rational design of multifunctional carbon nanomaterials and highlight the potential of carbon dots as versatile platforms for next-generation optical sensors and biomedical technologies.

Keywords: *Carbon dots, Photoluminescence, Optical sensing, Bioimaging, Fluorescence thermometry.*

O-10 Ontological Validation of Non-Stationary Cardiac Electrodynamics via Pushdown Automata and Topological Invariants in Ultra-Lightweight Edge Architectures

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Abstract:

Background: Myocardial electrical propagation is governed by synchronized ionic flux across cellular membranes, generating continuous non-stationary phase-space trajectories. Conventional data-driven artificial intelligence models minimize empirical loss functions without incorporating physical conservation laws. Consequently, when exposed to out-of-distribution physical perturbations, such as mechanical electrode pop or baseline wander from respiration, these black-box models suffer phase-space trajectory collapse, producing ungrounded hallucinations that compromise safety in real-time edge telemetry.

Methods: We address this vulnerability by establishing a physics-constrained symbolic dynamical engine that converts continuous electrodynamic trajectories into discrete symbolic sequences over an alphabet of cardiac biophysical states. An ontological pushdown automaton (PDA) serves as the core validation engine. To account for biological diversity, the automaton's stack memory dynamically holds individual baseline parameters derived from Rasch measurement theory for eliminating inter-individual variance. The transition rules strictly enforce biophysical conservation principles and topological invariants across cardiac phases. Any input sequence that violates fundamental physical dynamics is deterministically routed to a refusal state, executing an immediate veto at the input gate before downstream processing.

Results: Evaluated on the PTB-XL database (21 837 records) injected with severe MIT-BIH NSTDB noise (negative SNR dB), the PDA-validated symbolic engine achieved a Matthew Correlation Coefficient (MCC) of 0.9375 under extreme electrode pop disturbances (versus 0.1520 for black-box AI) and MCC = 0.7172 under severe baseline wander during early ischemia. Quantized into an asymmetric dual-layer edge architecture, the engine requires < 50000 static parameters and < 200 KB SRAM, delivering deterministic inference latencies under 10 milliseconds per cycle on bare microcontrollers.

Conclusion: This study bridges non-linear biophysics, symbolic dynamics, and formal automata theory, establishing a computable paradigm for syntactically verified, hallucination-free biomedical telemetry on resource-constrained edge devices.

Keywords: *Biophysical Electrodynamics, Symbolic Dynamics, Pushdown Automata, Topological Invariants, Edge Computing, Physics-Informed Validative System.*

O-11 Mucoadhesive, antioxidant, and lubricant catechol-functionalized poly(phosphobetaine) as biomaterial nanotherapeutics for treating ocular dryness

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Abstract: Dry eye disease (DED) is associated with ocular hyperosmolarity and inflammation. The marketed topical eye drops for DED treatment often lack bioavailability and precorneal residence time. In this study, we investigated catechol-functionalized polyzwitterion p(MPC-co-DMA), composed of 2-methacryloyloxyethyl phosphorylcholine (MPC) and dopamine methacrylamide (DMA) monomers, as potential topical nanotherapeutics for DED. The copolymers were synthesized via random free-radical copolymerization, producing different proportions of catecholic functionalization. All as-prepared polymer compositions displayed good ocular biocompatibility. At a feeding ratio of 1:1, p(MPC₁-co-DMA₁) can facilitate a robust mucoadhesion via Michael addition and/or Schiff base reaction, thus prolonging ocular residence time after 4 days of topical installation. The hydration lubrication of MPC and radical-scavenging DMA endow the nano-agent to ease tear-film hyperosmolarity and corneal inflammation. A single dose of p(MPC₁-co-DMA₁) (1 mg/mL) after 4 days post-instillation can protect the cornea against reactive oxygen species, inhibiting cell apoptosis and the over-expression of pro-inflammatory factors (IL-6 and TNF- α). In clinical assessment, DED-induced rabbit eyes receiving p(MPC₁-co-DMA₁) could increase lacrimal fluid secretion by 5-fold higher than cyclosporine A. The catechol-functionalized polyzwitterion with enhanced lubricity, mucoadhesion, and anti-oxidation/anti-inflammation properties has shown high promise as a bioactive eye drop formulation for treating DED.

Keywords: Multifunctional polyzwitterion, Catechol, Poly(phosphobetaine), Biomaterial nanotherapeutics, Ocular dryness.

O-12 Distinct Effects of Mechanical Pressure and HepG2 Paracrine Signaling on Hepatic Stellate Cell Activation

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Abstract: *Background:* Hepatic stellate cell (HSC) activation involves the transition from a quiescent state to an activated phenotype (such as myofibroblasts or cancer-associated fibroblasts) during liver injury. While paracrine factors within the liver microenvironment are well-established drivers of HSC activation, the impact of mechanical stimuli remains less characterized. This study aims to compare the distinct effects of mechanical pressure and HepG2-derived paracrine factors on HSC activation. *Methods:* CFSC cells (a rat HSC line) were subjected to 8 kPa of pressure using a pressure-controlled chamber or co-cultured with HepG2 cells in a compartmentalized system permitting paracrine signaling. After 24 hours of culture, CFSC morphology, cell function (lipid droplet retention via Oil Red O staining), cell migration, and key activation markers (collagen and α -SMA expression) were evaluated. *Results:* Compared to control conditions, both 8 kPa pressure and HepG2 co-culture successfully induced CFSC activation after 24 hours. However, the activation profiles differed significantly between the two stimuli. HepG2 paracrine factors induced greater cell migration ($p < 0.05$) and increased cell surface area ($p < 0.01$), whereas mechanical pressure elicited a stronger reduction in lipid droplet area ($p < 0.05$) and higher expression of fibrotic markers (collagen and α -SMA, $p < 0.001$). *Conclusion:* Mechanical pressure and HepG2 paracrine factors induce HSC activation with distinct phenotypic characteristics. These findings demonstrate that both biophysical and biochemical signals in the liver microenvironment play complementary roles in modulating HSC behavior during liver damage.

Keywords: *Mechanobiology, liver fibrosis, hepatic stellate cell activation, liver stiffness, HepG2*

O-13 Berberine susceptibility depends on bacterial cell shape rather than Gram type or cell wall architecture

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Abstract: Berberine, a plant-derived isoquinoline alkaloid, has well-documented antibacterial activity; nevertheless, the characteristics controlling its species selectivity are unknown and often associated with Gram type. To test whether selectivity is determined by cell wall architecture or cell shape, we used a broad taxonomic screen in conjunction with a morphology control panel. Berberine extract was tested against 29 clinical strains - 17 Gram-negative bacilli, 11 Gram-positive cocci, and *Haemophilus influenzae* - using a two-fold broth dilution in BHI across a ten-point series with growth and sterility controls and read after 24 hours. A targeted panel was established to differentiate morphology from Gram reaction, comparing cocci (*S. aureus*, *S. epidermidis*), Gram-positive bacilli (*B. subtilis*, *L. plantarum*), and Gram-negative bacilli (*E. coli*, *P. aeruginosa*) by OD₆₀₀ growth curves over 24 hours at 0.004-1 mg/mL. After 24 hours of exposure in 96-well plates, CFU enumeration on Mueller-Hinton agar was used to assess viability. MBC was defined as a ≥ 3 log₁₀ reduction compared to untreated controls. The screen revealed that activity was limited to coccoid organisms. Streptococci were most susceptible (*S. pyogenes*, *S. pneumoniae*), while staphylococci were only inhibited at the highest dosages, leaving *Enterococcus faecalis*, *E. faecium*, and *S. capitis* unaffected. Sixteen of 17 Gram-negative bacilli grew well at all concentrations examined; only *Sphingomonas paucimobilis* was inhibited at the maximum concentration. *H. influenzae*, a coccobacillus, was inhibited over the entire range. The targeted panel had MICs of 125 μ g/mL for *S. aureus* and *S. epidermidis* and 1000 μ g/mL for *E. coli* and *P. aeruginosa*, with MBCs of 250 μ g/mL for the former two cocci species. The Gram-positive bacilli *B. subtilis* and *L. plantarum* exhibited only partial inhibitions and were indistinguishable from the Gram-negative bacillus. Susceptibility was determined by cell shape rather than Gram response or wall architecture: coccoid organisms were suppressed, but bacilli were only moderately impacted, regardless of envelope type. Partial suppression of bacilli is compatible with previously reported berberine-induced cell elongation, as elongating cells continue to gain optical density, but cocci rely on the divisome machinery for nearly all peptidoglycan syntheses. Uninhibited enterococci may represent efflux, for which berberine is a known substrate.

O-14 Cation-Substituted Zinc Cobaltite Spinel for Enhanced Electrochemical Sensing Performance of Small Molecules: A Combined DFT and Experimental Study

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Abstract: In this work, Mn and Ni cations were successfully incorporated into the ZnCo₂O₄ spinel lattice via a simple microwave-assisted hydrothermal method. The physicochemical properties of the as-prepared spinels were systematically investigated through a combination of experimental characterization and density functional theory (DFT) calculations. The obtained results demonstrated that cation incorporation significantly modulated the electronic structure and enhanced the electrical conductivity of ZnCo₂O₄ spinel, thereby facilitating interfacial electron transfer kinetics and strengthening small-molecule adsorption. Notably, tuning the substituted-cation ratio significantly altered the electrochemical response and analytical performance of ZnCo₂O₄ spinel, enabling improved selectivity towards dopamine and uric acid. The Mn-substituted ZnCo₂O₄-based sensor exhibited excellent sensing performance towards dopamine and uric acid. This work offers an innovative strategy based on a reliable theoretical and experimental basis for selective electrochemical sensors of small molecules.

Keywords: *Mn substitution, Cobaltite, Electrocatalytic activity, Uric acid, Dopamine*

O-15 Investigating lipid sensitivity of ToxA and ToxB toxins causing Acute Hepatopancreatic Necrosis Disease in shrimp using High-speed Atomic Force Microscopy

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Abstract: Acute Hepatopancreatic Necrosis Disease (AHPND) is a lethal disease in shrimps and prawns, which causes severe economic losses on the global shrimp farming industry annually. The ToxAB toxin complex is the primary causative agent of AHPND, which causes necrosis effect on the hepatopancreatic system of shrimp. It is produced by the bacterium *Vibrio parahaemolyticus* and is composed of two individual toxins, ToxA and ToxB. Despite numerous studies on the structure and pathogenic mechanism of this toxin, all existing research just provided prediction models, including heterodimeric and heterotetrameric models. To date, no experimental studies have been published that employ advanced microscopy techniques to directly visualize the interaction between the toxins and lipid membranes, as well as the oligomeric structures formed by the toxins. Therefore, in this research, we utilized High-speed atomic force microscopy (HS-AFM) to understand the oligomerization and interaction between the toxins with lipid bilayer membrane. We investigated six liposome compositions representing major lipid components of animal and shrimp epithelial cell membranes: POPC, POPC/PIP2, POPC/Liver PI, POPC/DOPE, POPC/DHA, and POPC/Triglycerides. The liposomes were prepared using the thin-film hydration method and subsequently immobilized onto mica substrates for imaging. The results demonstrated that both toxins exhibit non-specific interactions with all investigated lipids through binding, oligomerization, and membrane disruption. Contrary to previous studies, ToxA alone displays pore-forming and membrane-damaging properties, which intensify with higher concentrations or in the presence of ToxB. The membrane-disruption patterns of ToxA are diverse and tend toward membrane tearing. While ToxB individually also possesses pore-forming and membrane-damaging abilities, its mechanism differs from ToxA and is less diverse. These findings provide an initial perspective for the mechanisms of ToxA/ToxB and the ToxAB complex as pore-forming toxins.

Keywords: *Toxin oligomerization, pore-forming mechanism, lipid bilayer model, protein dynamics, HS-AFM*

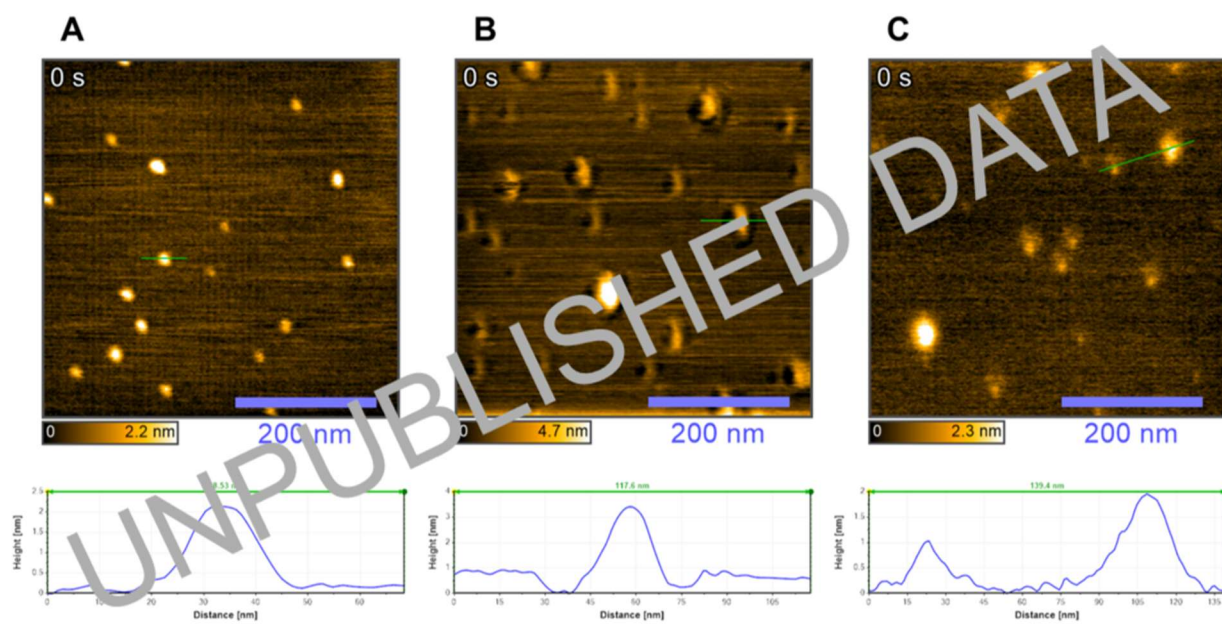


Figure 1:
ToxB molecule on HS-AFM images and cross-section profiles measuring heights of one representative ToxB molecule on (A) POPC, (B) POPC/PIP2, and (C) POPC/Liver PI lipid membrane

O-16 Computational Investigation of Curcumin/ β -Cyclodextrin Drug Delivery Systems for Potential Cancer Therapy Applications

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Abstract: Curcumin (CUR) is a natural polyphenolic compound with diverse biological activities, including antioxidant, anti-inflammatory, antiproliferative, and pro-apoptotic effects, highlighting its potential for cancer therapy applications. However, its practical use remains limited by poor water solubility, low aqueous stability, and limited bioavailability under physiological conditions. β -Cyclodextrin (β -CD), which possesses a hydrophobic inner cavity and a hydrophilic outer surface, has attracted considerable interest as a molecular carrier capable of improving the solubilization, stabilization, and delivery of hydrophobic therapeutic compounds, such as CUR. In this study, the molecular interactions, structural stability, and encapsulation behavior of CUR/ β -CD inclusion complexes were investigated using a combination of density functional theory (DFT) calculations and molecular dynamics (MD) simulations. Molecular models of CUR, β -CD, and their inclusion complexes were geometrically optimized using ORCA at the B3LYP/6-31G(d) level. The optimized structures converged successfully and showed no imaginary vibrational frequencies, confirming that they correspond to stable energy minima. Frontier molecular orbital analysis further indicated that complex formation altered the electronic characteristics of the system and provided insight into the electronic stability of the resulting host-guest assemblies. An MD simulation in an aqueous environment revealed that the host-guest assemblies remained structurally stable after initial molecular rearrangements, while CUR was effectively retained within the β -CD region throughout the simulation. These findings demonstrate the ability of β -CD to encapsulate and protect CUR in aqueous environments and provide molecular-level insight into the interactions governing the stability of CUR/ β -CD drug-carrier systems. Overall, this study provides a computational basis for the development of β -CD-based delivery platforms aimed at improving CUR stability, aqueous dispersibility, and transport for potential applications in cancer therapy.

Keywords: *Curcumin, β -cyclodextrin, density functional theory, molecular dynamics, drug delivery, cancer therapy.*

O-17 Within-host evolution of *Pseudomonas aeruginosa* during antibiotic therapy in fatal ICU infections.

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Abstract:

Background: The within-host evolution of *Pseudomonas aeruginosa* has been extensively studied in chronic infections, but its dynamics in acute fatal ICU infections remain poorly understood. We investigated the genotypic and phenotypic evolution of sequential *Pseudomonas aeruginosa* strains isolated from three ICU fatal patients under antibiotic treatment.

Methods: We analyzed six paired *Pseudomonas aeruginosa* isolates collected longitudinally during antibiotic treatment from tracheal aspirates of three fatal ICU patients at the Hospital of Tropical Diseases, Ho Chi Minh City, Vietnam. Species identification was performed using MALDI-TOF MS and clinical data retrieved from patient records. Susceptibility to nine antibiotics representing five antibiotic classes was determined using the broth microdilution method. Whole-genome sequencing (WGS) was performed using long-read Oxford Nanopore sequencing. MLST, AMRFinderPlus were applied to identify sequence types and antimicrobial resistance genes respectively. Genetic, phenotypic, and clinical data were integrated to assess the evolutionary changes within the host during antibiotic treatment.

Results: All three patients were elderly male ICU patients (65–100 years) who died despite antimicrobial treatment. Regimens differed but all received carbapenems and cephalosporins. WGS identified three unrelated sequence types (ST277, ST773, and ST313), confirming each patient was infected by a distinct lineage. ST277 and ST773 are recognized international high-risk clones, whereas ST313 is a less frequently reported lineage. All converged on similar chromosomal mechanisms of carbapenem resistance but exhibited different within-host evolutionary patterns. In patient F1 (ST277), cefepime resistance emerged under cefepime treatment and coincided with an *ampD* E120 deletion and replacement of the chromosomal *blaPDC* allele, suggesting β -lactam adaptation. In patient F2 (ST773), the later isolate exhibited an apparent reversion to carbapenem susceptibility

despite continuous imipenem exposure. WGS showed that it carried a distinct full-length *oprD* allele with lineage-associated polymorphisms, rather than restoration of *OprD*. In patient F3 (ST313), the later isolate lacked the *oprD/mexR* loss-of-function changes seen in the earlier isolate yet remained carbapenem-resistant. Thus, F1 demonstrated resistance emergence during therapy, whereas F2 and F3 showed genotype–phenotype discordance consistent with possible within-host heterogeneity. Despite differences in lineage, treatment regimen, and evolutionary pattern, all three infections remained resistant to the β -lactams administered, and all three patients died.

Conclusion: The within-host evolution of *Pseudomonas aeruginosa* during fatal ICU infections follows distinct adaptive trajectories, including diverse resistance patterns. Integrating longitudinal WGS with susceptibility testing provides additional insights into bacterial adaptation and highlights that single-isolate testing may miss resistant subpopulations relevant to treatment.

Keywords: *Pseudomonas aeruginosa*, antibiotic resistance, within-host evolution, whole genome sequencing, ICU infection.

O-18 Topography-Aware Adaptation of Vision Foundation Models for AFM

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Abstract: Atomic Force Microscopy (AFM)[1] produces two-dimensional images in which pixel intensity corresponds to surface height, thereby encoding three-dimensional topography at the nanometer scale. Vision foundation models (VFMs)[2–7] have achieved state-of-the-art performance across many computer-vision tasks; however, because they are predominantly pretrained on natural images, their representations may not fully exploit the quantitative topographic nature of AFM data. This study investigates an effective adaptation strategy for transferring VFMs to AFM analysis. The proposed framework introduces topographic information at three levels: a geometry-explicit input representation using height and local gradients, a lightweight topography-aware attention mechanism based on height differences and local surface orientation, and a geometry-preserving learning objective using masked topography reconstruction. Experiments on a High-Speed AFM dataset of α -hemolysin show that the adapted DINO achieves a macro-F1 of approximately 0.76 for oligomer/pre-pore/pore classification, while the adapted SAM achieves an F1-score of approximately 0.87 and an IoU of 90% for segmentation. These results indicate that explicitly incorporating topographic geometry can improve the adaptation of VFMs pretrained on natural images to AFM.

Keywords: *AFM, HS-AFM, Vision Foundation Models, DINO, SAM, Topography-Aware Learning, Artificial Intelligence*

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POSTER PRESENTATIONS

PP-01 Applications of an oil-free nanoemulsion method in magnetic-fluorescent nanosphere production for bio-separation and bioimaging.

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Abstract: A two-phase ethanol-water inverse nanoemulsion method using TSC as a surfactant was proposed and investigated to fabricate multi-core/silica (SiO₂) shell nanoparticles exhibiting both magnetic and fluorescent properties, with potential in bio-applications. By replacing the oil phase used in conventional emulsion methods with ethanol and employing TSC, which is low-solubility in ethanol and highly soluble in water, an environmentally friendly, oil-free approach was successfully developed to overcome the common limitations of conventional microemulsion methods. In this study, the critical micelle concentration (CMC) of the system was systematically evaluated using UV-Vis spectroscopy by monitoring the dependence of the optical response on the TSC concentration. Using this synthetic approach, core-shell structures were successfully fabricated as uniform spherical nanoparticles with diameters ranging from 300 to 500 nm. The multi-core/shell materials retained the inherent superparamagnetic properties of the NiFe₂O₄ cores while preserving the fluorescent characteristics of the ZnO components. These results highlight the strong potential of these bifunctional core-shell nanoparticles for bio-separation and bioimaging applications.

Keywords: *Inverse microemulsion method, Core-shell SiO₂ nanoparticles, Bioimaging applications.*

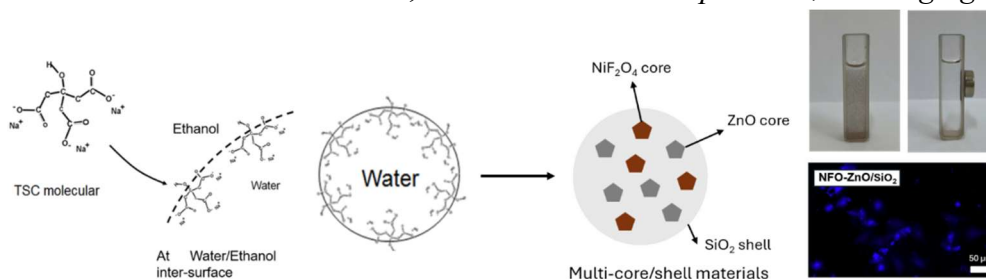


Figure: *An oil-free nanoemulsion method in magnetic-fluorescent nanosphere production*

PP-02 Benchmarking Multi-Generation AI Models and Physics-Based Simulations to Discover Dual-Target SARS-CoV-2 Mpro Inhibitors with Favorable CYP3A4 Clearance Profiles from Natural Products

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Abstract

Background: The discovery of novel antiviral agents against SARS-CoV-2 is severely hindered by high attrition rates due to poor pharmacokinetic profiles, particularly rapid Cytochrome P450 3A4 (CYP3A4) hepatic clearance. Although artificial intelligence (AI) has accelerated virtual screening, state-of-the-art models frequently fail when predicting complex, bulky natural products due to 'Out of-Distribution' (OOD) extrapolation errors, leading to false positives. This study establishes a dual branch screening pipeline to address potency and metabolic stability simultaneously.

Methods: We systematically benchmarked three generations of AI models—XGBoost (2D classical), Chemprop (2D GNN), and Uni-Mol (3D Spatial Transformer)—in predicting both pharmacodynamics (inhibitory potency against SARS-CoV-2 Mpro) and pharmacokinetics (CYP3A4 intrinsic clearance). To eliminate AI 'hallucinations,' predictions were cross-validated using structure-based GNINA molecular docking with 3D CNN scoring to overcome size bias. High-scoring leads and controls were subjected to 100-ns molecular dynamics (MD) simulations. Key analyses included Mpro binding energy calculations via MM-PBSA, residue-specific energy decomposition, as well as dynamic C-Fe distance and catalytic angle (θ) measurements in CYP3A4.

Results: For SARS-CoV-2 Mpro, MD and MM-PBSA identified Quercetin ($\Delta G_{\text{bind}} = -21.27 \pm 3.71$ kcal/mol) and Liquiritigenin ($\Delta G_{\text{bind}} = -19.92 \pm 2.60$ kcal/mol) as potent inhibitors, exhibiting competitive affinities compared to the FDA-approved control Nirmatrelvir ($\Delta G_{\text{bind}} = -23.46 \pm 3.70$ kcal/mol). These leads were anchored by key hydrogen bonds with Glu166 (occupancy: 31.69% for Quercetin, 19.14% for Liquiritigenin). In contrast, the bulky glycoside Rutin exhibited steric clashes with Glu166 (+1.60 kcal/mol), and the small fragment Favipiravir failed to maintain stable binding ($\Delta G_{\text{bind}} = -11.79 \pm 2.96$ kcal/mol). For CYP3A4 clearance, dynamic simulation successfully corrected AI 'hallucinations.' Nirmatrelvir, falsely predicted by AI as high clearance (119.11 mL/min/kg), was proven 'Safe by Physics' due to a stable dynamic C-Fe distance exceeding 6.0 Å (6.185 Å static) and an unfavorable catalytic angle ($\theta < 135^\circ$). Remdesivir was confirmed as a highly active substrate, hovering in the reactive zone (C-Fe < 5.0 Å, static 4.01 Å) with a highly favorable catalytic angle ($\theta > 135^\circ$). Among the natural ligands, Quercetin ($\Delta G_{\text{bind}} = -24.17 \pm 2.11$ kcal/mol, static C-Fe = 7.172 Å) and Liquiritigenin ($\Delta G_{\text{bind}} = -19.88 \pm 2.69$ kcal/mol, static C-Fe = 4.929 Å)

were validated as dual-target leads by MD simulations, exhibiting safe-to-moderate dynamic behaviors and moderate-to-low clearances. Oroxylin A and Hispidulin represent promising predicted dual-target candidates with outstanding static profiles from the virtual screening phase.

Conclusion: Integrating multi-generation AI with structure-based docking and dynamic physics based filters provides a robust, bifurcated pipeline that accurately filters out false positives and accelerates the discovery of potent, metabolically stable dual-target antivirals.

Keywords: SARS-CoV-2 Mpro, Cytochrome P450 3A4, GNINA CNN score, Out-of-Distribution (OOD), Natural Products, Drug Metabolism

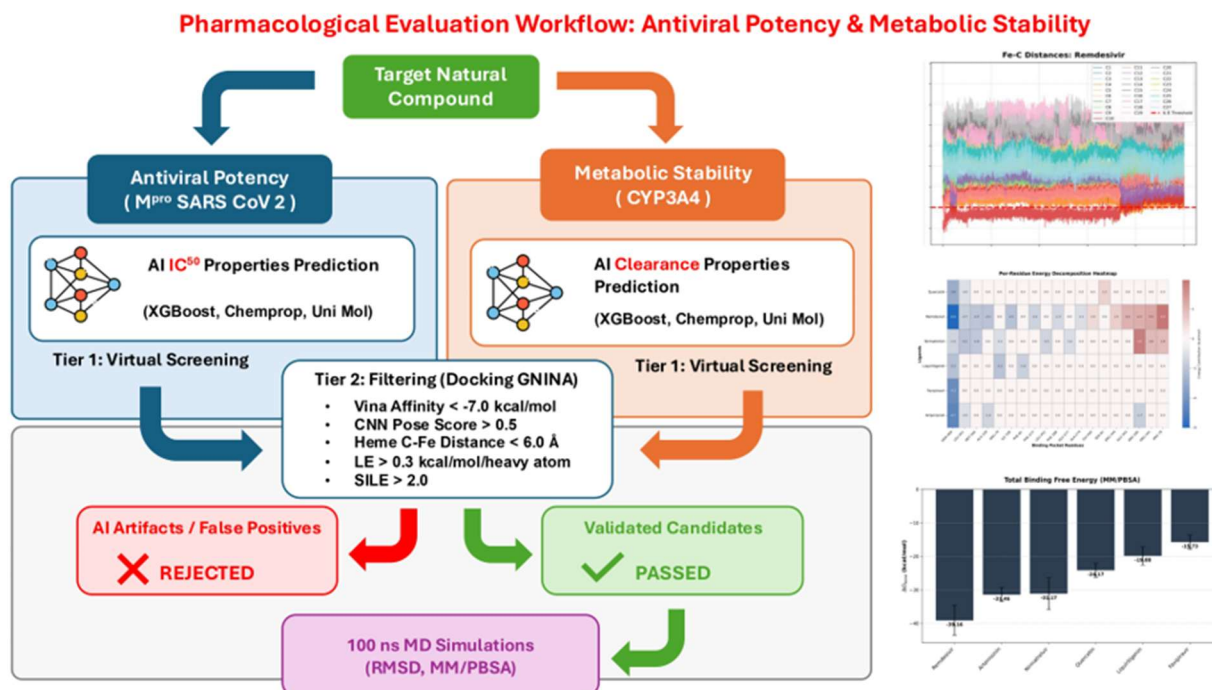


Figure 1. Integrated dual-branch virtual screening pipeline and 3D molecular validation. The workflow showcases a hierarchical strategy bridging ligand-based AI screening with structure-based physics constraints. The pipeline branches into: (i) the Pharmacodynamics (PD) arm evaluating SARS-CoV-2 Mpro inhibitory potency, and (ii) the Pharmacokinetics (PK) arm predicting CYP3A4-mediated clearance. Discrepancies and OOD hallucinations from multi-generation AI models (XGBoost, Chemprop, and Uni-Mol) are resolved through deep learning-based GNINA docking (CNN scoring) and 100-ns molecular dynamics (MD) simulations. Quercetin and Liquiritigenin are highlighted as MD-validated dual-target leads, while Oroxylin A and Hispidulin represent top-predicted candidates.

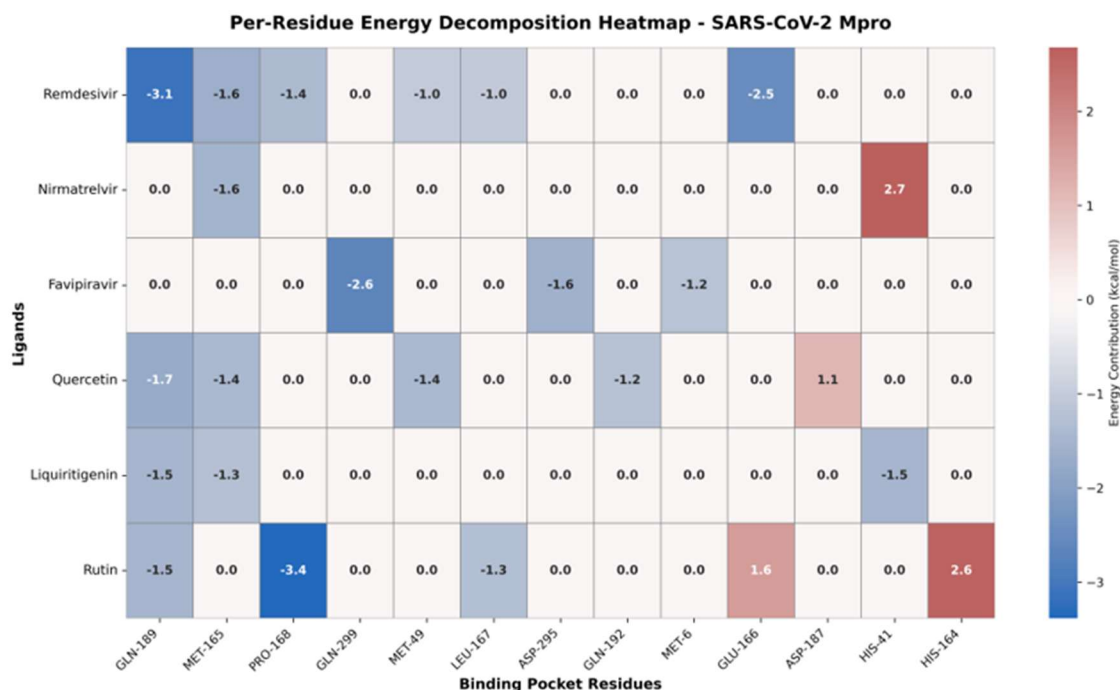


Figure 2: Per-residue binding free energy decomposition of SARS-CoV-2 Mpro complexes. The heatmap illustrates the thermodynamic contribution (in kcal/mol) of key active-site residues during 100-ns MD simulations. Highly favorable stabilizing interactions are highlighted in cool colors (e.g., MET-165 in the S2 pocket and GLN-189), while unfavorable steric or electrostatic clashes are depicted in warm/positive values, such as the bulky glycoside Rutin with GLU-166 (+1.60 kcal/mol) and HIS-164 (+2.62 kcal/mol), and non covalent Nirmatrelvir with HIS-41 (+2.68 kcal/mol).

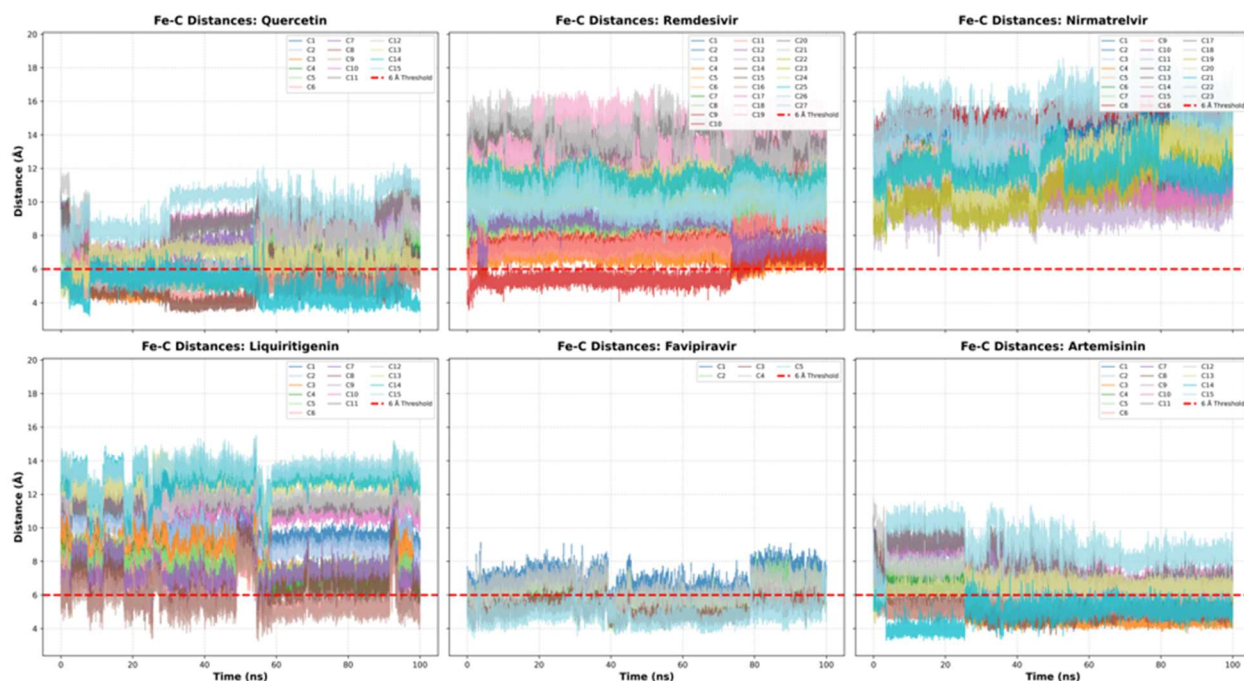


Figure 3: Dynamic trajectories of minimal Heme-Fe to ligand carbon (C-Fe) distances over 100-ns MD simulations. The red dashed lines define the critical biophysical thresholds, the Reactive Zone (<6.0 Å), where enzymatic oxidation is highly favorable, and the Safe Zone (>6.0 Å), where steric hindrance prevents metabolic oxidation.

PP-03 Composition-Optimized CuO/Ag-4-MPBA SERS Platform for Glucose Detection

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Abstract: Nanomaterial-based sensing platforms offer promising opportunities for sensitive detection of biologically relevant molecules. In this work, a series of CuO/Ag nanomaterials with different CuO:Ag ratios were developed for surface-enhanced Raman scattering (SERS)-based glucose sensing, with Ag used as a reference. The materials were functionalized with 4-mercaptophenylboronic acid (4-MPBA), which provides molecular recognition of glucose through interactions between its boronic acid group and the cis-diol groups of glucose. The glucose responses of the functionalized nanomaterials were systematically compared to evaluate the influence of CuO/Ag composition on sensing performance. The incorporation of CuO improved the glucose response compared with Ag, and the 20:80 CuO/Ag composition exhibited the most favorable performance among the investigated materials. The optimized CuO/Ag-4-MPBA system enabled sensitive glucose detection with a limit of detection of 2.6×10^{-5} M. These findings demonstrate how compositional engineering of metal-semiconductor nanomaterials combined with surface molecular recognition can provide an effective strategy for SERS-based glucose sensing.

Keywords: *CuO/Ag nanomaterials; surface-enhanced Raman scattering; glucose sensing; 4-mercaptophenylboronic acid; nanobiosensing.*

PP-04 Curvature-Aware Interpolation for Microtubule Filament Tracing in Cryo-EM

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Abstract: Cryo-electron microscopy (cryo-EM) analysis of continuous helical assemblies, such as microtubules, frequently suffers from extraction gaps along individual filaments due to regional low contrast, local defocus variations, or picking algorithm thresholding. These missing coordinates compromise lattice continuity and down-stream reconstruction quality. Here, we present a curvature-aware local fitting algorithm designed to restore missing particle coordinates across microtubule datasets within CryoSPARC. Using a threshold-guided framework based on local linear and quadratic fitting, we processed 88,229 initial particles distributed across 1,717 global filaments from 768 micrographs. The algorithm identified 1,696 structural gaps and evaluated them under predefined straightness criteria (linear threshold = 0.85, quadratic threshold = 0.5). A total of 1,632 gaps (96.2%) were successfully filled—comprising 1,565 linear interpolations for straight segments and 67 quadratic interpolations for moderately bent regions. To prevent spatial distortion, 64 gaps were strictly skipped due to excessive localized curvature (straightness ≥ 0.5). This quality-filtered interpolation strategy augmented the dataset by +4,720 high-confidence particles (+5.35%), resulting in a final consolidated output of 92,949 particles. This automated, geometry-validated pipeline effectively recovers missing lattice information while preserving true biological curvature, providing a robust dataset for high-resolution cryo-EM structure determination of filamentous complexes.

Keywords: Cryo-EM, Microtubule, Filament tracing, Curvature-aware interpolation, CryoSPARC.

PP-05 Desentanglement of Single-Cell Raman Spectra in Tensor-Product Hilbert Spaces with Galois Adjunction Operators

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Abstract:

Background: Single-cell optical biophysics relies on vibrational Raman spectroscopy to non-destructively probe cellular biomolecules. However, observed biophysical spectra are non-commutatively entangled with high-entropy environmental noise, including severe autofluorescence baselines, laser power decay, and biomass concentration fluctuations. Standard data-driven neural networks and empirical smoothing algorithms treat these perturbations as flat, decoupled additive noise. Consequently, under physical domain shifts, they suffer geometric feature collapse, eroding localized molecular peak ratios and generating ungrounded hallucinations that compromise diagnostic integrity.

Methods: We present a physics-constrained algebraic paradigm named Ontological Subspace Mapping Optimization (OSMO) implemented via the closed-form Subspace-Orthogonal Adjunction and Recovery (SOAR) engine. Unlike legacy algorithms that assume decoupled additive noise, we model physical observations as a tensor-product Hilbert space, capturing the non-commutative entanglement between target molecular states and environmental context drift. Rather than empirical curve fitting, we construct Galois Adjunction operator pairs over closed subspace lattices. The closing operator projects the raw entangled spectrum into the target subspace by mapping non-linear autofluorescence baselines directly into its mathematical kernel, completely annihilating baseline artifacts without eroding fine molecular vibrational signatures. Multiplicative laser power fluctuations are decoupled through log-linear group transformations, while common-mode genomic spectral overlaps are isolated using orthogonal null-space projections.

Results: Evaluated on a benchmark dataset of 82 000 single-cell Raman spectra across 30 clinical pathogens, the OSMO-SOAR engine demonstrated exceptional resilience under extreme physical degradation. Under a 40% laser power reduction and a 150% background noise surge, the system maintained 89.13% classification accuracy, whereas deep neural networks collapsed to 0.07% due to feature hallucination. In resolving six closely related *Staphylococcus* sibling strains sharing over 95% biophysical spectral overlap, the framework achieved 42.00% accuracy (compared to 18.67% random chance and < 18.00% for traditional deep learning) while preserving 100% of peak amplitude ratios. Compiled onto an ARM Cortex-M4 microcontroller, the entire validative engine operates within 178.5 KB of SRAM with zero dynamic memory allocation.

Conclusion: This study proves that Galois adjunction operators and Hilbert subspace ontologies provide an exact, hallucination-free foundation for molecular biophysical telemetry, enabling real-time, deterministic pathogen identification on resource-constrained micro-edge hardware.

Keywords: *Molecular Biophysics, Raman Spectroscopy, Galois Adjunction, Hilbert Subspace, Invariant Operators, Edge Computing.*

PP-06 Development of Ag/AZO Hybrid Thin Films for Sensitive SERS Detection of Metronidazole in Shrimp

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Abstract: Surface-enhanced Raman scattering (SERS) has attracted considerable interest as a rapid and highly sensitive analytical technique for detecting trace contaminants in complex matrices. In this work, Ag/Al-doped ZnO (Ag/AZO) hybrid thin films were synthesized as efficient SERS substrates for the detection of metronidazole (MNZ) residues in shrimp. AZO thin films were fabricated by dc magnetron sputtering with systematically varied substrate temperatures and Al doping concentrations to optimize their structural, electrical, and surface properties. The AZO film deposited at 200 °C with 2 wt.% Al exhibited the highest carrier concentration and Hall mobility, together with increased effective surface area and defect density, providing favorable conditions for charge transfer induced Raman enhancement. Ag nanoparticles were subsequently deposited onto the optimized AZO film by dc magnetron sputtering, generating hybrid substrates that combine localized surface plasmon resonance with semiconductor-assisted charge transfer to achieve synergistic electromagnetic and chemical enhancement. The optimized Ag/AZO thin film substrate enabled highly sensitive detection of MNZ, achieving a limit of detection (LOD) of 0.001 ppm for standard solutions with an enhancement factor (EF) of approximately 2.5×10^6 . In MNZ-spiked shrimp samples, the substrate achieved an LOD of 0.05 ppm, with a linear response ($R^2 = 0.993$) and satisfactory recoveries ranging from 94% to 109%, demonstrating reliable analytical performance in a complex food matrix. These results highlight the effectiveness of engineering Ag/AZO hybrid thin films to improve SERS sensitivity and demonstrate their strong potential as practical sensing platforms for rapid monitoring of antibiotic residues in seafood.

Keywords: *Surface-enhanced Raman spectroscopy; Ag/AZO hybrid thin films; metronidazole detection; electromagnetic enhancement; semiconductor-assisted charge transfer.*

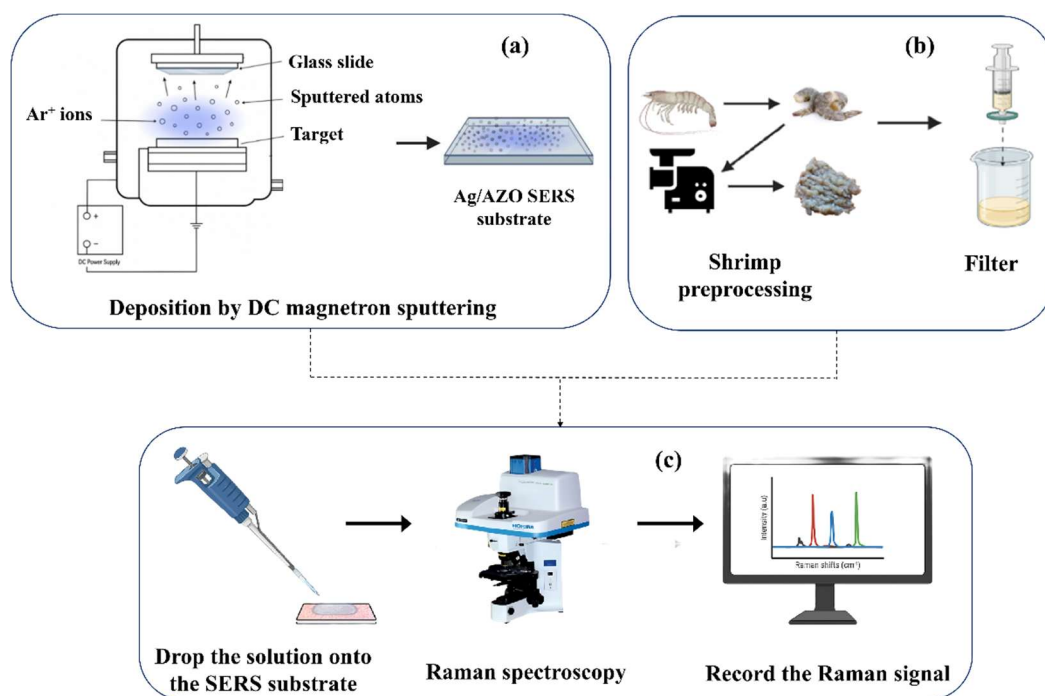


Figure: Schematic illustration of the fabrication of the Ag/AZO thin-film SERS substrate by DC magnetron sputtering (a), sample preparation (b), and Raman measurements of standard and shrimp samples (c).

PP-07 Eco-Friendly Biosynthesis and Comprehensive Physicochemical Characterization of *Annona reticulata*-Derived Silver Nanoparticles with Potential Anticancer Activity Against MCF-7 Cells

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Abstract: The present study investigated the green synthesis of silver nanoparticles using the ethanolic leaf extract of *Annona reticulata* and evaluated their physicochemical characteristics and anticancer potential. Fresh leaves of *A. reticulata* were subjected to Soxhlet extraction using ethanol to obtain a phytochemical-rich extract, which was subsequently employed as a reducing and stabilizing agent for the synthesis of silver nanoparticles through the reduction of silver nitrate under controlled conditions. The formation of nanoparticles was initially indicated by a gradual color change from light yellow to dark brown, suggesting the reduction of silver ions by bioactive constituents present in the extract. Comprehensive characterization of the synthesized nanoparticles (AREEAgNPs) was performed using UV–Visible spectroscopy, FTIR, XRD, DLS, zeta potential analysis, FESEM, EDS, and HR-TEM. UV–Visible analysis revealed a distinct surface plasmon resonance peak at approximately 370 nm, confirming nanoparticle formation, while a strong absorption band between 250–290 nm indicated the presence of phytochemicals associated with nanoparticle stabilization. FTIR analysis demonstrated the presence of hydroxyl, aliphatic, aromatic, and carbonyl-containing functional groups, confirming the involvement of plant-derived biomolecules in the reduction and capping processes. XRD analysis exhibited well-defined diffraction peaks with a prominent reflection at 25.8°, confirming the crystalline nature of the synthesized nanoparticles. DLS analysis revealed a Z-average particle size of 100.3 nm and a low polydispersity index of 0.105, indicating a narrow particle size distribution and good dispersion characteristics. The nanoparticles exhibited a zeta potential value of –10.44 mV, suggesting surface stabilization by phytochemical constituents. FESEM and HR-TEM analyses revealed predominantly spherical to quasi-spherical nanoparticles, with HR-TEM showing particles largely within the range of 10–20 nm, while FESEM measurements indicated particle diameters of approximately 44.99–55.57 nm. EDS analysis confirmed the elemental composition of the nanoparticles through the presence of a characteristic silver signal at approximately 3 keV. The biological activity of AREEAgNPs was assessed against MCF-7 human breast adenocarcinoma cells. MTT assay results demonstrated concentration-dependent inhibition, increasing from 7.05% at 0.973 µg/mL to 79.01% at 125 µg/mL. Furthermore, AO/EB staining revealed distinct apoptotic morphological changes, including increased orange-red fluorescence, membrane permeability alterations, and cellular condensation in treated cells compared with untreated controls. These findings demonstrate that *Annona reticulata*-derived silver nanoparticles possess favorable physicochemical properties and significant cytotoxic activity against MCF-7 cells, highlighting their potential for further investigation as phytochemical-assisted nanotherapeutic agents for cancer-related biomedical applications.

Keywords: *Annona reticulata*, Silver Nanoparticles, Green Nanotechnology, Nanomedicine, MCF-7, Anticancer Activity, Phytochemical-Assisted Synthesis

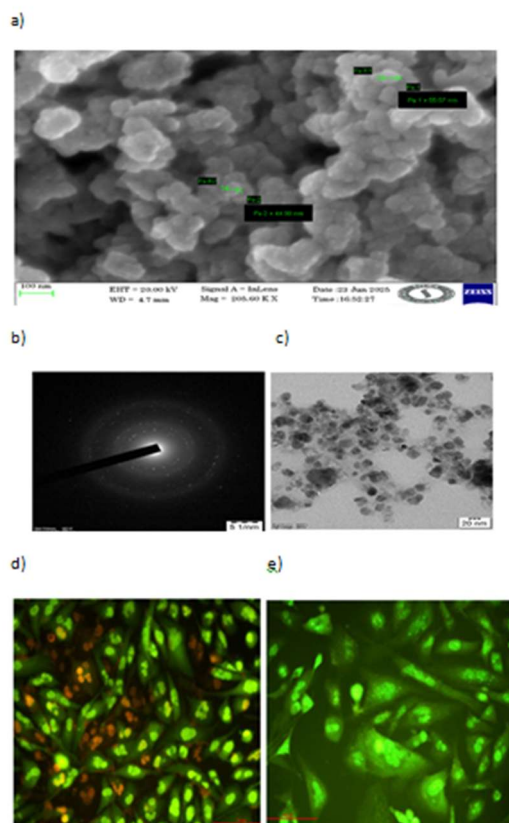


Figure: a) FESEM micrograph of silver nanoparticles synthesized using *Annona reticulata* ethanolic extract (AREEAgNPs), b), c) HR-TEM image of silver nanoparticles synthesized using *Annona reticulata* ethanolic extract (AREEAgNPs), showing predominantly spherical to quasi-spherical nanoparticles with nanoscale dimensions and slight agglomeration, d), e) AO/EB fluorescence staining of control and *Annona reticulata* ethanolic extract-mediated silver nanoparticle (AREEAgNP)-treated cells showing increased apoptotic cell death in the treated group compared with the control

PP-08 Effect of Polar Solvents on the Photoluminescent Properties of Carbon Dots

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Abstract: Nowadays, the synthesis of carbon dots (CDs) and research into their potential applications as optical sensors represent one of the most promising areas of modern nanotechnology and materials science. Owing to their high photostability, low toxicity, good biocompatibility and pronounced photoluminescent properties, CDs are widely used for the detection of various chemical substances, including polar organic solvents and alcohols of varying concentrations. In this study, CDs were synthesized using the solvothermal method. The structural, morphological and optical properties of the resulting nanoparticles were investigated using TEM, XPS, FTIR, UV-Vis and PL. The synthesized CDs were then dispersed in solutions of isopropyl alcohol, methanol, ethanol and water at various volume concentrations, after which changes in their photoluminescence characteristics as a function of solvent polarity were investigated. The results of the studies showed that the average size of the synthesized CDs is approximately 8-10 nm $\pm$ 0.5 nm. It was found that a change in the polarity of the medium significantly affects the photoluminescence spectra of the CDs. As the water content increases and the percentage ratio of polar solvents changes, a bathochromic (red) shift of the photoluminescence peak is observed from 500 to 530 nm. The results obtained demonstrate the high sensitivity of CDs to the polarity of the surrounding environment and confirm the potential for their use as optical sensors for determining the composition and concentration of polar solvents.

Keywords: *Carbon dots, Polar solvents, Photoluminescence, Optical properties, Red shift*

PP-09 Electrical validation of stepwise surface functionalization and real-time specific toxin detection on a label-free semiconductor biochip.

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Abstract: This work presents a stepwise surface modification protocol, oxygen-plasma activation, APTES silanization, and A8 nanobody immobilization, for capturing the botulinum neurotoxin light chain (LC/A) and evaluating each step using a lock-in-based differential amplitude readout on a resistive Wheatstone-bridge sensor architecture. Across two functionalized chips, A8 nanobody immobilization consistently produced an increase in differential amplitude relative to baseline, confirming successful bilayer formation; however, the magnitude of this shift varied substantially between chips (1.6-1.8-fold versus 3.5-6.0-fold baseline), indicating that absolute amplitude values are not yet quantitatively reproducible across devices. Subsequent LC/A exposure induced a further amplitude change (1.1- to 3.9-fold baseline) that scaled qualitatively with bound analyte concentration (2.7 ppm versus 0.1 ppm, a ~27-fold difference), although the response direction relative to the preceding A8 step differed between chips - a continued increase on one chip versus a partial decrease from an anomalously high A8 signal on the other. A preliminary real-time kinetic assay on one chip showed that specific LC/A binding produced a smooth, non-monotonic, U-shaped relaxation over 2-3 minutes, clearly distinguishable from the monotonic upward drift observed for a non-specific buffer control on the reference channel. These results indicate that the oxygen-plasma/APTES/nanobody route reliably yields an LC/A-responsive capture surface, and that differential lock-in readout can qualitatively discriminate specific binding from non-specific drift, even though chip-to-chip variability in absolute signal magnitude currently limits the present dataset (n = 2 chips) to qualitative and comparative interpretation. Ongoing work therefore focuses on three directions: expanding the chip cohort to establish statistically robust bounds on reproducibility; introducing on-chip reference normalization to suppress device-to-device baseline variance; and replicating the real-time kinetic assay across multiple chips and analyte concentrations to define a quantitative discrimination threshold between specific binding and non-specific drift.

Keywords: surface functionalization, label-free biosensor, biochip, differential lock-in readout, botulinum neurotoxin

PP-10 Enhancing Exosomal Loading and Cytosolic Delivery of Recombinant Proteins via Structural Cyclization

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Abstract: Effective cytosolic delivery of therapeutic proteins is impeded by endosomal entrapment and subsequent degradation. While exosomes are promising nanocarriers capable of direct cytosolic release, their application is restricted by low exogenous loading efficiency. Here, we present a synergistic strategy utilizing protein cyclization and saponin permeabilization to overcome both loading and intracellular delivery barriers. Using enhanced green fluorescent protein (EGFP) as a model, carrying N-terminal tetra- arginine (R4) as cell penetrating peptide and a C-terminal His-6 tag, we demonstrated that saponin-assisted loading increased the exosomal encapsulation efficiency of cyclized proteins from 11% to 33%, compared to an increase from 6% to 13% for their linear counterparts. Crucially, *in vitro* cellular assays demonstrated that exosomes loaded with these cyclized proteins bypassed endosomal entrapment, achieving functional cytosolic delivery into HeLa cells. By simultaneously addressing low encapsulation rates and endosomal degradation, this combinatorial approach establishes a potent platform for protein therapeutics.

Keywords: endosomal entrapment, cyclized protein, EGFP, saponin, exosome.

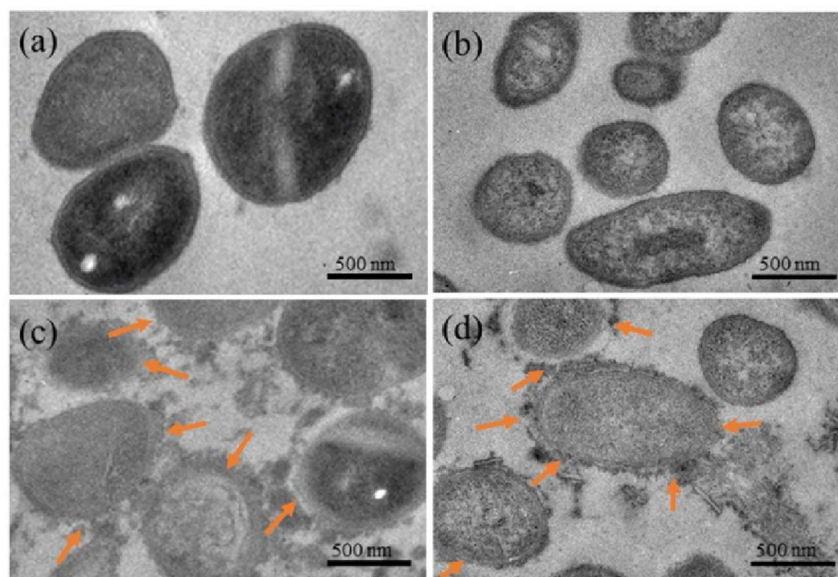


Figure: The caption of the figures

PP-11 Green Synthesis and Physicochemical Characterization of Silver Nanoparticles Using Pomegranate Peel (*Punica granatum*)

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Abstract: Background: Green synthesis of metallic nanoparticles using plant-derived phytochemicals has emerged as an eco-friendly and sustainable alternative to conventional chemical methods. Pomegranate peel (*Punica granatum*), rich in polyphenols, flavonoids, and tannins, serves as an effective natural reducing and stabilizing agent. This study investigates the green synthesis of silver nanoparticles (PPAgNPs) using pomegranate peel ethanolic extract and evaluates their physicochemical characteristics. **Methods:** Ethanolic extract of pomegranate peel was prepared using Soxhlet extraction and employed for the synthesis of silver nanoparticles by reducing aqueous silver nitrate solution. The synthesized PPAgNPs were characterized using UV–Visible spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Dynamic Light Scattering (DLS), Zeta Potential Analysis, X-ray Diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), and High-Resolution Transmission Electron Microscopy (HR-TEM). **Results:** UV–Visible spectroscopy confirmed nanoparticle formation, while FTIR analysis revealed the involvement of phytochemicals in nanoparticle reduction and stabilization. DLS analysis showed a Z-average particle size of 38.3 nm with a polydispersity index of 0.427. The nanoparticles exhibited a zeta potential of –20.7 mV, indicating acceptable colloidal stability. XRD confirmed the crystalline nature of the nanoparticles, whereas FE-SEM and HR-TEM revealed predominantly spherical nanoparticles with slight aggregation. **Conclusion:** The study demonstrates the successful green synthesis of stable silver nanoparticles using pomegranate peel ethanolic extract. The phytochemical-rich extract acted as both a reducing and capping agent, producing crystalline nanoparticles with favourable physicochemical properties. These findings highlight the potential of pomegranate peel-mediated silver nanoparticles for biomedical, antimicrobial, and nanobiotechnology applications while promoting the valorisation of agricultural waste.

Keywords: *Green synthesis, silver nanoparticles, Pomegranate peel extract, Characterization, Nanobiotechnology, Phytochemical capping.*

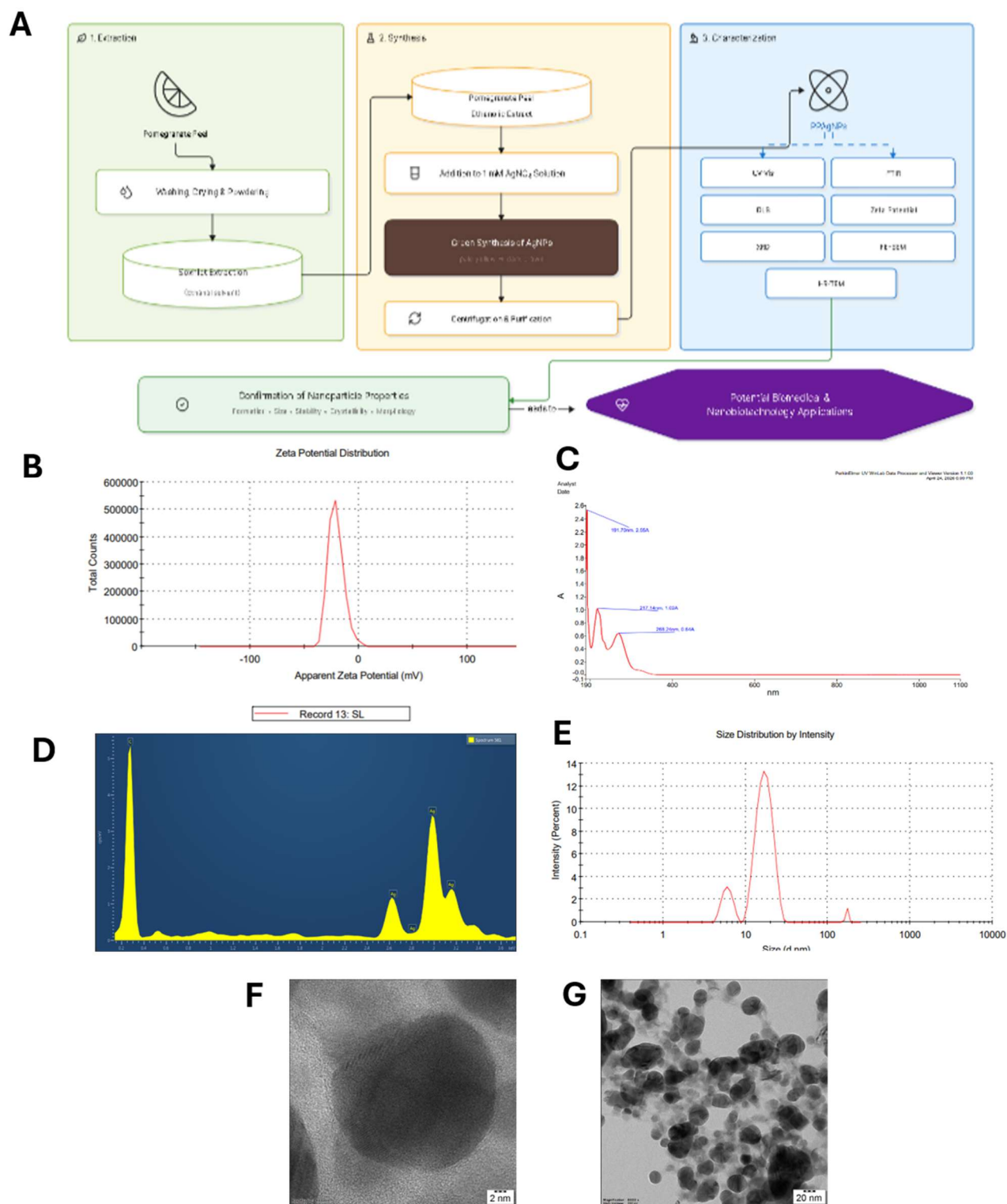


Figure 1: Graphical representation of PPAgNPs synthesis and characterization: (A) Green synthesis workflow of Silver Nanoparticles, (B) Zeta Potential Analysis (-20.7 mV), (C) UV-Visible Spectrum, (D) FTIR Spectrum, (E) Dynamic Light Scattering (Particle Size Distribution), (F) HR-TEM (Single Nanoparticle), (G) HR-TEM (Overall Morphology and Dispersion)

PP-12 Green Synthesis of Fe₃O₄, MgO, and Fe₃O₄–MgO Nanoparticles Using *Psidium cattleianum* Leaf Extract: Evaluation of Antibacterial and In Vitro Antioxidant Activities

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Abstract: This study investigates the green synthesis, characterization, and biological activities of metal oxide nanoparticles using *Psidium cattleianum* leaf extract as a sustainable phytochemical reducing and stabilizing agent. Rich in phenolic compounds and natural antioxidants, the leaf extract provides an eco-friendly alternative to conventional chemical synthesis methods. Initially, copper nanoparticles (CuNPs) were synthesized using an aqueous leaf extract and copper sulfate solution. Their formation and stability were confirmed through UV–Visible spectroscopy and FTIR analysis, while antioxidant activity was evaluated using the DPPH assay. The synthesized CuNPs exhibited significant antibacterial activity against clinically relevant pathogens, including *Enterococcus* spp., *Enterobacter* spp., methicillin-resistant *Staphylococcus aureus* (MRSA), and *Acinetobacter baumannii*.

Further studies involved the synthesis of Fe₂O₃, MgO, and Fe₂O₃–MgO nanoparticles under controlled stirring and thermal conditions. Characterization techniques confirmed successful nanoparticle formation, and antibacterial efficacy was assessed using agar well diffusion and minimum inhibitory concentration (MIC) methods. To enhance functional performance, Fe₃O₄, MgO, and Fe₃O₄–MgO nanocomposites were subsequently synthesized and evaluated. Among the tested materials, Fe₃O₄–MgO nanocomposites demonstrated superior antibacterial activity, particularly against MRSA and *A. baumannii*, likely due to synergistic interactions between the constituent metal oxides. A comparatively lower effect was observed against *Enterobacter* spp.

Overall, the findings highlight the potential of *P. cattleianum* leaf extract as a cost-effective and environmentally friendly resource for nanoparticle synthesis. The synthesized nanoparticles possess promising antibacterial and antioxidant properties, indicating their potential applications in biomedical, industrial, and environmental sectors while supporting the development of sustainable nanotechnology strategies to combat antimicrobial resistance.

Keywords: *Green synthesis, Metal oxide nanoparticles, Psidium cattleianum, Antibacterial activity, Nanobiotechnology.*

PP-13 Green Synthesis, Physicochemical Characterization, and Anti-Hemolytic Activity of Pepper-Derived Copper Nanoparticles (PCuNPs) Using *Piper nigrum* Ethanolic Extract

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Abstract

Background: Green synthesis of metal nanoparticles using plant extracts has emerged as an environmentally friendly approach for producing nanomaterials with desirable physicochemical and biological properties. In the present study, copper nanoparticles (PCuNPs) were synthesized using the ethanolic extract of *Piper nigrum* (black pepper), where the phytochemicals present in the extract acted as reducing and stabilizing agents.

Methods: Pepper ethanolic extract was prepared by Soxhlet extraction and used for the green synthesis of copper nanoparticles by mixing 10 mL of extract with 90 mL of 1 mM copper sulfate solution under continuous stirring at room temperature for 45–60 minutes. Formation of nanoparticles was confirmed by a visible colour change. The synthesized PCuNPs were characterized using UV–Visible spectroscopy, Fourier Transform Infrared Spectroscopy (FTIR), Dynamic Light Scattering (DLS), zeta potential analysis, X-ray diffraction (XRD), Field Emission Scanning Electron Microscopy (FE-SEM), High-Resolution Transmission Electron Microscopy (HR-TEM), and Energy Dispersive X-ray Spectroscopy (EDAX). The biological activity of PCuNPs was evaluated by a human red blood cell membrane stabilization assay to determine anti-hemolytic activity.

Results: UV–Visible spectroscopy showed characteristic absorption peaks at **191.74 nm** and **450.61 nm**, confirming the formation of copper nanoparticles. FTIR analysis revealed the presence of hydroxyl, alkane, amide, C–N, and C–O functional groups, indicating the involvement of phytochemicals in nanoparticle reduction and stabilization. DLS analysis showed a Z-average particle size of **38.3 d.nm** with a polydispersity index of **0.427**, indicating moderate particle size distribution. The synthesized nanoparticles exhibited a zeta potential of **–20.7 mV**, suggesting moderate colloidal stability. XRD analysis confirmed the crystalline nature of the nanoparticles. FE-SEM analysis revealed irregular and clustered nanoparticles with rough surface morphology, whereas HR-TEM showed predominantly spherical to nearly oval nanoparticles with slight agglomeration. EDAX confirmed copper as the major elemental constituent of the synthesized nanoparticles. The anti-hemolytic assay demonstrated concentration-dependent membrane stabilization, with **78.05% protection against hemolysis at 100 µg/mL**, indicating effective erythrocyte membrane protection.

Conclusion: The study demonstrates the successful green synthesis of copper nanoparticles using *Piper nigrum* ethanolic extract. The synthesized PCuNPs exhibited desirable physicochemical characteristics and significant anti-hemolytic activity, indicating their potential for further investigation in biomedical and pharmaceutical applications.

Keywords:

Copper nanoparticles, Green synthesis, Piper nigrum, Pepper extract, Physicochemical characterization, Anti-hemolytic activity, Nanomedicine

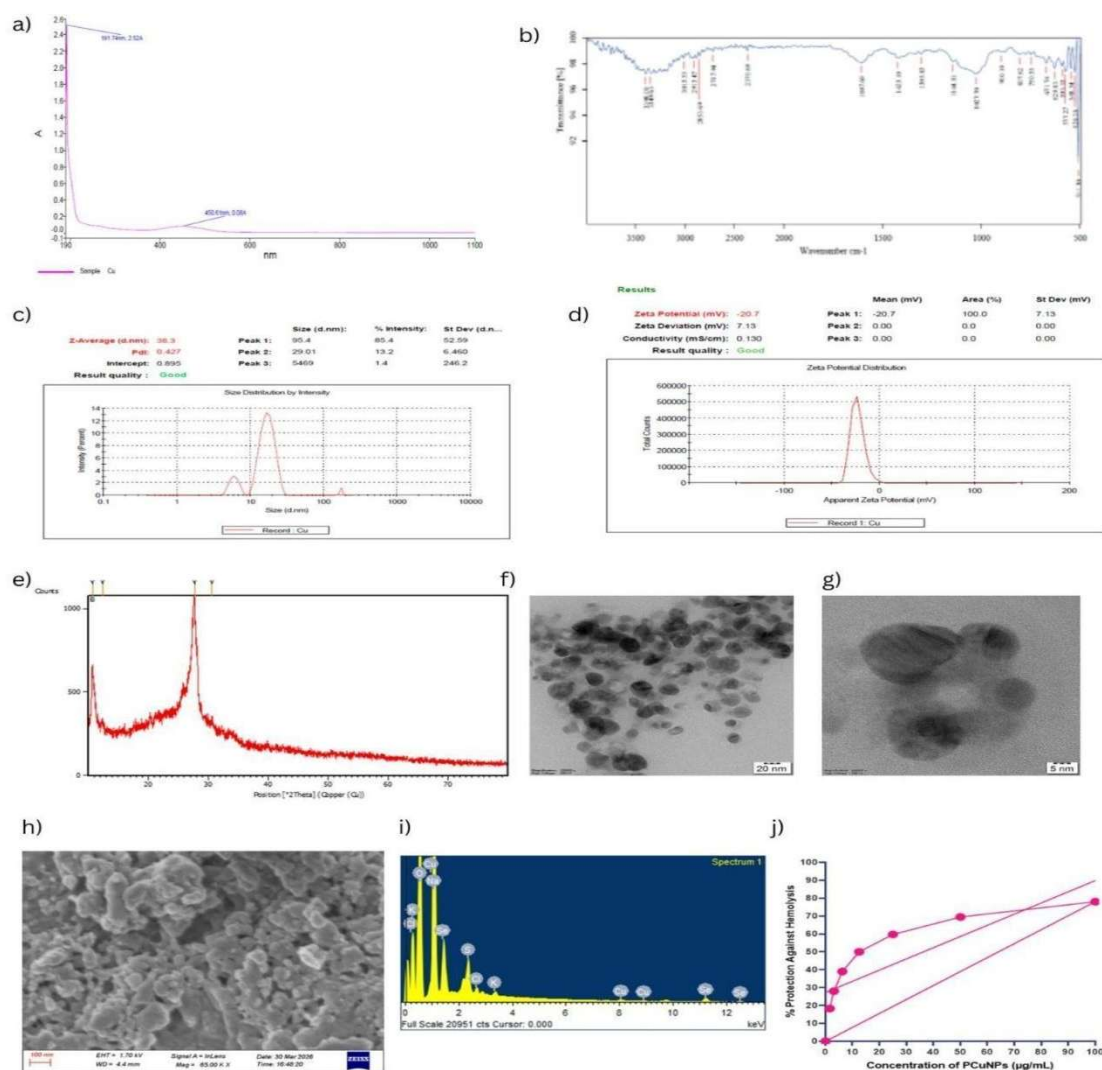


Figure: Representative characterization of PCuNPs: **(a)** UV–Visible absorption spectrum showing characteristic absorption peaks at 191.74 and 450.61 nm; **(b)** FTIR spectrum illustrating the functional groups involved in the reduction and stabilization of copper nanoparticles; **(c)** Dynamic Light Scattering (DLS) particle size distribution (Z-average: 38.3 d.nm; PDI: 0.427); **(d)** Zeta potential distribution showing a surface charge of -20.7 mV; **(e)** X-ray diffraction (XRD) pattern confirming the crystalline nature of the synthesized nanoparticles; **(f, g)** HR-TEM micrographs showing predominantly spherical to nearly oval nanoparticles with nanoscale dimensions; **(h)** EDAX spectrum confirming copper as the major elemental constituent; **(i)** FE-SEM micrograph revealing the surface morphology of the synthesized copper nanoparticles; **(j)** Anti-hemolytic activity of phytogenic copper nanoparticles (PCuNPs) determined by the human red blood cell membrane stabilization assay.

PP-14 Green Synthesis, Physicochemical Characterization, and Biological Activity of Clove-Derived Selenium Nanoparticles (CSeNPs) using *Syzygium aromaticum* Ethanolic Extract

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Abstract: The escalating demand for eco-friendly and sustainable nanomaterial synthesis has prompted significant interest in green nanotechnology. Selenium nanoparticles (SeNPs) have gained considerable attention owing to their distinctive physicochemical properties and promising biological activities. In this study, selenium nanoparticles were synthesized using the ethanolic extract of clove buds (*Syzygium aromaticum*) as a green reducing and capping agent, a cost-effective and environmentally benign approach. Clove extract was prepared via Soxhlet extraction with ethanol for 6–8 hours, and nanoparticles were synthesised by adding 10 mL of the extract to 90 mL of 1 mM sodium selenite solution containing ascorbic acid, under constant stirring at 25°C for 45–60 minutes. A characteristic colour change confirmed successful nanoparticle formation. Comprehensive physicochemical characterization was performed using UV–Vis spectroscopy, FTIR, DLS, zeta potential analysis, XRD, FE-SEM, HR-TEM, and EDAX. UV–Vis spectroscopy revealed a characteristic absorption peak at 193.79 nm (absorbance: 2.93 A), confirming the optical properties of the synthesized CSeNPs. FTIR analysis identified key functional groups, including O–H stretching (3287.52 cm^{-1}), C=O/C=C stretching (1637.02 cm^{-1}), and Se–O vibrations (563.48 and 528.02 cm^{-1}), attributable to phytochemicals such as eugenol and phenolic compounds, which act as natural capping agents. DLS analysis showed a Z-average particle size of 104.6 nm with a PDI of 0.269, indicating a narrow, uniform size distribution. The zeta potential of -44.7 mV confirmed excellent colloidal stability through strong electrostatic repulsion. XRD analysis confirmed the crystalline nature of CSeNPs, with a prominent diffraction peak at $2\theta \approx 26\text{--}27^\circ$, indicative of well-defined crystalline selenium. FE-SEM revealed spherical to irregular, nanoscale morphology with slight agglomeration, while HR-TEM confirmed the nanoscale dimensions and crystalline structure of the particles. EDAX verified selenium as the dominant elemental component, along with carbon and oxygen signals from phytochemical capping agents. Biological evaluation demonstrated that CSeNPs and clove extract exhibit concentration-dependent DPPH radical scavenging activity, with 71.00% inhibition at $100\text{ }\mu\text{g/mL}$ compared to 97.22% for ascorbic acid. Antibacterial activity was assessed against selected pathogenic strains by the agar well diffusion method, and inhibition zones were recorded. These findings collectively establish that clove-mediated selenium nanoparticles represent a promising green nanomaterial with significant antioxidant and antibacterial potential, offering prospective applications in nanomedicine and biomaterial sciences.

Keywords: *Selenium nanoparticles, Green synthesis, Syzygium aromaticum, Clove extract, Physicochemical characterization, Antioxidant activity, Antibacterial activity, Nanomedicine*

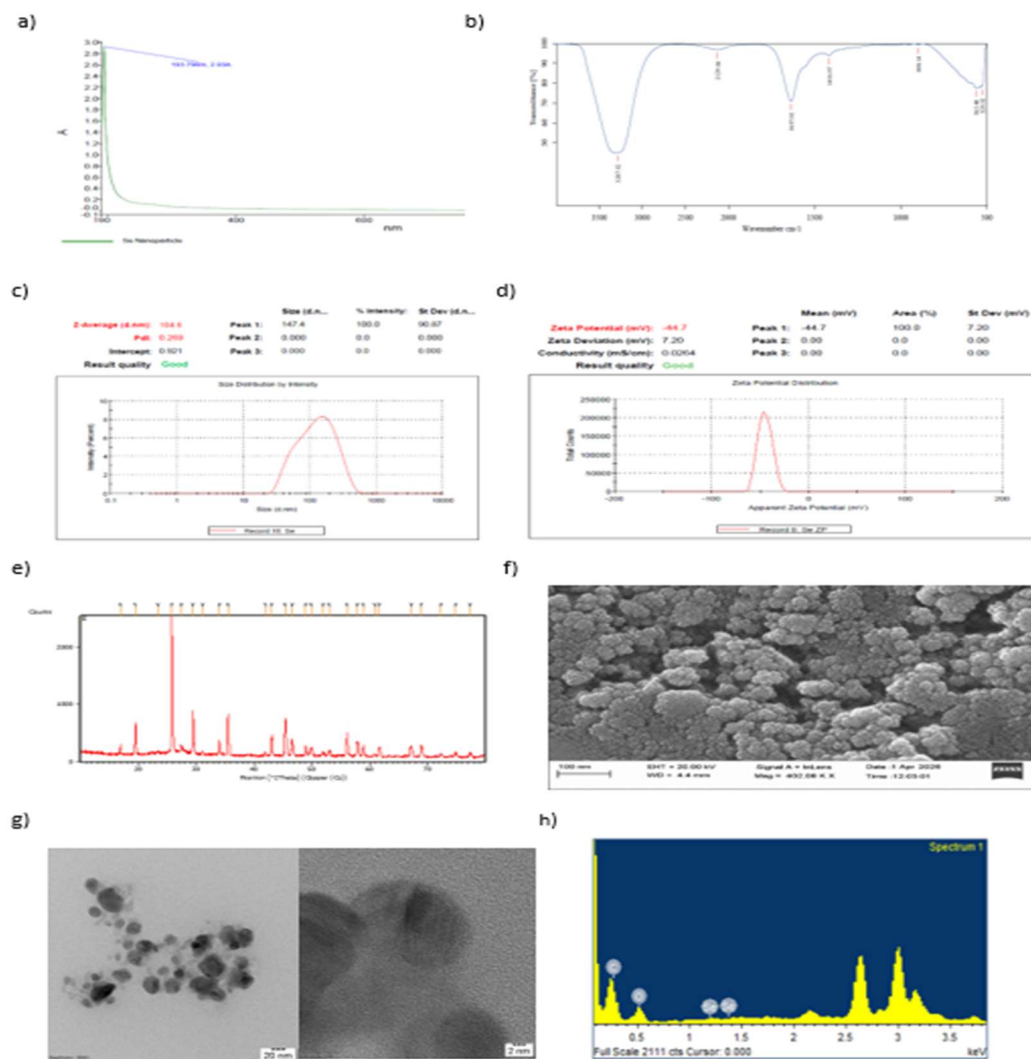


Figure 1: Representative characterization of Coens: (a) UV–Vis absorption spectrum showing peak at 193.79 nm; (b) FTIR spectrum revealing phytochemical functional groups; (c) DLS particle size distribution (Z-average: 104.6 nm, PDI: 0.269); (d) Zeta potential distribution (−44.7 mV); (e) XRD pattern confirming crystallinity; (f) FE-SEM micrograph showing nanoscale morphology; (g) HR-TEM image; (h) EDAX spectrum confirming elemental selenium composition.

PP-15 Investigation of Controllable Cooling for Improved Thermal Response in a Peltier-Based PCR Thermal Cycler

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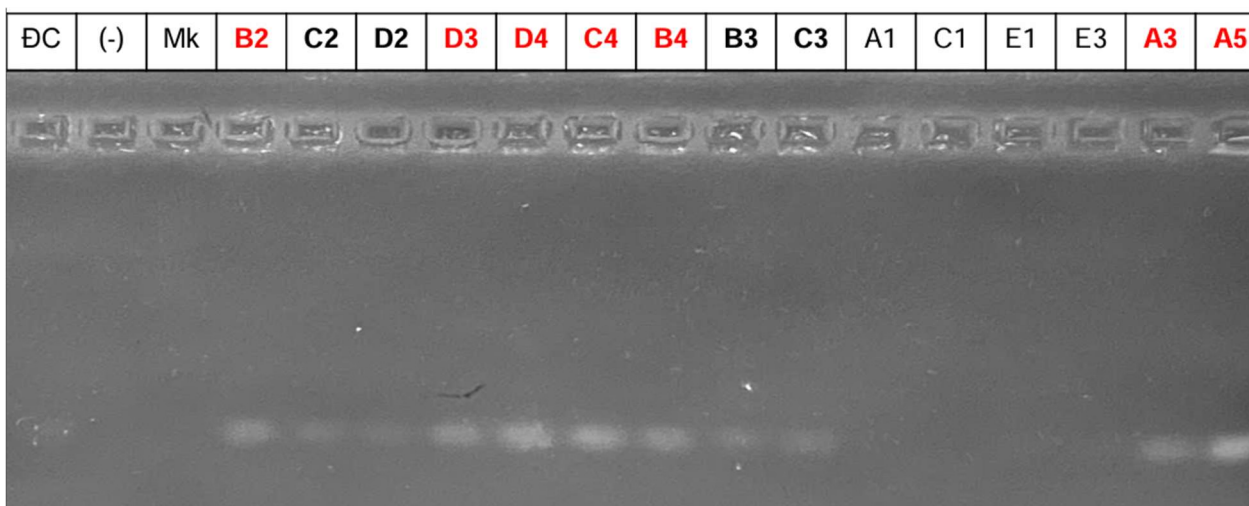
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Abstract: Polymerase chain reaction (PCR) requires precise temperature control for efficient and reproducible DNA amplification. Peltier thermoelectric modules provide compact and bidirectional temperature control, but their thermal performance is strongly affected by the cooling boundary conditions. In this study, we developed a Peltier-based PCR thermal cycling system with a controllable-temperature cooling unit to investigate the influence of cooling conditions on the thermal response of the sample chamber. The system was fabricated using a Peltier thermoelectric module, an aluminum sample chamber, and a temperature-controlled cooling unit. An NTC thermistor-based thermometer was developed and calibrated over 25-95 °C for real-time temperature monitoring. The transient temperature response was investigated under different electrical input powers, and the temperature-time data were fitted using an exponential heat-transfer model. The NTC thermistor showed a measurable and reproducible response, with a calibration relationship of exponential function. The fitted thermal parameters exhibited a linear relationship with the supplied electrical power. The prototype PCR system achieved denaturation, annealing, and extension temperatures of 90 °C, 60 °C, and 72 °C, respectively, with a temperature deviation of less than 0.5 °C. Before implementation of the controllable cooling unit, PCR validation over 30 cycles successfully produced amplification products at 10 positions, with samples B2, D3, D4, C4, B4, A3, and A5 showing approximately 2-4 times higher product levels than the control. We expect that increasing the cooling-unit temperature during heating will reduce heat dissipation from the Peltier module and increase the heating rate of the sample chamber. The controllable cooling unit will subsequently be evaluated experimentally to quantify its effect on thermal cycling performance.



Hình 1. Kết quả điện di sản phẩm PCR trên gel agarose 3% TBE
 ĐC: đối chứng dương máy Astec, (-): đối chứng âm, Mk: marker 100bp
 Chu trình nhiệt: 80-1p, 40x(80-40s, 60-20s)

Keywords: *Peltier effect; thermoelectric module; PCR thermal cycler; thermal cycling; temperature control; heat transfer; thermoelectric cooling*

PP-16 Investigation of the effects of BPA on the expression levels of DNA methyltransferase genes in zebrafish (*Danio rerio*) embryos

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Abstract: Bisphenol A (BPA) is a widespread endocrine-disrupting chemical that raises significant concerns regarding its potential toxicity to aquatic organisms. This study evaluated the effects of BPA exposure on the expression of DNA methyltransferase genes (*dnmt1*, *dnmt3aa*, *dnmt3ba*, and *dnmt3bb.1*), which play key roles in establishing and maintaining DNA methylation patterns during embryonic development. Zebrafish (*Danio rerio*) embryos were exposed to 0, 20, 2500, and 5000 µg/L BPA for 96 hpf. While BPA exposure caused no significant morphological alterations or changes in hatching rate, RT-qPCR analysis revealed clear molecular responses. All *dnmt* genes were significantly upregulated at 5000 µg/L, with expression increases of approximately 3-6-fold. Notably, *dnmt1* responded significantly at 2500 µg/L, whereas *dnmt3aa* showed particularly high sensitivity, with an approximately 3-fold increase at only 20 µg/L. These findings demonstrate that BPA can induce molecular alterations related to DNA methylation in zebrafish embryos at concentrations where overt developmental toxicity is not observed, highlighting the potential sensitivity of epigenetic biomarkers for detecting early effects of BPA exposure.

Keywords: Bisphenol A; *Danio rerio*; DNA methyltransferases; Gene expression; Epigenetics; Embryonic toxicity

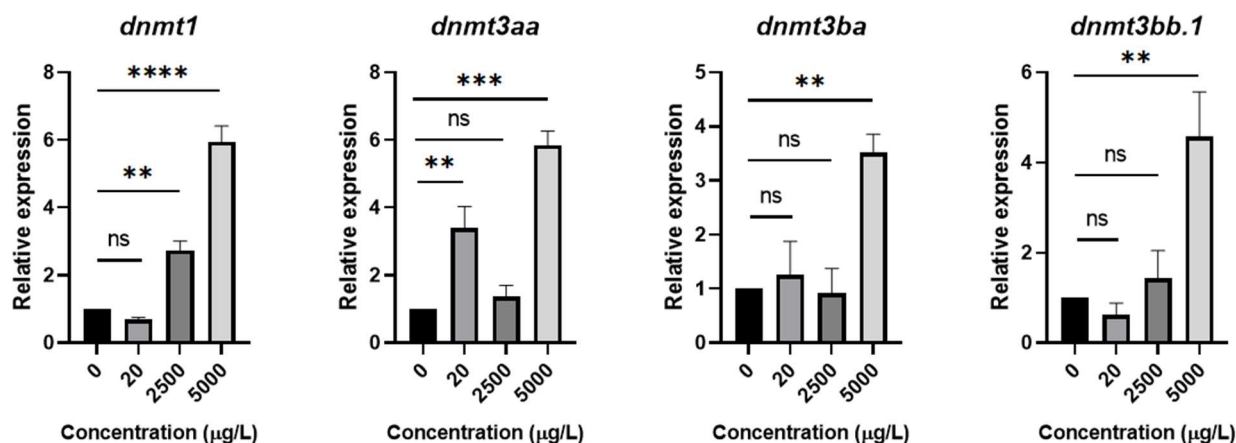


Figure: Relative mRNA expression of DNA methyltransferase genes (*dnmt1*, *dnmt3aa*, *dnmt3ba*, and *dnmt3bb.1*) in zebrafish embryos exposed to BPA (0, 20, 2500, and 5000 µg/L) for 96 hpf, measured by RT-qPCR.

PP-17 Local Microenvironment as a Conformational Selector: Impact of pH and Membrane Phase State on Early Folding of Amyloid- β 42

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Abstract: The toxicity of amyloid- β 42 (A β 42) in Alzheimer's disease is inextricably linked to its interaction with lipid bilayers. However, the role of the local microenvironment—namely, the phase state of the membrane and local pH variations—in the early stages of peptide folding remains only partially understood. In this work, we map the conformational landscape of A β 42 in model zwitterionic DPPC membranes, integrating experimental Raman spectroscopy, circular dichroism (CD), and atomistic molecular dynamics (MD) simulations.

We investigated the secondary structure of A β 42 under two distinct sets of conditions: varying pH (5.5, 7.4, 9.5) and inducing the lipid phase transition from the gel phase (25°C) to the fluid phase (48°C). Deconvolution of the Amide I bands in Raman spectra and CD data revealed that an acidic environment (pH 5.5) strongly stabilizes the α -helical conformation (up to 80%), suppressing the formation of disordered random coils. The most dramatic structural rearrangements are observed during the thermal phase transition of DPPC: in the rigid gel phase, the peptide localizes at the membrane surface, exhibiting a heterogeneous profile with an increased contribution of β -structures and random coils. The transition of the membrane to the fluid phase (48°C) triggers deep hydrophobic insertion of A β 42 into the acyl chains, as confirmed by MD trajectories. This insertion shields the peptide backbone from water, promoting the formation of intramolecular hydrogen bonds and stabilizing α -helices (up to 64% in MD), while simultaneously reducing the population of β -aggregation precursors.

Comparison of the three methods revealed high convergence in estimating the dominant structural motifs, despite methodological differences in sensitivity to transient β -turns. We demonstrate that the lipid bilayer acts not as a passive matrix, but as an active conformational selector. Bilayer fluidity and local pH independently dictate the early folding pathway of A β 42, shifting the equilibrium away from β -prone states. These data indicate that membrane phase dynamics must be incorporated as a critical variable in algorithms predicting the membrane-mediated toxicity of amyloids.

Keywords: Amyloid- β 42; Raman spectroscopy; CD; MD; membrane fluidity

PP-18 $\text{Mn}_x\text{Zn}_{1-x}\text{Co}_2\text{O}_4$ Nanosheets as an Efficient Electrocatalytic Platform for the Electrochemical Detection of Cd^{2+} in Nutritional Cereal Samples

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Abstract: Herein, we successfully synthesized and employed $\text{Mn}_x\text{Zn}_{1-x}\text{Co}_2\text{O}_4$ ($x=0.1-0.5$) (MZCO) nanosheets as an efficient electrocatalytic platform for the sensitive detection of Cd^{2+} in nutritional cereal samples. The incorporation of Mn into the ZnCo_2O_4 spinel structure was designed to regulate the electronic structure, facilitate interfacial electron transfer, and enhance the electrochemical response toward Cd^{2+} . The MZCO-based electrochemical sensor exhibited a wide linear response range of 1-1000 ppb for Cd^{2+} , with a sensitivity of $17 \mu\text{A ppm}^{-1}$ and a low detection limit of 0.66 ppb. The practical applicability of the MZCO/SPE sensor was evaluated by determining of Cd^{2+} in nutritional cereal samples. With their excellent electronic and electrochemical properties, $\text{Mn}_x\text{Zn}_{1-x}\text{Co}_2\text{O}_4$ nanosheets hold considerable promise as efficient electrocatalytic platforms for developing high-performance electrochemical sensors for monitoring toxic heavy metals in food products.

Keywords: *Electrochemical sensors, heavy metal, spinel oxide, $\text{Mn}_x\text{Zn}_{1-x}\text{Co}_2\text{O}_4$.*

PP-19 Molecular-Size-Selective ZIF-8/Ag SERS Nanoplatform for Ultrasensitive Urea Detection

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Abstract: Urea is an important small-molecule analyte in biological and food-related systems, creating a need for sensitive and selective analytical approaches. In this study, a ZIF-8/Ag nanostructure was developed as a surface-enhanced Raman spectroscopy (SERS) platform for ultrasensitive urea detection. The porous ZIF-8 framework was combined with plasmonic Ag nanoparticles to promote molecular enrichment near SERS-active regions while providing size-dependent accessibility to the sensing interface. To investigate this effect, urea was compared with the larger molecules methylene blue (MB) and Congo red (CR). Urea, whose molecular dimensions are compatible with the ZIF-8 pore structure, exhibited substantially enhanced SERS signals on ZIF-8/Ag, whereas MB and CR showed weaker responses than on Ag nanoparticles alone. Adsorption measurements further supported the preferential uptake of urea by the porous nanostructure, while disruption of the ZIF-8 framework reduced the additional enhancement observed for urea, highlighting the importance of the intact porous architecture. Under optimized conditions, the ZIF-8/Ag platform enabled urea detection over a broad concentration range with a limit of detection of 1.48×10^{-10} M. These results demonstrate how the integration of porous and plasmonic nanomaterials can provide molecular-size-dependent enrichment and highly sensitive SERS detection, offering a promising nanotechnology-based sensing strategy for life-science and food-related analytical applications.

Keywords: ZIF-8/Ag; surface-enhanced Raman spectroscopy (SERS); urea detection; size-selective sensing; molecular enrichment; nanomaterials.

PP-20 Multicore@Shell Ag@UiO-66-Based SERS Platform for Sensitive and Selective Salicylic Acid Detection via Machine Learning Analysis

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Abstract: Surface-enhanced Raman spectroscopy (SERS) has emerged as a powerful analytical platform for rapid and ultrasensitive molecular fingerprinting, offering distinctive vibrational signatures at trace concentrations and enabling broad applications across biomedical, environmental, and agricultural fields. Nevertheless, the reliable detection of molecules with intrinsically low Raman scattering cross-sections remains challenging, owing to their inherently weak Raman responses and susceptibility to spectral interference. Herein, we report a novel multicore-shell Ag@UiO-66 SERS platform that integrates intense plasmonic amplification from Ag nanoparticles (NPs) with the molecular enrichment and selective recognition capability of UiO-66, a metal-organic framework (MOF) for ultrasensitive detection of salicylic acid (SA), a naturally occurring phenolic compound involved in plant immune signaling and widely utilized in pharmaceutical and cosmetic applications. The Ag@UiO-66 architecture was fabricated through a facile room-temperature self-assembly strategy, enabling the *in-situ* formation of a porous UiO-66 shell around multiple AgNP cores. This unique configuration spatially confines the AgNPs within the porous framework, generating abundant electromagnetic hotspots while preserving their plasmonic activity. More importantly, the UiO-66 shell selectively enriches SA through synergistic interactions involving coordination with Zr sites, hydrogen bonding, and π - π interactions, thereby driving target molecules toward the plasmonically enhanced regions and facilitating efficient SERS amplification. Consequently, the Ag@UiO-66 substrate achieves an ultralow detection limit of 1 nM for SA, corresponding to an approximately improvement over conventional SERS substrates (~ 1 μ M), while delivering excellent signal reproducibility and measurement stability, with RSDs of 2.90% and 5.38% for repeatability and reproducibility, respectively. Furthermore, machine learning (ML)-assisted spectral analysis provides robust molecular discrimination, enabling reliable identification of SA across a broad concentration range and in complex mixtures.

Keywords: *SERS, Salicylic Acid, Machine Learning*

PP-21 Phytochemical-Shielded Iron Nanoparticles: A Structure-Property-Function Analysis of Ajwain (*Trachyspermum ammi*) Mediated CSFeNPs and their Apoptotic Efficacy against SK-MEL Skin Cancer Cells

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Background: Melanoma remains one of the most aggressive forms of skin cancer, necessitating the development of targeted, biocompatible therapeutic agents. Green nanotechnology offers a sustainable pathway for synthesizing metallic nanoparticles with enhanced bioactivity. This study explores the bio-fabrication of iron nanoparticles (CSFeNPs) using the polyphenol-rich ethanolic extract of Ajwain (*Trachyspermum ammi*) and evaluates their structural properties in correlation with their anticancer potential. **Methods:** CSFeNPs were synthesized via a green reduction method. Structural characterization was performed using UV-Vis, FTIR, XRD, and HR-TEM. The colloidal stability was assessed via Zeta potential analysis. The anticancer efficacy was evaluated against human skin melanoma (SK-MEL) cells using the MTT cell viability assay at concentrations of 10-50 µg/mL. Apoptotic induction was visually confirmed through Acridine Orange/Ethidium Bromide (AO/EB) dual staining. **Results:** Characterization confirmed the formation of crystalline iron nanoparticles (96.3 nm) with a unique "phytochemical shield" provided by Ajwain's monoterpenes. This shielding resulted in an exceptional zeta potential of -42.7 mV, indicating superior colloidal stability. The CSFeNPs exhibited potent, concentration-dependent cytotoxic activity, achieving a maximum growth inhibition of 71% at 50 µg/mL with an estimated IC₅₀ of ~35 µg/mL. AO/EB staining revealed significant morphological changes, including membrane blebbing and chromatin condensation, confirming that cell death occurred via the apoptotic pathway. **Conclusion:** The results demonstrate that the unique structure-property relationship of Ajwain-mediated iron nanoparticles, specifically their high surface charge and organic capping, directly facilitates their potent anticancer function. These findings position CSFeNPs as a promising, eco-friendly candidate for non-invasive melanoma therapy.

Keywords: *Green Synthesis, Ajwain extract, Iron Nanoparticles, SK-MEL cells, Apoptosis, Nanomedicine.*

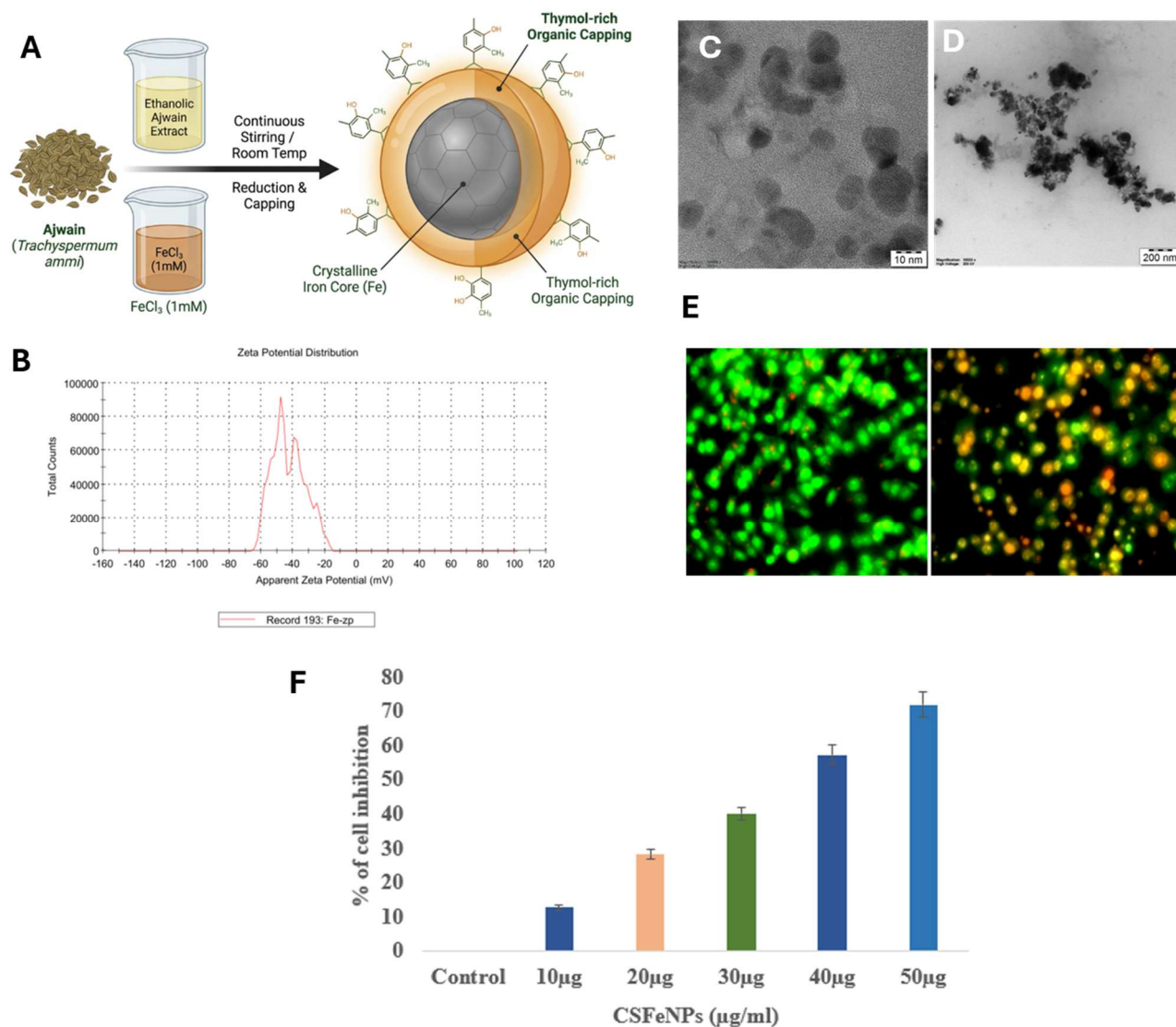


Figure 1: Graphical representation of CSFeNPs synthesis and characterization: **(A)** Schematic of phytochemical capping by Ajwain extract; **(B)** Zeta potential distribution confirming exceptional colloidal stability at -42.7 mV; **(C)** HR-TEM image showing spherical morphology, 10nm; **(D)** HR-TEM image showing spherical morphology, 200nm; **(E)** AO/EB dual staining showing apoptotic induction in treated cancer cells; **(F)** Concentration-dependent cytotoxic effect of CSFeNPs on SK-MEL melanoma cells

PP-22 Plasma-Engineered Carbon Quantum Dots: From Surface-Dependent Optical Properties to Antibacterial Activity and Fluorescence Sensing

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Abstract: Carbon quantum dots (CQDs) and nitrogen-doped carbon quantum dots (N-CQDs) were synthesized using environmentally friendly plasma-assisted approaches and explored as fluorescent probes for heavy metal ion detection. CQDs derived from *Citrus nobilis deliciosa* via microplasma treatment exhibited excitation-dependent photoluminescence and strong antibacterial activity, with inhibition rates of 99.24% against *Staphylococcus aureus* and 98.12% against *Escherichia coli*. The CQDs enabled fluorescence-based detection of Cd(II) over a linear range of 1–14 $\mu\text{g mL}^{-1}$, with a detection limit of 0.12 $\mu\text{g mL}^{-1}$. In parallel, N-CQDs synthesized through plasma–liquid interaction showed highly sensitive fluorescence quenching in response to Cu^{2+} , with a linear range of 0–6 nM and a detection limit of 2.3 nM. Time-resolved photoluminescence revealed enhanced non-radiative relaxation, while Stern–Volmer analysis indicated the coexistence of dynamic and static quenching at higher Cu^{2+} concentrations. DFT and TD-DFT calculations further demonstrated that Cu^{2+} adsorption induces redistribution of frontier molecular orbitals, supporting an orbital-mediated $\pi \rightarrow \text{Cu}^{2+}$ charge-transfer mechanism. Collectively, these results demonstrate that green plasma-assisted synthesis provides an effective strategy for tailoring the surface and optical properties of CQDs, enabling sensitive fluorescence-based detection of different heavy metal ions. The combination of facile synthesis, tunable photoluminescence, and mechanistic understanding highlights the potential of plasma-engineered CQDs for environmental monitoring and biomedical sensing applications.

Keywords: Carbon quantum dots; Plasma-assisted synthesis; Photoluminescence; Fluorescence sensing; Antibacterial activity

PP-23 Probe-Sonicated Nanostructured Lipid Carriers for Encapsulation and Sustained Release of Curcumin

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Abstract: Curcumin has poor aqueous solubility, which substantially limits its bioavailability and practical applications despite its well-established biological activities. This study aimed to develop curcumin-loaded nanostructured lipid carriers (Cur-NLCs) using high-temperature emulsification followed by probe sonication. A primary emulsion was prepared at an elevated temperature and subsequently subjected to probe sonication to produce nanoscale lipid particles. The optimized formulation achieved a curcumin loading concentration of 0.8 mg/mL and an encapsulation efficiency of $88.33 \pm 0.19\%$. The Cur-NLCs had a mean particle size of 112.2 nm, a polydispersity index of 0.287, and a zeta potential of -59.9 mV. In vitro release was evaluated using the dialysis membrane method in a pH 7.4 buffer. The formulation exhibited a sustained-release profile, with a cumulative curcumin release of 29.42% over 48 h. These findings demonstrate the feasibility of probe-sonicated NLCs for efficient curcumin encapsulation and sustained release, supporting their potential as a lipid-based delivery system for poorly water-soluble bioactive compounds.

Keywords: Curcumin; nanostructured lipid carriers; probe sonication; encapsulation efficiency; sustained release; drug delivery

PP-24 Reutilization of Fly Ash in the Fabrication of Protein Extraction Columns for Biomedical Applications

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Abstract: Protein purification plays an essential role in biological research and biomedical applications; however, current methods are often complex and costly. The reuse of fly ash as a raw material for developing functional materials has the potential to reduce waste and add value to industrial by-products. In this study, fly ash (FA) was functionalized with amino groups (NH₂) to generate the FA_NH₂ material, which was then immobilized within a filter column and combined with a vacuum pumping system to construct a net - zero protein extraction column. The protein solution was passed through the filter column, allowing the protein to be captured on the surface of FA_NH₂ through electrostatic interactions between the material surface and the charged regions of the protein. The results show that the protein extraction column using FA_NH₂ material is capable of both adsorbing and desorbing protein, with changes in protein content demonstrated by UV-Vis and SDS-PAGE results. The electrostatic interaction mechanism plays an important role in protein capture, while changing the desorption conditions allows the protein to be separated from the material. These results demonstrate the feasibility of the FA_NH₂-based protein extraction column, opening a direction for reutilizing fly ash to develop a low-cost, sustainable protein purification material with potential applications in the biomedical field.

Keywords: *Protein purification; Protein adsorption; Electrostatic interactions; Adsorption–desorption; Functionalized materials.*

PP-25 SiO₂ – coated NiFe₂O₄ functionalized with NH₂ and immobilized with carbon quantum dots for extraction and biosensing applications

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Abstract: In this report, carbon quantum dots (QDs) were immobilized on the surface of SiO₂ – coated NiFe₂O₄ functionalized with NH₂ (NSi - NH₂), yielding a multifunctional magneto – fluorescent nanomaterial for extraction and biosensing applications. The magnetic SiO₂ – coated NiFe₂O₄ (NSi), synthesized via a microemulsion method in a biphasic alcohol – water system, producing uniform particle size, was subsequently functionalized with amino groups NH₂ (NSi – NH₂). Carboxyl – functionalized QDs were covalently attached to surface NH₂ groups (NSi – QDs). Vibrating sample magnetometry (VSM) confirmed the superparamagnetic behavior, indicating strong potential for magnetic bioseparation. In addition, photoluminescence (PL) signals demonstrated excellent fluorescence properties, suitable for labeling in biosensing. Overall, the combination of magnetic responsiveness and fluorescence emission in SiO₂ – coated NiFe₂O₄ functionalized with NH₂ and immobilized with carbon quantum dots highlights its promise for diverse biomedical applications, including extraction, sensing, and bioimaging.

Keywords: *Superparamagnetic nanoparticle, Carbon QDs, multifunctional magneto – fluorescent nanomaterial.*

PP-26 Synthesis and Antibacterial Evaluation of Gold Nanorods Encapsulated in Zeolitic Imidazolate Framework-8 (Au NRs/ZIF-8) Nanocomposites against Escherichia coli and Staphylococcus aureus

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Abstract: The escalating prevalence of bacterial infections and antibiotic resistance presents a critical challenge to global public health, driving the urgent development of alternative antimicrobial agents. This study aim to synthesize gold nanorods integrated into zeolitic imidazolate framework-8 (Au NRs/ZIF-8) and subsequently evaluate for its antibacterial efficacy against both Gram-negative (*Escherichia coli*) and Gram-positive (*Staphylococcus aureus*) pathogens. Initially, Au NRs were prepared via a seed-mediated growth method using HAuCl₄, CTAB, AgNO₃, and ascorbic acid. Next, the nanorods encapsulated within the ZIF-8 matrix by stirring with Zn²⁺ and 2-methylimidazole precursors for 16 hours. The antibacterial performance was quantitatively evaluated across various composite formulations and dilution gradients, with tetracycline and DI water serving as positive and negative controls, respectively. The antibacterial assay results demonstrated that the Au NRs/ZIF-8 nanocomposites exhibited strong, concentration-dependent inhibitory activity against both bacterial strains ($p < 0.001$). Notably, the Au NRs/ZIF-8 formulation prepared with 12.5 mL demonstrated the highest antibacterial potency, exhibiting an inhibition zone comparable to that of standard tetracycline. Furthermore, *S. aureus* showed slightly higher sensitivity to the nanocomposites than *E. coli* ($p < 0.001$). These findings highlight the superior bactericidal capabilities of Au NRs/ZIF-8 nanocomposites, demonstrating their promising potential as effective alternative antibacterial agents against pathogenic bacteria.

Keywords: *Antibacterial activity, Au NRs/ZIF-8, Escherichia coli, Nanocomposite synthesis, Staphylococcus aureus*

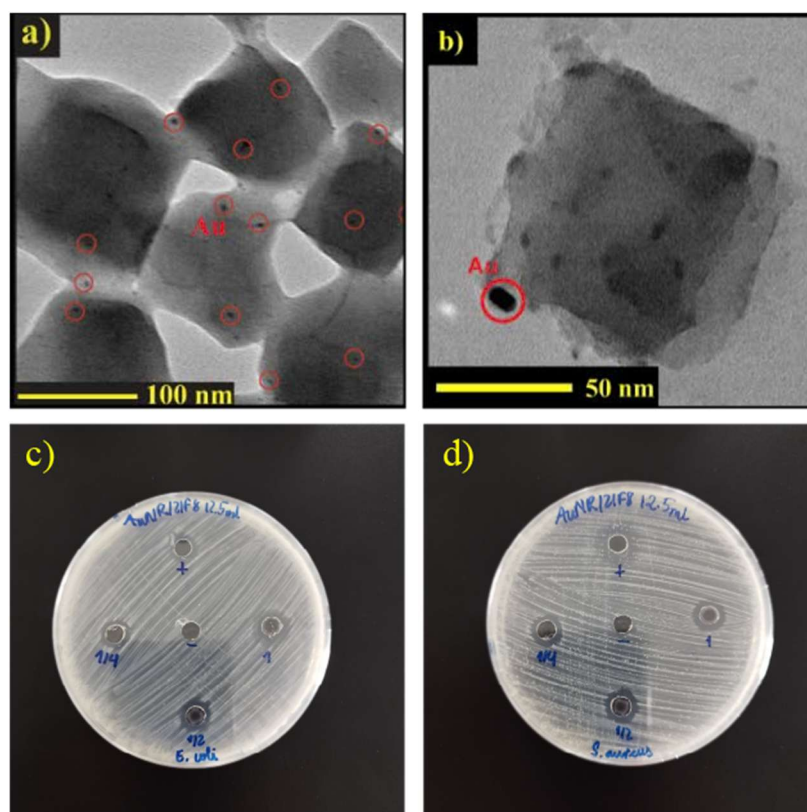


Figure: a, b) TEM images of AuNR/ZIF-8 at different magnifications with Au nanoparticles highlighted in red circles; (c, d) Antibacterial zone of inhibition against (c) *Escherichia coli* and (d) *Staphylococcus aureus* via the agar well diffusion method.

PP-27 The influence of CAA interruptions on the formation of open states in the ATXN2 gene

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Abstract: The *ATXN2* gene (ataxin-2) plays an important role in neurodegenerative diseases, including spinocerebellar ataxia type 2 (SCA2), amyotrophic lateral sclerosis, and parkinsonism. The stability of the trinucleotide repeat region depends on whether the CAG tract is continuous or contains CAA interruptions. A CAG tract without interruptions exhibits a tendency toward expansion, which triggers the development of SCA2.

The precise mechanisms underlying these expansions remain unknown, although it has been hypothesized that one such mechanism involves the propensity of trinucleotide repeats in single-stranded DNA to form hairpin structures, which give rise to a "slippage" effect during information readout.

CAA interruptions within the trinucleotide repeat region represent sequence alterations that do not affect the resulting protein product. Nevertheless, CAA interruptions may play an important role in stabilizing the CAG tract in the *ATXN2* gene. The presence of even a single CAA interruption can exert a discernible influence on the secondary structure of DNA. Moreover, CAA interruptions may be associated with other neurodegenerative conditions, such as parkinsonism.

In the present work, the stability of the CAG tract in the presence of CAA interruptions was investigated as a function of their localization using mathematical modeling approaches. The study was carried out by means of coarse-grained DNA modeling, which enables the investigation of processes that are inaccessible to all-atom models.

Our findings demonstrate that CAA interruptions affect the stability of the CAG tract, and that this effect—depending on the interruption location—can either increase or decrease CAG-tract stability [1]. It was established that CAA interruptions positioned near the center of the CAG tract lead to a reduction in CAG-tract stability, as reflected by an increased probability of occurrence of additional large open-state zones within the CAG tract. In contrast, CAA interruptions located near the boundaries of the CAG tract have a lesser destabilizing effect or may even enhance stability.

A CAA interruption replaces the G nucleotide with an A nucleotide within one of the CAG triplets, resulting in a moderate alteration of the mechanical properties of the nucleotide in question and a substantial change in the energy of complementary hydrogen bonding. This would intuitively be expected to reduce the stability of the CAG tract; however, the computational results indicate that certain localizations of CAA interruptions actually stabilize the CAG tract. This points to the important role of DNA dynamics, whereby even a single-nucleotide substitution can lead to significant changes in the nucleation zones of open states.

Furthermore, a distinct asymmetry is observed: CAA interruptions located near the left boundary of the CAG tract result in a modest decrease in stability only at $k = 35$, whereas at other CAG-tract lengths k , such interruptions increase stability. CAA interruptions situated near the right boundary

enhance CAG-tract stability only at $k = 55$; in all other cases, they reduce stability, albeit to a lesser extent than interruptions positioned in the middle of the CAG tract.

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Keywords: CAA interruption, ATXN2, torque, parkinsonism, open states

PP-28 The MnCo₂O₄-modified electrochemical sensing platform for ultrasensitive detection of Carbendazim residue in fruit and vegetable samples

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Abstract: A spinel cobaltite MnCo₂O₄ (MCO) nanomaterial was successfully synthesized via a facile microwave-assisted hydrothermal method and employed as an electrocatalytic modifier for screen-printed electrodes toward carbendazim (CBZ) detection. The fabricated MCO/SPE sensor exhibited remarkable electrocatalytic activity for the electro-oxidation of CBZ, resulting in excellent analytical performance. Differential pulse voltammetry measurements revealed two linear detection ranges of 0.05 - 5 μM and 25 - 500 μM , together with a low detection limit of 0.02 μM and a high sensitivity of 6.46 $\mu\text{A } \mu\text{M}^{-1} \text{ cm}^{-2}$. The superior sensing behavior is attributed to the synergistic contribution of the Co²⁺/Co³⁺ and Mn²⁺/Mn³⁺ redox couples, which promote charge-transfer processes and enhance the electrocatalytic oxidation of CBZ. In addition, the one-dimensional nanorod morphology provides efficient diffusion pathways for CBZ molecules, further improving the sensing response. The practical applicability of the proposed sensor was validated through CBZ determination in fruit and vegetable samples, and the obtained results showed good agreement with those obtained using liquid chromatography-tandem mass spectrometry (LC-MS/MS). These findings demonstrate the strong potential of the MCO/SPE platform as a simple and effective electrochemical sensing system for pesticide monitoring and food safety applications.

Keywords: Spinel structures, MnCo₂O₄, Electrochemical sensor, Carbendazim, Pesticide residue

PP-29 Tripeptides inhibit dual targets AChE and BACE-1: a computational study

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Abstract: Alzheimer's disease (AD) is a progressive neurodegenerative disorder characterized by cognitive decline and memory loss, with amyloid-beta (A β) plaques and acetylcholine deficits being central pathological features. Inhibition of dual targets including acetylcholinesterase (AChE) and beta-site amyloid precursor protein cleaving enzyme 1 (BACE-1) represents a promising strategy to address cholinergic deficits and amyloid pathology. In this study, we used computational approaches to evaluate 8000 tripeptides as potential dual inhibitors of AChE and BACE-1. Machine learning models, for which RMSE = 1.357 ± 0.096 kcal/mol for AChE and 1.01 ± 0.05 kcal/mol for BACE-1, revealed the four top-lead tripeptides, including WHM, HMW, WMH, and HWM. Molecular docking simulations indicated that WHM possessed the most favorable interactions through hydrogen bonds, π - π stacking, and salt bridges with key catalytic residues in both enzymes. The docking scores of WHM were -16.6 and -14.4 kcal/mol for AChE and BACE-1, respectively. Molecular dynamics simulations, with RMSD values stabilizing around 0.2 nm, confirmed the stability of the protein-ligand complexes, with WHM exhibiting the most consistent conformations and significant disruption of catalytic residue geometries. Free energy perturbation analysis further supported WHM's superior stability across both targets, with binding energies of -33.31 ± 8.31 and -38.30 ± 1.96 for AChE and BACE-1, respectively. ADMET predictions suggested moderate oral absorption and limited brain penetration, consistent with the typical behavior of peptide-based compounds. Overall, WHM demonstrated the strongest potential as a dual inhibitor of AChE and BACE-1, offering a promising lead for future therapeutic development in AD.

Keywords: *Alzheimer's disease, AChE, BACE-1, Machine learning, Molecular docking, Molecular dynamics.*

PP-30 Vortex-Associated Platelet Accumulation in Arterial and Venous Microfluidic Models: Role of Flow Recirculation Beyond Wall Shear Stress

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Background: Thrombus formation in stenotic arteries and cardiovascular devices is often linked to elevated wall shear stress (WSS). However, platelet-rich thrombi can also develop in low-shear venous regions, including valve pockets and bifurcations, where flow recirculation occurs. Because WSS describes near-wall loading, it may not fully capture volumetric rotational flow features that influence platelet transport, residence time, and local accumulation. This study examined whether recirculation zones co-localize with thrombus formation across arterial- and venous-like microfluidic flow regimes.

Methods: An 80% arterial stenosis model and a 20% venous contraction model were designed to investigate hemodynamics based on physiological relevance. Computational fluid dynamics (CFD) simulations were performed using standard blood properties ($\mu = 3.5$ cP, $\rho = 1060$ kg/m³) to characterize flow streamlines, velocity, and shear rate. Following flow pattern validation with 1.5 - 3 μ m fluorescent microbeads, the microfluidic chips were coated with collagen type I. Citrated platelet-rich plasma (PRP) was fluorescently labeled with 10 mM Mepacrine, recalcified in-line using 2 mM CaCl₂, and perfused through the devices to observe thrombus formation within the recirculation zones.

Results: CFD analysis of the venous model revealed a distinct post-stenotic circulation zone characterized by a low shear rate (<500 s⁻¹). Fluorescence microscopy confirmed that platelet activation and aggregation heavily localized within this vortex core rather than in areas of peak wall shear stress. Quantitative analysis showed that fluorescent platelets covered 49.4% of the venous circulation zone, demonstrating massive, localized clot formation compared to surrounding linear-flow regions. Furthermore, similar enstrophy-driven platelet trapping was observed in the 80% arterial stenosis model at flow rates of 1 and 3 mL/min. These findings provide direct quantitative evidence that flow recirculation universally promotes thrombosis across diverse vascular environments.

Conclusion: This imaging-based study demonstrates that platelet-rich thrombus accumulation strongly co-localizes with recirculating vortex regions across both arterial and venous microfluidic models. By quantifying significant platelet trapping within low-shear zones (nearly 50% coverage in the venous model), these findings highlight the importance of using recirculation-based metrics alongside traditional WSS to accurately predict thrombosis-prone locations. Future work will quantify enstrophy distributions, investigate real-time thrombus growth dynamics, and assess direct platelet-activation markers.

Keywords: *platelet accumulation, hemodynamic vorticity, microfluidics, thrombosis, stenosis, flow recirculation, wall shear stress*

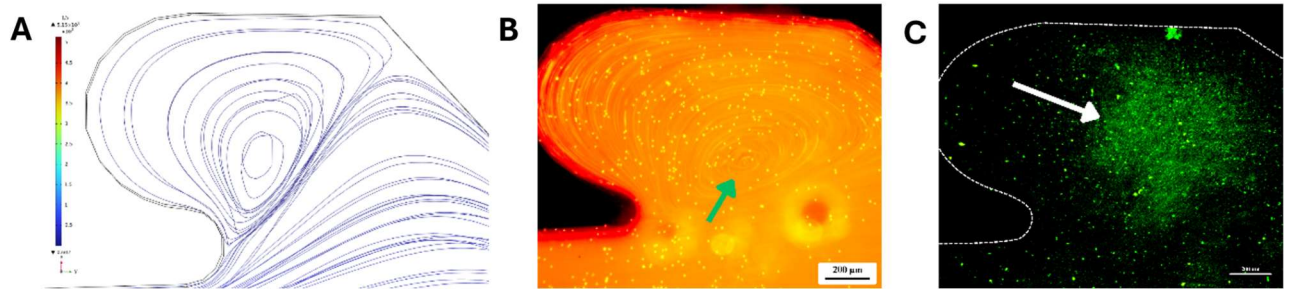


Figure 1: Vortex-localized platelet accumulation in the venous microfluidic model at 5 mL/min. (A) CFD streamlines colored by shear rate, demonstrating a distinct low-shear core ($<500 s^{-1}$) within the recirculation vortex. (B) Fluorescent microbead visualization confirms the predicted recirculation pattern. (C) Fluorescence imaging of labeled platelets reveals massive thrombus accumulation heavily co-localized with the vortex region, resulting in 49.4% area coverage; the channel wall is outlined by a dashed line. Scale bars: 200 μm

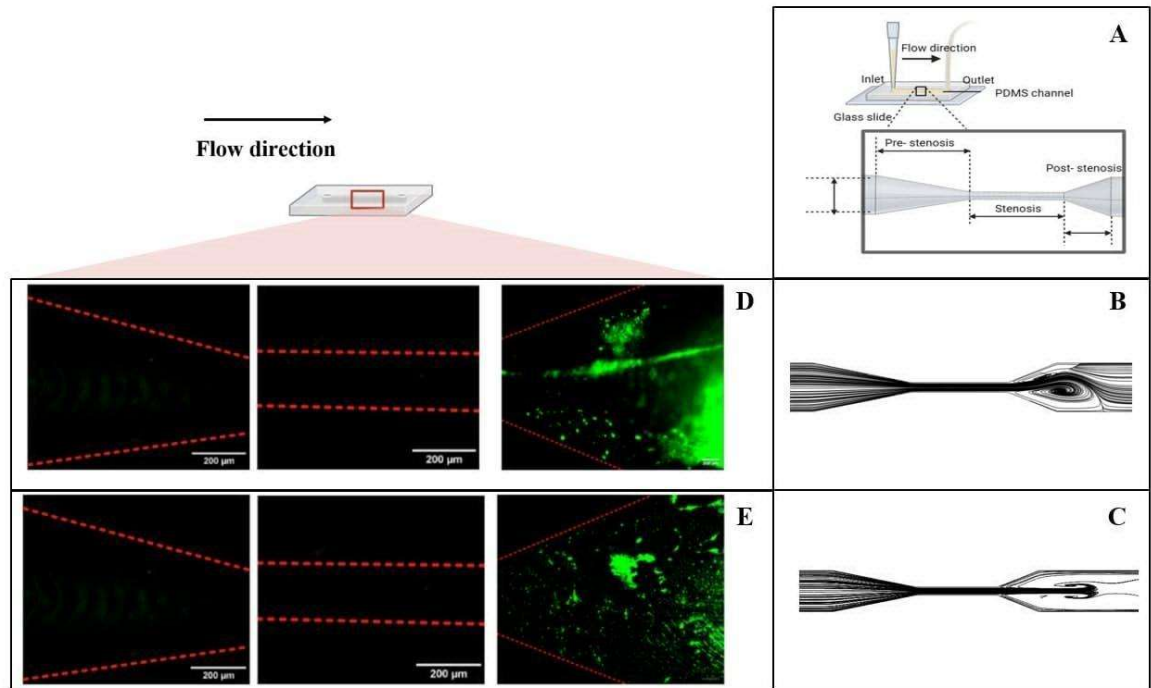


Figure 2: Arterial stenosis microfluidic model and flow-dependent platelet accumulation. (A) Schematic of stenosis model design. CFD-predicted flow patterns at (B) 1 mL/min and (C) 3 mL/min. Representative fluorescence images of platelet accumulation at (D) 1 mL/min and (E) 3 mL/min. Scale bars: 200 μm .

PP-31 Length-dependent DNA flexibility of the ATXN2 CAG tract

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Abstract: The human *ATXN2* gene at 12q24.12 encodes ataxin-2, a protein abundant in brain neurons. Pathology arises when the *ATXN2* gene undergoes CAG trinucleotide repeat expansion. Healthy individuals typically have 22–23 CAG repeats; when repeats exceed ~33–34 copies, spinocerebellar ataxia type 2 (SCA2) develops. In SCA2, ataxin-2 acquires an elongated polyglutamine tract, misfolds, and accumulates in neurons, especially in the cerebellum and brainstem.

Disease mechanisms from CAG expansion are incompletely understood. Evidence suggests pathogenic effects arise both from altered protein function and from DNA-level structural changes. Since cytosine pairs with guanine, bent DNA strands can form intra-strand hydrogen bonds, producing stable noncanonical secondary structures (hairpins, quadruplexes) instead of the canonical double helix. Hairpins within the *ATXN2* CAG tract generate genetic instability that can drive SCA2. Formation of such structures is associated with large regions of open states (OS) in the CAG tract.

Bending and flexibility in DNA segments are strongly correlated, and torsional stiffness of the double helix changes markedly under twisting. Therefore, collective states of nucleotide pairs can reveal alterations in DNA's structural properties. We used mathematical modelling to study how CAG-tract length affects formation of zones of collective conformational states in an *ATXN2* gene fragment under weak torsional perturbations.

Our model represents an angular representation of DNA, analogous to two interconnected chains of pendulums, an approach developed by Englander et al. and later by Yakushevich, and modernized by us. These results show that small external torsional perturbations, insufficient to create open states, still induce conformational states marked by a distinctive bend in the CAG region. For a fixed repeat count, bend amplitude increases with torsional magnitude. The data indicate that an *ATXN2* region with a pathologically expanded CAG tract forms a unique, vulnerable “hot spot” in DNA structure that responds differently to mechanical perturbations than a normal tract. Large-amplitude bends within the expanded tract signal increased flexibility and intrinsic instability, making the region more susceptible to stress and to formation of additional OS zones at higher torsional loads.

More broadly, three-dimensional DNA organization is a critical regulatory layer linking spatial genome structure, epigenetic mechanisms, and cellular adaptive responses. The structural distortions we observe in expanded CAG tracts likely contribute to the genetic instability and pathological cascade leading to SCA2.

Funding: The research is carried out with the financial support of the Russian Science Foundation and the Kuban Science Foundation in the framework of the scientific project Num. 24-14-20014.

Keywords: *SCA2, ATXN2, CAG repeats, DNA flexibility, torque*

PP-32 Facile fabrication of Melaleuca alternifolia essential oil-impregnated chitosan/poly(vinyl alcohol) films for wound-healing applications

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Abstract: This study aimed to fabricate Melaleuca alternifolia essential oil (MAEO)-impregnated chitosan/poly(vinyl alcohol) (CS/PVA) films and evaluate their potential for wound-healing applications. CS and PVA were blended at a fixed 1:1 ratio, followed by the incorporation of MAEO at concentrations of 0, 0.5, and 1.0% (v/v) to produce M0, M1, and M2 films, respectively, using a facile solvent-casting method. MAEO incorporation maintained the overall physical and mechanical integrity of the CS/PVA films while markedly enhancing their antibacterial activity against Staphylococcus aureus. In an in vivo wound model, MAEO-impregnated films accelerated wound closure and significantly shortened the time required for complete epithelialization. Notably, the M2 film containing 1.0% MAEO achieved complete epithelialization within 12.8 ± 1.1 days, compared with 15.8 ± 1.3 days in the control group. The enhanced wound-healing performance may result from the synergistic functions of the CS/PVA matrix and MAEO: the polymeric film provides a protective interface for the wound, while the incorporated essential oil enhances antibacterial activity, particularly against S. aureus, thereby potentially reducing bacterial interference and creating a favorable microenvironment for tissue repair and re-epithelialization. These findings highlight MAEO-impregnated CS/PVA films as promising multifunctional materials for wound-healing applications.

Keywords: *Melaleuca alternifolia, wound-healing, S. aureus, chitosan/poly(vinyl alcohol) film, epithelialization.*

PP-33 Synergistic Enhancement of UV Protection and Antioxidant Activity in Cosmetic Systems Based on Natural Extract-Metal Oxide Hybrids

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Abstract: The growing demand for multifunctional, sustainable cosmetic products has driven extensive research into natural bioactive compounds and inorganic UV-filter materials. However, natural extracts generally exhibit poor photostability and limited UV-shielding properties, whereas metal oxide nanoparticles, such as ZnO and TiO₂, may generate reactive oxygen species (ROS) under UV irradiation. In this study, a hybrid cosmetic system based on natural plant extracts and metal oxide nanoparticles was developed to investigate their synergistic effects on UV protection, antioxidant activity, and antibacterial performance. Polyphenol-rich plant extracts were combined with ZnO and TiO₂ nanoparticles to fabricate multifunctional hybrid formulations. The physicochemical interactions between natural compounds and metal oxide surfaces were characterized using FTIR, UV-Vis spectroscopy, XRD, SEM/TEM. Cosmetic-related performances, including UV absorption capability, antioxidant activity (DPPH/ABTS assays), antibacterial activity against skin-related bacteria, and formulation stability were systematically evaluated. The results demonstrated that incorporating natural extracts significantly improved nanoparticle dispersion and enhanced UV absorption efficiency. The synergistic interaction between plant polyphenols and metal oxide nanoparticles contributed to improved photostability and multifunctional cosmetic performance. This work provides a promising strategy for developing next-generation green cosmetic materials with enhanced safety, stability, and multifunctionality.

Keywords: *metal oxide, plant extracts, skin protection*

PP-34 pH-Responsive Colorimetric Indicator Membrane Based on CMC/Chitosan/Anthocyanin for Pork Freshness Monitoring

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Abstract: During storage, microbial degradation of pork proteins releases ammonia and other volatile basic compounds, leading to a change in the environmental pH. This study evaluated the ability of A CMC/Chitosan/Anthocyanin (CMC/CS/ATH) colorimetric indicator membrane to monitor pork freshness in real-time under room (27–28°C) and refrigerated (4–5°C) conditions. At room temperature, pH and TVB-N increased from 5.50 and 10.60 mgN/100g at 0h to 7.27 and 65.99 mgN/100g after 36 h, respectively. The pork remained within the acceptable quality range during the first 12 h, after which signs of spoilage were indicated by pH and TVB-N values above the threshold levels. In cold storage, TVB-N exceeded 20 mg N/100 g on day 3, while pH exceeded 6.2 on day 4. There was a strong correlation between pH and TVB-N ($r > 0.99$), and the membrane showed clear color changes matching spoilage of the pork. The color changes from pink/red to green at room temperature, while more gradual color changes were observed under refrigeration. These findings highlight the potential of the CMC/CS/ATH membrane as a simple, non-destructive visual tool for evaluating pork freshness.

Keywords: *Polymer membrane; Anthocyanin; colorimetric indicator; pH-responsive; pork freshness monitoring.*

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