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PEERS ALLEY MEDIA

7TH EDITION OF

ADVANCED CHEMISTRY WORLD CONGRESS

26-27 MARCH 2026

ROME, ITALY

BOOKMARK DATES

8TH EDITION OF

ADVANCED CHEMISTRY WORLD CONGRESS

March 2027 | Vienna, Austria

SCIENTIFIC PROGRAM

DAY 01

THURSDAY

MARCH 26, 2026

08:00-08:30	**Registrations**
08:30-08:40	**Inaugural Ceremony**

Sessions: Analytical Chemistry | Industrial Chemistry | Agricultural Chemistry | Medicinal Chemistry | Chemical Engineering | Green Chemistry | Environmental Chemistry | Biochemistry | Organic Chemistry | Physical Chemistry |Geochemistry | Food Chemistry | Materials Science | Molecular Biology | Polymer Chemistry and Technology

Distinguished Speaker Talks	
Session Chair	**Carlos Alberto Guerrero-Fajardo,** *Universidad Nacional de Colombia, Colombia*
Session Chair	**Ranu Gadi,** *Indira Gandhi Delhi Technical University for Women, India*
08:40-09:00	Title: Pea Pod Valorization: Exploring the Influence of Biomass/Water Ratio, Particle Size, Stirring, and Catalysts on Chemical Platforms and Biochar Production
	Carlos Alberto Guerrero-Fajardo, *Universidad Nacional de Colombia, Colombia*
09:00-09:20	Title: Evaluation of Hydrogen Adsorption on Zn–Ni Alloy Coating by the Electrochemical Desorption Technique and its Permeability on AISI 1020 Steel
	Eudesio Oliveira Vilar, *UFCG - Federal University of Campina Grande, Brazil*
09:20-09:40	Title: Adsorption of Heavy Metals from Aqueous Solutions using Polysaccharides Hydrogels
	Adi Wolfson, *Sami Shamoon Collage of Engineering Israel*

09:40-10:00	Title: Neural Circuit Formation and Decision Making in the Mouse Olfactory System **Hitoshi Sakano,** *The University of Tokyo, Japan*
10:00-10:20	Title: Demystifying AI: Neural Networks, Transformers, and Agents for Modern Chemists **Safwan Omari,** *Lewis University, USA*
GROUP PHOTO 10:20-10:30	
REFRESHMENT BREAK 10:30-10:50	
10:50-11:10	Title: Docosahexaenoic Acid Increases the Pro-Resolving Brain Lipid Mediators of Inflammation in Rat Pups Prenatally Exposed to Alcohol **Enrique M. Ostrea Jr.,** *Wayne State University School of Medicine, USA*
11:10-11:30	Title: Antibacterial and Prooxidant Activity of Sol-Gel Prepared Copper - Silica Nanocomposite Materials **Iliana Atanasova Ivanova,** *Sofia University "St. Kliment Ohridski", Bulgaria*
11:30-11:50	Title: Preparation and Characterization of Novel Lignosulfonate-Based Starch-Silica Nanocomposite (LS-SSNC) Hybrid Material for Drilling Stability **Muhammad-Noorul-Anam Mohd-Norddin,** *Universiti Teknologi Malaysia (UTM), Malaysia*
11:50-12:10	Title: Incorporating Quantum Mechanical Effects into Molecular Dynamics Simulations: A Novel Approach **Yoshiaki Teranishi,** *National Yang Ming Chiao Tung University, Taiwan*
12:10-12:30	Title: Timing Matters: An Observational Study on Circadian Effects of Spinal Anesthesia in Cesarean Delivery **Evangelia Nikouli,** *General Hospital of Komotini, Greece*
12:30-12:50	Title: The Effects of the Environment (Medium) on Nuclear Reaction Yields **Houria Salah,** *Centre de Recherche Nucleaire d'Alger, Algeria*

GROUP PHOTO 12:50-13:00	
LUNCH BREAK 13:00-13:40	
13:40-14:00	Title: Multicenter Clinical Trial for the Treatment of Obstructive Sleep Apnea with a Non-Permanent Orthodontic Intraoral Device in Children **Tammarie Heit,** *The University of Alberta, Canada*
14:00-14:20	Title: Plant Extracts Mediated Syntheses of Nanoparticles and their Effectiveness on Agricultural Pathogens **Graciela M. L. Ruiz-Aguilar,** *University of Guanajuato, Mexico*
14:20-14:40	Title: Photoregulation in *Xanthomonas campestris*: Integration of Red/Far Red and Blue Light Signals **Valeria P. Conforte,** *Instituto de Ciencia y Tecnología Dr. César Milstein (CONICET - Fundación Pablo Cassará), Argentina*
14:40-15:00	Title: Transposition and Implementation of European Union Renewable Energy Legislation in France, Italy, and Germany: A Regulatory Perspective and a Comprehensive Analysis of Opportunities and Challenges **Ana Maria Fagetan,** *University of Rome "La Sapienza", Italy*
15:00-15:20	Title: Removal of Uranium from Aqueous Systems using Green Cellulose Biosorbent Derived from Banana (Musa paradisiaca) Leaves **Rohit Mehra,** *Dr. B. R. Ambedkar National Institute of Technology, India*
15:20-15:40	Title: Morphological Characterization and Health Risk Assessment of Fine Particulate Matter over the National Capital Region of India **Ranu Gadi,** *Indira Gandhi Delhi Technical University for Women, India*
15:40-16:00	Title: The Influence of Powder Particle Shape on the Macrostructure of Material Obtained by Direct Energy Deposition (DED) **Oleksandr Radchenko,** *Frantsevich Institute for Problems of Material Science NAS of Ukraine, Ukraine*

REFRESHMENT BREAK 16:00-16:20	
16:20-16:40	Title: Unraveling the Structural and Functional Characteristics of Cocoonase, Trypsin, and Sericin: An Approach Towards Cocoon Softening for the Benefit of the Silk Industry
	Dev Mani Pandey, *Birla Institute of Technology, India*
16:40-17:00	Title: Synthesis and Characterization of a New CrMOF using Captopril as a Linker and its Integration into Chitosan for Enhanced Optoelectronic Properties
	Diary Ibrahim Tofiq, *University of Sulaimani, Iraq*
17:00-17:20	Title: Development of Rapid Chromogenic and Fluorescence Spectroscopy-Based Test Protocol to Determine Proper Heat Treatment in Goat Milk
	Mangroliya Parita Alpeshbhai, *Parul University, India*
17:20-17:40	Title: Environmentally Friendly Methods for Enhancing the Biological Functions of Certain Transition Metals
	Jovana Bogojeski, *University of Kragujevac, Serbia*
17:40-18:00	Title: Plant-Microbe Interactions: A Gateway to Sustainable Agriculture and Enhanced Crop Resilience
	Beema Jainab S.I, *Justice Basheer Ahmed Sayeed College for Women (Autonomous), India*
NETWORKING	
END OF DAY 1	

SCIENTIFIC PROGRAM

DAY 02

FRIDAY

MARCH 27, 2026

08:30-08:40	**Introduction**

Sessions: Analytical Chemistry | Industrial Chemistry | Agricultural Chemistry | Medicinal Chemistry | Chemical Engineering | Green Chemistry | Environmental Chemistry | Biochemistry | Organic Chemistry | Physical Chemistry |Geochemistry | Food Chemistry | Materials Science | Molecular Biology | Polymer Chemistry and Technology

Distinguished Speaker Talks	
Session Chair	**Tamara POTLOG,** *Moldova State University, Republic of Moldova*
Session Chair	**Rina Ghosh,** *St. Xavier's College, India*
08:40-09:00	Title: RUNX1: A Novel Therapeutic Target for Myocardial Infarction and Cerebral Infarction
	Weihong He, *Sichuan University, China*
09:00-09:20	Title: Re-orientating Research to Deliver Innovation
	David Dent, *Dent Associates Ltd, UK*
09:20-09:40	Title: CFD Simulation of the Claus Reaction Furnace with Operating Conditions: Temperature and Excess Air for Sulfur Recovery
	Pablo Vizguerra Morales, *Centro Mexicano para la Producción más Limpia, Mexico*
09:40-10:00	Title: Reflections on the Role of Procedural Knowledge in the Teaching of Science
	Elizabeth Vergis, *University of Alberta, Canada*

10:00-10:20	Title: The Designing of Coordination Polymers Consisting of Late-Transition Metals and Lanthanide Ions for Luminescence Enhancement **Zerihun Assefa,** *North Carolina Agricultural and Technical State University, USA*
GROUP PHOTO 10:20-10:30	
REFRESHMENT BREAK 10:30-10:50	
10:50-11:10	Title: Interaction of "Tryptophans" with Excited State Proton Transfer Probes – An Insight through Experiments and Theory **Rina Ghosh,** *St. Xavier's College, India*
11:10-11:30	Title: Diagnostic and Therapeutic Outcomes in Spinal Tuberculosis: A Retrospective Study Integrating GeneXpert MTB/RIF, Histopathology, and Clinical Management Strategies **Eldin Karaikovic,** *Ascension St Joseph Hospital, Chicago, USA*
11:30-11:50	Title: Comparative Economic Analysis of Batch vs. Continuous Manufacturing in Catalytic Heterogeneous Processes: Impact of Catalyst Activity Maintenance and Materials Costs on Total Costs of Manufacturing in the Production of Fine Chemicals and Pharmaceuticals **Felix Mendoza Suarez,** *Auburn University, USA*
11:50-12:10	Title: Influence of Peripheral Carboxy Group Number on Zinc Phthalocyanine Photophysics **Tamara POTLOG,** *Moldova State University, Republic of Moldova*
12:10-12:30	Title: Transmembrane Homodimers Interface Identification: Predicting Interface Residues in Alpha-Helical Transmembrane Protein Homodimers using Sequential and Structural Features **Bander Almalki,** *University of Bisha, Saudi Arabia*

12:30-12:40 (Poster)	Title: Unravelling the Specific Interactions of Drugs with the Intrinsic Tryptophan Residues in Multi-Tryptophan Proteins: Spectrofluorimetric and Theoretical Approaches
	Priyanka Mukherjee, *Asutosh College, India*
	Title: Sustainable Rubber Compounds with Incorporated Biopolymer Filler
	Ján Kruželák, *Slovak University of Technology in Bratislava, Slovakia*
GROUP PHOTO 12:40-12:50	
LUNCH BREAK 12:50-13:30	
13:30-13:50	Title: Preclinical Evaluation of Sodium Copper Chlorophyllin: Chemical Basis, Pharmacokinetics, and Therapeutic Potential in Chemotherapy-Associated Toxicities
	Neha Ramani, *Bhabha Atomic Research Centre, India*
13:50-14:10	Title: Eltrombopag Olamine Induces Apoptosis in Human Breast and Hepatocellular Carcinoma Cells by the Modulation of MAPK, WNT and Caspase-Dependent Signaling Pathways
	Mohammad Taufiq Alam, *University of Barisal, Bangladesh*
14:10-14:30	Title: Assessment of Physicochemical and Antibacterial Properties of Structured Water Samples from Ota, Ogun State, Nigeria
	Abiodun H. Adebayo, *Covenant University Ota, Nigeria*
14:30-14:50	Title: Rapid and Reliable Characterization of Supersaturated Brines and Prediction of their Mining Potential – Cases of Algerian Brines
	Merzouk Zatout, *Kasdi Merbah University, Algeria*
14:50-15:10	Title: Organic Amendments Influence Soil Properties, Soil Microbial Diversity, and Winter Barley Traits in a Five-Year Field Trial with Contaminated Soils at a Former Wood Preservation Site
	Claudia Chiodi, *University of Padua, Italy*

15:10-15:30	Title: Theoretical Study of the Enhancement of the Photoconversion Efficiency on Zinc Porphyrins Dyes by Combining Electron Donor-Acceptor Theory with the BCL Model
	Mauricio Barrera, *Independent, Chile*
15:30-15:50	Title: Translational Quantitative Two-Photon Microscopy of Extracellular Matrix Remodeling Distinguishes Esophageal Squamous Cell Carcinoma from High-Grade Dysplasia
	I-Chen Wu, *Kaohsiung Medical University Hospital, Taiwan*
15:50-16:10	Title: Natural Products as Promising Chemotherapeutic Agents: Anti-Proliferative Effects of Coffee Extracts and Chlorogenic Acid in Hepatocellular Carcinoma Independent of Wnt/β-Catenin Modulation
	Manuel Jaime Moreno Ceballos, *Universidad de Antioquia, Colombia*
REFRESHMENT BREAK 16:10-16:30	
16:30-16-50	Title: Unusual Nanofluids: Properties and Applications
	Valery Ya. Rudyak, *Novosibirsk State University of Architecture and Civil Engineering, Russia*
16:50-17:10	Title: Stem Cell Therapy for Hypoplastic Left Heart Syndrome: Safety, Efficacy, and Future Directions
	Michael Joy Dara, *Zaporizhzhia State Medical University, Ukraine*
17:10-17:30	Title: An Experimental Investigation into using Sewage Effluent to Capture CO_2
	Salam K. Al-Dawery, *University of Nizwa, Sultanate of Oman*
17:30-17:50	Title: Beyond Formal Law: Harnessing African Indigenous Knowledge to Foster Green Marketing Governance and Sharing Economy
	Chipo Mutongi, *Midlands State University, Zimbabwe*
NETWORKING	
END OF DAY 2	

PEERS ALLEY MEDIA

DAY 01

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SPEAKER TALKS

Pea Pod Valorization: Exploring the Influence of Biomass/Water Ratio, Particle Size, Stirring, and Catalysts on Chemical Platforms and Biochar Production

Carlos Alberto Guerrero-Fajardo and **Alejandra Sophia Lozano Pérez**

Universidad Nacional de Colombia, Colombia

This study delves into the valorization of pea pod waste using hydrothermal processes, focusing on optimizing key parameters such as temperature, biomass-to-water ratio, particle size, and catalyst influence. Noteworthy findings include the significant impact of temperature variations on product yields, with 180 °C favoring sugars, HMF, and furfural, while 220 °C and 260 °C led to distinct platform chemical productions. The utilization of a 1:20 biomass-to-water ratio consistently enhances yields by 10%, underscoring its importance in promoting efficient hydrolysis without excessive product degradation. Furthermore, the investigation into particle size reveals that smaller dimensions, particularly 1 mm particles, improved heat and mass transfer, reduced diffusion barriers, and enhanced digestibility, ultimately boosting overall efficiency in platform chemical production. Moreover, the study sheds light on the role of catalysts in the hydrothermal processes, showcasing the differential impact of acid and basic catalysts on product yields. Acid catalysts demonstrate a notable increase of up to 135.5% in the production of platform chemicals, emphasizing their crucial role in enhancing reaction efficiency. The complex relationship between agitation, temperature, and product formation is elucidated, with experiments revealing varying outcomes based on the presence or absence of agitation at different temperatures. These findings provide valuable insights into optimizing pea pod waste valorization, offering a pathway towards sustainable and efficient conversion of agricultural residues into valuable platform chemicals.

Presenter:

Carlos Alberto Guerrero-Fajardo

Universidad Nacional de Colombia, Colombia

Evaluation of Hydrogen Adsorption on Zn–Ni Alloy Coating by the Electrochemical Desorption Technique and its Permeability on AISI 1020 Steel

E. O. Vilar, J. R. Jovelino Torres and **G. Carvalho Lira**
UFCG - Federal University of Campina Grande, Brazil

This study evaluated the influence of nickel content in zinc-nickel coatings on hydrogen retention and permeability in low-carbon steel. A modified electrochemical desorption method was used to quantify hydrogen adsorption on the coatings. A dual-cell electrochemical setup analyzed the hydrogen permeation behavior. Scanning electron microscopy and X-ray diffraction characterized the coatings' morphology and composition. The results indicate that increasing nickel content refines the grain structure and enhances corrosion resistance. A significant decrease in hydrogen permeability was observed for the intermediate composition of 17.27 wt% Ni, suggesting a synergistic effect that increased irreversible hydrogen traps. Moreover, a gradual decrease in the apparent diffusivity of hydrogen was observed as the nickel content in the coating increased. This suggests the development of more resistant barriers to the diffusion process. These findings suggest that optimizing alloy composition is of significant importance for improving the resistance of steel substrates to hydrogen embrittlement.

Table 1- Estimation of the breakthrough time (t_b), apparent diffusivity (D_{app}), permeability (P) and solubility (S), BM - Base Metal.

	t_b (s)	$D_{app} \times 10^5$ ($cm^2\ s^{-1}$)	$P \times 10^{10}$ ($mol\ cm^{-1}\ s^{-1}$)	$S \times 10^8$ ($mol\ cm^{-3}$)
BM	5	15.40	3.28	2.13
BM/Zn-Ni_x (x – wt%)				
11.32	17	4.53	3.63	8.02
17.27	36	2.14	1.25	5.85
19.54	129	0.15	2.74	45.8

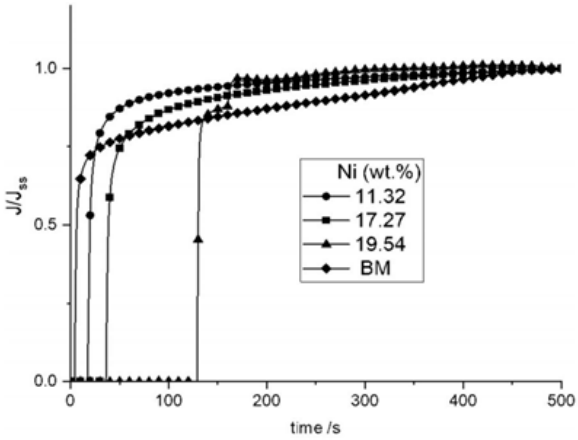

Fig. 2- Hydrogen permeation curves normalized for different nickel compositions by weight (%). BM - Base metal, J- current density, J_{ss}- current density at stationary state.

Presenter:
Eudesio Oliveira Vilar
UFCG - Federal University of Campina Grande, Brazil

Adsorption of Heavy Metals from Aqueous Solutions using Polysaccharides Hydrogels

Adi Wolfson and **Oshrat Levy-Ontman**
Sami Shamoon Collage of Engineering, Israel

Adsorption has been found to be highly effective for removing heavy metals from polluted industrial wastewater. Adsorbents of biological origin, such as negatively charged polysaccharides, e.g., alginate and carrageenan, have at-tracted a lot of attention recently. In this study, I- and K-carrageenan, which contain sulfate ester and hydroxyl groups, and A, which contains carboxyl and hydroxyl groups, were successfully used to adsorb six representative metal ions (Ce3+, Eu3+, Nd3+, Dy3+, Ru3+, and Rh3+), either individually or in var-ious mixtures, from aqueous solutions. All three polysaccharides effective-ly adsorbed the metal ions. The sorption yields for the four lanthanide ions were similar across all polysaccharides, likely due to their comparable ionic radii and valency. The I-carrageenan, however, which has a higher sulfate ester content than the K-carrageenan, exhibited greater sorption yields for all metal ions. The sorption capacities for Ru3+ and Rh3+ were similar to or low-er than those of the lanthanides. These findings suggest that the sorption mechanisms of the lanthanide ions differ from those of the platinum-group metal ions. However, when a binary mixture containing both lanthanide ions (Ce3+ and Eu3+) and platinum-group ions (Ru3+ and Rh3+) was tested, all three polysaccharides exhibited higher selectivity for the platinum-group ions. In some cases, the addition of light metal ions (Na+, K+, Ca2+ and Mg2+) to the heavy metal ion solutions led to a reduction in heavy metal sorption due to competition for binding sites. This reduction was dependent on both the type and concentration of the light metal ions. Finally, FTIR, SEM/EDS, and TGA analyses confirmed that all metal ions were adsorbed onto all types of polysaccharides.

Presenter:
Adi Wolfson
Sami Shamoon Collage of Engineering, Israel

Neural Circuit Formation and Decision Making in the Mouse Olfactory System

Hitoshi Sakano

Department of Animal Behaviors, School of Veterinary Medicine, The University of Tokyo, Japan
Department of Brain Function, School of Medical Sciences, University of Fukui, Japan

In mammals, the olfactory system plays an important role in searching for food, avoiding danger, and finding mating partners for survival of the individuals and species. Odor information is detected by odorant receptor (OR) molecules expressed by olfactory sensory neurons (OSNs) in the olfactory epithelium. In each OSN, only one functional OR gene is expressed in a monoallelic manner and OSN axons expressing the same OR species converge to specific target sites in the OB forming glomerular structures. Thus, binding signals of odorants are converted to map information of activated glomeruli in various combinations. The OB is not simply a projection screen to generate odor maps, but also composed of functional domains for innate odor qualities. The map information is then conveyed by tufted cells (TCs) to the anterior olfactory nucleus to identify the input odor and to recollect the associated memory of odor experience. The recalled odor scene further activates the valence network in the amygdala that was previously connected to the memory engram for learned decisions. Separately from the memory-based learned decisions, odor signals from a specific functional domain of the OB are directly transmitted by mitral cells (MCs) to valence regions in the amygdala to elicit innate olfactory responses. Although the basic architecture of hard-wired circuits is generated according to a genetic program, stereotyped decisions can be modified by olfactory experiences during the critical period. Neonatal odor exposure to environmental odors affects olfactory perception later in life. This odor-induced imprinting imposes the positive quality on imprinted memory, even when the odor quality is innately aversive. In response to the olfactory signals, secondary MCs and TCs are separately activated in the exhalation and inhalation phases, respectively. Thus, each odor input is differentially processed in the separate respiratory phases by distinct sets of projection neurons.

In my presentation, I will provide an overview of the recent progress made in understanding the olfactory circuitry and odor perception in mice.

Presenter:
Hitoshi Sakano
The University of Tokyo, Japan

Demystifying AI: Neural Networks, Transformers, and Agents for Modern Chemists

Safwan Omari
Lewis University, USA

In an era where artificial intelligence is revolutionizing scientific discovery, this presentation demystifies the core technologies powering today's AI breakthroughs and equips chemists with practical tools to integrate them into their workflows. Delving into neural networks, we'll explore their historical roots and non-linear capabilities that enable arbitrary function approximation, from image classification to text generation. The spotlight falls on the transformer, the massively successful model behind GPT and similar systems, with intuitive visualizations of attention mechanisms (resolving ambiguities like "bank" in context) and a peek at code implementations. Discover emergent abilities from billion-parameter scales, tempered by recent power-law insights favoring efficient, fine-tuned models.

A rapid overview of leading large language models (LLMs) like GPT-5, Llama 4, Grok 3, DeepSeek V3, Qwen 2.5-Max, and Gemini 2.0 compares parameter sizes, training corpora, and benchmark performances, including advanced evals from FrontierMath. Hands-on demos *via* Google Colab notebooks show black-box LLM usage with Ollama and Hugging Face—querying explanations or generating text in minutes—escalating to ReAct agents that reason, act with tools (web searches, databases), and integrate domain-specific APIs for practical tasks.

Additionally, I will present my original research results on applying AI, particularly LLMs, to software engineering challenges—such as code comprehension, repair, and conversion between paradigms—as one example of the successful use of these technologies in a diverse field, underscoring their broad potential.

Attendees will leave with actionable code, resources, and confidence to wield AI as a collaborative tool—leaping into the AI era to elevate their work. Join us for an interactive journey blending theory, code, and application—perfect for curious practitioners eager to accelerate workflows.

Presenter:
Safwan Omari
Lewis University, USA

Docosahexaenoic Acid Increases the Pro-Resolving Brain Lipid Mediators of Inflammation in Rat Pups Prenatally Exposed to Alcohol

Enrique M. Ostrea Jr.[1], Deepak Yadav[1], Charlie T. Cheng[1], Esther D. Kisseih[1], Krishna R. Maddipati[2] and **Ronald L. Thomas[1]**

[1]Department of Pediatrics, Hutzel Women's Hospital and Children's Hospital of Michigan, Wayne State University School of Medicine, USA
[2]Bioactive Lipids Research Program, Wayne State University, USA

The fetal alcohol spectrum disorder (FASD/FAS) is a chronic inflammatory process of the fetal brain induced by alcohol and mediated by pro-inflammation (PILM) and pro-resolu- tion (PRLM) lipid mediators of inflammation. DHA (Docosahexaenoic acid) is an essential precursor of PRLM. A study of the response by the lipid mediators of inflammation to alcohol insult and DHA supplementation can provide vital information on the pathogenesis of FASD/FAS and the potential ameliorative role of DHA.

Methods: Four groups of timed pregnant rats were studied: Control, low dose (1.6 g/kg/day) and high dose (2.4 g/kg/day) alcohol and high dose alcohol (2.4 g/kg/day) + DHA, (1250 mg/kg/day of DHA). The pups were delivered on day 20, and their whole brain was examined for lipid mediators by liquid chromatography mass spectroscopy.

Results: The following biomarkers of brain lipid mediators were studied, *viz*., PILM (LTB4, PGE2, PGF2a, TXB2) and PRLM (LXA5, 4- HDoHE,17-HDoHE and MaR1n-3, DPA). The brain PILM and PRLM concentrations de- creased significantly ($p<0.001$) with high dose alcohol. However, high dose alcohol + DHA resulted in a significant ($p<0.001$) increase in PRLM levels, *viz*, LXA5, MaR1n-3 DPA, 17- HDoHE and threefold increase in 4-HDoHE.

Conclusion: We conclude that brain lipid inflammation can be ameliorated by DHA by mobilizing PRLM.

Presenter:
Enrique M. Ostrea Jr.
Wayne State University School of Medicine, USA

Antibacterial and Prooxidant Activity of Sol-Gel Prepared Copper - Silica Nanocomposite Materials

Iliana Ivanova[1], Lilia Yordanova[1], Elitsa Pavlova[2], Yoanna Kostova[3], Miroslav Metodiev[4], Lora Simeonova[4] and **Albena Bachvarova-Nedelcheva[5]**

[1]Faculty of Biology, Sofia University "St. Kliment Ohridski", Bulgaria
[2]Faculty of Physics, Sofia University "St. Kliment Ohridski", Bulgaria
[3]Institute of Metal Science, Equipment and Technologies with Hydro- and Aerodynamics Centre "Acad. A. Balevski", Bulgarian Academy of Sciences, Bulgaria
[4]Department of Virology, The Stephan Angeloff Institute of Microbiology, Bulgarian Academy of Sciences, Bulgaria
[5]Institute of General and Inorganic Chemistry, Bulgarian Academy of Sciences, Bulgaria

The present work is devoted to the sol-gel synthesis of copper-silica hybrid nanomaterials. Tetramethyl ortosilane (TMOS) was used as a silica precursor, while copper was introduced as a solution in ethanol with $Cu(OH)_2$ or $CuSO_4$. The phase formation, structure and morphology of the samples were studied by XRD, IR, UV-Vis and SEM.

The antibacterial activity of four copper-silica nanocomposites was tested on *Staphylococcus aureus ATCC25923, Bacillus cereus NBIMCC1090, Escherichia coli ATCC 25922, Salmonella typhimurium ATCC BAA-2162,* and *Pseudomonas aeruginosa ATCC 27853*. The results showed that the nanocomposites exhibited concentration-dependent effects; they depended on the composite type, gel form, or heat treatment when tested against Gram-positive and Gram-negative bacteria. The composites obtained from $CuSO_4$ were more toxic to all tested bacteria in comparison to those obtained by $Cu(OH)_2$. *P. aeruginosa* was the most resistant strain to the new synthesized hybrid nanocomposites.

All materials were tested for their prooxidant activity at pH 7.4 in three model chemical systems for the generation of various ROS (·OOH, ·OH and O_2·- radicals) or containing H_2O_2 - an oxidant and a ROS. The obtained results explain the antibacterial properties of the new materials. All data suggest clinical implementations of the as-prepared hybrids.

Acknowledgements: *This study is financed by the European Union-Next-GenerationEU, through the National Recovery and Resilience Plan of the Republic of Bulgaria, project SUMMIT BG-RRP-2.004-0008-C01 contract* 70-123-661/16.04.2024 GREEN SYNTHESIS ON NANOPARTICLES AND STUDY ON THE ANTIMICROBIAL AND CYTOTOXIC EFFECT

Presenter:
Iliana Atanasova Ivanova
Sofia University “St. Kliment Ohridski”, Bulgaria

Preparation and Characterization of Novel Lignosulfonate-Based Starch-Silica Nanocomposite (LS-SSNC) Hybrid Material for Drilling Stability

M. Noorul Anam Mohd-Norddin, Samuelson I. Okwaraku and **Azad A. Rasol**

Department of Petroleum Engineering, Faculty of Chemical and Energy Engineering, Universiti Teknologi Malaysia (UTM), Malaysia

The development of advanced hybrid additives is crucial for enhancing applications that require high-temperature, high-salinity (HTHS) conditions. A novel lignosulfonate–starch–silica nanocomposite (LS-SSNC) was synthesised *via* graft polymerisation of acrylamide using potassium persulfate as initiator, with acid-modified potato starch, nanoprecipitated lignosulfonate (LS), and sol-gel derived silica nanoparticles as building blocks. Then, the morphology, size distribution, crystalline structure, stability and thermal properties of the LS-SSNC was determined. Likewise, the adsorption capacity of LS-SSNC was evaluated and fitted into known adsorption models. The LS-SSNC exhibited a mesoporous structure from Brunauer-Emmett-Teller results (mean surface area 77.73 $m^2 g^{-1}$, mean pore volume 0.53 $cm^3 g^{-1}$, mean pore diameter 27.88 nm) with abundant functional groups. Dynamic light scattering revealed Z-average diameters of 120–1900 nm with polydispersity indices between 0.24–0.37, and LS-SSNC-3 being enriched in nanosized fractions (214 nm). Stable dispersions were confirmed by zeta potentials of –20 to –30 mV across pH 2–10. Adsorption equilibrium with bentonite (BT) was achieved at 180 min, yielding capacities of 468–477 mg g^{-1} and more than 5 grams(g) BT removal per gram of LS-SSNC. Kinetics followed the pseudo-second-order model (R^2 was 1), while isotherms fitted the Langmuir model (R^2 was 0.998). Thermodynamic analysis ($\Delta H°$ was –1.19 kJ mol^{-1}) indicated predominant chemisorption with physisorption contributions. Strong thermal stability was confirmed by thermogravimetric analysis, which displayed a multi-stage degradation pattern with little weight loss up to 800 °C. LS-SSNC demonstrates dual adsorption mechanisms, high binding efficiency, and environmental compatibility for oil and gas, water treatment, and related industries.

Presenter:
Muhammad-Noorul-Anam Mohd-Norddin
Universiti Teknologi Malaysia (UTM), Malaysia

Incorporating Quantum Mechanical Effects into Molecular Dynamics Simulations: A Novel Approach

Yoshiaki Teranishi[1], **I-Yun Hsiao**[2] and **Hiroki Nakamura**[3]

[1]Institute of Physics, National Yang Ming Chiao Tung University, Taiwan
[2]Physics Division, National Center for Theoretical Sciences, Taiwan
[3]Institute for Molecular Science, Institute of Natural Sciences, Japan

Molecular dynamics (MD) simulation is a powerful computational method for predicting physical and chemical phenomena, with applications ranging from drug design to material science. While modern MD techniques have achieved significant success, they rely on the Born-Oppenheimer approximation, which treats nuclei as classical particles on an empirical potential energy surface. This approach, however, often fails to accurately describe phenomena where quantum mechanical effects—such as atomic tunneling, interference, and nonadiabatic transitions—play a crucial role, especially at low temperatures or in systems with close-lying electronic states.

To overcome these limitations, new theories of quantum many-body dynamics are being developed. These theories can be broadly classified into two categories: wave function-based and trajectory-based methods. Wave function-based methods, which solve the time-dependent Schrödinger equation, face significant computational challenges due to the exponential scaling of computational resources with the number of particles. This "curse of dimensionality" makes them impractical for large systems.

In contrast, trajectory-based methods offer a more scalable approach. By solving equations of motion for multiple independent trajectories, these methods drastically reduce memory requirements and are highly suitable for parallel computation. Our proposed method falls into this category, leveraging recent advances in semiclassical theories. We introduce a novel framework that incorporates three key quantum effects into a trajectory-based MD simulation.

First, we address **quantum interference** using the Initial Value Representation (IVR) method, which approximates the quantum mechanical path integral using classical trajectories. Second, we incorporate **tunneling effects** through a new method proposed by Nakamura et al. This approach efficiently identifies tunneling paths and caustics, overcoming limitations of older methods like instanton theory. Finally, we account for **nonadiabatic transitions**—which occur when the Born-Oppenheimer approximation breaks down—using the Zhu-Nakamura Trajectory Surface Hopping (ZN-

TSH) method. This method treats nuclear motion classically but handles transitions probabilistically in regions of avoided crossing.

By combining these three novel approaches, our method provides a comprehensive and computationally efficient framework for accurate molecular dynamics simulations that fully incorporate essential quantum mechanical effects. This represents a significant step toward bridging the gap between classical MD and full quantum dynamics for many-body systems. We will present the theoretical foundations of our method, supported by illustrative examples.

Presenter:
Yoshiaki Teranishi
National Yang Ming Chiao Tung University, Taiwan

Timing Matters: An Observational Study on Circadian Effects of Spinal Anesthesia in Cesarean Delivery

Evangelia Nikouli[1], Nikoleta Koutlaki[2], Kostas Anagnostopoulos[3], Christina Tsigalou[4] and **Pelagia Chloropoulou[5]**

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Background: The timing of anesthesia administration may affect drug efficacy and recovery outcomes. Understanding these variations is important for optimizing anesthetic care.

Aim: To assess how spinal anesthesia timing affects block duration, postoperative pain, and CRP and cortisol levels in cesarean deliveries.

Methods: Ninety women were divided into three groups based on spinal anesthesia timing: Group A (08:00–16:00), Group B (16:00–00:00), and Group C (00:00–08:00). Standardized spinal anesthesia was administered. Sensory/motor blockade and pain (NRS) were assessed every 10 min. Blood samples for CRP and cortisol were collected preoperatively and at 2, 4, 24, and 48 h post operation.

Results: Group C showed shorter sensory and motor blockade than Groups A and B ($p < 0.05$). The time to first analgesic request was longest in Group A, while Group C reported the highest pain scores ($p < 0.05$). CRP levels were significantly higher in Group B vs. Group A at 24 and 48 h, and vs. Group C at 48 h ($p < 0.05$). Group B demonstrated the steepest CRP velocity, indicating a more rapid physiological stress response. BMI differences may have influenced biomarker dynamics.

Conclusions: Spinal anesthesia timing significantly impacts block duration, pain experience, and the rate of the physiological stress response. CRP velocity may offer additional insights into perioperative inflammation. Circadian considerations should be integrated into anesthetic planning for cesarean deliveries.

Presenter:
Evangelia Nikouli
General Hospital of Komotini, Greece

The Effects of the Environment (Medium) on Nuclear Reaction Yields

Houria Salah
Centre de Recherche Nucleaire d'Alger, Algeria

The borderline between atomic and nuclear is governed by processes related to electromagnetic and weak interactions. These involve electrons as is the case in internal conversion and electron capture. In solid state environment coulomb interaction can lead to the occurrence of what is called solid state internal conversion process and may assist the fusion reaction at low energy nuclear reactions.

Understanding the dependence of the nuclear reactions cross sections on the involved environments [*i.e.* screening] and the experimental results obtained with low energy nuclear reactions especially with deuterated metals requires a deeper studies of the intrinsically generated electromagnetic fields within the nuclei vicinity.

Further to the suggestions concerning the involvement of target effects in screening phenomenon, observed for C^{12}(d,p)C^{13} and C^{12}(d,d)C^{12} reactions at MeV energy in polyethylene, we present here interesting results that could provide first proof of principle experiment of the role played by electrons in nuclear phenomena. Evidence of nuclear reaction rate alteration is also demonstrated in graphite when the sample is irradiated with fast electrons. We also emphasize the possibility of nuclear excitation and solid state electron conversion that may appear with the emergence of collectivity behavior.

Presenter:
Houria Salah
Centre de Recherche Nucleaire d'Alger, Algeria

Multicenter Clinical Trial for the Treatment of Obstructive Sleep Apnea with a Non-Permanent Orthodontic Intraoral Device in Children

Tammarie Heit[1], Clete A Kushida[2], James Stevens[3], Michael Bennett[4], Dennis Klemp[5], Dean Raio[6], Jesse Cozean[7] and **Colette Cozean[7]**

[1]The University of Alberta, Canada
[2]Stanford University Division of Sleep Medicine, USA
[3]Stevens Health Alliance, USA
[4]Advanced Dental Care, USA
[5]Klemp Family Dentistry, USA
[6]Raio Dental, USA
[7]The EyeDeas Company, USA

The development of an OSA (obstructive sleep apnea) treatment that is simple, affordable, comfortable, noninvasive, effective at all severity levels, and accepted but most patients is still the holy grail of sleep medicine. (Kirsch) OSA is a serious medical condition with a solution found in dentistry.

This presentation is a multicenter clinical trial in dentistry done on children that demonstrated an improvement of obstructive sleep apnea closer to the above objective. It was demonstrated that the DNA oral device was safe and effective. There was an anatomical change in the oral cavity and upper airway allowing for better eating and breathing functions.

Through academic multidisciplinary collaboration at this conference, the search for a mechanism of action can be explored to simplify treatment in dentistry and improve prevention clinically. Then protocols to help make it available for everyone through medicine and dentistry can be taught. The DNA device is thought to allow the full genetic expression of maxillary development making room for the teeth and improving the anatomy of the upper airway resulting in the resolution of sleep apnea in both adults and children.

Collaborative exploration in the area of molecular biology and neurochemistry to determine a mechanism of action of this treatment could provide the breakthrough needed in research and development. This can direct clinical

protocols in the fields of medicine and dentistry to help achieve treatment and prevention of obstructive sleep apnea in humans.

I will present this paper and show images of clinical results in children (and adult samples) to stimulate thought in the experts of molecular biology, neurochemistry and other influencers in an effort to move research and development toward closer collaboration of academia and clinical work.

Presenter:
Tammarie Heit
The University of Alberta, Canada

Plant Extracts Mediated Syntheses of Nanoparticles and Their Effectiveness on Agricultural Pathogens

Graciela M. L. Ruiz-Aguilar[1], Nanh Lovanh[2] and **Byung-Taek Oh[3]**

[1]Department of Environmental Sciences, Division of Life Sciences, University of Guanajuato, Mexico
[2]ARS, FAESRU, USA (retired)
[3]Division of Biotechnology, BK21 Plus, College of Environmental and Bioresource Sciences, Chonbuk National University, South Korea

The high demand for protein consumption in the ever-increasing population has put great pressure on food animal and crop production systems. To increase profit margin along with productivity, the utilization of antibiotics to promote animal growth and reduce mortality has contributed to the emergence of resistant bacteria that may affect humans as well as the animals themselves. Thus, it is necessary to find a simple and economical way to counter or reduce the proliferation of these antibiotic resistant bacteria. Nanoparticles with antimicrobial properties hold a great promise in this arena. This study utilized silver nanoparticles synthesized from bitter melon (*Momordica charantia*) and sugar cane (*Saccharum officinarum*) extracts to test against common agricultural pathogens (e.g., fungi and *Escherichia coli*). The synthesized nanoparticles were characterized and confirmed as silver nanoparticles by using the UV spectroscopy, FTIR, and SEM analysis. The results show that these silver nanoparticles are effective against agricultural fungi and pathogens such as *Phytophthora capsici, Colletotrichum acutatum*, *Cladosporium fulvum*, and *Escherichia coli*.

Presenter:
Graciela M. L. Ruiz-Aguilar
University of Guanajuato, Mexico

Photoregulation in *Xanthomonas campestris*: Integration of Red/Far Red and Blue Light Signals

Valeria P. Conforte[1,2], Hernán R. Bonomi[3,4], Jimena Rinaldi[3,5], Lisandro H. Otero[6], Ariel E. Festa[1], Dana Garacoche[7], Sabrina A. Foscaldi[3,5,8,] Emilia Castagnaro[1,2], Adrián A. Vojnov[1,2] and **Florencia Malamud[6,9]**

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[6]Departamento de Biología Molecular, Facultad de Ciencias Exactas, Fisicoquímicas y Naturales, INBIAS - CONICET, Universidad Nacional de Río Cuarto, Argentina
[7]PECSI, Departamento de Ciencias Básicas, Universidad Nacional de Luján, Argentina
[8]Inmunova S.A., Argentina
[9]CONICET, Argentina

Xanthomonas campestris pv. campestris (Xcc), the bacterial agent of black rot, employs light as a key environmental cue to regulate virulence. The *Xcc* genome encodes two main photoreceptors: a red/far-red-sensing bacteriophage (*Xcc*BphP) and a blue-light- responsive LOV histidine kinase (LOV-HK).

Previous studies from our group revealed that *Xcc*BphP acts as a negative regulator of virulence factors such as xanthan production and biofilm formation through a reversible light-dependent mechanism. Crystallographic and spectroscopic analyses identified *Xcc*BphP as a bathy type phytochrome characterized by a thermally stable Pfr ground state and an exceptionally slow dark reversion. This molecular stability provides a robust conformational switch that connects illumination to virulence control.

In our latest work, we examined the photochemical behaviour of *Xcc*BphP under blue light and uncovered an additional layer of regulation. Spectroscopic analyses showed that blue illumination partially converts the stable Pfr population into Pr, reaching a photostationary state with approximately 19 % residual Pfr. Site-directed mutagenesis confirmed that this blue-light-induced transition drives the reduction in xanthan synthesis and cell aggregation ob-

served in *Xcc* wild-type strain. These results demonstrate that *Xcc*BphP, although primarily a red/far-red sensor, also perceives blue wavelengths, broadening its role in environmental signal transduction.

Moreover, we found that the LOV-HK is activated under the same blue-light conditions, and that both photoreceptors cooperate to regulate motility and plant colonization efficiency. Together, these findings reveal that *Xanthomonas* integrates spectral information through interconnected photochemical pathways. This dual photoregulatory system enables a fine tuning of virulence according to light quality and intensity, representing a sophisticated example of environmental adaptation in bacterial pathogenesis.

Presenter:
Valeria P. Conforte
Instituto de Ciencia y Tecnología Dr. César Milstein (CONICET - Fundación Pablo Cassará), Argentina

Transposition and Implementation of European Union Renewable Energy Legislation in France, Italy, and Germany: A Regulatory Perspective and a Comprehensive Analysis of Opportunities and Challenges

Ana Maria Fagetan
University of Rome "La Sapienza", Italy

This presentation will provide a detailed comparative analysis of the transposition and implementation of the Renewable Energy Directives II and III (RED II and RED III), REPowerEU Plan, and the 'Fit for 55' package in France, Italy, and Germany. The analysis highlights the objectives, key legislative provisions, and national-scale achievements, challenges, advantages, and disadvantages — including implications for investment conditions and renewable energy financing mechanisms — associated with these pivotal European Union legislative frameworks, which, to a certain extent, induced a paradigm shift with varying degrees of impact in every Member State. The work is divided into four parts that follow this brief introductory outline of the problem. The introduction presents legal developments in renewable energy law in the European Union. The second part offers a comprehensive and in-depth examination of the European Union's renewable energy regulatory framework and research gaps that hinder doctrinal tensions within the EU's renewable energy legislative framework. In the third part, we analyze the transposition and implementation of each mentioned directive in the selected countries. The last part highlights commonalities, divergences, challenges, best practices, and lessons learned from each nation's approach. This comparative analysis predicts that implementation success is inversely linked to administrative divergence, with France's centralized legal system facilitating effective bureaucratic streamlining and higher predicted deployment, while the fragmented governance structures of Germany and Italy serve as structural impediments that critically undermine the EU's acceleration mandate.

Presenter:
Ana Maria Fagetan
University of Rome "La Sapienza", Italy

Removal of Uranium from Aqueous Systems using Green Cellulose Biosorbent Derived from Banana (*Musa paradisiaca*) Leaves

Rohit Mehra
Dr. B. R. Ambedkar National Institute of Technology, India

The contamination of groundwater by uranium has emerged as a major environmental and public-health challenge owing to its combined radiological and chemical toxicity. Although uranium occurs naturally in geological matrices, its elevated concentrations in water bodies are often associated with anthropogenic influences such as excessive fertilizer usage, industrial discharge, and fuel combustion. In aqueous media, uranium primarily exists as uranyl ions (UO22+), which are highly soluble and mobile, thereby increasing the risk of human exposure through drinking water. Chronic ingestion can lead to kidney dysfunction and other systemic toxic effects.

In alignment with the principles of Green Chemistry, which emphasize sustainability, biodegradability, and the minimization of hazardous substances, this study explores a biobased approach for uranium removal using natural cellulose extracted from banana (*Musa paradisiaca*) leaves. The cellulose adsorbent was utilized under varying experimental conditions—adsorbent doses (10–50 mg), uranium concentrations (10–100 µg/L), pH values (2–7), and contact durations (15–60 minutes)—to evaluate its performance in an aqueous system. The highest removal efficiency of 97.69% was recorded at an optimum combination of 10 mg adsorbent dose, 55 µg/L uranium concentration, pH 4.5, and 15 minutes of contact time.

The adsorption process was further optimized using Response Surface Methodology (RSM) to investigate the interactive influence of operating parameters and to determine statistically significant conditions for maximum removal. The findings reveal that cellulose derived from banana leaves acts as an efficient, low-cost, and eco-benign biosorbent, offering a promising alternative to conventional chemical treatments. This work supports the Green Chemistry paradigm by promoting waste-to-resource conversion, utilizing renewable plant-based materials, and minimizing secondary pollution during remediation. The study provides valuable insight into sustainable technologies for uranium decontamination and contributes to the development of green water-purification strategies for radiotoxic contaminants.

Presenter:
Rohit Mehra
Dr. B. R. Ambedkar National Institute of Technology, India

Morphological Characterization and Health Risk Assessment of Fine Particulate Matter over the National Capital Region of India

Ranu Gadi and **Shobhna Shankar**
Indira Gandhi Delhi Technical University for Women, India

Fine Particulate Matter ($PM_{2.5}$) in the National Capital Region (NCR) of India exhibits significant spatial and temporal variability in its morphology and toxicity. Through integrated morphological characterization and health risk assessment, this study provides insights into the sources, composition, and potential health impacts of fine particulate matter in the region. The chemical characteristics (including semi-volatile organic compounds and elemental composition), infra-red spectral signatures, and morphological features indicates for diverse sources of origin of the pollutants. The source apportionment models, additionally confirm the sources' contribution of the pollutants. The SVOCs have been traced to possess diverse sources of anthropogenic origin, whereas, the elemental composition revealed the mixed impact of anthropogenic activities as well as natural sources of origin and the meteorological impact in the region. Numerous functional groups obtained in FTIR results helped in characterization of various organic compounds. The spherical and irregular shapes of the fine particulate matter indicated and confirmed for high-temperature anthropogenic activities and other sources (including traversed particles). The diverse irregular shapes hold huge information on their own revealing the respective sources and the chemical composition as well.

The health aspect of the study indicated Boron exhibiting the highest Hazard Quotient for all routes of exposure at both the sites. The high molecular weight polycyclic aromatic hydrocarbons prevailed throughout the study period at both the sites. Consequently, it was observed that these contributed significantly (88-91%) to the total toxic equivalent quotient at both the sites. The obtained range of cancer risk remained in safer range ($<10^{-4}$), and the order of cancer risk through all exposure routes was inhalation> dermal> ingestion. It is speculated that the increasing trend of accumulation of pollutants may show enhanced synergistic impacts of the pollutants. These are potent enough to possess chronic impact on different physiological systems of the human body. Hence, the sources need to be monitored regularly. Additionally, the inhalation exposure needs revised implementation in the policies related to pollutant reduction from the ambient atmosphere.

Presenter:
Ranu Gadi
Indira Gandhi Delhi Technical University for Women, India

The Influence of Powder Particle Shape on the Macrostructure of Material Obtained by Direct Energy Deposition (DED)

Oleksandr Radchenko, Kazbek Gogaev, Oleksandr Umanskyi, Oleksandr Terentiev and **Oleksii Kushchev**

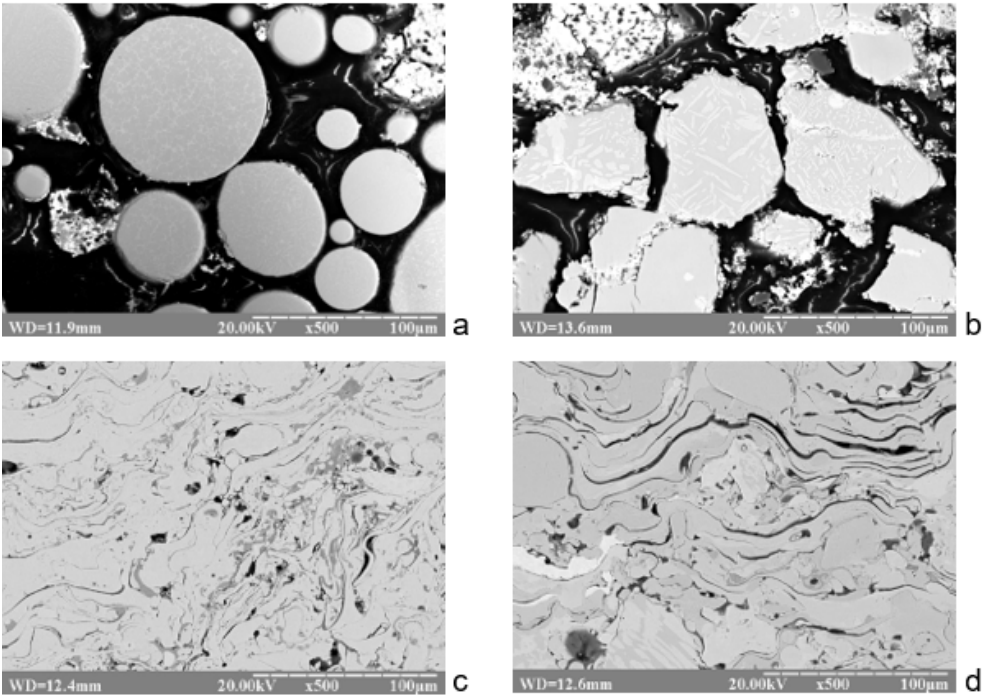
Frantsevich Institute for Problems of Material Science NAS of Ukraine, Ukraine

Additive technologies do not require the creation of new equipment for the production of new parts, but only require a 3D printer and powder of the appropriate chemical composition, size and shape of particles. The powder has rather strict requirements. This applies in particular to the shape of the particles. In most cases, it must be spherical. Grinding methods that produce a fairly large amount of powder do not allow obtaining spherical particles. Therefore, additional processing is carried out for them, which increases the cost of the powder and can worsen its chemical properties. It is of interest to establish the possibility of using non-spherical powders in additive technologies.

The work used high-speed steel powder P6M5K5 with a spherical particle shape (Fig. a) and cobalt alloy powder CoCrAlYSi with a non-spherical particle shape (Fig. b). The steel powder was obtained by spraying molten metal with nitrogen gas. The alloy powder was obtained by grinding in the rolls of a rolling mill under harsh grinding conditions (the magnitude of the contact stresses exceeded the strength limit of the alloy at room temperature). Both powders had the same size (15 - 50 μm), but different particle shapes.

The compact material was obtained by applying the powder to the substrate by plasma method in an open environment) using a mixture of argon and hydrogen as plasma-forming gases. The substrate was made of steel 3. The figure shows electron micrographs of powder sections and the resulting material without etching, made in the Compo mode at a magnification of 500 times. In the macrostructure of the resulting materials, several unmelted or partially melted particles can be seen (Fig. c, d). In the material from the ground powder, there are more defects in the form of interface surfaces, which increase the total porosity.

Both spherical and non-spherical powders in the case of the DED process allow for the production of a fairly dense material in which the starting particles are almost absent.



Electronographic images of powder sections (a, b) and material obtained by the DED method (c, d): P6M5K5 steel (a, c), CoCrAlYSi alloy (b, d)

Presenter:
Oleksandr Radchenko
Frantsevich Institute for Problems of Material Science NAS of Ukraine, Ukraine

Unraveling the Structural and Functional Characteristics of Cocoonase, Trypsin, and Sericin: An Approach Towards Cocoon Softening for the Benefit of the Silk Industry

Dev Mani Pandey[1], Nishi Prakash Tiwari[1], Sneha[1], Aruna Rani[1,2], Preeti Anand[1], Smita Lata[1] and **Jay Prakash Pandey[2]**

[1]Birla Institute of Technology, India
[2]Central Tasar Research and Training Institute, India

Cocoonase is a proteolytic enzyme capable to dissolve silk cocoon shell to exit the silk moth. Cocoon silk fiber contains mainly fibroin protein and sericin protein. Chemicals like sodium carbonate, soap, soda etc. are used for silk cocoon shell degumming. During cocoon degumming sericin protein solubility is increased that result in sericin release from silk fibroin protein. However, chemical-based degumming cause loss of natural silk color and softness. Cocoonase enzyme soften silk sericin protein at the cocoon's anterior area while fibroin protein of silk is not affected. Likewise, trypsin is another universal enzyme belonging to the proteases family capable to hydrolyze proteins into amino acids and serine hydroxyl an active site is regenerated. The sericin is a preferred substrate of trypsin enzyme. Catalytic triad (serine, aspartic acid and histidine) present at the substrate binding site of this enzyme is important for its catalytic activity. However, no comprehensive study on structural and functional characterization of *Antheraea mylitta* cocoonase, trypsin and sericin protein were carried out. In the present research computational and experimental based approaches were applied to elucidate comprehensive characteristics of cocoonase, trypsin, and sericin. Here, *A. mylitta* cocoonase gene cloning and expression, transcriptome based differential gene expression analysis, mechanism of interaction between the cocoonase enzyme and sericin protein, and trypsin enzyme and sericin protein were studied by applying experimental and various computational based methods. Additionally, Optical Coherence Tomography based analysis of cocoonse enzyme and chemical-treated silk cocoon sheets were also studied. Because of similar proteases both cocoonase and trypsin have an important role in silk cocoon softening. Detailed work carried out on structural and functional characteristics of cocoonase, trypsin, and sericin as well as on silk cocoon degumming will be presented.

Presenter:
Dev Mani Pandey
Birla Institute of Technology, India

Synthesis and Characterization of a New CrMOF using Captopril as a Linker and its Integration into Chitosan for Enhanced Optoelectronic Properties

Diary I. Tofiq[1], Karzan A. Abdalkarim[1] and **Shujahadeen B. Aziz[1,2]**

[1]Department of Chemistry, College of Science, University of Sulaimani, Iraq
[2]Research and Development Center, University of Sulaimani, Iraq

This study describes the synthesis of a new Chromium(III)-based metal-organic framework (CrMOF) with a high surface area of approximately 430 m^2/g, using captopril (CP) as a linker for the first time. The CrMOF is employed for the first time to improve the optical properties of chitosan (CS), a natural polymer. Various characterization techniques, including FTIR, UV-vis. Spectroscopy, TGA, DSC, BET, DLS, XRD, FESEM, and EDX were examined on the samples to analyze the synthesized MOF and chitosan composites' structural, thermal, and optical properties. The Tauc method was employed to evaluate the onset optical energy band gap (OEBG) for all the films, revealing a significant reduction in the band gap from 5.5 eV to approximately 3 eV. The optical dielectric losses were also utilized to establish the OEBG and characterize the type of electron transition in each thin film. Furthermore, the Urbach energy (EU) was found to increase with rising CrMOF concentration from 0.4394 to 0.9497 eV. Our results demonstrate that incorporating CrMOF into chitosan significantly reduces the band gap, enhancing its optical properties. The doped CS films enhance the refractive index and optical dielectric constant. This innovative approach opens a new field for polymer composite fabrication, which differs from traditional filler particle methods.

Presenter:
Diary Ibrahim Tofiq
University of Sulaimani, Iraq

Development of Rapid Chromogenic and Fluorescence Spectroscopy-Based Test Protocol to Determine Proper Heat Treatment in Goat Milk

Parita Mangroliya[1], Tanmay Hazra[2] and **Rohit Sindhav[3]**

[1]Parul Institute of Technology, Parul University, India
[2]Department of Dairy Chemistry, College of Dairy Science, Kamdhenu University, India
[3]Department of Dairy Technology, College of Dairy Science, Kamdhenu University, India

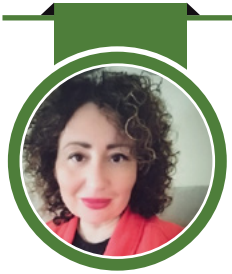
Goat milk is increasingly preferred due to its superior digestibility and suitability for individuals with cow milk protein allergy; however, ensuring its microbiological safety through proper pasteurization remains challenging. Conventional alkaline phosphatase (ALP)–based assays are often unreliable for goat milk because of the inherently low ALP activity. The present study aimed to develop and validate rapid, sensitive, and reliable alternative test protocols targeting lactoperoxidase (LPO) enzyme activity to ascertain proper heat treatment of goat milk.

Raw goat milk samples were subjected to low-temperature long-time (63°C/30 min), high-temperature short-time (72°C/15 s), and higher heat treatments ranging from 74°C to 80°C for 15 s. LPO activity was assessed using a modified rapid chromogenic assay based on color development in the presence of phenol, 4-aminoantipyrine, and hydrogen peroxide. In parallel, fluorescence spectroscopy was employed to monitor structural changes in LPO, with emission spectra recorded at an excitation wavelength of 295 nm. Multivariate data analysis was performed using principal component analysis (PCA) to differentiate raw and heat-treated samples.

The chromogenic assay revealed a progressive reduction in pink color intensity with increasing heat severity, with complete disappearance at 80°C for 15 s, indicating total LPO inactivation. Fluorescence spectroscopy showed a marked increase in emission intensity at 343 nm following heat treatment, attributed to exposure of tryptophan residues during LPO denaturation. PCA clearly discriminated raw milk from heat-treated samples, with PC1 and PC2 explaining over 93% of the total variance.

In conclusion, both chromogenic and fluorescence spectroscopy-based methods demonstrated 100% accuracy in identifying high-temperature pasteurized goat milk. These rapid, simple, and cost-effective techniques offer robust alternatives to ALP-based assays and are well suited for routine application in dairy quality control laboratories.

Presenter:
Mangroliya Parita Alpeshbhai
Parul University, India



Environmentally Friendly Methods for Enhancing the Biological Functions of Certain Transition Metals

J. Bogojeski[1], A. Caković[1], A. Kesić2, A. Gigić[1], N. Srećković[1] and **V. Mihailović[1]**

[1]Faculty of Science, University of Kragujevac, Serbia
[2]Department of Science, Institute for Information Technologies Kragujevac, University of Kragujevac, Serbia

Malignant tumors remain a major obstacle in modern medicine due to high mortality rates and the limitations of conventional therapies, such as systemic toxicity and drug resistance. In the search for more targeted and effective alternatives, transition metal complexes have gained increasing attention for their unique reactivity and biological versatility. [1] This study focuses on Rh(III), Os(II), and Cu(II) complexes coordinated with various nitrogen-donor ligands, which were synthesized and extensively characterized. Rh(III) and Os(II) complexes were selected for their structural flexibility and high affinity for biological targets, while Cu(II) complexes were examined for their ability to generate reactive oxygen species (ROS), bind to DNA, and exhibit lower toxicity than platinum-based drugs. The adaptable coordination environment of these metals enables fine-tuning of biological behavior through ligand design. The investigation included studies of substitution kinetics with biologically relevant ligands, DNA and serum albumin binding, lipophilicity analysis, and *in vitro* cytotoxicity assays on selected cancer cell lines. A key feature of this work is the incorporation of environmentally friendly methods. The impact of ionic liquids on the reactivity and bioactivity of Rh(III) and Os(II) complexes was explored to assess their potential as green solvents.[2] In parallel, Cu(II) complexes were evaluated in the presence of *Salvia pratensis* and *Lythrum salicaria* plant extracts to investigate possible synergistic effects within a green chemistry context. The results emphasize the promise of eco-conscious strategies in the development of transition metal-based anticancer agents and highlight how sustainable approaches can complement and enhance the biological activity of these compounds.

Presenter:
Jovana Bogojeski
University of Kragujevac, Serbia

Plant-Microbe Interactions: A Gateway to Sustainable Agriculture and Enhanced Crop Resilience

Beema Jainab S. I[1], Rashmi Mohapatra[2], B. Saritha[3], Jaiminee Jhankar[4], Sumitha. J[5] and **Shweta Kailash Pal[6]**

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[2]School of Comparative Indic Studies and Tribal Science, Kalinga Institute of Social Sciences (KISS), Deemed to be University, India
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[4]Department of Botany, Kalinga Institute of Social Sciences (KISS), Deemed to be University, Bhubaneswar, India
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[6]Department of Biotechnology, School of Bioengineering, SRM Institute of Science and Technology, India

Plant-microbe interactions play a pivotal role in shaping plant health, productivity, and ecosystem sustainability. These interactions span mutualistic, commensal, and pathogenic relationships involving diverse microorganisms such as bacteria, fungi, and viruses. Symbiotic associations—like those between rhizobia and legumes or mycorrhizal fungi and plant roots—are instrumental in enhancing nutrient uptake, promoting plant growth, and strengthening resistance to both biotic and abiotic stresses. Beneficial endophytic microbes contribute further by synthesizing growth-promoting substances and offering protection against pathogens. Conversely, pathogenic microbes challenge plant health, necessitating a comprehensive understanding of host immune responses and microbial virulence mechanisms. This review delves into the molecular signaling networks and regulatory pathways that govern these complex interactions. It also examines real-world applications, including microbial inoculants and integrated biological management strategies that have successfully improved crop performance. While promising, the practical use of plant-microbe systems in agriculture faces hurdles such as environmental variability, host specificity, and ecological risks. Overcoming these barriers requires a multidisciplinary approach combining genomics, microbial ecology, and sustainable agronomic practices. Advancing research in this field will be crucial for reducing chemical inputs, improving soil health, and fostering a resilient and sustainable agricultural future.

Table 1. Types of plant-microbe interactions

Interaction Type	Key Examples	Key Mechanisms	Benefits to Plants	Challenges/Considerations
Symbiotic	Rhizobia and legumes, Mycorrhizal fungi	**Rhizobia:** Nitrogen fixation in root nodules **Mycorrhizae:** Nutrient uptake via hyphal network	**Rhizobia:** Enhanced nitrogen availability **Mycorrhizae:** Improved phosphorus and water uptake	Specificity to host plants Soil nutrient variability
Commensal	Endophytic bacteria and fungi	**Endophytes:** Producing growth-promoting substances, enhancing stress tolerance	Enhanced growth, stress tolerance, and disease resistance	Limited to specific plant tissues or types
Pathogenic	Bacterial pathogens, Fungal pathogens, Viruses	**Pathogens:** Direct infection, toxin production, hijacking plant processes	Resistance to diseases, activation of plant immune responses	Disease management and

Presenter:
Beema Jainab S.I
Justice Basheer Ahmed Sayeed College for Women (Autonomous), India

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SPEAKER TALKS

RUNX1: A Novel Therapeutic Target for Myocardial Infarction and Cerebral Infarction

Weihong He[1], Si Wang[2], Hengshu Chen[3] and **Simiao Wu[3]**

[1]Department of Physiology, Sichuan University, China
[2]Department of Cardiology, West China Hospital, Sichuan University, China
[3]Department of Neurology, West China Hospital, Sichuan University, China

Ischemia of organs can have severe consequences such as myocardial infarction (MI) and cerebral infarction. In the clinical setting, ischemic stroke and MI are both life-threatening conditions with narrow therapeutic time-window that leads to poor patient prognosis. Pharmacological approaches against these diseases remain limited and thus new therapeutic targets are urgently needed. RUNX1, the Runt-related transcription factor-1, is an emerging target for cardiovascular diseases. RUNX1 is a member of the core-binding factor family of transcription factors. It is a master regulator transcription factor which works at top levels of signaling cascades and dictates cell fate during development. RUNX1 was classically characterized for its involvement in hematopoietic system and blood cancer genesis. Recently, a role that RUNX1 plays in the heart has come prominence and it represents a promising therapeutic target for MI, adverse cardiac remodeling, and heart failure. Here, we present our recent progress in the study of RUNX1 using animal disease models of MI and ischemic stroke. Our data show that targeting RUNX1 reduces infarct size and improves cardiac function following MI. The protective effect is associated with the repression of a key type of lysosomal proteases, cathepsins. Inhibition of RUNX1 reduces the expression of cathepsins and prevents the activation of cathepsin-mediated cell death signaling following ischemic injury. Based on our data and recent findings from other groups, we envisage that the usage of RUNX1 as a therapeutic target for tissue protection has the potential to be translated into clinical application for the treatment of MI and ischemic stroke.

Presenter:
Weihong He
Sichuan University, China

Re-orientating Research to Deliver Innovation

David Dent
Dent Associates Ltd, UK

Innovation can deliver impact for any scientific discipline as well as economic, social and environmental benefits for a nation. Innovation should then, be a primary driver of scientific endeavor. Innovation as a process has however, become a vague concept that means different things to different people, not least researchers. In addition, different categories of research and their relationship to innovation is likewise vague and lacks relevance. A different set of terms to describe types of research relating to outputs pertinent to innovation are described - namely: scholarly, practitioner, trade and custom research. The relationships between discovery, invention and innovation are then defined and the reasons for differentiation explained. A new systematic typology for innovation that encompasses earlier definitions (including those of the OECD) emphasising the embodiments of products, processes and services, is also presented. A case for adopting this new typology is made.

The origins of innovation achieved through institutional search, emergence of problems, market opportunities and emerging technologies is made. Three of these four categories of origin of innovation are well represented by our research capacities but one of these is generally under supported - knowledge of market gaps and opportunities. A different problem exists for technological opportunities, in particular those much sought-after general-purpose technologies. These GPTs, the scale and scope of their multiple applications in different sectors, can transform markets and significantly impact on an economy. However, predicting their emergence is key to capturing economic value and currently this is not possible. Comparative scales like the one presented and use of AI may provide the means to map and predict emergence of GPTs to enable their protection and better exploitation.

Change is essential to re-orientate our thinking and scientific research towards more productive innovative outputs - that is - if we really want to generate economic, social and environmental impact.

Presenter:
David Dent
Dent Associates Ltd, UK

CFD Simulation of the Claus Reaction Furnace with Operating Conditions: Temperature and Excess Air for Sulfur Recovery

Pablo Vizguerra Morales[1], Miguel Ángel Morales Cabrera[2] and **Fabian S. Mederos Nieto[1]**

[1]Instituto Politécnico Nacional, Centro Mexicano para la producción más limpia, México
[2]Facultad de Ciencias Químicas Región Xalapa Universidad Veracruzana, México

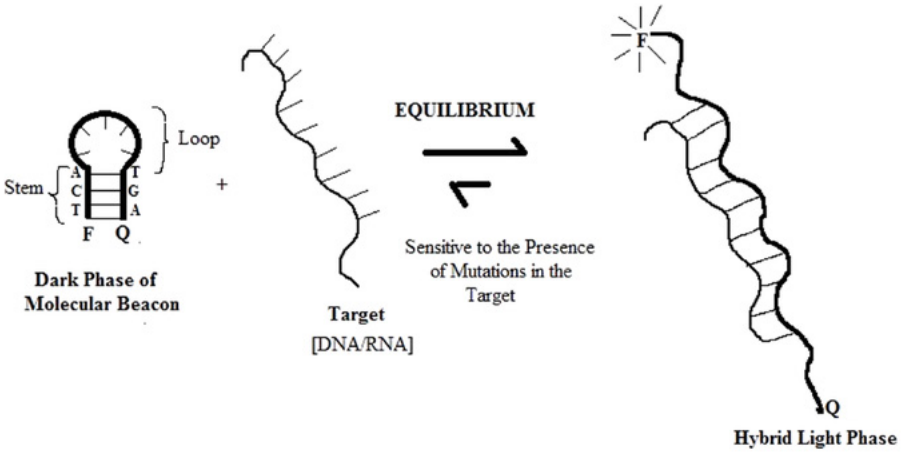
In this work, a Claus reaction furnace was analyzed in a sulfur recovery unit (SRU) of the Abadan Oil Refinery where the combustion operating temperature is important since it ensures optimal performance in the reactor, the novelty of the research focused on temperature control of 1400, 1500 and 1600 K and excess air of 10, 20 and 30% to improve the reaction yield and H_2S conversion and the CFD simulation was carried out in Ansys Fluent in transitory state and in 3 dimensions, considering the turbulence model *k*- ϵ estándar, energy model with transport by convection and mass transport with chemical reaction using the Arrhenius Finite-rate/Eddy - Dissipation model for a kinetic model of destruction of acid gases H_2S and CO_2, obtaining a good approximation with the experimental results of the industrial process of the Abadan Oil refinery, Iran. The percentage between experimental and simulated results varies between 0.5 at 6% depending on the species. The temperature of 1600 K and with excess air of 30% was the best, with one a mol fraction of 0.055 of S_2 at the outlet and with a conversion of the acid gas (H_2S) of 96.64%, which is quite good compared to the experimental one.

Presenter:
Pablo Vizguerra Morales
Centro Mexicano para la Producción más Limpia, México

Reflections on the Role of Procedural Knowledge in the Teaching of Science

Elizabeth Vergis
University of Alberta, Canada

Adapted primary literature (APL) is a genre that retains the canonical form and authentic results of primary literature but is made readable and understandable for a target population, which in this study consists of first-year university undergraduate students. My objective was to use APL in order to probe the understanding of Concepts of Evidence held by first-year undergraduate students and investigate whether and how a pedagogic intervention could develop this understanding further. Concepts of Evidence are ideas that dictate how evidence can be collected, verified, analyzed, and interpreted. To achieve my goal I had to: (a) identify one piece of primary literature (b) compose an APL based on this primary literature; (c) devise a measure of Concepts of Evidence called the "Evidence Survey," comprised of a pre-test questionnaire and a post-test questionnaire; (d) identify college/university classes where the instructors teaching first-year chemistry courses read the APL and agreed to be interviewed; (e) enlist students from these classes who were willing to participate in this study; (f) distribute the APL to these students followed by the administration of the pre-test questionnaire; (g) render a pedagogic intervention to the participating students on the Concepts of Evidence followed by the post-test questionnaire; (h) analyze the data from the two questionnaires to make the desired comparisons; after transcribing interviews and coding the transcripts. Thematic content analysis was carried out on the coded transcripts and the main emerging themes were identified. Four themes emerged from the student interviews and five from interviewing the instructors. My findings from the Evidence Survey showed that the majority (86%) of the student participants performed better on the post-test, suggesting that the teaching intervention was effective in furthering the understanding of both the content knowledge of the APL and the Concepts of Evidence embedded in it.



Presenter:
Elizabeth Vergis
University of Alberta, Canada

The Designing of Coordination Polymers Consisting of Late-Transition Metals and Lanthanide Ions for Luminescence Enhancement

Zerihun Assefa[1] and **Richard Sykora**[2]

[1]Department of Chemistry, North Carolina Agricultural and Technical State University, USA
[2]Department of Chemistry, University of South Alabama, USA

Lanthanide ions have sharp characteristic emission in the visible and near-infrared (NIR) ranges, long luminescence lifetimes, and large Stokes shifts, which makes them very attractive candidates for the development of optical devices, including as light conversion materials. The potential for these and other applications requires a new approach in the choice of chromophores suitable for lanthanide sensitizations. In this study we have followed a cooperative energy transfer methodology where the donor light harvesting range has been broadened highly efficient lanthanide luminescence systems have been established. A class of chromophores involving transition metal complexes is emerging as a suitable choice as sensitizer for lanthanide ion acceptors. A major advantage afforded by these chromophores is their ability to sustain a better energy match-up with most Ln3+acceptor states. Unique advantages of metal complexes over organic chromophores are that they provide a relatively high triplet quantum yield due to the rapid intersystem crossing inherent within the system (due to the heavy-atom effect), and the possibility of a facile detection of both quenching of the d-block chromophores and the sensitized emission from the lanthanide centers. Two classes of donor groups that can cooperatively enhance the lanthanide emission are discussed in this talk. One class involves N-containing multidentate donor ligands and the second class of donors involves selected group 10 and 11 transition metal complexes. The choice of donor groups is established based on the presence of strongly overlapping absorption regions that will provide the added advantage of broadening the usable excitation range and promote tunability to the emission. The structural and photophysical details as well as the energy transfer mechanisms and the sensitization efficiency are studied through temperature dependent, life-time, time-resolved, quantum yield and luminescence experiments.

Presenter:
Zerihun Assefa
North Carolina Agricultural and Technical State University, USA

Interaction of "Tryptophans" with Excited State Proton Transfer Probes – An Insight through Experiments and Theory

Rina Ghosh[1], Priyanka Mukherjee[2] and **Titas Kumar Mukhopadhyay[3]**

[1]Department of Chemistry, St. Xavier's College, India
[2]Department of Biochemistry, Asutosh College, India
[3]Department of Chemistry, National Institute of Technology Jamshedpur, India

In this study, tryptophan, the intrinsic fluorophore present in proteins, is our target molecule, primarily because the difference in ground and excited state dipoles make it an extremely environment sensitive probe. However, what would be the situation in a molecule constituted entirely of Tryptophans? Therefore, questions pertaining to structure becomes very important. We have chosen the homopolymer, poly-L-Tryptophan and to add to experimental insight, we have carried out both steady-state (fig 1) and time-resolved fluorescence studies along with low-temperature phosphorescence (LTP) of poly-L-tryptophan and the globular proteins BSA and HSA. The nature of the emitting Tryptophan (Trp) residue in the former has been characterized based on a comparison with the emission features of the parent monomer. The emitting moieties are the core Trps which are present within the highly hydrophobic environment of the polymeric molecule where solvent molecules are unable to penetrate. The very large red-shift of the (0–0) band of phosphorescence in poly-L-Tryptophan has been explained through triplet-triplet energy transfer along with the structure of the latter. This data substantiates surface-core Trp interactions. Hence this necessitated some molecular dynamic simulation studies (fig 2).

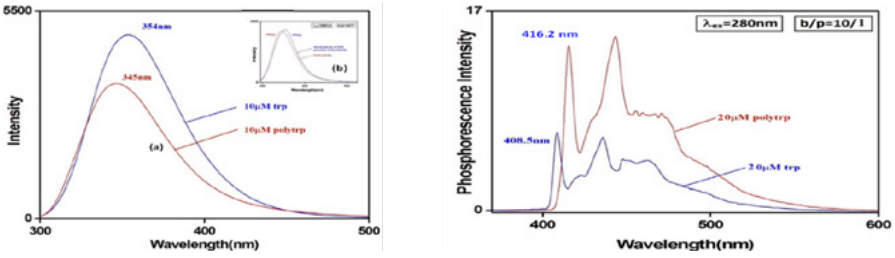


Fig 1: Fluorescence and Phosphorescence spectra of Trp and poly-L-Trp.

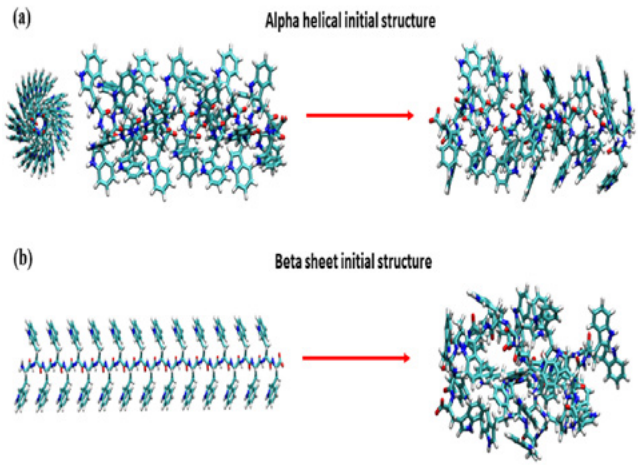


Fig 2: Initial and final structures of the 25-mer of the poly-L-Trp peptide having (a) alpha-helical (front and side views) and (b) beta-sheet structures before and after 600 ns of production simulations, respectively.

The interactions with ESIPT probe 3-hydroxynaphthoic acid (*via* triplet-triplet energy transfer) has also been investigated (fig 3). The results have been compared with the interaction of the former with different globular proteins like BSA and HSA (Table 1).

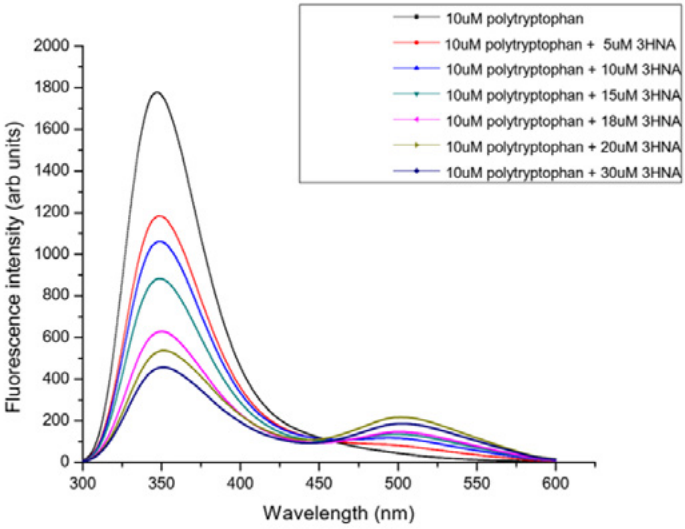


Fig 3: Plot of F0/F against [3-HNA] in aqueous buffer at λex = 280nm

Table 1: Binding constants of Serum Albumins and 3-HNA complexes and poly-L-trp and 3-HNA complexes at 300K

System	Quenching Studies (monitoring the protein emission) k_q ($M^{-1}sec^{-1}$)	Modified Benessi-Hildebrand Equation (monitoring ESIPT emission of 3HNA) K (M^{-1})	ΔG(kJ/mole)
BSA-3HNA	7.2×10^{12}	5.3×10^{5}	-14.3
HSA-3HNA	1.5×10^{13}	2.2×10^{5}	-13.3
Poly-L-Trp-3HNA	7.39×10^{12}	6.53×10^{4}	-27.2

Molecular dynamics studies show π-π stacking interaction between the aromatic Trp residue of the polymer and the naphthalene ring of 3-HNA. These interactions are further stabilized by intramolecular hydrogen bonds. This study highlights two significant aspects: (i) structural details of the homopolymer as indicated by simulation and (ii) binding interactions between polymeric Trps and aromatic ligands and their comparison with globular proteins.

Presenter:
Rina Ghosh
St. Xavier's College, India

Diagnostic and Therapeutic Outcomes in Spinal Tuberculosis: A Retrospective Study Integrating GeneXpert MTB/RIF, Histopathology, and Clinical Management Strategies

Eldin Karaikovic[10], Prashant Adhikari[1], Isha Amatya[2], Pradeep Regmi[3], Jeevan Kumar Sharma[4], Raju Pangeni[5], Nishma Pokharel6, Smriti Bhatta[7], Deepak Shrestha[8], Bhaskar Raj Pant[5], Sandeep Bhandari[5], Arun Dhakal[9] and Emre Acaroğlu[11]

[1]Hospital for Advanced Medicine and Surgery (HAMS), Nepal
[2]Patan Academy of Health Sciences, Nepal
[3]Department of Radiodiagnosis, Tribhuvan University Teaching Hospital, Nepal
[4]Spine Services, Indian Spinal Injuries Center, India
[5]Hospital for Advanced Medicine and Surgery (HAMS), Nepal
[6]MercyOne Medical Center, USA
[7]Aarus Lifestyle Hospital, Nepal
[8]Sushma Koirala Memorial Hospital, Nepal
[9]University of Medicine and Health Sciences, Saint Kitts and Nevis
[10]Ascension St Joseph Hospital, Chicago, USA
[11]Ankara Spine Center, Turkey

Purpose: Spinal tuberculosis (STB) remains prevalent in developing nations and significantly contributes to morbidity, often resulting in kyphotic deformity and neurological deficits. In this study, we correlate the diagnostic, therapeutic and prognostic factors according to the current standard of management of STB.

Methods: This retrospective study evaluated diagnostic and prognostic factors in 77 patients with STB treated surgically (37.7%) or non-surgically (62.3%) between 2018 and 2023. Diagnostic tools included GeneXpert MTB/RIF(GX-MTB/RIF)- a rapid molecular test for detecting Mycobacterium tuberculosis and rifampicin resistance- and histopathological confirmation via biopsy. Clinical outcomes were assessed using Visual Analogue Scale, Oswestry Disability Index, inflammatory markers (ESR, CRP), kyphotic deformity correction, and neurological improvement.

Results: GeneXpert MTB/RIF detected Mycobacterium tuberculosis in 94.8% of cases, with 5.2% showing rifampicin resistance. Histopathology revealed granulomatous infiltration in 96.1% of biopsies, underscoring the impor-

tance of combining diagnostic methods. Both groups showed significant improvement over 12 months, with surgical patients exhibiting higher baseline kyphosis angles (47.41° vs. 19.27°, $p < 0.001$) and greater post-treatment correction (14.14° vs. 2.71°, $p = 0.04$). Neurological status, evaluated via ASIA Impairment Scale improved post-treatment, with 93.5% achieving normal neurology. Deformity presence strongly correlated with surgical intervention (51.9% vs. 8%, $p < 0.001$).

Conclusion: The study highlights the efficacy of anti-tubercular therapy (ATT) and the role of surgery in severe deformity or neurological compromise. Notably, rare discrepancies between GXMTB/RIF and histopathology (5.2% GXMTB/RIF - negative but histopathology- positive) emphasize the need for clinical judgment alongside laboratory findings. Surgical intervention is pivotal for deformity correction and neurological recovery, while ATT remains the cornerstone.

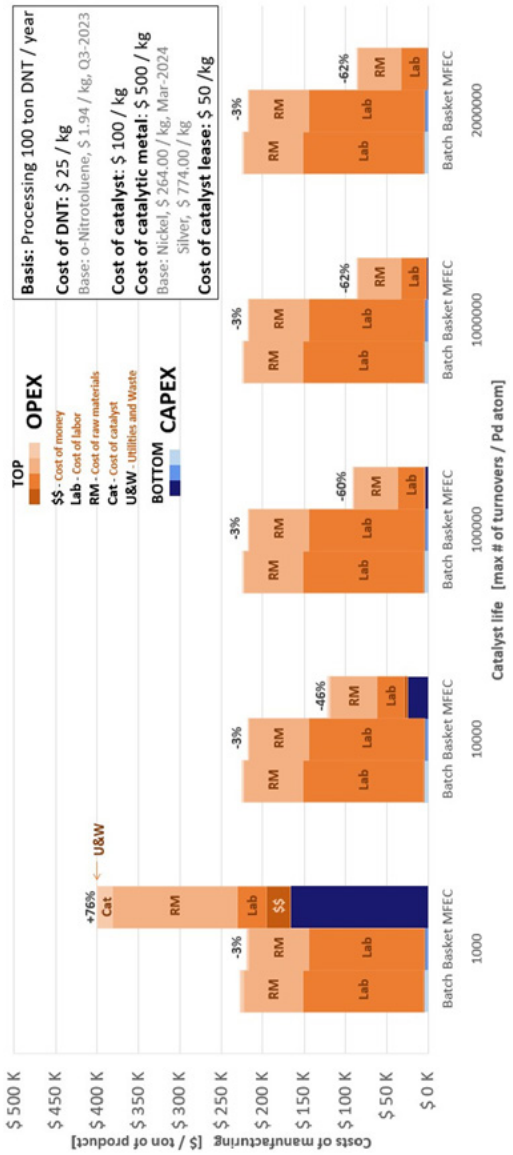
Presenter:
Eldin Karaikovic
Ascension St Joseph Hospital, Chicago, USA

Comparative Economic Analysis of Batch vs. Continuous Manufacturing in Catalytic Heterogeneous Processes: Impact of Catalyst Activity Maintenance and Materials Costs on Total Costs of Manufacturing in the Production of Fine Chemicals and Pharmaceuticals

Felix Mendoza Suarez and **Bruce Tatarchuk**

Center for Microfibrous Materials Manufacturing (CM3), Auburn University, USA

To evaluate the feasibility of transforming batch manufacturing processes in the fine chemicals and pharmaceutical industries to continuous synthesis, Capex, Opex and the total cost of manufacturing are estimated for production facilities for the hydrogenation of a nitro compound to its final amino counterpart. Two cases are evaluated: First, a high annual production dedicated plant, designed on the basis of processing 100,000 kg of the principal raw material per year, where raw materials cost, catalyst cost, and catalyst activity maintenance are varied over a broad range for typical industrial cases. Second, a “short campaign” model for a small volume production trial setup designed for the manufacture of only 100 kg of the final product, as a way to evaluate relevant industrial scenarios of scale-up and process development. A comparison is made between slurry batch, catalyst basket batch reactor and fixed bed continuous reactor manufacturing facilities. The hydrogenation of 2,4-dinitrotoluene was chosen as a probe reaction for the development of the manufacturing processes, with costs of the key raw material varying between $5 and $100 per kilogram, costs of catalyst varying between $100 and $1,500 per kilogram, and catalyst activity maintenances varying between 1,000 and 2,000,000 total turnovers before a change in catalyst load is necessary. For low catalyst activity maintenance, the total manufacturing costs for the fixed bed reactor process were always found to be higher than those of the two other alternatives. As catalyst activity maintenance increases, the manufacturing costs for the continuous alternative rapidly fall, reaching savings between 37 and 75% compared to the base batch reactor case, depending on the combination of costs of the key raw material and catalyst used.



Presenter:
Felix Mendoza Suarez
Auburn University, USA

Influence of Peripheral Carboxy Group Number on Zinc Phthalocyanine Photophysics

Tamara Potlog[1], Ion Lungu[1], Radu Tigoianu[2], and **Anton Airinei[2]**

[1]Moldova State University, Republic of Moldova
[2]Petru Poni Institute of Macromolecular Chemistry, Romania

Metallophthalocyanines, particularly zinc phthalocyanine (ZnPc), are among the most promising photosensitizers for photodynamic therapy (PDT) due to their intense absorption in the red to near-infrared region, high photostability, and efficient triplet-state formation that enables effective singlet oxygen generation. Despite these favorable photophysical properties, the direct biomedical application of ZnPcs remains challenging because of their poor solubility in aqueous media, strong tendency toward aggregation driven by π–π stacking interactions, and limited biocompatibility, all of which significantly compromise photodynamic efficiency through aggregation-induced quenching. To address these limitations, peripheral functionalization with hydrophilic groups and incorporation into nanostructured carriers have been widely explored. In this paper, we present a comparative photophysical investigation of tetra- and octa-carboxy zinc phthalocyanines, $ZnPc(COOH)_4$ and $ZnPc(COOH)_8$, together with their dextran-coated Fe_3O_4 hybrid nanocomposites ($ZnPc–Dx–Fe_3O_4$). The effects of peripheral carboxyl group density and hybridization on aggregation behavior and excited-state dynamics were systematically examined using steady-state and time-resolved spectroscopic techniques. Both molecular ZnPc derivatives exhibited mixed H- and J-type aggregation in solution, whereas immobilization within the magnetic polymeric matrix promoted dominant H-type aggregation accompanied by pronounced fluorescence quenching, attributed to interfacial energy and charge transfer processes. Time-resolved fluorescence studies revealed lifetimes in the nanosecond range (τ = 4–10 ns), while phosphorescence decay and transient absorption measurements demonstrated long-lived triplet states with microsecond average lifetimes (τ ≈ 9 μs). Enhanced intersystem crossing and accelerated excited-state deactivation were observed in the hybrid systems, highlighting their potential for improved PDT performance through controlled photophysical modulation. MTT assay used to determine the vitality of the cells show that cell reduction was not significantly evident in all $ZnPc(COOH)_4$, $ZnPc(COOH)_8$ and $ZnPc–Dx–Fe_3O_4$ hybrid nanocomposites.

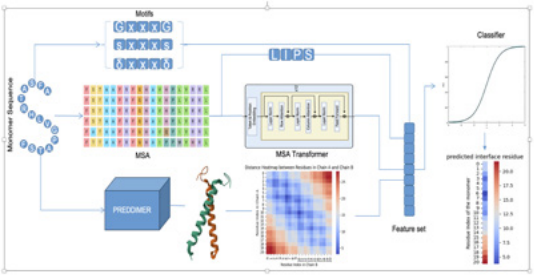
Presenter:
Tamara POTLOG
Moldova State University, Republic of Moldova

Transmembrane Homodimers Interface Identification: Predicting Interface Residues in Alpha-Helical Transmembrane Protein Homodimers using Sequential and Structural Features

Bander Almalki[1,2] and **Li Liao**[2]

[1]University of Bisha, Saudi Arabia
[2]University of Delaware, USA

Most bitopic transmembrane proteins associate with one another through interface residues to form dimers, which facilitate or activate specific cellular functions. Therefore, accurately identifying interface residues, in a given dimer, is crucial for understanding its function and has been a challenging pursuit for many computational methods. These methods can be broadly categorized into two approaches: general-purpose ones for dimerization and specialized ones for interface residues. In this study, we develop a machine learning method that integrates both approaches by integrating sequential and structural features extracted from predicted structures and various domains. The results from cross-validation on a benchmark dataset show that our method, despite utilizing significantly fewer features, outperforms the state-of-the-art methods by more than three percentage points in performance, as measured by the F1 score. Furthermore, we evaluated the performance of the proposed model on a benchmark dataset as compared to the state-of-the-art multimeric structure predictors, including RoseTTAFold2, AlphaFold2Multimer, and PREDDIMER. The results show the superiority of the proposed model by outperforming all the other models, highlighting the effectiveness of integrating both structural and sequential features within the proposed framework.



Presenter:
Bander Almalki
University of Bisha, Saudi Arabia

Unravelling the Specific Interactions of Drugs with the Intrinsic Tryptophan Residues in Multi-Tryptophan Proteins: Spectrofluorimetric andTheoretical Approaches

Priyanka Mukherjee[1], Sanjukta Chatterjee[2], Archisman Banerjee[2] and **Rina Ghosh[2]**

[1]Department of Biochemistry, Asutosh College, India
[2]Department of Chemistry, St. Xavier's College, India

In this study, we have chosen Bovine serum Albumin (BSA) as our target macromolecule. It is a globular protein with 586 amino acids. It has two Trp residues at positions 134 and 213 with characteristic fluorescence and phosphorescence spectra (Fig 1).

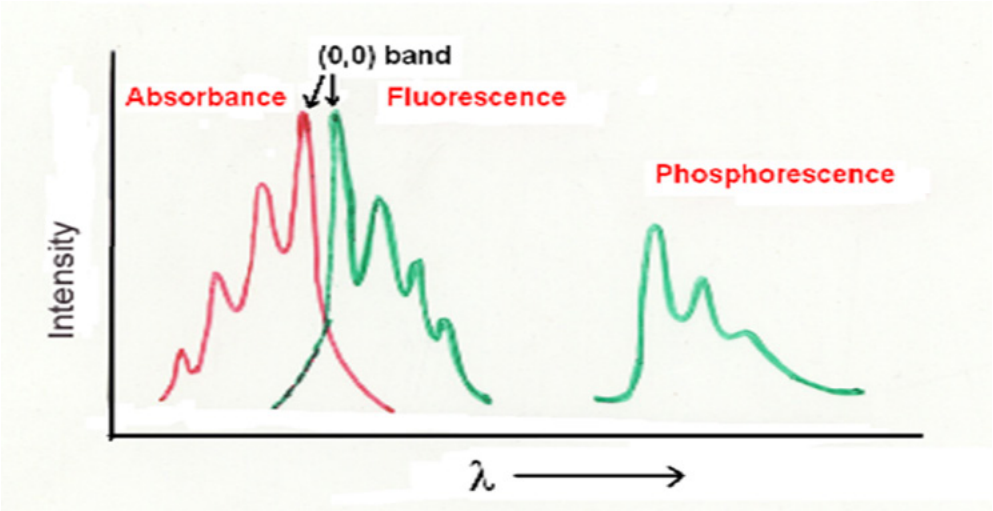


Fig 1: Fluorescence and phosphorescence pectra of BSA

The former Trp is partially solvent exposed while the latter is buried (conclusion drawn from other multi-tryptophan phosphorescence studies).

We have investigated the quenching of the intrinsic fluorescence of Trp residues of BSA by different antibacterial drugs like norfloxacin (Fig 2) doxycycline, cephalexin, moxifloxacin (Fig 3).

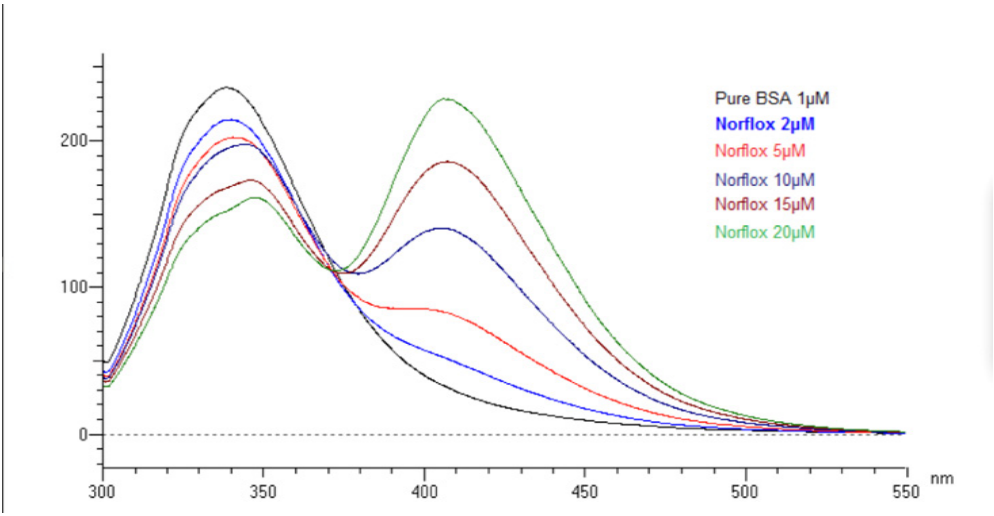


Fig 2: Fluorescence quenching of BSA with Norfloxacin

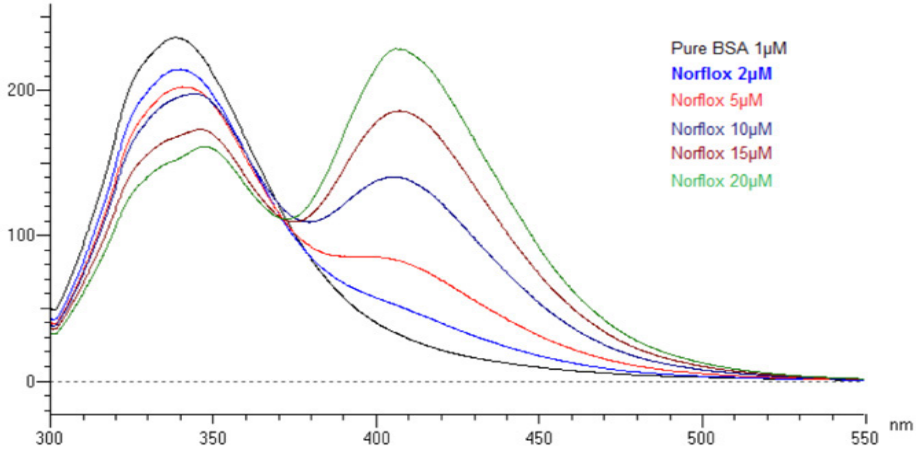


Fig 3: Fluorescence quenching of BSA with Moxifloxacin

The interaction of BSA with a different line of drug like febuxostat which is a xanthine oxidase inhibitor, has also been studied. We tried to compare the binding and energy transfer efficiencies from the respective Stern-Volmer plots (Fig 4). Both steady-state and time-resolved fluorescence studies have been performed to analyze such drug-protein interactions. The quenching studies provide information

about the emitting Trp residues in the protein. Stern-Volmer plots for norfloxacin, cephalexin and doxycycline are linear but an upward curvature has been observed in case of Moxifloxacin (Fig 5). This is indicative of both static and dynamic quenching. This has also been established by lifetime measurements. The modified Benessi-Hildebrand equation has been employed to extract the binding constant for our ligands.

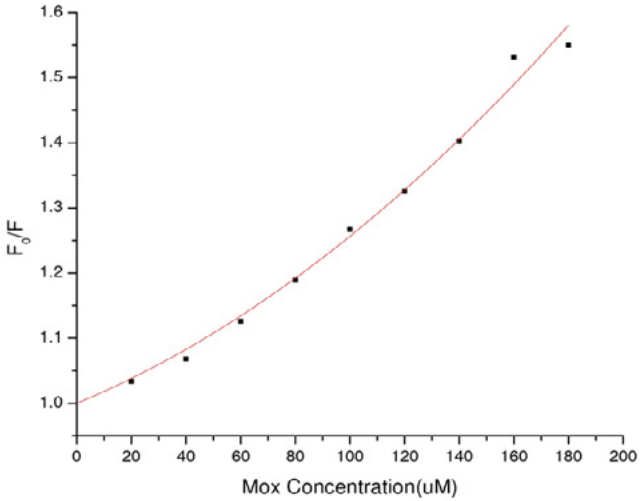


Fig 4: Stern Volmer plot (BSA and Norfloxacin)

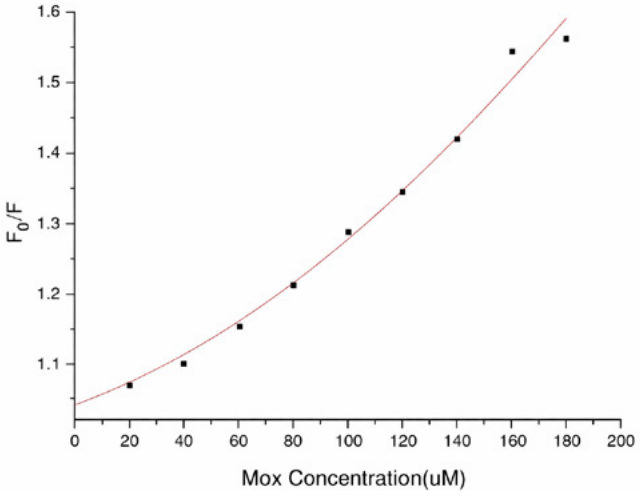


Fig 5: Stern Volmer plot (BSA and Moxifloxacin

From the theoretical point of view, molecular docking studies yielded results that corroborate well with the experimental investigations suggesting a significant role of Trp 213 in binding to these drugs (Fig 6).

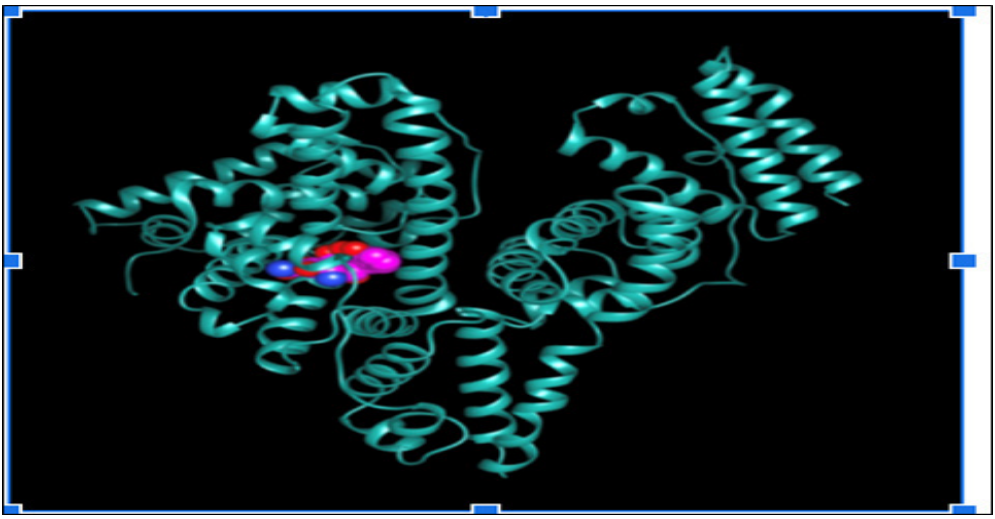


Fig 6: Docking studies of BSA with Doxycycline

In this figure, Trp 213 is located at a very efficient energy transfer distance and Trp 134 is not visible in this regard. Since the interaction of the protein with different drugs elucidate different binding patterns, the results should provide a basis for drug design and molecular dynamics simulation studies, which are atpresent being processed.

Presenter:
Priyanka Mukherjee
Asutosh College, India

Sustainable Rubber Compounds with Incorporated Biopolymer Filler

Ján Kruželák, Lucia Balcerčíková, Michaela Džuganová and **Ivan Hudec**

Department of Plastics, Rubber and Fibres, Faculty of Chemical and Food Technology, Slovak University of Technology in Bratislava, Slovakia

Lignin is the second most abundant renewable natural polymer globally, following cellulose, and possesses immense industrial potential. Despite its unique attributes, such as biodegradability, antioxidant properties, and low cost, only a fraction of worldwide production is currently utilized commercially, while the remainder is largely discarded as waste fuel. A significant barrier to the broader application of lignin as a filler in the rubber industry is its strong tendency toward intramolecular interaction, which leads to poor dispersion and the subsequent degradation of the physico-mechanical properties of non-polar composites.

The present study focuses on an effective and cost-efficient solution to this challenge through the incorporation of low-molecular-weight polar plasticizers. The primary objective was to improve the homogeneity and interfacial adhesion between the elastomer phase and the biopolymer. Acrylonitrile-butadiene rubber (NBR) filled with 50 phr of calcium lignosulfonate served as the model system. Four types of hydrophilic plasticizers, namely 1,4-butanediol, ethylene glycol, and two types of glycerol (99% purity and an 86% aqueous solution), were incorporated into the compounds in concentrations ranging from 5 to 30 phr.

The results demonstrated that these additives effectively plasticize both the rubber matrix and the biopolymer filler, with the intensity of the plasticizing effect correlating directly with the plasticizer's polarity (increasing in the order: 1,4-butanediol < ethylene glycol < glycerols). Structural analysis confirmed that the softened lignosulfonate forms finely dispersed domains within the matrix, exhibiting significantly improved interfacial adhesion. This synergistic effect resulted in a marked increase in the tensile characteristics of the vulcanizates, particularly when using ethylene glycol and glycerol. This work demonstrates a viable pathway for developing high-performance "green" composites while maintaining industrial feasibility.

Acknowledgement: This work was supported by the Slovak Research and Development Agency under the contract No. APVV-19-0091 and APVV-22-0011

Presenter:

Ján Kruželák
Slovak University of Technology in Bratislava, Slovakia

Preclinical Evaluation of Sodium Copper Chlorophyllin: Chemical Basis, Pharmacokinetics, and Therapeutic Potential in Chemotherapy-Associated Toxicities

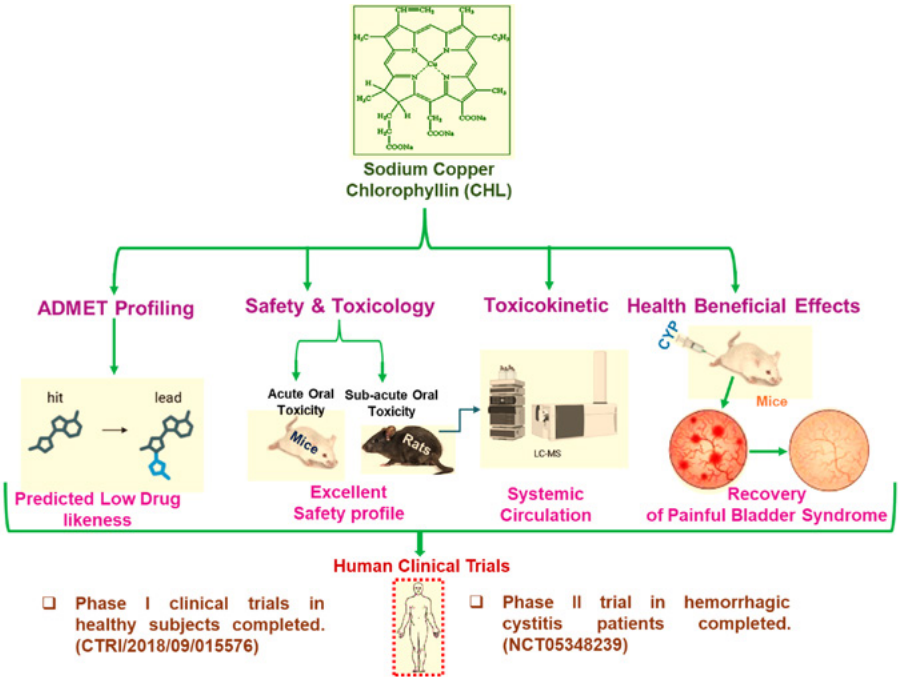
Neha Ramani[1,2,3,4], Raghavendra S. Patwardhan[1,2] and **Deepak Sharma[1,2]**

[1]Radiation Biology & Health Sciences Division, Bhabha Atomic Research Centre, India
[2]Homi Bhabha National Institute, India
[3]ACTREC–Tata Memorial Centre, India
[4]East Ocyon Bio Pvt. Ltd., India

Sodium copper chlorophyllin, generally known as Chlorophyllin (CHL), is a semi-synthetic, water-soluble copper porphyrin complex derived from a green plant pigment chlorophyll, characterized by a redox-active metalloporphyrin core and high chemical stability. Owing to its widespread nutraceutical use, understanding its chemical pharmacokinetic behavior and translational safety is critical for broader therapeutic applications. This study aims to present a chemistry-driven preclinical evaluation of CHL, integrating in silico ADMET prediction, physicochemical profiling, toxicokinetic, and health beneficial effects in chemotherapy-associated models.

Computational ADMET analysis revealed that CHL possesses high molecular weight and polarity, resulting in low predicted oral drug-likeness, yet exhibits a favorable medicinal chemistry profile with no PAINS or CYP inhibition alerts. Experimental toxicology studies conducted under OECD-GLP guidelines demonstrated exceptional chemical safety, with CHL being well tolerated at acute doses up to 5000 mg/kg body weight and a NOAEL exceeding 1000 mg/kg body weight upon repeated oral exposure. LC-MS/MS-based toxicokinetic studies confirmed systemic exposure and sustained tissue distribution, consistent with its hydrophilic metalloporphyrin chemistry. Functionally, CHL acted as a chemotherapy response modulator, enhancing cyclophosphamide-induced cytotoxicity in triple-negative breast cancer cells while simultaneously mitigating cyclophosphamide-induced bladder toxicity *in vivo*. Proteomic analyses linked these effects to redox modulation, disruption of DNA damage repair pathways, mitochondrial stress induction, and activation of antioxidant signaling. Importantly, CHL demonstrated selective protection of normal tissues without compromising anticancer efficacy.

Collectively, this work highlights how metalloporphyrin chemistry, redox behavior, and pharmacokinetic characteristics converge to define the therapeutic utility of CHL. The findings position Sodium Copper Chlorophyllin as a chemically robust, biologically safe adjunct with potential translational relevance in chemotherapy-associated toxicity management.



Presenter:
Neha Ramani
Bhabha Atomic Research Centre, India

Eltrombopag Olamine Induces Apoptosis in Human Breast and Hepatocellular Carcinoma Cells by the Modulation of MAPK, WNT and Caspase-Dependent Signaling Pathways

Mohammad Taufiq Alam[1,2], Md. Asaduzzaman[2] and **Syed Rashel Kabir[3]**

[1]Vice-Chancellor, University of Barisal, Bangladesh
[2]Department of Applied Chemistry and Chemical Engineering, University of Rajshahi, Bangladesh
[3]Department of Biochemistry and Molecular Biology, Faculty of Science, University of Rajshahi, Bangladesh

In light of the global inadequacies in cancer treatment, there is a pressing need for the development of more efficacious drugs. This study explores the potential of Eltrombopag olamine, a compound recognized for its ability to boost platelet levels, as an anticancer agent against human breast (MCF-7) and hepatocellular (SMMC-7721) carcinoma cell lines. Eltrombopag olamine exhibited significant inhibition of MCF-7 and SMMC-7721 cells with IC_{50} values of 31 and 154 μg/ml, respectively. The antiproliferative activities against both cells were due to the induction of apoptosis that was detected by Hoechst 33342 staining. Early and late apoptosis was detected in both cells by FITC-annexin V/PI staining. Involvement of caspase-3,-8 & -9 in the apoptotic regulatory mechanism was confirmed by caspase-3,-8 & -9 inhibitors. 'S' cell cycle arrest was detected in both cell lines by flow cytometry after treatment with Eltrombopag olamine. Several gene expressions were checked for both types cells using real-time PCR. FAS, p53, Bax, TNFα, and cytochrome-C gene expression was raised with the reduction of ERK gene expression in MCF-7 cells. While TNFα, p53 Bax gene expression was enhanced with the loss of STAT3, MAPK, Notch1, PARP, EGFR, and ERK gene expression in SMMC-7721 cells. The results show the involvement of several signaling pathways, including intrinsic, EGFR-MAPK-ERK, WNT and death receptor signaling pathways in the apoptosis process. Interactions between Eltrombopag olamine and proteins were clarified by the molecular docking simulation. In conclusion Eltrombopag olamine can be attractive to researchers for further studies.

Presenter:
Mohammad Taufiq Alam
University of Barisal, Bangladesh

Assessment of Physicochemical and Antibacterial Properties of Structured Water Samples from Ota, Ogun State, Nigeria

Abiodun H. Adebayo[1], Okukwe C. Obode[2], Bosede T. Adekeye[3] and **Bamidele Durodola[4]**

[1]Department of Biochemistry, College of Science and Technology, Covenant University Ota, Nigeria
[2]Nutrition and Toxicology Division, Food Technology Department, Federal Institute of Industrial Research Oshodi, Nigeria
[3]Microbiology Programme, Department of Biological Sciences, Covenant University Ota, Nigeria
[4]Chemistry Department, Covenant University Ota, Nigeria

We investigated the effect of structuring potable water with QNET Amezcua Bio Disc 3 (BD3). Seven water samples, including public tap, borehole, rain, bottled (2 brands), distilled, and sachet water, obtained from Ota, Nigeria, were analyzed for their physicochemical and antibacterial properties. The water samples were placed on the BD3 for 15 and 30 minutes, 1, 6, 12, 24, and 48 hours respectively, with the unstructured water serving as the control. Physicochemical properties were evaluated using standard methods described by the Association of Official Analytical Chemists (AOAC), elemental analysis was executed using the inductively coupled plasma atomic emission spectroscopy (ICP-OES), while microbial analysis was done using the most probable number method. Results showed that the samples' appearance, color, taste, and odor were clear, colorless, and unobjectionable. The alkalinity of the sachet (160 ± 2.01mg/l) and bottled (240 ± 1.12mg/l) water samples after treatment with BD3 was enhanced compared to the control sample (124 ±1.00mg/l). Furthermore, supercharging with BD3 significantly (p<0.05) increased the pH and alkalinity of the water. There was a significant (p<0.05) increase in electrical conductance of all structured water samples when compared with the control groups except in sachet and borehole water samples. No significant (p>0.05) effect was observed for total dissolved solids when comparing the structured samples with the control. Most parameters assayed for were within the allowable limits. No heavy metals were detected. Supercharging up to 5 times enhanced the concentrations of calcium, potassium, iron, and magnesium ions significantly (p<0.05) across the groups compared to the control samples, while the sodium ion was significantly (p<0.05) reduced as the water samples were serially charged with the BD3. Supercharging of the infected autoclaved distilled water samples

significantly (p<0.05) reduced the total viable count at low concentrations of *E. coli*. In conclusion, BD3 impacts high electrical conductivity on the structured water samples with increased efficacy of solved minerals and a potential antibacterial effect.

Presenter:
Abiodun H. Adebayo
Covenant University Ota, Nigeria

Rapid and Reliable Characterization of Supersaturated Brines and Prediction of their Mining Potential – Cases of Algerian Brines

Merzouk Zatout
Kasdi Merbah University, Algeria

In addition to NaCl salt, natural inland supersaturated brines of Algerian saline lakes contain huge quantities of oceanic salts such as Na_2SO_4, K_2SO_4, and $MgSO_4$. To attract investment in natural resource development, it is necessary to characterise and evaluate their mining potential. For this aim, the isothermal evaporation experiment is a powerful tool currently used worldwide, enabling the determination of precipitation sequences for different salts as a function of the brine's density and ionic composition. However, it is challenging to implement due to the presence of metastable solutions, and it requires numerous facilities, including specialized devices and analytical equipment, as well as expensive reagents and a relatively long operational time. In this study, the alternative proposed tools are the Mg-corner diagram of the five-fold diagram Na^+, K^+, Mg^{2+}, Cl^-, $SO_4^{2-}//H_2O$, at fixed temperature, the solubility diagrams of salts evolving the supersaturated brine, and the Phreeqc modeling with the Pitzer thermodynamic database. Indeed, during evaporation, the evaporation rate, the density, the pH, and major ion content of the brine obtained by Phreeqc and by experimental work yielded similar results. Furthermore, similar crystallization salts sequences are obtained by Phreeqc, Mg-corner diagram, and experimental results. The succession salts sequences are halite (NaCl) → halite and leonite ($K_2Mg(SO_4)_2 \cdot 4H_2O$) → halite, leonite, and sylvite (KCl). A negligible deviation was reported regarding the presence of epsomite in the solid assembly recovered in the final stages of experimental evaporation. This is because supersaturated brine tends to capture moisture from the atmosphere rather than lose water to the atmosphere. In conclusion and based on the major ion content of a single brine sample, the supersaturated brine of the Algerian Salt Lake has been reliably characterized and its exploitation potential has been very well determined in qualitative terms.

Presenter:
Merzouk Zatout
Kasdi Merbah University, Algeria

Organic Amendments Influence Soil Properties, Soil Microbial Diversity, and Winter Barley Traits in a Five-Year Field Trial with Contaminated Soils at a Former Wood Preservation Site

C. Chiodi[1], G. Zardinoni[1], P. Stevanato[1], L. Giagnoni[2], P. Carletti[1], N. Oustrière[3], A. Sæbø[4], T. Persson[4], W. Szulc[5], B. Rutkowska[5], M. Mench[3] and **G. Renella[1]**

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[2]Department of Civil, Environmental, Architectural Engineering and Mathematics (DICATAM), University of Brescia, Italy
[3]University of Bordeaux, France
[4]NIBIO-Norwegian Institute of Bioeconomy Research, Norway
[5]Institute of Agriculture, Warsaw University of Life Sciences, Poland

Soil contamination with metal(loid)s and organic pollutants creates environmental and health concerns, driving the need for remediation strategies. Organic amendments can mitigate contamination effects and enhancing soil quality; however, their long-term influence remains an open question. In a five-year field experiment at a former wood-preservation site, this study evaluates the effects of five organic amendments - fresh pig manure (PM), biodigested pig manure (PD), compost (C), compost pellets (Pt), and green waste compost (G) - on Cu-contaminated soils. We evaluated their impacts on soil properties, metal bioavailability, microbial community, plant growth and soil fertility. All amendments led to an overall soil improvement. The amendments promoted the concentration of soil bacterial genes and improved the yield of winter barley cultivated in the plots. The most abundant phyla detected across soil samples were *Actinobacteriota*, with *Bacillus among* the dominant genera. Compost-based amendments at 5% w/w addition rate (C5 and Pt5) showed the most promising results, significantly increasing soil carbon, nitrogen, and phosphorus contents, while reducing bioavailability of Cd, Ni, Pb, and Zn compared with untreated control plots ($p < 0.01$). A decrease in Cu availability was observed but it was not significant. Both compost and compost pellets amendments enriched microbial communities associated with soil quality and plant yield, leading to significant improvements in soil fertility and barley yield (+ 200% on average). This integrative approach identified organic amendments that effectively contribute to soil remediation from multiple perspectives: chemical properties (pH, organic

content, nutrients), reduction of bioavailable soil Cd and Zn, enzyme activities, microbial abundance and diversity, and winter barley yield. The study evidenced signature biomarkers characteristic of healthy soils and polluted soils. Our findings support the use of compost as a balanced approach for phyto-managing metal-contaminated soils, reducing 1 M NH_4NO_3-extractable soil Cd and Zn while enhancing microbial activity and soil fertility.

Presenter:
Claudia Chiodi
University of Padua, Italy

Theoretical Study of the Enhancement of the Photoconversion Efficiency on Zinc Porphyrins Dyes by Combining Electron Donor-Acceptor Theory with the BCL Model

Mauricio Barrera[1] and **Irma Crivelli**[2]

[1]Independent, Chile
[2]Faculty of Sciences, University of Chile, Chile

In order to increase the efficiency of dye sensitized solar cells (DSSC), we propose to study the influence of maximizing the push-pull effect by quantifying the donor force (Ds) and the acceptor capacity (Ap) calculated as functions of the Electrophilicity, Orbital Hardness and Polarizability. The sum of the donor force and the acceptor capacity is the inductive force, which allows the push-pull effect to be maximized.

With this approach, we applied the Barrera-Crivelli-Loeb (BCL) model to a series of eleven Zinc Porphyrins to correlate the Global Efficiency Index (GEI) with the experimental measurement of Photo Conversion Efficiency (PCE) (Fig.1)

The use of this strategy together with the use of siloles and siloxanes allows the design of two new dyes, BCL 516 and BCL 520 (Fig. 2), with theoretically calculated efficiencies of 10.64% and 10.61%.

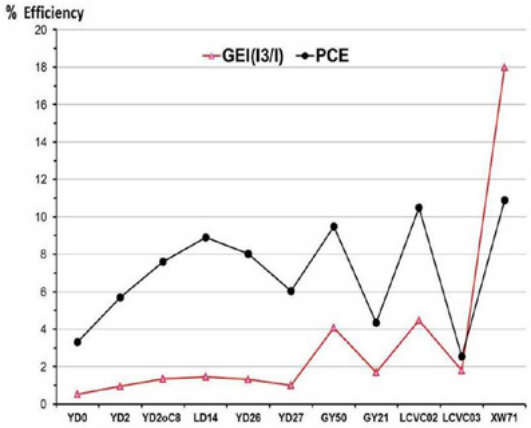

Fig. 1

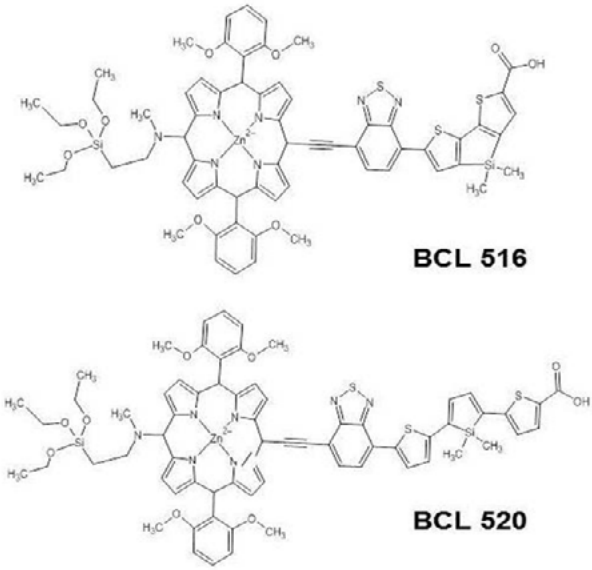

Fig. 2

Presenter:
Mauricio Barrera
Independent, Chile

Translational Quantitative Two-Photon Microscopy of Extracellular Matrix Remodeling Distinguishes Esophageal Squamous Cell Carcinoma from High-Grade Dysplasia

I-Chen Wu[1], Guan-Yu Zhuo[2] and **Wei-Chung Chen[1]**

[1]Department of Internal Medicine, Division of Gastroenterology, Kaohsiung Medical University Hospital, Kaohsiung Medical University, Taiwan
[2]Institute of Biophotonics, National Yang Ming Chiao Tung University, Taiwan

Esophageal squamous cell carcinoma (SCC) and high-grade dysplasia (HGD) are biologically distinct lesions that can exhibit overlapping histologic architecture, particularly in clinically complex settings such as metachronous disease. Because diagnostic uncertainty can directly influence surveillance intensity and treatment selection, there is a need for objective, reproducible approaches that complement conventional pathology by capturing microstructural signatures of malignant transformation. Two-photon microscopy enables label-free interrogation of tissue architecture, yet subtle stromal changes relevant to cancer progression often require quantitative analysis and machine learning (ML) to be detected reliably. We evaluated whether quantitative features derived from two-photon imaging of the extracellular matrix (ECM) can distinguish SCC from HGD with translational potential. Tissue samples were organized into two clinically informative comparisons: Group 1, primary SCC versus metachronous HGD (SCC-HGD), and Group 2, primary HGD versus metachronous HGD (HGD-HGD). Second harmonic generation (SHG) and two-photon fluorescence (TPF) signals were acquired to characterize ECM organization and tissue autofluorescence. Texture features were extracted using gray-level co-occurrence matrix (GLCM) analysis, and support vector machine (SVM) models were trained to classify pathology based on these quantitative descriptors. SHG-based classifiers achieved accuracies of 75% and 84.21% for Group 1 and Group 2, respectively, and improved to 95% for primary SCC versus primary HGD. Notably, metachronous HGD from Group 1 versus Group 2 was classified with 95.65% accuracy, suggesting that ECM remodeling patterns reflect not only histologic grade but also clinical context. This quantitative imaging–ML framework supports translational development of objective ECM biomarkers that may aid risk stratification and diagnostic decision-making, with future adaptability to real-time, endoscopy-adjacent workflows in esophageal oncology.

Presenter:
I-Chen Wu
Kaohsiung Medical University Hospital, Taiwan

Natural Products as Promising Chemotherapeutic Agents: Anti-Proliferative Effects of Coffee Extracts and Chlorogenic Acid in Hepatocellular Carcinoma Independent of Wnt/β-Catenin Modulation

Manuel Moreno-Ceballos[1,2], Fabian M. Cortes-Mancera[2,3], Han Moshage[1,3] and **Johanna C. Arroyave-Ospina[1,3]**

[1]Universidad de Antioquia, Colombia
[2]Instituto Tecnológico Metropolitano, Colombia
[3]University Medical Center of Groningen, The Netherlands

Hepatocellular carcinoma (HCC) remains the most common primary liver malignancy and is associated with poor prognosis and limited therapeutic success, particularly in advanced disease stages. Given the molecular complexity of HCC and the frequent activation of oncogenic pathways such as Wnt/β-catenin, the identification of multi-target compounds is urgently needed. Natural products constitute a rich and unexplored source of bioactive molecules with potential chemotherapeutic value.

Epidemiological studies associate coffee consumption with hepatoprotective effects: however, the molecular mechanisms underlying these benefits remain poorly understood. This study evaluated the *in vitro* effects of green (GC) and roasted coffee (RC) extracts, and chlorogenic acid (CGA), on HepG2 hepatocellular carcinoma cells.

Both coffee extracts and CGAs significantly reduced cell viability and cell proliferation in a dose-dependent manner (Figure 1, D). GC at 500 µg/mL and CGA at 400 and 800 µM markedly increased caspase-3 activity, indicating induction of apoptosis. Additionally, treatment with coffee extracts (500 and 1000 µg/mL) promoted membrane permeabilization (Figure 1, A, B, C), leading to an increased necrotic cells. Despite these anti-proliferative effects, TOP/FOP luciferase assays revealed minimal modulation of Wnt/β-catenin transcriptional activity. Among canonical Wnt target genes, only c-Myc expression was significantly downregulate, while β-catenin protein levels and subcellular localization remained largely unchanged.

Collectively, these findings demonstrated that coffee-derived compounds exert significant anti-cancer effects in HCC cells, even in the context of constitutive Wnt pathway activation. This study underscores the importance of systematically investigating natural products as potential chemotherapeutic agents for complexes malignancies such as HCC, where multi-mechanistic interventions may provide therapeutic advantage.

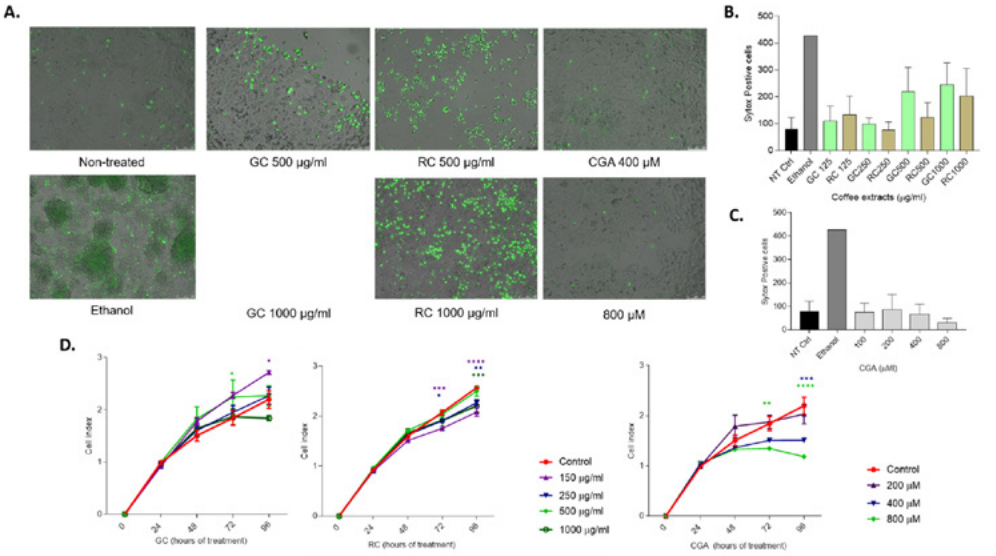

Figure 1. Cell death and proliferation assessment: HepG2 cells treated with Green Coffee (GC) or Roasted Coffee extracts (RC) 125-1000ug/ml, or Chlorogenic Acid (CGA) 100-800uM. **A**. SYTOX Green staining of HepG2 cells treated with GC, RC and CGA during 48h. Green: necrotic cells. **B**. Relative quantification of SYTOX green-positive cells compared to the BSA control of HepG2 cells treated with GC, RC and **C**. CGA (SYTOX green-positive cell counting was also normalized according to the confluence of the cell cultures). **D**. Cell confluence kinetic measured by XCelligence during 96h. Results were obtained from three independent experiments (n = 3, ** $p \leq 0.01$).

Presenter:
Manuel Jaime Moreno Ceballos
Universidad de Antioquia, Colombia

Unusual Nanofluids: Properties and Applications

Valery Ya. Rudyak
Novosibirsk State University of Architecture and Civil Engineering, Russia

Nanofluids are suspensions with a characteristic particle size of 1 to 100 nm or with carbon nanotubes. These are unusual and wonderful fluids. Their properties are not described by the classical theories for coarse-dispersed liquids, at the origins of which stood J. Maxwell and A. Einstein. The purpose of this report is to introduce the colleagues to the properties and applications of nanofluids. The current understanding this subject is presented in my last book (Rudyak, 2025). The viscosity, thermal conductivity and electrical conductivity of nanofluids are considered. The necessary experimental data are presented, and the features of the transport processes are revealed using the molecular dynamics method. It is shown that, unlike coarse-dispersed liquids, the viscosity and thermal conductivity of nanofluids depends not only on the concentration of dispersed particles, but also on their size and material. The reasons for such dependence are explained. In the case of nanofluids with carbon nanotubes, viscosity and thermal conductivity significantly depend on whether they are single-walled or multi-walled. Then the issue of possible change in the rheology of the nanofluid is discussed and the reasons for such change are identified. It is shown that for any liquids and nanofluids, change in rheology is a threshold phenomenon. The dependence of the critical shear rate of rheology changes on the concentration of nanoparticles, their size and material is determined. At sufficiently high shear rates, the viscosity of all nanofluids decreases sharply and their viscosity is practically no different from the viscosity of the base fluid which is also decreases monotonically. Using the molecular dynamics method, an explanation of this effect is given. In conclusion, the existing and potential possibilities for the practical use of nanofluids are discussed.

Presenter:
Valery Ya. Rudyak
Novosibirsk State University of Architecture and Civil Engineering, Russia

Stem Cell Therapy for Hypoplastic Left Heart Syndrome: Safety, Efficacy, and Future Directions

Michael Joy Dara[1], Kavya Thayappa[2], Aman Bazarov[3], Gresa Puwar[4], Sri Divya Vasupalli[5], Jamil Nasrallah[6], Talha Farooq[7] and **Priyansh Patel[8]**

[1]Zaporizhzhia State Medical University, Ukraine
[2]MVJ Medical College and Research Hospital, India
[3]Kyrgyz State Medical Academy, Kyrgyzstan
[4]GMERS Medical College, India
[5]Dr. NTR University of Health Sciences, India
[6]Lebanese University, Lebanon
[7]Jinnah Sindh Medical University, Pakistan
[8]University of Miami Miller School of Medicine, USA

Hypoplastic Left Heart Syndrome (HLHS) is a severe congenital heart disease requiring staged surgical palliation. Despite advances in surgical care, long-term morbidity and mortality remain significant, prompting investigation into regenerative therapies. Stem cell–based interventions have emerged as a promising adjunct to improve myocardial function and outcomes. Evidence from clinical and observational studies demonstrates favorable safety profiles, with improvements in right ventricular function and heart failure status. Larger multicenter trials are required to confirm long-term benefit.

Presenter:
Michael Joy Dara
Zaporizhzhia State Medical University, Ukraine

An Experimental Investigation into using Sewage Effluent to Capture CO_2

Salam K. Al-Dawery and **Saima Farooq**
University of Nizwa, Sultanate of Oman

The current project's objective is to examine the possibility of CO_2 sequestration using sodium hydroxide (NaOH) sewage solution in a semi-batch column with an integrated gas lift tower. Our technique achieves a 50% CO_2 gas capture rate by using sewage sludge and sludge supernatant (filtered wastewater). The effectiveness of CO_2 removal at different concentrations (0.05 and 0.1M), NaOH volumes (2, 3, and 4 L), and CO_2 gas flow rate (3 L/min) was assessed in preliminary experiments. The results demonstrated that the concentration of NaOH has a substantial effect on the CO_2 capture rate. The results showed that after neutralizing the sewage sludge and supernatant without the use of NaOH, the pH value dropped more quickly (in 30 seconds) than it did for tap water to get close to a pH of less than 7. The pH value dropped rapidly after neutralization, approaching pH 7 in 1 minute for the tap water solution, indicating a faster reaction rate, according to the results of the volume 2L NaOH (0.05 M) solution with a 3 L/min CO_2 gas flow rate. In contrast, it took longer for the sludge and supernatant solutions to reach pH 7 in 3 minutes. According to the data, the reaction of the sewage sludge solution including NaOH, the residence time for CO_2 is 73 seconds, while the solution without NaOH takes 49 seconds. The results showed minimal difference between supernatant solutions 0.05 and 0.1M for pH decrease to neutrality within 2 minutes, with the exception of the initial neutralization phase, which was a bit slower for solution 0.1 than for solution 0.05M. With 0.05 and 0.1M NaOH sludge solutions, it took longer to reach pH 7, requiring a substantial amount of gas consumption in just 4 minutes.

Presenter:
Salam K. Al-Dawery
University of Nizwa, Sultanate of Oman

Beyond Formal Law: Harnessing African Indigenous Knowledge to Foster Green Marketing Governance and Sharing Economy

Chipo Mutongi and Theo Tsokota
Midlands State University, Zimbabwe

There is a wide range of knowledge and wisdom in the indigenous systems. As the world grapples with the challenges of environmental degradation and climate change, indigenous wisdom offers a wealth of indigenous knowledge that can inform sustainable green marketing practices. This presentation explores the potential of indigenous knowledge and wisdom to drive innovation and transformation in green marketing, highlighting the importance of decolonizing the mind and dominant Western perspectives and embracing diverse worldviews that are sustainable. The whole marketing mix may be implemented through the use of indigenous knowledge. Indigenous preservation can be implemented in bio-degradation items. There are indigenous proverbs, riddles, songs and ceremonies that preach and teach the power of maintaining the eco-system. Indigenous foods also carry all the health and medical aspects for longevity. Through a critical review of existing literature and case studies, we examine how indigenous knowledge can inform sustainable consumption patterns, eco-friendly product development and culturally sensitive marketing communications. We argue that by unlocking the power of indigenous wisdom, marketers can develop more effective and sustainable green marketing strategies that not only reduce environmental damage but also promote cultural diversity and social justice. Ultimately, this presentation aims to inspire a new generation of marketers to embrace indigenous knowledge and wisdom to create a more sustainable and equitable green marketing future. This chapter therefore responds to increased calls to go beyond formal environmental laws and harness the potential power of African indigenous knowledge to foster green marketing governance.

Presenter:
Chipo Mutongi
Midlands State University, Zimbabwe

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