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6th Global Summit on

Advances in Medicinal Chemistry and Pharmacology

April 03-04, 2025 | Amsterdam, Netherlands

Theme:

Innovations Shaping the Future: Transformative Technologies in Medicinal Chemistry & Pharmacology

ADV. MED CHEM 2025

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2 DAYS WITH MORE THAN 45 SESSIONS, KEYNOTES & ORAL PRESENTATIONS

12+ INNOVATIVE FEATURED SPEAKERS

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- Structural Biologists
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- Clinical Researchers
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- Biotech Entrepreneurs
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Title: Aqueous two-phase partitioning: science and applications for biomarkers discovery and early cancer detection

Speaker Name: Boris Y. Zaslavsky

Affiliation: Cleveland Diagnostics, USA

Abstract:

This presentation covers the fundamentals of protein partitioning in aqueous two-phase systems (ATPS) and analytical application of solute partitioning in ATPS.

Multiple examples of experimental data providing evidence that phase-forming polymers do not interact with solutes partitioned in ATPS.

The partitioning of solutes is governed by the differences in solute interactions with aqueous media in the two phases. Solvent properties of the aqueous media in these two phases may be characterized and manipulated. The solvent interaction analysis (SIA) method, based on the solute partitioning in ATPS, may be used for characterization and analysis of individual proteins and their interactions with different partners.

The current state of clinical proteomics regarding the discovery and monitoring of new protein biomarkers is discussed, and it is argued that the protein expression level in a biological fluid may be not the optimal focus of clinical proteomic research. Multiple examples of application of the SIA method for discovery of changes in protein structure and protein–partner interactions in biological fluids are described. The SIA method reveals new opportunities for discovery and monitoring structure-based protein biomarkers.

Title: Water clarification and impact transfer on tissues in wet contact

Speaker Name: Juhani H. Pylkkanen

Affiliation: SansOx Ltd., Finland

Abstract:

Water is a pure substance that picks up a huge load during its cycles on the earth, bio systems, in washing and cleaning, as well as in industrial and agricultural processes. Water can be clarified and loaded again with desirable gases like clean air within seconds by the new integrated clarification technology in tube condition. The clarified and reloaded water is able to transfer impact of the load on tissues in wet contact, and pick in slag from the tissue due to reduced surface tension. The water clarification technology is presented briefly, and selective case studies of air impact transfer on bio tissues in wet contact are reported briefly here.

OxTube, a new water treatment innovation, clarifies water matrices in tube condition within seconds by four seamless phases; (1) separation of dissolved substances, (2) activation of molecules, (3) clarification and (4) post dissolving and refreshing. It separates and removes dissolved gases like radon, carbon dioxide, hydrogen sulfide and hydrocarbon, and dissolved solids like iron, manganese compounds, calcium, fluorine and phosphorus within seconds. Combined removal of pharmaceutical residues, disinfection and clarification in one within seconds is verified by ozone feed. Efficiency is based on kinetic energy of the flow converted to high dynamic pressure, even mixing and high collision probability of molecules in tube condition.

Health and wellness impacts of clean air can be dissolved in to the water such a way that exchange of slag and air gas between bio systems and the water initiates immediately in wet contact. Comparable iron gets rusted right away in this treated water but it could take years in dry air.

Title: Primary Side Effect Mechanisms of Covid-19 Vaccines and Serious Pathologies

Speaker Name: Beril ANILANMERT

Affiliation: Institute of Forensic Sciences and Legal Medicine

Abstract:

Most of the current SARS-CoV-2 vaccines are based on producing or introducing the spike (S) protein, which is responsible from the main pathology of vaccines and even COVID-19. It causes pathologies due to hypercoagulable state, hyperinflammation, autoimmune reactions and cell damages in the organs or systems where it is localized. To assess the side effects experienced after vaccinations, the mechanisms of the spike proteins introduced by the vaccines should be evaluated. The primary pathological mechanisms and some serious side effects are presented under the light of literature.

Spike protein has multiple pathways of causing pathologies: After it binds to Angiotensin Converting Enzyme2 (ACE2), fusion peptide is released after a series of cleavages of spike protein. Synctia occurs via the pores formed by the aid of fusion peptide [1]. Different lymphocytes remain inside syncytia to form cell-in-cell structure and such cells die rapidly. Downregulation of ACE2 by spike protein causes dysregulation of the renin–angiotensin–aldosterone system (RAAS) which increases pulmonary vasoconstriction and induction of tissue factor (TF) and plasminogen activator inhibitor 1 (PAI-1) expression on platelets and the endothelium. Endothelial cell damage, immunothrombosis or thromboinflammation, hypertension occurs. Immune response is dysregulated and the hyperinflammation appears, proinflammatory cytokines, particularly IL-6 and TNFα are overproduced. Spike protein act as infectious prion-like protein, which can replicate using PrPC (via inducing misfolding in normal variants of the same protein). It also crosses the human brain endothelial cell barrier effectively, while it can exist in peripheral blood monocytes for 15 months. Spike used some vaccines has been made less fusogenic, however, none of the vaccine inventors mutated the S2' site of the protein, which releases the fusion peptide after its breakage.

RNA molecule is unstable, however mRNA vaccines are attached to lipid nanoparticles, graphene etc. for stability. The composition of the lipid nanoparticles, the formulation components, the sequence selection for the vaccine mRNA and the amount of RNA also may influence the side-effect profile. While the ratio is 36% in natural SARS-CoV-2 virus, mRNA exists in the most well known two mRNA vaccines in a ratio of 53% and 61% with higher reactogenity. Replacing uridines with pseudouridines or methyl-pseudouridine, overcomes the recognition of mRNA by the Toll-Like Receptors, so mRNA can progress into cell easily. This replacement and addition of a long poly(A) tail and the 30 UTR from human globin stabilizes and improve its translation.

mRNA was shown to replicate itself in 6 hours via endogenous reverse transcriptase in hepatic cells upon mRNA vaccine exposure [2]. mRNA vaccines strongly trigger IFN-I. Especially after multiple administration, IFN-I can also lead to depression, cognitive slowing and cause symptoms of chronic fatigue syndrome and stimulation of synthesis of cytokines and chemokines.

Pathologies occur in the sites where the spike proteins are more localized. Dyspnea, deep fatigue, headache and muscle/joint pains, extremity weakness, reduced mental clarity/concentration, heat/cold intolerance, menstrual changes and palpitations are among the mild and most frequent side effects of these vaccines. However, it should not be forgotten that such symptoms may be related with more serious vaccine pathologies related to cerebrovascular, kidney, heart diseases, etc., even Long Covid. Among the more reported serious adverse events with fatal income after COVID-19 vaccination, there were anaphylaxis, myocarditis, Guillain–Barré Syndrome (GBS) acute transverse myelitis (TM) and a specific pathology called vaccine-induced thrombotic thrombocytopenia (VITT), which has been arised after vaccination period. Serious side effects also include; kidney injuries, facial (Bell's) palsy, autoimmune hepatitis, Creutzfeldt-Jakob disease, and even cancers as lymphoblastic/lymphoblastic lymphoma and axillary lymphadenopathy.

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Title: Discovery of antibodies that modulate macrophage functions in boosting cancer immunotherapy

Speaker Name: Jianyong Wang

Affiliation: Genentech, USA

Abstract:

As one of the most abundant cell types in many solid tumors, tumor-associated macrophages (TAMs) play critical roles in cancer progression. TAM is a type of immune cells characterized as high plasticity with both pro- and anti-tumor functions, depending on the environmental stimuli. On one hand, TAMs are capable of engulfing dying tumor cells, leading to the clearance of associated tumor antigens, which helps the tumor escape the host immune surveillance. TAMs also secret immune-suppressive cytokines that maintain a pro-tumor microenvironment. Consequently, TAMs contribute to the resistance of checkpoint inhibitors, chemotherapeutic agents, and adoptive T cell immunotherapies in clinic. On the other hand, when TAMs are properly activated, they can also actively engulf and destroy cancer cells and other pro-tumor immunosuppressive cells, acting as a defensive mechanism against tumors by killing them directly and indirectly. Thus, modulation of TAMs functions in tumors represents an attractive approach for cancer immunotherapy. Here, we share two case studies to exemplify that antibody drugs enhance cancer immunotherapy by modulating macrophage functions. First, we outline the discovery of anti-MerTK monoclonal antibodies (mAbs) that inhibit macrophage-mediated phagocytosis of apoptotic cancer cells both in vitro and in vivo. Dosing of anti-MerTK mAb in syngeneic mouse models resulted in robust anti-tumor responses when combined with anti-PD-L1, a checkpoint inhibitor that by itself only exhibited modest anti-tumor activity. Second, we will discuss how to exploit the antibody-dependent cellular phagocytosis (ADCP) function of TAMs to destroy regulatory T (Treg) cells, the major immunosuppressive cell type in tumors. More specifically, we discovered a specific mAb with enhanced antibody-dependent cellular cytotoxicity (ADCC) and ADCP that depletes the tumor-infiltrating Treg cells. In a syngeneic mouse tumor model, this specific mAb showed anti-tumor effects as a single agent and enhanced anti-tumor activities when combined anti-PD-L1.

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Title: Topical delivery of drugs in the treatment of high-grade cervical squamous intraepithelial lesions: A meta-analysis

Speaker Name: Jianlan Zheng

Affiliation: Chenggong Hospital of Xiamen University

Abstract:

Objective: The present study aims to evaluate the efficacy and effect of localized delivery of drugs in the treatment of high-grade squamous intraepithelial lesion (HSIL) based on a meta-analysis.

Study Design: Databases including Cochrane Library, PubMed, Embase, Scopus, CNKI, and Wanfang were searched from their inception till August 2022. Randomized controlled trials (RCTs) that compared the efficacy of drugs and surgery in the treatment of HSIL were collected. A meta-analysis was performed using the software of Review Manager (version 5.4.1).

Results: Eight RCTs involving 523 patients were included in the meta-analysis. For HSIL, the rate of cervical lesions histological regression was 69.85% in the surgery group and 59.88% in the drug group, there was no significant difference between the two groups [OR=0.45, 95% CI (0.07, 3.03), P=0.41]. The histological regression rate of cervical lesions in the placebo group was 37.76%, and the difference between the drug group and the placebo group was statistically significant [OR=4.94, 95% CI (2.65, 9.20), P<0.00001].

Conclusion: A total of four drugs were involved in the eight RCTS included in this study, which were imiquimod, 5-fluorouracil (5-FU), cidofovir and interferon. The results showed that although drug administration was effective in the histological regression of HSIL, the efficacy was less than about 10% of surgical treatment. Considering the recurrence of the disease after surgery and the problems of abortion, premature delivery and premature rupture of membranes after cervical conization in reproductive women, drug therapy can be used as a supplement to surgery or conservative treatment to promote the histological regression of cervical lesions in patients with HSIL.

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Title: Unraveling the bidirectional relationship between muscle inflammation and satellite cells activity: influencing factors and insights

Speaker Name: Esmail Karami

Affiliation: Baqiyatallah University of Medical Sciences

Abstract:

Inflammation stands as a vital and innate function of the immune system, essential for maintaining physiological homeo-stasis. Its role in skeletal muscle regeneration is pivotal, with the activation of satellite cells (SCs) driving the repair and generation of new myofibers. However, the relationship between inflammation and SCs is intricate, influenced by various factors. Muscle injury and repair prompt significant infiltration of various immune cells, particularly macrophages, into the muscle tissue. progenitors, and SCs, further shapes the inflammation-SCs dynamic. While some studies suggest heightened inflammation associates with reduced SC activity and increased fibro- or adipogenesis, others indicate an inflammatory stimulus benefits SC function. Yet, the existing literature struggles to delineate clearly between the stimulatory and inhibitory effects of inflammation on SCs and muscle regeneration. This paper comprehensively reviews studies exploring the impact of pharmacological agents, dietary interventions, genetic factors, and exercise regimes on the interplay between inflammation and SC activity.

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Title: NMR-based metabolomics and biochemical analyses as tools for precision medicine in fighter pilots

Speaker Name: Grace Barros de Sá

Affiliation: IBMR University Center, Brazil

Abstract:

Fighter pilots face a range of physical, psychological, and environmental stressors. NMRbased metabolomics provides a reliable and comprehensive approach to map the metabolic profile analysing associated to acute and chronic effects of aviation of aviation. We evaluated 34 subjects: FP1 (n = 7, fighter pilots with less than 1,100 hours of accumulated flight time), FP2 (n = 6, fighter pilots with 1,100 or more flight hours), and NP (n = 21, military non-pilots). Data collected included total blood count, lipid profile, oxidative stress markers, and serum NMR-based metabolomics. Compared to NP ($p < 0.05$), pilots showed reduced levels of leucocytes (−13%), neutrophils (−15%), lymphocytes (−20%), alpha-glucose (−13%), lactate (−26%), glutamine (−11%), histidine (−20%), and tyrosine (−11%). However, they had higher isobutyrate concentrations (+10%). FP1 exhibited signs of immune-metabolic dysregulation, which appeared to improve in FP2 pilots. A previous study assessed the acute metabolic effects before and after A-29 flights in trainees (n = 12) and instructors (n = 20). Post-flight, trainees showed increased segmented neutrophils (12%) and salivary glucose (49%), alongside a 23% reduction in serum lactate. Instructors displayed a rise in lymphocytes (15%) and decreases in serum lactate (12%) as well as key metabolites, notably choline (−23%) and lactate (−15%). Additionally, urinary L-anserine levels increased by 200% in trainees and by 4.2% in instructors, while trigonelline levels rose by 53% in instructors. These findings highlight the acute metabolic responses to flight stressors in combat pilots, underscoring the importance of personalized monitoring to optimize interventions related to training, diet, supplements, medications, chronic fatigue management, and personnel selection based on metabolic adaptations.

Title: Intratumoral Delivery of Genetically Engineered Anti-IL-6 Trans-signaling Therapeutics

Speaker Name: Raphaela Bento

Affiliation: Rutgers University, NJ, USA

Abstract:

Scope: Interleukin-6 (IL-6) is a highly pro-inflammatory cytokine involved in the etiopathology of several inflammatory diseases and cancer. As so, the inhibition of IL-6 signaling pathways has emerged as an attractive therapeutic avenue for the treatment of several chronic diseases. The pathological role of IL-6 trans-signaling has led to the development of selective inhibitors, with next-generation variants offering increased specificity and potency while minimizing offtarget effects. However, the costly and time-consuming processes of recombinant protein production have limited the clinical advancement of anti-cytokine therapies. This study aimed to develop and validate gene therapeutic modalities of IL-6 trans-signaling inhibitors as alternatives for local and sustained recombinant protein delivery.

Methods: Engineered cells were generated via stably lentiviral transduction to constitutively express the anti-IL-6-trans-signaling molecule sgp130Fc and or its second-generation variant sgp130FlyRFc, as well as a secreted bioluminescent biomarker probe (Gaussia Luciferase, Gluc) for easy detection in solution. IL-6-dependent cells (DS-1 cells) were used to validate the bioactivity and selectivity of the gene therapeutics in vitro. IL-6-dependent lymphoma cell line and xenograft tumor model were used to test the superior inhibitory potential of sgp130FlyRFc in vivo. The efficiency of distinct gene delivery modalities was tested using GLuc secretion as a readout of protein production via cell-based delivery.

Results: In a comparative study, the second-generation inhibitor sgp130FlyRFc exhibited approximately ten-fold greater inhibitory capacity, demonstrated by a significant reduction in IL-6-dependent cell proliferation (Figure 1A-B). In vivo pharmacokinetics revealed that cell-based delivery outperformed direct gene transfer, showing enhanced secretion of the anti-cytokine molecule over time, even at lower doses. Intratumoral delivery of sgp130FlyRFc-secreting cells significantly reduced tumor burden and improved animal survival (Figure 1C-D), highlighting the potential of cell-based delivery for sustained gene therapy.

Conclusion: Herein, we established a proof-of-concept framework that enables local cell-based delivery of anti-cytokine therapeutics, yielding high levels of soluble protein with mensurable inhibitory effects. This approach represents a promising avenue for clinically relevant gene delivery applications.

Title: Combined Experimental and Computational Analysis of Drug Resistance in HIV-1 Protease Conformational Landscape

Speaker Name: Gail E. Fanucci

Affiliation: University of Florida, USA

Abstract:

HIV-1 Protease (PR) is a current drug target in the treatment of HIV-1 infection, although drug-resistance continues to emerge with virological failure. We utilize both experimental pulsed-electron paramagnetic resonance distance measurements and computational approaches to evaluate how natural polymorphisms (NPs) and drug-pressure (DP) selected mutations impact the conformational landscape of HIV-1 PR. Several NPs found in African and Brazilian PR variants alter the conformational landscape towards a closed conformation, whereas those in the African Subtype C and several drug-resistance combinations stabilize an open like conformations of HIV-1 PR. These conformational insights provide a hypothesis for why drug resistance mutational patterns vary in HIV-1PR throughout the world.

Title: Skin and soft tissue nontuberculous mycobacteria infection: A retrospective case series of 49 patients after procedures

Speaker Name: Huijuan Fu

Affiliation: Peking University People's Hospital, China

Abstract: The incidence of skin and soft tissue nontuberculous mycobacteria infection (SSTNI) is increasing and emerging, evidence suggests there is association between plastic and cosmetic procedures and SSTNI.

Objective: To summarize wound healing process, clinical features, diagnosis and treatment of SSTNI and explore the association between SSTNI and plastic and cosmetic procedures.

Methods: A retrospective case series study was conducted among patients diagnosed with SSTNI after plastic and cosmetic procedures. The medical history was collected, wound healing process and disease characteristics were summarized and analyzed.

Results: A total of 49 patients were collected. Among them, 39 (80%) patients were infected with Mycobacterium abscesses. 40 (82%) patients had a history of fat-related procedures, including 17 (35%) lipolysis injection and 23 (47%) fat transplantation and liposuction. The median and interquartile range of onset time were 15 and 43 days (1-100). Time from first visit to diagnosis was 82±57 days (23-308). Wound healing time was 161±92 days (30-545). The symptoms were non-specific and the most common infected site was head and neck, followed by breasts. Only 6 (12.5%) patients were diagnosed clearly before admission to our department. Only 10 (28%) patients showed positive acid-fast bacilli (AFB) smears among 36 patients. Treatment included debridement surgeries, vacuum sealing drainage (VSD) and multiple antibiotics.

Conclusion: Though the specific mechanism is not clear yet, it seems that fat-related procedures increase susceptibility of SSNTI. Every patient presenting with unspecific clinical symptoms and long course of disease should be considered as SSTNI. Results of AFB smears are frequently negative after empirical antibiotic therapy so that molecular diagnostic techniques are required for rapid and accurate identification. Debridement surgeries, VSD combined with long-term sensitive antibiotics are effective for SSTNI. Drug safety and psychological status should also be paid attention during treatment.

Title: Comparing the Generalizability of Reliability-Based vs. Accuracy-Based Diagnostic Models in Medical and Healthcare Applications.

Speaker Name: Sepideh Etemadi

Affiliation: University of Minnesota Duluth, USA

Abstract: Various approaches with different structures and characteristics have been proposed as tools to address diverse health and medical prognostic and diagnostic issues. Despite the differences among these modeling methods, they all focus on maximizing the accuracy or reliability of the outcomes to obtain the most generalizable model. Although reliability theoretically plays a crucial role in enhancing generalization capability, especially in high-risk decisions, many models for tasks such as causal prediction, time-series forecasting, and classification have primarily been developed with a focus on maximizing accuracy. Hence, the primary objective of this study is to emphasize the relative importance of accuracy- and reliability-based methodologies on the quality of medical decisions made in intelligent and statistical decision support systems, as well as to determine their impact. To achieve this, 33 diverse datasets from the UCI database, spanning causal, classification, and time series categories, have been analyzed. These datasets cover various scopes, including cancer and disease diagnosis, experimental therapy, and fertility prediction. Empirical results indicate that the reliability-based methodology achieved improvements over the accuracy-based approach: 2.26% in causal prediction cases, 13.49% in classification cases, and 3.08% in time-series forecasting cases. Overall, the reliability-based approach resulted in a 6.28% improvement compared to similar accuracy-based models. As a result, the findings of this study indicate that reliability is a more effective factor than accuracy in improving the quality of decisions made by models in medical-related issues. Ensuring the reliability of model performance is essential for achieving stable and appropriate predictions in medical areas such as disease prediction, medical diagnosis, and clinical data modeling, thereby facilitating decision-making. Consequently, reliability-based models with the capability to model uncertainty are more suitable for addressing real-world medical decision-making problems.

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Title: Hypothalamic TRPM8 and TRPA1 ion channel genes in the regulation of temperature homeostasis at water balance changes

Speaker Name: Irina Petrovna Voronova

Affiliation: Novosibirsk State University, Russia

Abstract: The role of the hypothalamic cold-sensitive ion channels - transient receptor potential melastatin 8 (TRPM8) and transient receptor potential ankyrin 1 (TRPA1) in homeostatic systems of thermoregulation and water-salt balance – is not clear. The interaction of homeostatic systems of thermoregulation and water-salt balance without additional temperature load did not receive due attention too. On the models of water-balance disturbance, we tried to elucidate some aspect of these problems.

Body temperature (T_{body}), O_2 consumption, CO_2 excretion, electrical muscle activity (EMA), temperature of tail skin (T_{tail}), plasma osmolality, as well as gene expression of hypothalamic TRPM8 and TRPA1 have been registered in rats of 3 groups: 1-control; 2-water-deprived (3 days under dry–eating); 3-hyperhydrated (6 days without dry food, drinking liquid 4% sucrose). The MP100 set of instruments (BIOPAC Systems, USA) was used for continuous registration of physiological parameters. Osmolality of plasma was determined by the cryoscopic method. Gene expression was assayed by the method of quantitative RT-PCR.

No relationship was observed between plasma osmolality and gene expression of *Trpm8* and *Trpa1*. However, in water-deprived rats, the constriction of skin vessels, increased fat metabolism by 10% and increased EMA by 48% allowed the animals to maintain T_{body} unchanged. The hyperhydrated rats did not develop sufficient mechanisms, and their T_{body} decreased by 0.8 ^{o}C. The development of reactions was correlated with the expression of genes of thermosensitive ion channels in the anterior hypothalamus. T_{tail} had a direct correlation with the expression of the *Trpm8* gene (r=0.7 and r=0.8 for water-deprived and hyperhydrated animals, respectively), whereas EMA directly correlated with the expression of the *Trpa1* gene (r=0.68) in water-deprived group. The obtained data also attract attention from the point of view of management and correction of physiological functions by modulating the operation of ion channels under various influences, including the development of pathological processes.

Title: Seeking Molecular Biomarkers for Schizophrenia Using ROC Analysis

Speaker Name: Margareth Borges Coutinho Gallo

Affiliation: University of Campinas – UNICAMP, Brazil

Abstract: Schizophrenia Spectrum Disorders (SSD) represent a multidimensional and severe mental illness, characterized by abnormalities in molecular processes and dysregulated pathways. The pursuit of effective molecular biomarkers to diagnose this complex disorder has evolved over the past century. The primary objective of this work was to examine the molecular biomarkers associated with the hypotheses of the pathophysiology of SSD that underwent receiver operating characteristic (ROC) curve analysis in the past 12 years (2011-2023). The aim was to identify prevalent biomarkers within developed models, potentially forming a distinctive biomarker signature for SSD, as depicted in Table 1.

The conclusions drawn from this investigation reveal intriguing and promising insights. Out of 84 metabolic biomarkers identified from the studies, 17 significantly matched a disease signature for SSD (FDR 9.48E-27) in MetaboAnalyst 6.0. Overrepresentation analysis using RaMP-DB/2 entries showed significant enrichment for transport disorders and amino acid metabolism/catabolism (Figure 1). Thirty metabolites from blood/fecal samples associated with dysbiosis in SSD corroborated the previous results, yielding a panel of 15 metabolites. Considering both results, 7 common metabolites emerged: tyrosine, arginine, glutamine, leucine, phenylalanine, tryptophan, and kynurenine. This panel secured the first position for SSD in the enrichment analysis with a notable significance (FDR 1.18E-14).

Moreover, the Bacillota phylum and Lachnospiraceae family emerged as the most prevalent in all studies, with genera such as *Roseburia* and *Dorea* significantly reduced in the feces of SSD patients. This family stands out as one of the most prevalent microbial families globally, underscoring its potential as a biomarker that transcends geographical and ethnic boundaries.

A panel of cognitive tests surpassed inflammatory markers in both diagnostic accuracy and transdiagnostic ability for distinguishing SSD patients. This indicates that future research may benefit from an integrated approach, combining various classes of biomarkers and clinical tools, to enhance the accuracy and reliability of predictive models.

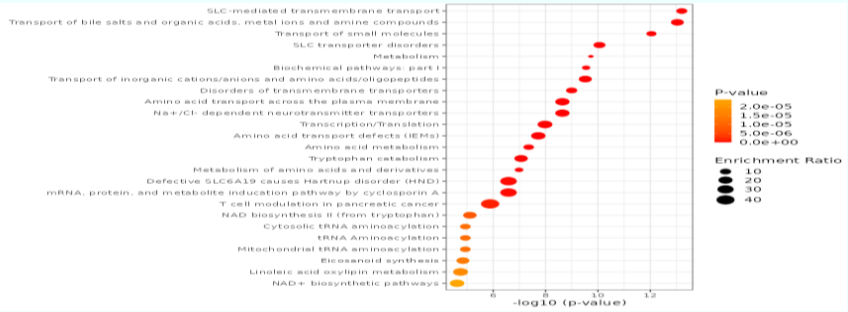

Figure 1. Overrepresentation analysis of 17 metabolites selected by ROC analysis across 32 articles to determine the most enriched pathways for schizophrenia

Title: Chitosane - Antibiotic Based Composites and Their Application In Medicine

Speaker Name: Dilyana Todorova Zvezdova

Affiliation: Prof. Dr. Assen Zlatarov University, Bulgaria

Abstract: Diabetes mellitus and its complications pose a number of socially significant problems for health care and require innovative approaches in the prevention and treatment of complications. The long-term prognosis and quality of life of diabetic patients depend on the development and severity of the latest complications. The most dangerous cases are when peripheral arterial disease (PAD) develops, leading to ischemia of the lower limb.

This process makes it difficult to control any superimposed infection, difficult wound healing, the appearance of phlegmon and devitalization of tissues due to the developing vascular-degenerative syndrome. In this direction, a motivating goal of the research is to create a therapy based on the biocarrier chitosan and sustained release antibiotics on the affected tissues with bacterial infection.

Chitosan derived from demineralization and deproteinization of raw material from the Black Sea was used in order to reach derivation of the composite membranes. In this study, the possibility of immobilizing antibiotics onto chitosan (CS) and chitosan/zeolite (CSZ) composite membranes for wound healing applications was investigated. The structure of the derived compounds has been confirmed by FTIR, NMR, DSC and SEM analysis. To study the loading capacity of antibiotics onto the CS/CSZ membranes UV- spectroscopy was employed. The main challenge was to provide antibacterial properties through a local delivery of antibiotics in order to prevent infection in wounds during the wound treatment procedures. The antibacterial activity against Escherichia coli ATCC 25922 and Staphylococcus aureus ATCC 29213 strains of the developed membranes was assessed through disk-diffusion method by means of Mueller-Hinton agar. The obtained results showed that chitosan/zeolite membranes loaded with antibiotics exhibited better antimicrobial properties compared to other studied objects.

Title: Gold Nanoparticle-Based Plasmonic Detection of Escherichia coli, Salmonella enterica, Campylobacter jejuni, and Listeria monocytogenes from Bovine Fecal Samples

Speaker Name: Ahmed Mohamed Ghazy

Affiliation: Veterinary Services Department of Egyptian Armed Forces

Abstract: Current diagnostic methods for detecting foodborne pathogens are time-consuming, require so-phisticated equipment, and have a low specificity and sensitivity. Magnetic nanoparticles (MNPs) and plasmonic/colorimetric biosensors like gold nanoparticles (GNPs) are cost-effective, high-throughput, precise, and rapid. This study aimed to validate the use of MNPs and GNPs for the early detection of Escherichia coli O157:H7, Salmonella enterica spp., Campylobacter jejuni, and Listeria monocytogenes in bovine fecal samples. The capture efficiency (CE) of the MNPs was de-termined by using Salmonella Typhimurium (ATCC_13311) adjusted at an original concentration of 1.5 × 108 CFU/mL. One (1) mL of this bacterial suspension was spiked into bovine fecal suspen-sion (1 g of fecal sample in 9 mL PBS) and serially diluted ten-fold. DNA was extracted from Sal-monella Typhimurium to determine the analytical specificity and sensitivity/LOD of the GNPs. The results showed that the CE of the MNPs ranged from 99% to 100% and could capture as little as 1 CFU/mL. The LOD of the GNPs biosensor was 2.9 µg/µL. The GNPs biosensor was also tested on DNA from 38 naturally obtained bovine fecal samples. Out of the 38 fecal samples tested, 81.6% (31/38) were positive for Salmonella enterica spp., 65.8% (25/38) for C. jejuni, 55.3% (21/38) for L. monocytogenes, and 50% (19/38) for E. coli O157:H7. We have demonstrated that MNP and GNP biosensors can detect pathogens or their DNA at low concentrations. Ensuring food safety throughout the supply chain is paramount, given that these pathogens may be present in cattle feces and contaminate beef during slaughter.

Title: Forging the path to precision medicine in Qatar: a public health perspective on pharmacogenomics initiatives

Speaker Name: Kholoud Bastaki

Affiliation: Qatar University, Qatar

Abstract: Pharmacogenomics (PGx) is an important component of precision medicine that promises tailored treatment approaches based on an individual's genetic information. Exploring the initiatives in research that help to integrate PGx test into clinical setting, identifying the potential barriers and challenges as well as planning the future directions, are all important for fruitful PGx implementation in any population. Qatar serves as an exemplar case study for the Middle East, having a small native population compared to a diverse immigrant population, advanced healthcare system, national genome program, and several educational initiatives on PGx and precision medicine. This paper attempts to outline the current state of PGx research and implementation in Qatar within the global context, emphasizing ongoing initiatives and educational efforts. The inclusion of PGx in university curricula and healthcare provider training, alongside precision medicine conferences, showcase Qatar's commitment to advancing this field. However, challenges persist, including the requirement for population specific implementation strategies, complex genetic data interpretation, lack of standardization, and limited awareness. The review suggests policy development for future directions in continued research investment, conducting clinical trials for the feasibility of PGx implementation, ethical considerations, technological advancements, and global collaborations to overcome these barriers.

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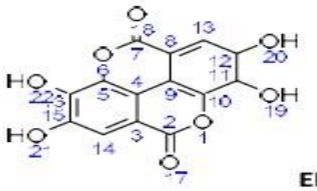
Title: DFT Investigation of the Antioxidant Capacity of Culinary Herbs Polyphenols

Speaker Name: André Mauricio de Oliveira

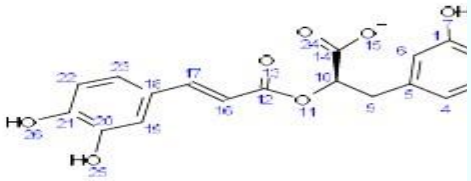
Affiliation: Federal Centre of Technological Education of Minas Gerais, Brazil

Abstract: This work investigates the antioxidant potential of two culinary herbs polyphenols, rosmarinic acid (RA) and ellagic acid (ELA), key inflammatory pathways enzymes inhibitors. RA can be found on sage, thyme, oregano, peppermint, rosemary, and EA has been detected in beverages, berries and nuts. The antioxidant capacity of ELA and RA was analysed using DFT (M06-2X/6-311G(2d,2p) and B3LYP/6-311G(2d,2p)). Enthalpies were determined for non-ionized (ArOH), ionized (ArO-), radical (ArO•), and cation radical (ArOH+•) forms. The scavenging activity was correlated with O-H bond dissociation enthalpy (BDE), adiabatic ionization potential (IP), proton dissociation enthalpy (PDE), proton affinity (PA), and electron transfer enthalpy (ETE)1 (Table 1). M06-2X showed overestimated values when compared to B3LYP. BDE favours RA over ELA. In RA, the 7-OH group, closer to the negative carboxylate group, is less reactive. Electron-donating groups such as OH diminishes the BDE, increasing antioxidant activity2 . Lower IP suggests stronger electron-donating ability. Discrepancies arise when different functionals are used with cation radicals, affecting the IP calculation of the 20-OH group in ELA, and M06-2X exhibiting better reproducibility.

Table 1. Parameters for estimating the scavenging activity of phenolic antioxidants.



ELA



Compound	Substitution	BDE		IP		PDE		PA	
		M06X	B3LYP	M06X	B3LYP	M06X	B3LYP	M06X	E
ELA	19-OH	0.1499	0.1183	0.2844	0.2698	0.3679	0.3508	0.5091	0
	20-OH	0.1193	0.1167	0.2902	0.0012	0.3314	0.6178	0.5128	0
RA	7-OH	0.1620	0.1139	0.8505	0.9593	-0.1863	-0.3431	0.6513	0
	8-OH	0.1250	0.0948	0.8284	0.9470	-0.2012	-0.3499	0.6763	0
	25-OH	0.1331	0.1100	0.8461	0.6725	-0.2108	-0.0602	0.6531	0
	26-OH	0.1636	0.1098	0.8489	0.7376	-0.1830	-0.1256	0.6183	0

HOMO/LUMO orbitals (M06X-6-311G(2d,2p); Figure 1) for RA in their ArO- and ArOH+• forms presents higher values of anion HOMO, which implies in higher PA. The carboxylate group in RA takes part in the LUMO electron delocalisation profile, due to the proximity of the electron loss centre.

Title: Antibacterial Activity of Silver Nanoparticles Derived from Extracellular Extract of Enterococcus

Speaker Name: Mohammed Abas Abd Ali

Affiliation: Misan University College, Iraq

Abstract:

Bacteria are known to have a high ability to manufacture many compounds with biological functions in a short time compared with eukaryotic cells due to the fact that bacterial cells possess efficient metabolic mechanisms for the manufacture of these compounds (intracellular or extracellular). Herein, the goal of this study is to use pathogenic Enterococcus aerogenes bacteria strains, namely, S1, S2, and S3, isolated from the mouths of individuals with dental decay to produce silver nanoparticles in an environmentally friendly and cost-effective manner.

Methods. These nanoparticles have been tested for antibacterial activity against Streptococcus mitis, an MDR bacterium, either alone or in combination with antibiotics. These bacteria were identified using morphological characteristics and bio chemical tests, in addition to molecular methods such as PCR and DNA sequences. Besides, their identification was done on the basis of their alignment with the reference strains in the NCBI blast to calculate the degree of similarity among these strains (S1, S2, and S3).

The results. The results of the current study showed a clear synergistic effect in the inhibition of Streptococcus mitis bacteria when mixing silver nanoparticles with some antibiotics, and it was found that there is a synergistic effect when mixing those AgNPs with erythromycin, followed by streptomycin and tetracycline. In contrast, the effect was antagonistic in the case of streptomycin and tetracycline antibiotics. Conclusion *Enterobacter aerogenes* AgNPs.

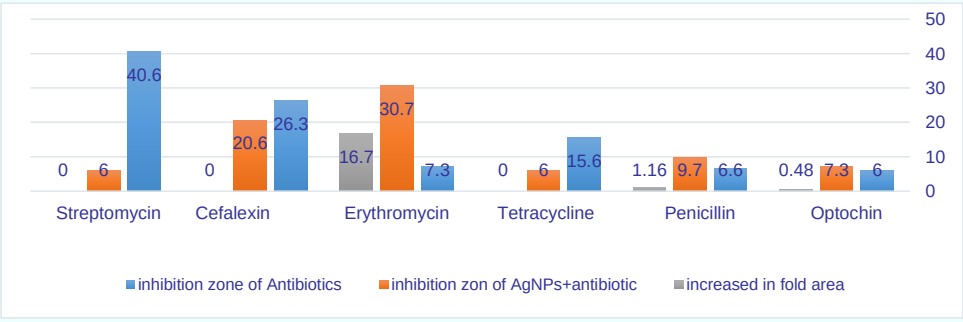


Fig. 2. Percentage fold increases of AgNPs produced by S2 strain in combination with antibiotics against MDR Streptococcus mitis

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Title: Mutagenic Azido Impurities in Drug Substances: A Perspective

Speaker Name: Sumit S. Chourasiya

Affiliation: IOL Chemicals and Pharmaceutical Ltd., India

Abstract: Contamination of drug products and substances containing impurities is a significant concern in the pharmaceutical industry because it may impact the quality and safety of medicinal products. Special attention is required when mutagenic impurities are present in pharmaceuticals, as they may pose a risk of carcinogenicity to humans. Therefore, controlling potential mutagenic impurities in active pharmaceutical ingredients (APIs) to an acceptable safety limit is mandatory to ensure patient safety. As per the International Council for Harmonization (ICH) M7(R2)3 Guideline, mutagenic impurities are those compounds or materials that induce point mutations. In 2018, the sartan class of drugs was recalled due to the presence of N-nitrosamine impurities, which are potential mutagens. In addition to the primary impurities being detected, this class of products, especially losartan, irbesartan and valsartan, have been identified as having organic azido contaminants, which are again highly reactive toward DNA, leading to an increased risk of cancer. These azido impurities form during the preparation of the tetrazole moiety via the reaction of a nitrile intermediate with sodium azide. Given that this is a newly raised issue in the pharmaceutical world, it should be noteworthy to review the related literature. Thus, this review article critically accounts for (i) the toxicity of azido impurities and the proposed mechanism of mutagenicity, (ii) the regulatory perspective, and (iii) the sources and control strategies used during the preparation of drug substances and (iv) future perspectives.

Title: *In vitro* Assessment of the Therapeutic Efficacy of Jania rubens Extract on Colorectal Cancer CaCo2 Cells

Speaker Name: Zeina Dassouki

Affiliation: Faculty of Health Sciences, Lebanon

Abstract:

Colorectal cancer (CRC) is a major cause of morbidity and mortality, driven by various environmental stressors and often treated with chemotherapeutic drugs. Due to its adverse effects, the need for natural biomolecules or extracts from plants and algae has gained prominence. Abundant phytochemicals in red algae have shown promise in addressing the multilayered mechanisms of cancer. Recently we have proven a potent antitumor potential of Jania rubens (J. rubens). In this study, we further investigated the antineoplastic properties of J. rubens active content against CaCo CRC cells.

Methods: In this study, total phenolic and flavonoid contents are quantified using the Folin-Ciocalteu and Aluminum chloride assays, respectively. Antioxidant activity is assessed through 2,2-diphenyl-1-picrylhydrazyl (DPPH) free radical scavenging assays. The antitumor effects of J. rubens extracts are evaluated on CRC CaCo2 cells using MTT, Trypan blue, and wound healing assays.

Results: Biochemical characterizations show that the highest phenolic content is attributed to proteins while lipids revealed the highest flavonoid content. The antioxidant activity is highest in proteins, followed by lipids and polysaccharides. Polysaccharides exhibit the highest anti-proliferative activity. Also, M soxhlet and DM soxhlet extracts demonstrate potent cytotoxicity against CaCo2 CRC cells. To further analyze the anti-migratory potential of the most cytotoxic extracts, a wound healing assay was performed showing that polysaccharide and M Soxhlet significantly inhibited CaCo2 wound healing at low concentrations and after a short exposure while no difference in the inhibition potency of DM Soxhlet and M Soxhlet after a longer exposure time.

Conclusion: Bioactive compounds in Lebanese J. rubens have proven a promising potential to enhance chemotherapy effectiveness. These findings could underline the proposed benefit of this algae and warrant broader clinical studies potentially leading to more effective and personalized CRC therapies.

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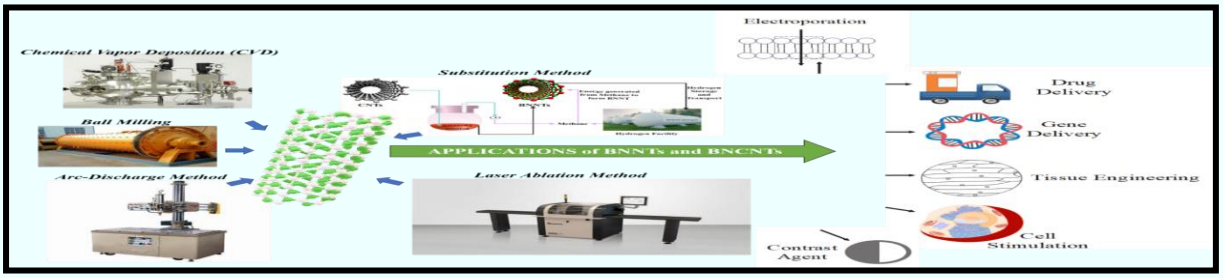
Title: Energy, Environment and Biomedical Applications of Boron Nitride and Boron Nitride Carbon Nanotubes: A Sustainable Industrial Scale-up Exegesis

Speaker Name: Harshit Mittal

Affiliation: Guru Gobind Singh Indraprastha University, India

Abstract: Boron-Nitride Nanotubes (BNNTs) are electrical insulators that usually have higher thermal and chemical properties than Carbon Nanotubes. Some of the most exceptional stiffness are shown by BNNTs, which shows potential applications in polymeric composites and ceramics. Such high stiffness also leads to lighter, more affordable, and faster transportation applications for lightweight ballistic armor and applications. When considering BNNTs' possible uses, focusing on their thermal and oxidative stability and their chemical inertness is essential. These properties can be logically used in capsules in which we have to protect nanomaterials that are unstable in the air or can be contaminated easily at standard atmosphere. This study discusses about the current trends, sustainable elucidation of synthesis methods, and prospective applications of boron nitride nanotubes. Through recent advancements, many new technologies are used in synthesizing and applying BNNTs and boron-nitride carbon nanotubes, giving higher yields and keeping the unique properties shown intact which align with the current United Nations Sustainable Development Goals. A balanced approach has been followed in the review to cover all the significant challenges, opportunities and economics of various industry-based production and application models associated with the BNNTs towards carbon neutrality.



An overview of the circular Solutions for Boron Nitride Nanotubes synthesis, production and applications.

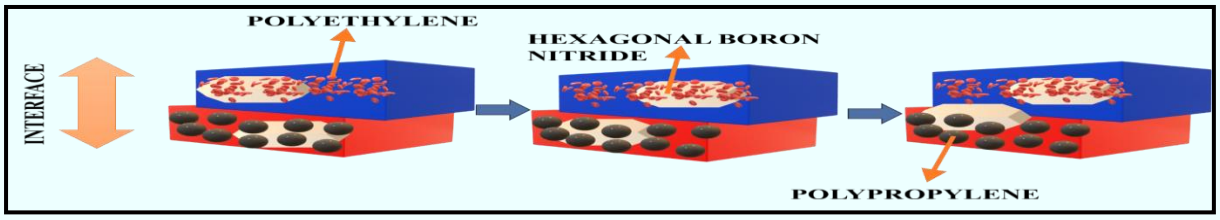


Figure 6: In-situ exfoliation mechanism of hexagonal boron nitride due to polyethene (PE) and polypropylene (PP) melt compounding.

Table 1: Characterization of surface tension values of PE, PP and Hexagonal boron nitride.

Material	Surface Tension Characterization
Polypropylene (PP)	39 mN/m
Polyethylene (PE)	37 mN/m
Hexagonal Boron Nitride	46 mN/m

Title: Models incorporating Inliers in Clinical trials

Speaker Name: K. Muralidharan

Affiliation: The Maharaja Sayajirao University of Baroda Vadodara, India

Abstract: When the failures patterns are subjected to many causes, a single failure time distribution may not be a good probability model for describing the system characteristics and patterns. This suggests strongly that the population is not homogeneous but rather it is made up of several subpopulations mixed in unknown proportions. Since, instantaneous/ immediate failures are a natural occurrence of a uncertain system or process, such failures usually discard the assumption of a unimodal distribution and hence the usual method of modelling and inference procedures may not be accurate in practice. Such failures are called *inliers,* and they can arise due to mechanical failures, wrong method of formulations, inferior quality or faulty construction of items and components.

We propose some inliers-prone models and study the likelihood estimation of the unknown parameters of the model along with Uniformly Minimum Variance Unbiased Estimator (UMVUE) for various parametric functions. With the support of some practical situations, specifically in clinical trials, the estimators and characteristics are studied and compared.

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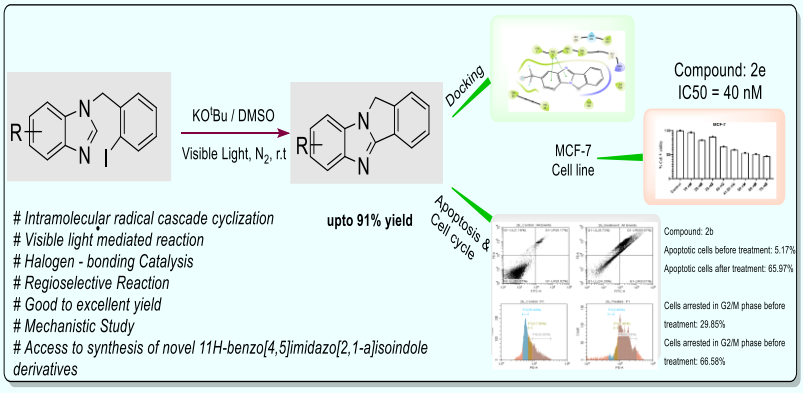
Title: Metal Free, Visible light mediated synthesis of tetracyclic benzimidazole: Regioselective C-H functionalization with in-vitro and computational study of potent compounds)

Speaker Name: Annu Abhishek Choudhary

Affiliation: Veer Narmad South Gujarat University, India

Abstract: Visible light mediated; highly efficient synthetic strategy has been developed for the synthesis of tetracyclic benzimidazole derivatives via regioselective intramolecular C-H functionalization. Halogen attached on aromatic nucleus is activated through KOtBu to generate aryl radical. The radical subsequently itself reacts to the vicinal position through intramolecular coupling in suffices benzimidazole nucleus. The overall results the formation of tetracyclic benzimidazoles moderate to fair yield. These metal free regioselective synthesis is confirmed by control experiments and density functional theory (DFT) calculations. Three compounds, namely 2a, 2b, and 2e have demonstrated promising anti-cancer properties across multiple assays. In the MTT assay, these compounds significantly inhibited cell viability, indicating potent cytotoxic effects. Cell cycle arrest analysis revealed that these agents effectively stopped the progression of cancer cells at specific checkpoints, and affected their proliferation. Furthermore, apoptosis assays confirmed that the compounds induced programmed cell death in cancer cells, highlighting their potential as effective anti-cancer agents. Interestingly, compound 2e showed least IC50 value of 40 nM and same compound showed the most robust cell cycle arrest results (almost 80% cells were arrested at G2/M phase). Alongwith this, compound 2b showed significant death percentage in apoptosis where 65% of the cells were in apoptosis after the treatment. These findings suggest that these compounds warrant further investigation as potential therapeutic options for cancer treatment.



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Title: A Mobile Robot with an Autonomous and Custom-Designed Control System

Speaker Name: Brwa Abdulrahman Abubaker

Affiliation: Bayan University, Iraq

Abstract: Teaching autonomous mobile robots (AMRs) to acquire knowledge independently has been a formidable challenge, characterized by protracted convergence times and computational intensity within traditional methods. This research introduces an innovative paradigm employing a customized spiking neural network (SNN) to address these challenges, fostering autonomous learning and control of AMRs within unfamiliar environments. The proposed model amalgamates spike-timing-dependent plasticity (STDP) with dopamine modulation to augment the learning process. Incorporating the biologically inspired Izhikevich neuron model imparts adaptability and computational efficiency to the control systems, particularly in response to dynamic environmental alterations. Evaluation through simulations elucidates initial challenges during the training phase, where the infusion of brain-inspired learning, dopamine modulation, and the Izhikevich neuron model introduces intricacies, notably manifesting in difficulties adapting to diverse obstacle scenarios. Initial performance metrics reveal a 73% accuracy rate in reaching the target with a 27% collision rate in single obstacle scenarios. However, progressing to the testing phase demonstrates substantial enhancement, culminating in a remarkable 98% accuracy in reaching the target and a marked reduction in collisions to 2% in single obstacle scenarios. These outcomes underscore the model's adaptive prowess and proficiency in navigating complex environments with varied obstacles. The innovative application of the customized SNN, integrating STDP and dopamine modulation, showcases promising potential in surmounting the challenges associated with reinforcement learning in AMRs. Furthermore, the proposed methodology paves the way for future advancements in autonomous robotics by leveraging biologically inspired mechanisms, thereby enhancing the robots' ability to learn and adapt in real-world settings. This research not only addresses the computational and convergence issues but also opens new avenues for integrating neurobiological principles into artificial intelligence, fostering more efficient and effective autonomous systems.

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Title: Mycobacterial ATP-Phosphoribosyl Transferase (HisG) Inhibition by the New Anti-TB Chemotypes Benzo[d]thiazole-2-carboxamides/carbanilides

Speaker Name: Dhameliya Tejas Manjibhai

Affiliation: National Institute of Pharmaceutical Education and Research (NIPER), India

Abstract: Targeting metabolic enzyme, unique to Mycobacterium tuberculosis, provides a novel approach to develop new drugs to eradicate Mtb via inhibition of the mycobacterial ATP-phosphoribosyl transferase (ATP-PRTase). Benzo[d]thiazole-2-carboxamides and benzo[d]thiazole-2-carbanilides with activity against Mtb having MIC of 0.78-25 µg/mL were identified as potential inhibitors of ATP-PRTase (HisG). The effect of benzo[d]thiazole-2-carboxamide and benzo[d]thiazole-2-carbanalide derivatives on the enzymatic inhibitory activity against ATP-PRTase was studied. The compounds 1n and 2a were found to be most potent which inhibited the activity of ATP-PRTase with EC50 of 20 ± 2.2 and 14 ± 1.8 µM, respectively. The compounds 1n and 2a bound to ATP-PRTase with a dissociation constant (Kd) of 11 ± 1.5 µM and 6.6 ± 1.2 µM, respectively, and perturbed the secondary structure of ATP-PRTase. The compound 1n exhibited a stronger competitive inhibition towards ATP (Ki = 19 ± 3 µM) as compared to 2a (Ki = 35 ± 2 µM). There was a recovery in the growth of M. smegmatis when the growth medium was complimented with histidine in the presence of 1n and 2a indicating that these compounds inhibit the growth of Mtb by targeting histidine biosynthesis pathway. The molecular modelling studies revealed the binding interactions of 1n and 2a in the active site of ATP-PRTase supporting the activity of these compounds through inhibition of ATP-PRTase. The time dependent molecular dynamics simulation studies further supported the stability of 1n and 2a bound to the active site of the enzyme. Thus, benzo[d]thiazole-2-carboxamides and carbanilides can be exploited for identification of anti-TB agents by targeting the mycobacterial ATP-phosphoribosyl transferase enzyme, to develop new and effective anti-TB drugs.

Title: Early-stage detection of furcation radiolucency in primary mandibular molars using Vision Transformer

Speaker Name: Naveen Aggarwal

Affiliation: Panjab University, India

Abstract: Early childhood caries (ECC) is a prevalent oral health issue globally, affecting infants and preschoolers. Its severity can lead to furcation involvement in primary molars, a critical dental concern. Furcation radiolucency, a dark shadow between tooth roots on X-rays, indicates bone loss in this region as shown in Figure 1. Its early detection is crucial for timely intervention, preventing tooth extraction. Studies till date have not focused on pediatric IOPA for diagnosis of furcational pathology. The present study aims to apply a deep learning based architecture for effective pre-processing of periapical radiograph followed by improved segmentation and classification to detect furcation radiolucency in primary mandibular molars. For effective training and validation of models, we have created a labelled dataset of 5000 images from Retrospective cohort data of IOPA images taken from the Oral Health Sciences Centre, PGIMER Chandigarh INDIA. At the time of screening, the images with region of interest are manually cropped and further divided into two groups for model training.

The detection stage utilizes Faster-RCNN to accurately identify deciduous teeth and areas of furcation involvement. Performance is further enhanced by a novel ensemble-based Deciduous Detection Boosting (DDB) technique. For effective classification of furcation areas, we propose a spatial attention-based Vision Transformer (ViT) that processes resized segmented areas. The model is trained over multiple epochs to optimize parameters, then fine-tuned with hyper parameter adjustments on a validation set. Figure 2 represents the performance of proposed model trained over multiple epochs achieving an accuracy of 98.91%. This study could significantly aid in the early detection of furcation radiolucency in primary mandibular molars using IOPA radiograph images. A web interface for visual representation of detectable furcation lesions is also designed to assists doctors in treatment planning and report generation.

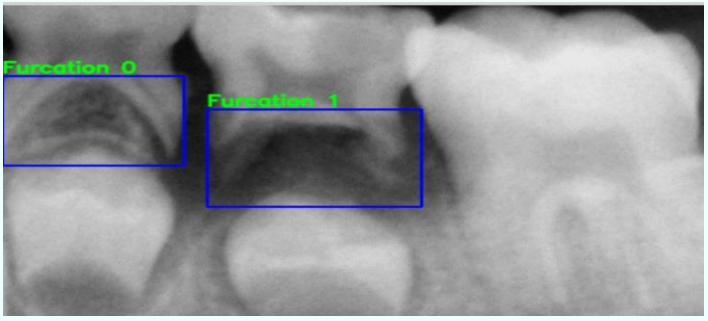
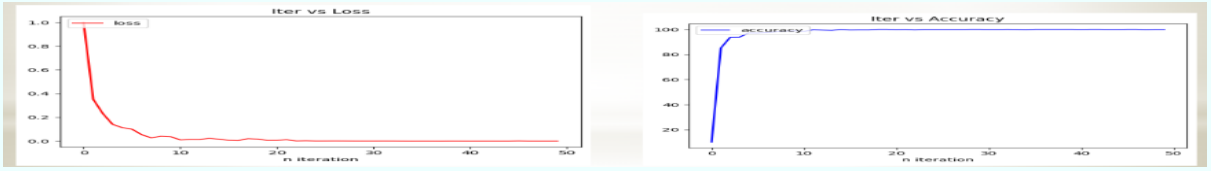


Figure 1: Deciduous teeth and the region of interest for furcation defects.



Title: De novo Design and Synthesis of dioate compounds: As a Novel and Preferable Antifungal Drugs

Speaker Name: Parisa Azerang

Affiliation: Pasteur Institute of Iran

Abstract: Objective: The primary objective of this study was to design, synthesize, and evaluate the antifungal properties of novel dioate compounds. These compounds were developed to overcome the limitations of current antifungal agents and to provide more effective treatment options.

Scope: The research focused on the de novo design of dioate molecules, leveraging molecular dynamics simulations and docking studies to predict their efficacy and stability. The scope included the synthesis of these compounds, followed by comprehensive biological testing to determine their antifungal activity.

Methodology: Initially, the drug design process involved computational methods, including molecular dynamics simulations and docking studies, to identify potential dioate structures with promising antifungal activity. These computational predictions guided the synthesis of the compounds in the laboratory. The synthesized compounds were then subjected to a series of biological assays to evaluate their antifungal properties. These assays included in vitro tests against various fungal strains to determine the minimum inhibitory concentrations (MICs) and the compounds' overall effectiveness compared to standard antifungal agents.

Results: The synthesized compounds exhibited significant antifungal activity in the biological assays. The results showed that these novel compounds had lower MIC values against a range of fungal strains, indicating higher potency compared to some existing antifungal drugs. The molecular dynamics and docking studies correlated well with the biological data, confirming the predicted interactions and stability of the compounds within the fungal cellular environment.

Conclusion: The study successfully demonstrated the potential of dioate compounds as effective antifungal agents. The de novo design approach, coupled with molecular dynamics and docking studies, proved to be a robust method for developing new antifungal drugs. The synthesized compounds not only showed excellent biological activity but also provided a promising foundation for further optimization and development as commercial antifungal treatments.

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Title: Exploring the therapeutic effects of sulforaphane: an in depth review on endoplasmic reticulum stress modulation across different disease contexts

Speaker Name: Samaneh Hajimohammadi

Affiliation: Mashhad University of Medical Sciences

Abstract: The endoplasmic reticulum (ER) is an intracellular organelle that contributes to the folding of proteins and calcium homeostasis. Numerous elements can disrupt its function, leading to the accumulation of proteins that are unfolded or misfolded in the lumen of the ER, a condition that is known as ER stress. This phenomenon can trigger cell death through the activation of apoptosis and inflammation. Glucoraphanin (GRA) is the predominant glucosinolate found in cruciferous vegetables. Various mechanical and biochemical processes activate the enzyme myrosinase, leading to the hydrolysis of glucoraphanin into the bioactive compound sulforaphane. Sulforaphane is an organosulfur compound that belongs to the isothiocyanate group. It possesses a wide range of activities and has shown remarkable potential as an anti-inflammatory, antioxidant, antitumor, and anti-angiogenic substance. Additionally, sulforaphane is resistant to oxidation, has been demonstrated to have low toxicity, and is considered well-tolerable in individuals. These properties make it a valuable natural dietary supplement for research purposes. Sulforaphane has been demonstrated as a potential candidate drug molecule for managing a range of diseases, primarily because of its potent antioxidant, anti-inflammatory, and anti-apoptotic properties, which can be mediated by modulation of ER stress pathways. This review seeks to cover a wealth of data supporting the broad range of protective functions of sulforaphane, improving various diseases, such as cardiovascular, central nervous system, liver, eye, and reproductive diseases, as well as diabetes, cancer, gastroenteritis, and osteoarthritis, through the amelioration of ER stress in both in vivo and in vitro studies.

Title: In vitro and In vivo effects of ethanolic extract of Fumaria parviflora Lam. embedded in chitosan nanoparticles against Leishmania major

Speaker Name: Azar Simin

Affiliation: Tarbiat Modares University

Abstract: Fumaria has been traditionally used to treat skin damages due to anti-inflammatory properties. In the present study, we evaluated the effect of the ethanolic extract of Fumaria parviflora Lam. (F. parviflora) against Leishmania major (L. major) using chitosan biopolymer drug delivery system both in vitro and in vivo models. The ethanolic extract of F. parviflora was analyzed by HPLC to determine its active ingredients content. The extract was then loaded on chitosan nanoparticles (CNPs). The parasite was treated with various concentrations of the ethanolic extract, CNPs and CNPs loaded with F. parviflora extract (CNPs@ F. parviflora). The size of lesions of treated mice were measured on a weekly basis. The parasite burden was evaluated eight weeks after treatment. The HPLC analysis showed the presence of Fumaric acid at a high concentration. The percentage of the drug released from CNPs@ F. parviflora within 24 and 72 hours were 65% and 90% respectively. The results showed that F. parviflora extract and CNPs@ F. parviflora caused 84% and 96% growth inhibition of L. major promastigotes as revealed by Neubauer chamber counting and MTT test respectively. The IC50 values of F. parviflora extract and CNPs@ F. parviflora were 450 and 68.4 µg/ml respectively. In amastigote assay the best results showed in CNPs@ F. parviflora that only 2% of macrophages were infected with amastigotes. In vivo experiments for mice treated with F. parviflora and CNPs @ F. parviflora in comparison to control group showed a significant reduction ($P<0.05$) in the mean diameter of the lesions (2.3 and 1.72 mm and 9.91 mm respectively). The ethanolic extract of F. parviflora both as standalone and loaded in CNPs showed promising inhibitory effects against L. major both upon in vitro and in vivo experimentation as well as therapeutic effects for wound healing in infected mice.

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Title: Review of fish protein hydrolysates: Production Methods, Antioxidant and antimicrobial activity and nanoencapsulation

Speaker Name: Mahrokh Nemati

Affiliation: Islamic Azad University

Abstract: Marine products are increasingly recognized for their valuable components, particularly proteins. However, the seafood industry generates significant waste due to the high perishability and low yield of these materials. Transforming low-value raw materials into high-value products is essential for sustainability, and protein hydrolysates have emerged as a leading solution in this regard. Fish Protein Hydrolysates (FPH), derived from various aquatic waste materials such as bones, scales, skin, and other by-products, are rich in proteins and peptides that can be utilized for a variety of value-added applications. Despite their numerous advantages, FPH face challenges, including undesirable taste profiles and high solubility, which can limit their broader application in food and nutraceuticals. Microencapsulation techniques present a promising scientific approach to overcome these limitations by protecting and stabilizing bioactive peptides, thus enhancing their functionality. This review systematically examines current research on the production methods of FPH, with a particular focus on their antioxidant and antibacterial activities. Among several production techniques, enzymatic hydrolysis using commercial enzymes has been identified as the most effective method for optimizing both the yield and functional properties of FPH. The antioxidant and antibacterial properties of FPH are substantiated through a range of in vitro studies, demonstrating their potential health benefits. Furthermore, microencapsulation using nanoliposomes has proven effective in prolonging the inhibitory activity of FPH while significantly enhancing their antioxidant and antibacterial capabilities. However, there remains limited information regarding the use of liposomes as nanocarriers for FPH to mitigate the bitter taste. Therefore, further research is necessary to enhance sensory attributes and reduce bitterness in protein hydrolysates, which is crucial for improving consumer acceptance and expanding their applications in the food industry.

Title: Mechanisms of Effectiveness of Intraosseous Therapy.

Speaker Name: Sokov Evgenii Leonidovich

Affiliation: Peoples' Friendship University of Russia - RUDN, Russia

Abstract: The intraosseous route of drug administration is equivalent to the intravenous route if the goal is to deliver the drug to the vascular bed of the body. When administered intravenously, the drug comes into contact with peripheral blood and the vascular wall. When administered intraosseously into spongy tissue, the drug acts: 1) on bone tissue, activating its reparative regeneration; 2) on bone marrow with stem cells; 3) on intraosseous afferent and efferent "slow" receptors, which are involved in the formation of pain, muscle-tonic, angio-spastic and other syndromes; 4) normalizes increased intraosseous pressure, which, irritating intraosseous receptors, creates pain and other symptoms; 5) the drug spreads into the blood vessels; 6) the drug spreads to the lymphatic vessels and nodes; 7) when introduced into the bones of the spine and pelvis, the drug penetrates the cerebrospinal valveless venous system, which is the central venous collector of the body and directly washes the central nervous system; 8) with intraosseous infusion into the iliac spine, the medicinal solution displaces bone marrow elements into the general bloodstream, distributing them throughout the body.

The impact of intraosseous infusion on such a large number of factors determines its high efficiency and can be called intraosseous therapy. We have been using intraosseous therapy since 1980 to treat a variety of conditions: low back and joint pain, headaches and facial pain, phantom and pelvic pain, complex regional pain syndrome and FBSS, diabetic polyneuropathy and erythromelalgia, pain and spasticity after stroke and multiple sclerosis, pain and plastic hypertonicity in parkinsonism, Modic 1-2 and post-Covid syndromes, other diseases.

Intraosseous therapy has shown a high degree of safety, effectiveness, and cost-effectiveness. The intraosseous therapy method is simple to perform and can be widely used in clinical practice.

The mechanisms of effectiveness of intraosseous therapy, especially the use of various drugs, require further research.

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Speaker Slots Filling Quickly

Title: A Novel Approach to Dementia Prediction of DTI Markers Using BALI, LIBRA, and Machine Learning Techniques

Speaker Name: Ahmad akbarifar

Affiliation: Islamic Azad University

Abstract: Early prediction of dementia and disease progression remains challenging. This study presents a novel machine learning framework for dementia diagnosis by integrating multimodal neuroimaging biomarkers and inexpensive and readily available clinical factors. Fractional anisotropy (FA) measurements in diffusion tensor imaging (DTI) provide microstructural insight into white matter integrity disturbances in dementia. However, the acquisition of DTI is costly and time-consuming. We applied Recursive Feature Elimination (RFE) to identify predictors from structural measures of the 7 factors of Brain Atrophy and Lesion Index (BALI) factors and 42 factors of Clinical Lifestyle for Brain Health (LIBRA) factors to estimate FA in DTI. The 10 most effective features of BALI/ LIBRA selected by RFE were used to train an interpretable decision tree model to predict the severity of dementia from DTI. A decision tree model based on biomarkers selected by RFE achieved an accuracy of 96.25% in predicting dementia in an independent test set. This integrated framework pioneers the prediction of white matter microstructural changes from available structural/ clinical factors using machine learning. By avoiding DTI acquisition, our approach provides a practical and objective tool to improve dementia screening and progress monitoring. The Identification of key predictive markers of BALI/ LIBRA will also provide information on the mechanisms of lifestyle-related disease mechanisms, neurodegeneration, and white matter dysfunction. This study aims to predict FA measures from DTI, which indicate white matter integrity and dementia severity, using inexpensive and readily available BALI and LIBRA factors through machine learning.

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Speaker Slots Filling Quickly

Title: The Role of Nutrition in Managing Hypertension: Strategies for a Heart-Healthy Diet"?

Speaker Name: Muhammad Akram

Affiliation: Government College University Faisalabad-Pakistan

Abstract: A significant fraction of the population suffers from hypertension, a serious worldwide health issue that is strongly associated with food habits and nutritional intake. The complex relationship between nutrition and hypertension is examined in this review, with a focus on the functions that different dietary components have in both treating and preventing high blood pressure. Fiber, potassium, calcium, and magnesium are important nutrients that support the diet's positive effects on vascular health and blood pressure regulation. On the other hand, high consumption of sodium, saturated fat, and refined sugar has always been associated with elevated blood pressure.

Oxidative stress, sodium-induced fluid retention, and endothelial dysfunction are the mechanisms that connect these dietary variables to hypertension. Furthermore, dietary regimens like the Mediterranean diet, which emphasizes ingesting a lot of healthy grains, nuts, seafood, and olive oil, have showed promise in lowering the prevalence of hypertension and improving cardiovascular outcomes. These dietary patterns have the potential to lower blood pressure because they include phytochemicals, antioxidants, and bioactive substances. In summary, altering eating habits is necessary for managing and preventing hypertension. By increasing the consumption of fruits, vegetables, whole grains, healthy fats, and lowering the intake of processed foods and sodium, it is feasible to considerably lower the prevalence of hypertension and the risks it poses for cardiovascular disease.

Title: Algae and Cyanobacteria as food supplements

Speaker Name: Abiola M. Asowata-Ayodele

Affiliation: University of Medical Sciences

Abstract: Microalgae have drawn a considerable interest of recent because of their importance in dietary food supplements and its potential applications in Biotechnology. Spirulina is one common and good example that has been extensively used as "health food" and is frequently purchased in supermarkets as tablets or dried powder.

Aim: Due to the fact that cyanobacteria contain nutrients like protein, amino acids, fructose, fatty acids, pigments, minerals, digestive and restricting enzymes, iron, and vitamin B6, consuming them as a food supplement has health, medicinal, nutraceutical, pharmaceutical, and therapeutic benefits to mentioned few. The work was done to give highlight on nutraceuticals gotten from algae origin.

Material and method: Series textbooks and articles were used to source for information online.

Result and Conclusion: Spirulina, which is typically accessible in supermarkets in the form of pills or powder that has been dried, is a well-known and superb example of a "health food" that has been used extensively. Because cyanobacteria are rich in nutrients like iron, vitamin B6, protein, amino acids, fructose, fatty acids, pigments, minerals, and digestive and restricting enzymes, using them as a food supplement has a multitude of health, medical, nutraceutical, pharmaceutical, and therapeutic effects. Microcystis aeruginosa and Thalassiosira weissflogii are two prevalent blue-green algae that have significant amounts of essential amino acid molecules in them. Numerous unique physiologically active chemicals are believed to be present in microalgae. Microcystis aeruginosa and Thalassiosira weissflogii are typical examples of blue-green algae with a significant amount of essential amino acid molecules. Microalgae have garnered significant attention recently because of their importance in dietary food supplements and potential applications in Biotechnology.

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Speaker Slots Filling Quickly

Title: Nanomaterials in Drug Delivery: Strengths and Opportunities in Medicine

Speaker Name: David Chukwu OBASI

Affiliation: London School of Hygiene and Tropical Medicine

Abstract: There is a myriad of diseases that plague the world ranging from infectious, cancer and other chronic diseases with varying interventions. However, the dynamism of causative agents of infectious diseases and incessant mutations accompanying other forms of chronic diseases like cancer, have worsened the treatment outcomes. These factors often lead to treatment failure via different drug resistance mechanisms. More so, the cost of developing newer drugs is huge. This underscores the need for a paradigm shift in the drug delivery approach in order to achieve desired treatment outcomes. There is intensified research in nanomedicine, which has shown promises in improving the therapeutic outcome of drugs at preclinical stages with increased efficacy and reduced toxicity. Regardless of the huge benefits of nanotechnology in drug delivery, challenges such as regulatory approval, scalability, cost implication and potential toxicity must be addressed via streamlining of regulatory hurdles and increased research funding. In conclusion, the idea of nanotechnology in drug delivery holds immense promise for optimizing therapeutic outcomes. This work presents opportunities to revolutionize treatment strategies, providing expert opinions on translating the huge amount of research in nanomedicine into clinical benefits for patients with resistant infections and cancer.

Title: Phytoremediation of Heavy Metals by Vetiver Grass near River Beds

Speaker Name: Leena Singh

Affiliation: Galgotia College of Engineering & Technology

Abstract:

Aquatic ecosystems worldwide are facing significant pollution challenges due to a wide range of contaminants, including heavy metals. These pollutants impact ecosystem structure, reducing population density, and species diversity, and altering community composition. Rapid urbanization, industrialization, and agricultural practices are contributing to deteriorating water quality, driven by both point and nonpoint pollution sources (Kusin et al., 2014; Chan, 2012). Given the toxic, persistent, and bio-accumulative nature of heavy metals, their presence in water bodies poses severe risks to both aquatic life and human health (Ali et al., 2019).

This study examines the effectiveness of vetiver grass (Chrysopogon zizanioides) in mitigating heavy metal contamination in aquatic environments. Vetiver grass has shown high potential in phytoremediation, a green technology using plants to extract, immobilize, and detoxify environmental pollutants. With its extensive root system, vetiver grass efficiently absorbs and stabilizes heavy metals such as cadmium, lead, and copper, reducing metal concentrations and the risk of leaching. Through water, sediment, and biological analysis, this research demonstrates that vetiver grass accumulates heavy metals primarily in its root tissues, offering a sustainable and cost-effective solution for improving water quality.

The results underscore the potential of vetiver grass-based phytoremediation as an eco-friendly alternative to traditional remediation techniques. This method minimizes secondary contamination risks, promoting safer and healthier aquatic ecosystems. Further research into large-scale applications of vetiver grass in contaminated riverbeds and other aquatic systems is recommended to validate its broader environmental benefits. Harnessing vetiver's phytoremediation capabilities can contribute to a sustainable approach in mitigating heavy metal pollution, thereby preserving aquatic biodiversity and promoting environmental health.

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Speaker Slots Filling Quickly

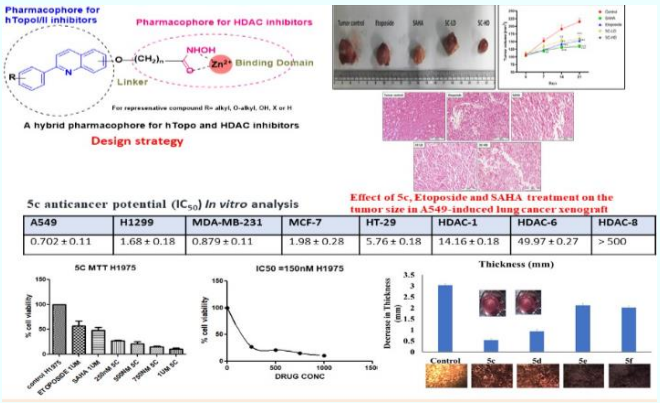
Title: Quinoline-hydroxamic acid inspired dual inhibitors of topoisomerase-histone deacetylase: Design, Synthesis, *in vitro* and *in vivo* anticancer potential

Speaker Name: Raj Kumar

Affiliation: Central University of Punjab

Abstract:

Topoisomerases (Topos) are among the most abundant proteins in the nucleus, second only to histone deacetylases (HDAC), both of which play crucial roles in regulating cellular processes. Despite the availability of several anticancer drugs that target these proteins, many have failed to deliver the desired therapeutic outcomes. These failures are often due to a lack of selectivity, low efficacy, excessive side effects, and the development of multi- drug resistance (MDR). Additionally, combination therapies face challenges such as varying pharmacokinetic profiles and drug-drug interactions. As a result, single-compound therapies with dual or multi-target inhibitory activity offer a more promising strategy for treating complex diseases like cancer. Synergistic effects between HDACs and human topoisomerases (hTopos) inhibitors have led to the development of multi-target inhibitors, which have garnered significant interest in cancer therapy.



A549	H1299	MDA-MB-231	MCF-7	HT-29	HDAC-1	HDAC-6	HDAC-8
0.702 ± 0.11	1.68 ± 0.18	0.879 ± 0.11	1.98 ± 0.28	5.76 ± 0.18	14.16 ± 0.18	49.97 ± 0.27	> 500

In this study, we aim to design and synthesize novel quinoline-bridged hydroxamate-based dual inhibitors targeting both hTopo and HDAC, and evaluate their potential as anticancer agents. The hybrid compounds demonstrated potent antiproliferative activity, with IC 50 values ranging from low micromolar to nanomolar concentrations. Among these, compound 5c exhibited the most robust inhibition of hTopo I/II and HDAC, with potency several times greater than the HDAC inhibitor SAHA. Furthermore, 5c was shown to modulate key oncogenic pathways and displayed favorable pharmacokinetic properties, including superior microsomal stability. In vivo studies revealed that compound 5c significantly inhibited tumor growth and improved survival in an A549 lung cancer xenograft model, outperforming standard anticancer drugs like vorinostat and etoposide. Compound 5c represents a promising lead for the development of dual Topo and HDAC inhibitors and may pave the way for further research into multi-target cancer therapies.

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Speaker Slots Filling Quickly

Title: Exploring the Role of Heme Oxygenase-1 in Cardiac Senescence and Myocardial Infarction: A Comprehensive Review of Triptych

Speaker Name: Tushar Ralhan

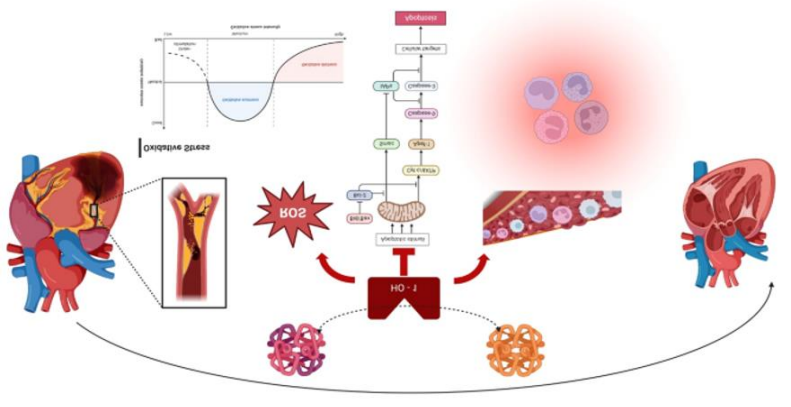
Affiliation: University of Missouri, USA

Abstract:

Background and Objectives: Heme oxygenase-1 (HO-1) is a vital enzyme in heme metabolism, breaking down heme into biliverdin, carbon monoxide, and free iron. Recognized for its cytoprotective properties, HO-1 has antioxidant, anti-inflammatory, and anti-apoptotic effects. This review aims to investigate the influence of HO-1 on cardiac senescence and its potential therapeutic implications in myocardial infarction (MI).

Methodology: A comprehensive literature review used scholarly databases including PubMed, Scopus, Google Scholar, Embase, and Web of Science. Relevant keywords were used to explore the evolving role of HO-1 in cardiac senescence and MI.

Results and Observations: Recent studies have revealed the critical role of HO-1 in cellular senescence, a process characterized by irreversible growth arrest and functional decline. Cardiac senescence, in particular, is now recognized as a critical factor in the progression of cardiovascular conditions such as MI. The accumulation of senescent cells, including vascular endothelial cells, smooth muscle cells, cardiomyocytes, and progenitor cells, contributes to diseases like vascular aging, atherosclerosis, and ventricular remodelling. HO-1 has been shown to mitigate cardiomyocyte senescence caused by ischemic injury and oxidative stress, thereby improving heart function. Evidence also links HO-1 genetic polymorphisms to cardiovascular outcomes, suggesting individual susceptibility to cardiac senescence. However, the role of HO-1 in obesity-related cardiovascular pathophysiology requires further investigation.



Conclusions: This review highlights potential strategies for upregulating HO-1, such as gene targeting and pharmacological agents, as promising therapeutic approaches. By synthesizing evidence from experimental models and clinical investigations, this study underscores the therapeutic potential of HO-1 in reducing cardiac senescence and improving outcomes in MI. Further research is necessary to fully realize HO-1's potential as a novel treatment strategy for cardiovascular diseases.

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Speaker Slots Filling Quickly

Title: Structural insights into trypanosomatid Mnk kinase orthologues (kMnks) suggest altered mechanism in the kinase domain

Speaker Name: Supratik Das

Affiliation: All India Institute of Medical Science (AIIMS)

Abstract:

Mitogen-activated protein kinase (MAPK) interacting protein kinases (Mnk1 and Mnk2) mediated phosphorylation of the eukaryotic initiation factor eIF4E is an important translation initiation control, in Mnk-mediated oncogenic activity and other disease conditions. Thus, Mnk kinases are an important target for therapy. Trypanosomatids are a class of kinetoplastids, some of which are protozoan parasites and cause diseases in humans. While protein translation initiation is well understood in eukaryotes and prokaryotes, there is a lack of sufficient structural information of this process in trypanosomatids. Here, we report that trypanosomatids have one orthologue of Mnk kinase with low overall sequence homology but high homology in the kinase domain and an additional C-terminal domain containing putative calmodulin binding site(s). We show that while many of the domains and motifs are conserved, homology modeling/structure prediction, docking analysis and molecular dynamics simulation studies suggest that trypanosomatid kMnk kinases, kinase domains are present in DFG-in conformation as opposed to the auto-inhibited DFD-out conformation of un-phosphorylated human Mnk1. Furthermore, we observed that several regulatory features are different in trypanosomatid kMnk kinases. Our study indicates that mechanism and regulation in the kinase domain of trypanosomatid kMnks are likely to be altered, and that they can be important drug targets.

Title: In vitro and in silico dynamic analysis of alkaloid extract of moringa oleifera leaf as a tocolytic agent.

Speaker Name: Ofulue Ofioritse Ogheneyoma

Affiliation: Delta State University

Abstract:

Background of Study: Tocolytics are substances which prevent preterm births by reducing or stopping uterine contractions. This study is aimed at using both in vitro and in silico docking in investigating Alkaloid extract of Moringa oleifera leaf (AML) as a tocolytic agent.
Method: The in vitro study was carried out on isolated uteri of albino wistar rats, a cumulative application of AML and its active fraction; chloroform fraction of AML (CAML) to the isolated uterine tissues was done. Compounds present in CAML were investigated via GC-MS. In the in silico study, compounds present in CAML were docked using the Autodock program to predict the most active compounds and possible binding sites between CAML and some target proteins (OXTR, ERs, COX-1 and TNF-α) associated with uterine contractions and the pharmacokinetic properties of the active compounds identified were investigated using lipinski rule of five (5).
Results and Discussion: In the in vitro study, the result showed that AML and CAML significantly inhibited spontaneous contractions. This suggests that CAML and AML may interact with calcium influx. CAML significantly inhibited oxytocin-induced, KCl-induced and calcium-free solution contractions. In silico study; 6 out of 47 compounds present in CAML had a strong binding affinity for OXTR, ERs, COX-1 and TNF-α as shown in the Table below and the pharmacokinetic investigation showed that these 6 compounds were likely oral drug candidates.
Table: Binding affinities of reference compounds and promising compounds to proteins associated with increased uterine contractions.

		Binding affinity (Kcal/mol)			
	Compounds	OXTR	ERs	COX-1	TNF-α
R	Retosiban	-10.2			
R	Clomiphene		-8.7		
R	Indomethacin			-8.6	
R	Curcumin				-7.9
1	Benzoic acid, 2-hydroxy-, phenylmethyl ester	-8.2	-8.2	-9.1	-6.1
2	Linolenic acid	-7.3	-6.8	-10.0	-6.9
3	Linoleic acid ethyl ester	-8.3	-7.0	-8.9	-6.6
4	trans-Geranylgeraniol	-7.4	-6.6	-8.7	-6.6
5	Phosphoric acid, trioctyl ester	-10.5	-7.9	-9.9	-7.4
6	Bis(2-ethylhexyl) phthalate	-10.3	-8.8	-8.9	-8.3

Reference Compound: R; Oxytocin Receptors - OXTR; Estrogen Receptors -ERs; Cyclooxygenase -COX-1; Tumor Necrosis Factor – Alpha - TNF-α.
Conclusion: CAML was observed to have the ability to prevent the release of calcium from the intracellular stores and also block its entry into the cytoplasm from the extracellular stores in the uterus, this makes it a strong tocolytic agent. The active compounds in CAML that are likely causing this tocolytic effect was also discovered. This discovery could enhance existing knowledge and act as a foundation which can be built up on in futher research in exploring compounds and substances from moringa oleifera leaves for the treatment of female reproductive problems associated with increase uterine contractions.

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Speaker Slots Filling Quickly

Title: Novel effect of topical Roquinimex and its combination with Clobetasol on an imiquimod- induced model of psoriasis in mice

Speaker Name: Abeer Mohammed Hasan Garma

Affiliation: Al-Nahrain University

Abstract:

Psoriasis is a chronic inflammatory skin condition affecting multiple systems and the skin, with topical therapy representing the fundamental treatment modality for psoriasis. Investigate the effect of topical Roquinimex (ROQ) alone and combined with Clobetasol propionate (CLO) on imiquimod (IMQ)-induced mouse model as a novel approach to treating psoriasis. Sixty male Swiss Albino mice were divided into six groups of ten mice; all groups except the negative control received IMQ cream 5% (62.5 mg) as a once-daily topical application for six days. On the seventh day, five groups (except negative control) received one of the following treatments for eight days: no treatment (positive control), Petrolatum gel 15% as a twice-daily topical application (Petrolatum control), CLO 0.05% ointment once daily, ROQ ointment 1% w/w twice daily topically, topical preparation of 0.025% CLO ointment combined with ROQ ointment 0.5% w/w twice daily; the total duration of the study is 14 days. The clinical, pathological, and laboratory effects were then measured. The use of ROQ ointment alone or combined with CLO resulted in significant improvement in psoriasis lesions (measured by Baker's and PASI scores) compared to positive control groups (2.15±1.08, 1.60±0.61, 9.00±0.00, and 7.60±0.84, respectively for Baker's score) (1.50±1.08, 1.30±0.95, 11.70±0.48, 9.30±0.67, respectively for PASI score), a similar improvement seen for various inflammatory markers, including interleukin (IL)-10 (140.53±60.68, 285.63±92.16, 31.83±3.03, and 92.50±27.13 pg/ml, respectively), IL-17 (126.58±40.98, 124.26±61.40, 553.04±141.32, and 278.52±100.27 pg/ml, respectively), tumor necrosis factor-α (72.34±23.40, 30.11±7.01, 807.13±500.06, and 281.79±240.17 pg/ml, respectively), and vascular endothelial growth factor (109.71±29.35, 80.96±24.58, 552.20±136.63, 209.56±73.31 pg/ml and respectively). Roquinimex exerts its antipsoriatic effect through multiple mechanisms; its combination treatment with Clobetasol is a promising therapy for managing psoriasis.

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Speaker Slots Filling Quickly

Title: Sodium citrate buffer improves pazopanib solubility and absorption in gastric acid-suppressed rat model

Speaker Name: Huda Jassim Muhammad

Affiliation: Karbala University, Iraq

Abstract:

The low solubility and variable absorption of pazopanib in gastric acid-suppressed conditions pose a significant challenge to its therapeutic efficacy. This study investigates the potential of a sodium citrate buffer system to improve pazopanib solubility and absorption in a gastric acid-suppressed rat model. The objectives of the study were to evaluate the solubility enhancement of pazopanib in the presence of sodium citrate buffer and its subsequent effect on absorption.

Methods included solubility studies conducted in different buffer solutions, followed by in vivo absorption tests in rats with induced gastric acid suppression. Preliminary studies were also carried out to determine the optimal dose of an acid-suppressing agent required to effectively inhibit gastric acid secretion in the animal model. The pharmacokinetic parameters of pazopanib, including plasma concentration and bioavailability, were analyzed after oral administration.

The results showed that pazopanib solubility significantly increased in sodium citrate buffer compared to standard conditions. In vivo absorption studies further demonstrated a marked improvement in the plasma concentration of pazopanib in gastric acid-suppressed rats when administered with sodium citrate buffer. The enhanced solubility and absorption were attributed to the buffering capacity of sodium citrate, which maintained an optimal pH environment for drug dissolution despite gastric acid suppression.

In conclusion, the sodium citrate buffer system effectively enhances pazopanib solubility and absorption under conditions of reduced gastric acidity. This approach holds promise for improving the oral bioavailability of pazopanib in patients on gastric acid-suppressing medications, providing a potential solution for overcoming drug absorption variability.

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Speaker Slots Filling Quickly

Title: Evaluation of the antimalarial properties of *Solanum incanum* L. leaf extract fractions and its ability to downregulate delta aminolevulinate dehydratase to prevent the establishment of malaria infection

Speaker Name: Ogochukwu Caroline Chiamah

Affiliation: Alex Ekwueme Federal University Ndufu-Alike

Abstract:

This study investigated the effectiveness of Solanum incanum leaf extracts as a curative and prophylaxis in malaria parasite infection and evaluated its ability to decrease δ-ALAD expression. The leaves of S. incanum were pulverized and subjected to a successive extraction protocol to obtain crude, hexane, ethyl acetate, and aqueous extract fractions. Phytochemical and GC-MS analyses were conducted on extract fractions. An acute toxicity study was also performed on the extracted fractions. The potency of the extract fractions as curative and prophylactic antimalarial was then evaluated using Plasmodium berghei-infected mice at 100 mg/kg. The extract fraction with the highest activity was further evaluated at varying doses and its effect on δ-ALAD was measured using RT-qPCR. Parasitemia, chemosuppression, and mean survival time were used as activity indices. Phytochemical analysis revealed the presence of terpenoids, flavonoids, and phenols in the ethyl acetate and aqueous extract fractions while alkaloids were only present in aqueous extract, and quinones were found in the crude extract. However, all extract fractions contained saponins but lacked tannins. While the plant extracts were found to be non-toxic, they did not exhibit curative antimalarial activity. However, all extract fractions showed prophylactic antimalarial activity, with the ethyl acetate extract having the highest chemosuppressive activity. In the negative control, the expression of δ-ALAD was 5.4-fold, but this was significantly reduced to 2.3-fold when mice were treated with 250 mg/kg of the ethyl acetate fraction. GC-MS analysis of the ethyl acetate fraction revealed the presence of 2-methyloctacosane, tetracosane, and decane. The fractions extracted from S. incanum leaves have been found to possess only antimalarial prophylactic properties, with the ethyl acetate extract fraction showing the most effective results. The activity of this fraction may be attributed to its ability to decrease the expression of δ-ALAD, as it contains an alkane compound implicated with enzyme-inhibitory activity.

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Speaker Slots Filling Quickly

Title: Impact of Photobiomodulation on IL1β and TGFβ-1 concentrations in patients with aphthous stomatitis

Speaker Name: Dalia Saleem Kareem

Affiliation: University of Baghdad, Iraq

Abstract:

Laser therapy has shown effectiveness in promoting wound healing by influencing various physiological factors such as blood flow, cytokines, histamine, nerve signals, lymphocyte function, tissue oxygenation, and cell growth. This study aims to evaluate the therapeutic efficacy of Photobiomodulation (PBM) treatment, by using diode laser, in modifying the levels of interleukin-1 beta (IL1β) and transforming growth factor beta-1 (TGFβ-1) in patients diagnosed with aphthous stomatitis. A before-after interventional design was conducted over 10 months with 20 subjects. Data on demographic details and serum concentrations of IL1β and TGFβ-1 were collected pre-treatment and on Days 3 and 7 post-treatments. The intervention involved a single session of four 30-second applications of a QuickLase dual-wavelength laser operating at 980 nm. Results show significant reductions in IL1β and TGFβ-1 levels after 7 days of treatment, indicating a time- dependent effect of PBM therapy on these inflammatory markers. The findings suggest that PBM therapy holds promise as an intervention for reducing inflammation associated with aphthous stomatitis.

Title: Flaxseed: A novel approach to enhanced wound healing

Speaker Name: Basma Ezzat Mustafa Alahmad

Affiliation: International Islamic University Malaysia

Abstract:

Delayed wound healing in diabetic patients remains a critical clinical challenge, driving the need for innovative and effective therapeutic approaches. Medicinal plants, including flaxseed, have gained increasing attention due to their regenerative properties and potential to address wound-healing complications. This study explores the therapeutic effects of flaxseed extract on wound healing in diabetic animal models, emphasizing its anti- inflammatory, antibacterial, antifungal, and antioxidant characteristics.

A total of forty-five male white New Zealand rabbits were included in the study, with four full- thickness, linear wounds created bilaterally on the dorsal skin of each animal. Tissue samples were collected on days 4, 7, and 14 post-wounding for histopathological analysis, evaluating key wound healing parameters such as inflammation, re-epithelialization, neovascularization, and surface closure rates. The results revealed that flaxseed extract significantly accelerates healing by enhancing keratinocyte and dermal fibroblast proliferation, promoting collagen deposition and maturation, facilitating new blood vessel formation, and reducing inflammation throughout the healing intervals.

Additionally, flaxseed extract improved skin elasticity and firmness during healing, providing further benefits beyond wound closure. These findings underscore the therapeutic potential of flaxseed extract as a promising topical agent for diabetic wound management. They suggest its applicability in developing advanced, efficient wound dressings for clinical use.

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Speaker Slots Filling Quickly

Title: Health hazards of waste water from mines in mining host communities in South east Nigeria

Speaker Name: Okoro, Chukwuemeka Ogbonna

Affiliation: David Umahi Federal University of Health Science

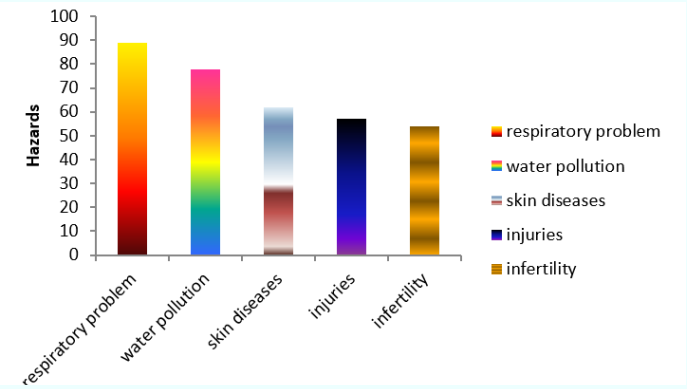
Abstract:

Background and Aim: Quarrying, mining and mineral processing in Nigeria are key activities that have had a great contribution to human civilization. Intentionally or unintentionally large volumes of water are used at mines and are released to the environment. The extractive sector in Nigeria has high magnitude of human rights violations and the urgent need for action is now. This study investigated the health hazards of waste water from mines.

Methodology: The research adopted mixed methods (both quantitative and qualitative) involving multiple sets of stakeholders (Mine Owners, Miners and Sorters, Civil Society Organizations, Community members and Government Officers) in the extractive minerals value chain. Purposive samples of respondents across the states were used based on their levels of involvement in the value chain. The key informant interviews of ten (10) in a group were both in person and phone calls and Focus Group Discussions (FGD), using interview and FGD guides.

Results: A little more than half 53.8% of the respondents interviewed stated that they were not aware of policies and health regulations governing mining sector, 38.5% said they were aware while 7.7% were indifferent. Those who were aware of the policies could only mention minerals act as the policies governing the sector. 90 % of our respondents agreed that people in Minerals value chain and miners are exposed to various forms of harms and abuses (respiratory problems (89 %), water pollution (78%) skin diseases (62%), injuries (57%) and infertility (45%).

Conclusion and recommendations: The result showed that our respondents believed that women, children were more vulnerable to health hazards associated with waste water from mining. It was attributed to their low level of information, drinking of contaminated water, eating of contaminated plants with toxins within the mines and long stay in exposed mining sites sorting and packaging and even warehousing the minerals such as lead without personal protective equipment. Treatment of waste water before discharge and Mechanized equipment for sorting and mining of minerals should be used. Collaboration with other researchers to find the level of waste water effect on biodiversity



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Title: Evaluation of oral and dermal health risk exposures of contaminants in groundwater resources for nine age groups in two densely populated districts

Speaker Name: Daniel Ayomikun Ayejoto

Affiliation: Texas Christian University, TX, USA

Abstract:

Human health and the sustainability of the socioeconomic system are directly related to water quality. As anthropogenic activity becomes more intense, pollutants, particularly potentially harmful elements (PHEs), penetrate water systems and degrade water quality. The purpose of this study was to evaluate the safety of using groundwater for domestic and drinking purposes through oral and dermal exposure routes, as well as the potential health risks posed to humans in the Nnewi and Awka regions of Nigeria. The research involved the application of a combination of the National Sanitation Foundation Water Quality Index (NSFWQI), HERisk code, and hierarchical dendrograms. Additionally, we utilized the regulatory guidelines established by the World Health Organization and the Standard Organization of Nigeria to compare the elemental compositions of the samples. The physicochemical parameters and NSFWQI evaluation revealed that the majority of the samples were PHE-polluted. Based on the HERisk code, it was discovered that in both the Nnewi and Awka regions, risk levels are higher for people aged 1 to 65 than for people aged 16 to Pb > Cu > Fe for Nnewi and Pb > Cd > Cu > Fe for water samples from Awka. Summarily, groups of middle age are less susceptible to possible health issues than children and elderly individuals. Hierarchical dendrograms and correlation analysis showed the spatio-temporal implications of the drinking groundwater quality and human health risks in the area. This research could help local government agencies make informed decisions on how to effectively safeguard the groundwater environment while also utilizing the groundwater resources sustainably.

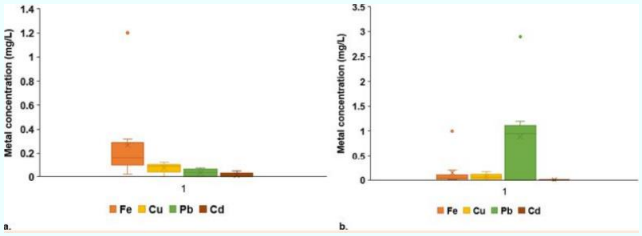

Fig. 1 Statistical distribution and variation of the heavy metals shown using box and whisker plots (a) Nnewi and (b) Awka

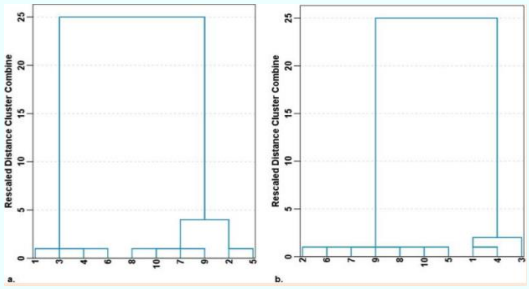

Fig. 2 Hierarchical dendrograms for classifying the water quality based on NSFWQI for (a) Nnewi and (b) Awka

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Title: Assessment of the antileishmanial activity of diallyl sulfide combined with meglumine antimoniate on *Leishmania major*: Molecular docking, *in vitro* and animal model

Speaker Name: Farzaneh Zarrinkar

Affiliation: Kerman University of Medical Sciences

Abstract:

Currently, no safe vaccine against leishmaniasis is available. So far, different control strategies against numerous reservoir hosts and biological vectors have not been environment friendly and feasible. Hence, employing medicinal components and conventional drugs could be a promising approach to developing novel therapeutic alternatives. This study aimed to explore diallyl sulfide (DAS), a dynamic constituent of garlic, alone and in a mixture with meglumine antimoniate (MAT as standard drug) using in vitro and animal model experiments against Leishmania major stages. The binding affinity of DAS and four major defence elements of the immune system (iNOS, IFN-γ, IL-12, and TNF-α) was used to predict the predominant binding mode for molecular docking configurations. Herein, we conducted a broad range of experiments to monitor and assess DAS and MAT potential treatment outcomes. DAS, combined with MAT, displayed no cytotoxicity and employed a powerful antileishmanial activity, notably against the clinical stage. The function mechanism involved immunomodulation through the induction of Th1 cytokine phenotypes, triggering a high apoptotic profile, reactive oxygen species (ROS) production, and antioxidant enzymes. This combination significantly decreased cutaneous lesion diameter and parasite load in BALB/c mice. The histopathological findings performed the infiltration of inflammatory cells associated with T-lymphocytes, particularly CD4+ phenotypes, as determined by biochemical markers in alleviating the amastigote stage and improving the pathological changes in L. major infected BALB/c mice. Therefore, DAS and MAT deserve further advanced therapeutic development and should be considered as possible candidates for treating volunteer cases with cutaneous leishmaniasis in designing an upcoming clinical trial.

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Title: Triclosan-induced histopathological alterations, oxidative stress, and immune dysfunction in the skin of the fish, *Cyprinus carpio*

Speaker Name: Usha Kumari

Affiliation: Banaras Hindu University

Abstract:

Triclosan (TCS), a widely used broad-spectrum antibacterial agent in several personal care and household products, is found in various aquatic environments at concentrations capable of causing detrimental effects to non-target organisms. Due to high lipophilicity, it can also be easily absorbed through the body surface of aquatic organisms. The study investigated the impact of three sublethal concentrations (1 µg/L, 10 µg/L and 100 µg/L) of TCS on the skin of fish Cyprinus carpio for 28 days. The histopathological alterations observed in the skin epidermis were hypertrophy, hyperplasia, and sloughing of epithelial cells. Intracellular vacuolisation, shrinkage, and degeneration in the content of club cells were also observed. The results of the biochemical analysis showed a significant ($p<0.05$) decrease in the activity of superoxide dismutase, catalase, glutathione-s-transferase, glutathione reductase, glutathione peroxidase, and reduced glutathione content. However, a significant ($p<0.05$) increase in the activity of acid phosphatase, alkaline phosphatase, lactate dehydrogenase; and the level of lipid peroxidation and nitric oxide was observed in the exposed groups till 28 d. In addition, TCS inhibited acetylcholinesterase activity from 7-28 d while significant accumulation in acetylcholine content was observed at the end of 28 d. A significant concentration-dependent increase in glucose, triglyceride, cholesterol and cortisol levels was observed at 28 d of exposure. Moreover, TCS exposure increased IL-6, TNF-α, and a decline in IL-10 at 28 d of exposure duration. This study reveals that TCS exposure alters the fish skin physiology affecting its barrier function.

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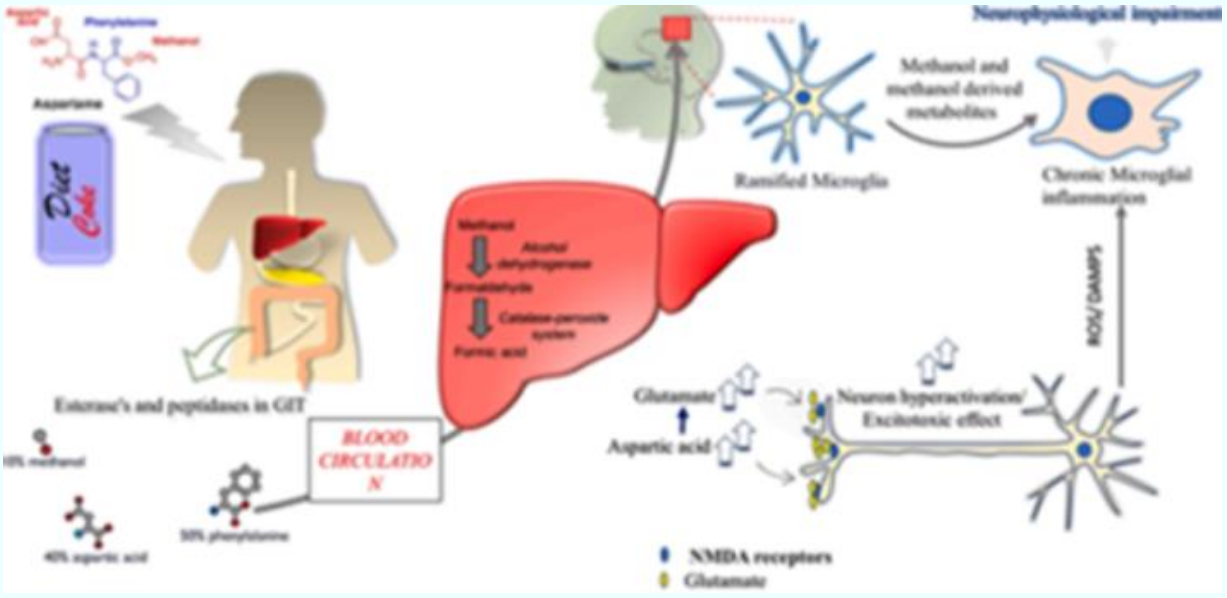
Title: Aspartame-induced cognitive dysfunction: Unveiling role of microglia-mediated neuroinflammation and molecular

Speaker Name: Waseem Dar

Affiliation: Shiv Nadar Institution of Eminence

Abstract:

Aspartame, an artificial sweetener, is consumed by millions of people globally. There are multiple reports of aspartame and its metabolites affecting cognitive functions in animal models and humans, which include learning problems, headaches, seizures, migraines, irritable moods, anxiety, depression, and insomnia. These cognitive deficits and associated symptoms are partly attributed to dysregulated excitatory and inhibitory neurotransmitter balance due to aspartate released from aspartame, resulting in an excitotoxic effect in neurons, leading to neuronal damage. However, microglia, a central immunocompetent cell type in brain tissue and a significant player in inflammation can contribute to the impact. Microglia rapidly responds to changes in CNS homeostasis. Aspartame consumption might affect the microglia phenotype directly via methanol- induced toxic effects and indirectly via aspartic acid-mediated excitotoxicity, exacerbating symptoms of cognitive decline. Long-term oral consumption of aspartame thus might change microglia's phenotype from ramified to activated, resulting in chronic or sustained activation, releasing excess pro-inflammatory molecules. This pro-inflammatory surge might lead to the degeneration of healthy neurons and other glial cells, impairing cognition. This review will deliberate on possible links and research gaps that need to be explored concerning aspartame consumption, ecotoxicity and microglia- mediated inflammatory cognitive impairment. The study covers a comprehensive analysis of the impact of aspartame consumption on cognitive function, considering both direct and indirect effects, including the involvement of microglia-mediated neuroinflammation. We also propose a novel intervention strategy involving tryptophan supplementation to mitigate cognitive decline symptoms in individuals with prolonged aspartame consumption, providing a potential solution to address the adverse effects of aspartame on cognitive function.



Title: Deep learning for prediction of cardiomegaly using chest X-rays

Speaker Name: Mrigakshi Gupta

Affiliation: Netaji Subhas University of Technology (NSUT)

Abstract:

In the past decade, deep learning in biomedical imaging has exponentially increased the accuracy of disease detection and improved the health standards. This research paper introduces a novel approach for the early detection and diagnosis of cardiomegaly using the cardiothoracic ratio (CT ratio) measurement in chest X-ray scans. Cardiomegaly is a serious cardiac condition that can lead to life-threatening complications if left undiagnosed. The proposed method involves segmenting the heart from a chest CT scan using a convolutional neural network model, ResNet-18, and calculating the CT ratio, which is the ratio of the maximum width of the heart to the maximum width of the thoracic cage. Studies have shown that increasing CT ratio leads to an increasing risk of heart diseases. Hence, a need to monitor the CT ratio for every individual arises, for if the ratio changes, an alert to take precautions can be rang. The method is evaluated using a dataset of 490 chest X-ray scans, and it achieves an accuracy of 84% and a precision of 93%.

The integration of CT ratio measurement in chest X-ray scan reports has the potential to aid in the early detection and diagnosis of cardiomegaly, allowing for prompt medical intervention and improving patient outcomes.

Title: Comparative analysis of intra and inter prediction compression techniques for endoscopic videos

Speaker Name: Heena Kouser Gogi

Affiliation: HKBK College Of Engineering, Bengaluru

Abstract:

The cloud-based health-care system has opened up new possibilities in the medical profession. By monitoring the whole digestive tract, endoscopic technology has improved the diagnosis of gastrointestinal illnesses and diseases. Image compression enhances the frame rate, which helps the diagnostic procedure. The aims of presenting this paper is to put light on brief review of image compression into two categories intra and inter prediction for endoscopy video compression, which is efficient and simple. Our research work shows an acceptable compression performance, the initial phase of work is an implementation of Intra prediction and the second phase of work is inter-prediction technique, which show a mark able performance in term of PSNR value, bit rate and compression ratio.

Title: Effect of Melia azedarach seed mediated nano-ZnO on growth performance, protein utilisation efficiency, haematology and nutritional status in pigs

Speaker Name: Enathi Dinga

Affiliation: North West University-South Africa

Abstract:

The current study was conducted to investigate the effect of Melia azedarach seed-mediated ZnO nanoparticles on growth performance, protein utilisation efficiency, haematology and nutritional status in pigs. A total of 48 pigs were allocated to the following six treatments replicated 8 times: Negative Control (NC, No antibiotic), Treatment 2: Positive control (PC) given a conventional antibiotic (Oxytetracycline, 40 mg/kg feed); Treatment 3: Nano-ZnO 300 mg/L (N300ZnO), Treatment 4: Group given 150 mg/L Melia azedarach seed mediated nano-ZnO (N150MA), Treatment 5: Group given 300 mg/L Melia azedarach seed mediated nano-ZnO (N300MA), Treatment 6: Group given 450 mg/L Melia azedarach seed mediated nano-ZnO (N450MA). The experiment was conducted over 7 weeks. Melia azedarach seed-mediated ZnO nanoparticles had no significant effect on growth performance apart from average daily feed intake (ADFI) with treatment 3 having the highest value. It also improved growth performance and cumulative weight gain when compared to conventional antibiotics. The green synthesized nanoparticles significantly affected protein consumption and growth efficiency but not protein efficiency ratio and specific growth rate. Melia azedarach seed-mediated ZnO nanoparticles had no significant impact on nutritional parameters, serum minerals apart from phosphorus which can negatively affect renal functioning.

Title: Design and synthesis of imidazoquinoxaline based fused heterocycles and in vitro assessment as anticancer agents

Speaker Name: Kapil Kumar Goel

Affiliation: Gurukul Kangri Deemed to Be university

Abstract:

Imidazoquinoxaline, one of the many azaheterocycles, is a special scaffold with a variety of pharmacological properties that has been thoroughly studied for its potential to treat cancer. Imidazoquinoxaline, being a synthon, offers numerous opportunities for structural alterations, drawing the interest of numerous researchers in the creation of novel anticancer compounds with enhanced target specificity and efficacy. The emergence of imiquimod and the subsequent derivatives EAPB203 and EAPB503 increased the recognition of this structural pharmacophore.

In the first goal, we used a pharmacophore mapping strategy to investigate the structural requirements needed for a synthetic to function as a tubulin inhibitor. We created a pharmacophore for one of the chemicals in our prototype, and the pharmacophore and its binding model may offer crucial insights for logical structure-based drug design.

To find a lead against tubulin as an anticancer drug, we rationally chose a library of 34 fused imidazo[1,2-a]quinoxaline and employed molecular docking, virtual screening, and molecular mechanics. The pharmacophoric attributes of Colchicine and EAPB203, approved and investigational drugs, respectively and known to inhibit the tubulin and possess potential anticancer assets. 1A2 was identified by computational analysis and pharmacophoric features as a possible lead against tubulin, since it possessed the highest affinity and binding score at the tubulin's colchicine binding site. Here, in silico methods were effectively used to determine which fused azaheterocycles produced the most likely leads.

The second goal involved creating a novel series of imidazole-based compounds with varied substitution patterns. These compounds include fused and non-fused imidazole-based compounds with distinct substituents at different imidazole and aryl ring points of interest. The modified compounds have been evaluated for their cytotoxic activity against four types of carcinogenic cell lines: MCF-7, MDA-MB-231 (breast cancer cell lines), A549 (lung cancer cells), and HCT-116 (colon cancer cells). Imidazoloquinoxaline-containing compound P2 and non-fused imidazole derivative compound P5 were identified as promising leads with cytotoxicity profiles against these cell lines resembling those of colchicine.

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Title: Urinary biomarkers ungal and kim-1: precision tools for early detection of acute kidney injury in canine leptospirosis and babesiosis

Speaker Name: Deepa PM

Affiliation: Kerala Veterinary and Animal Sciences University

Abstract:

Acute kidney injury (AKI) is a critical condition in dogs with leptospirosis and babesiosis, necessitating early detection for effective management. This study evaluated the diagnostic efficacy of urinary Neutrophil Gelatinase-Associated Lipocalin (uNGAL) and Kidney Injury Molecule-1 (uKIM-1) in detecting AKI at early stages.

Methods: AKI diagnosis was based on International Renal Interest Society (IRIS) guidelines, defined by an increase in serum creatinine ≥0.3 mg/dL within 48 hours. Dogs were categorized into AKI grades. Urinary NGAL and KIM-1 levels were compared with control dogs and traditional markers (serum creatinine and blood urea nitrogen). Statistical significance ($P<0.01$) across AKI grades was evaluated.

Results: Urinary NGAL and KIM-1 levels were significantly elevated in dogs with AKI compared to controls, with the highest sensitivity observed in non-azotemic cases (IRIS grade I; $P<0.001$). These biomarkers demonstrated superior diagnostic performance compared to traditional markers.(Table 1, Figure1).

Conclusion: uNGAL and uKIM-1 are promising early, non-invasive biomarkers for detecting AKI in dogs, particularly in subclinical stages. Their use in clinical settings could facilitate early intervention and improve outcomes. Further validation in larger cohorts is needed to confirm their broader utility in veterinary medicine.

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Title: A Novel Combination of Plant Quercetin and Drugs with anticancer potential

Speaker Name: Mary Shobha Rani Inala

Affiliation: Sri Devaraj Urs Academy of Higher Education and Research

Abstract:

Objectives: To screen the efficacy of plant derived quercetin with synthetic drugs against breast, colon and prostate cancer cell-lines.

Scope: Screening of anticancer potential helps to identify new treatment options for the cancers.

Methods: Quercetin was extracted from Anethum graveolens L. and Raphanus sativus L. by maceration, digestion and column chromatography procedures. Confirmed by thin layer and checked for purity by High performance Liquid Chromatography. The pure compound was then screened for anticancer potencies. Anticancer ability was checked against MCF-7, PC- 3 and COLO 320 cell-lines by determining its cytotoxicity, mitochondrial membrane potential, caspase-3 activity, apoptosis by dual stain method and cell cycle arrest.

Results: Quercetin in combination with Anastrozole on breast cancer (MCF-7); Capecitabine on colon cancer (COLO 320) showed potent cytotoxic effect and hence can be considered as an adjuvant for synthetic drugs in chemotherapy. Quercetin in combination with drugs displayed morphological changes in nuclei of both breast and colon cancer cells indicating damage to the cells.

Conclusion: To conclude, the combination of quercetin with chemotherapeutic drugs, Anastrozole and Capecitabine is reported for the first time.

Title: Clinical and sub-clinical features of *talaromyces marneffei* infection in hiv/aids patients treated at national hospital for tropical disease

Speaker Name: Bùi Văn Nam

Affiliation: National Hospital for Tropical Diseases

Abstract:

Talaromyces marneffei is a fungus that causes important opportunistic infections (OI) and increases mortality in people with HIV/AIDS. Objectives: We assessed the clinical and laboratory characteristics in HIV/AIDS patients infected with T. marneffei. Methods: 57 HIV/AIDS patients infected with T. marneffei treated at the National Hospital of Tropical Diseases, from January 2023 to April 2024, were studied. Results: The disease occurs in all ages, concentrated in the group under 40 years old and men. Patients are more distributed in the midlands than in the plains and mountains. The median time to admitted hospital from fever onset was 14 days. Common systemic manifestations were fever (94.7%), fatigue (84.2%), weight loss (64.1%), peripheral lymph nodes (54.4%) and skin lesions (52.6%). Organs with lesions included respiratory, digestive, anemia, hepatomegaly, coagulation index disorders and electrolyte disorders. The number of patients with 1 - 4 other OI was 70.2%, CD4 < 200 cells was 97.7% (less than 50 cells was 79.1%). In 57 patients with positive blood culture results, T. marneffei was also detected on skin papules (36.8%), sputum (19.8%), lymph nodes, bone marrow, urine and abdominal fluid. Conclusion: T. marneffei infection was very severe and diagnosis was often delayed, so in people with HIV/AIDS, along with early treatment with ARV, it was necessary to guide hygiene measures to prevent this fungus. Techniques for early detection of T. marneffei should also be implemented.

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Title: Use of bioactive compounds from plants as therapeutics in preventing Cancer

Speaker Name: Kanu Priya

Affiliation: School of Basic Sciences and Research, Sharda University

Abstract:

With the passage of time, we have seen the colossal upsurge of the use of bioactive compounds derived from plants for cancer prevention. This therapy has established significant attention in recent years. Traditional methods like chemotherapy are single targeted approach to combat cancer, however, cancer includes various factors like genes or epigenetics. Because of which the methods which comes with the holistic approach has drawn attention of scientists. Asian countries like China, India, Taiwan, Japan has been extensively used the natural products in day-to-day life. There are certain substantial bioactive components which play important role in preventing cancer, which includes polyphenols, terpenoids, alkaloids, saponins. These natural compounds, found in various plant sources, have demonstrated potential in modulating multiple pathways involved in cancer development and progression. Certain bioactive compounds for targeting different cancers includes taxanes, podophyllotoxin, vincristine and vinblastine. There is one compound named resveratrol, which was intensively studied for its anti-tumour activities, produced by several plants such as grapes, peanuts, blueberries, cranberries and red wine. Plant bioactive compounds are extensively benefited for human health because of the following properties: antioxidant, antitumor, antimutagenic, and antimicrobial. Usage of natural plant-based compound has several advantages over conventional one as it has fewer side effects. Advances in computer aided drug designing have given an impetus to the medicinal chemists to take the advantage of the natural products and use them as a good lead that can be optimized for treating different diseases. Natural products would be a good candidate to design the new drugs in the area of drug discovery. The major work which is to be done is to optimize these natural products for suitable pharmacokinetic properties so that their safety and efficacy could be relied in in vivo trials in humans.

Title: *Foeniculum Vulgare* Leaf Extract Loaded Synthesis of Silver Nanoparticles in Different Volume Ratios for Antimicrobial and Antioxidant Activities: Comparative Study of Composition

Speaker Name: Defaru Negera Duke

Affiliation: Adama Science and Technology University

Abstract:

Current world exposed to immense classes of challenges, of which antimicrobial caused infectious diseases has been ranked the third killer disease due to their high resistance capability. Oxidative stress is also the other problem faced by the world. In the current study, leaf of Foeniculum Vulgare was employed for the synthesis of Ag NPs within the 1:3, 1:1, and 3:1 composition using 0.1 M of AgNO3. The calculated average crystalline size was found to be 12.6-21.6 nm. SEM-EDS analysis depicts the quasi-spherical shape with intense Ag peak at around 3.00 eV. TEM-HRTEM with SAED showed spherical shaped Ag NPs. The electronic bandgap energy was calculated as 3.1-3.3 eV. Of the three ratios of Ag NPs, 1:3 showed enhanced antibacterial, antifungal, and antioxidant activity as compared to the counterpart volume ratios of Ag NPs.

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Title: Genomic analysis for the identification of therapeutic target against *Helicobacter pylori*

Speaker Name: Chaman Ara Keya

Affiliation: North South University

Abstract:

Helicobacter Pylori causes infection in the stomach and results in severe inflammation, gastritis, peptic ulcers, and a higher gastric cancer risk. The critical need to investigate new therapeutic targets is highlighted by the worldwide rise in antimicrobial resistance to drugs. In this investigation, a genomic approach was used to find unique H. pylori sites that might be possible targets for novel drugs. Genomic analysis and subsequent screening through different bioinformatics techniques revealed vacuolating cytotoxin (VacA) as a promising novel putative drug target. Several sets of ligand libraries from PubChem were used for blind docking with vacA using Autodock Vina in PyRx. Based on docking affinity scores validated by ADMET analysis, two cannabinergic ligands were selected for molecular dynamics (MD) simulation analysis. The binding affinity score of VacA with ligand 1(Pub Chem CID: 121283200) was -7.7 kcal/mol and with ligand 3(PubChem CID: 195772) was -7.0kcal/mol. The MD simulation analysis like RMSD, RMSF, RG, SASA also confirmed the stability of the desired drug candidates to the targeted protein. These findings demonstrate the potentiality of these two ligands to be used as highly effective inhibitors of VacA leading to better management and treatment of H. pylori infection. However, additional studies using in vitro and in vivo models are necessary before these findings can be applied in clinical applications.

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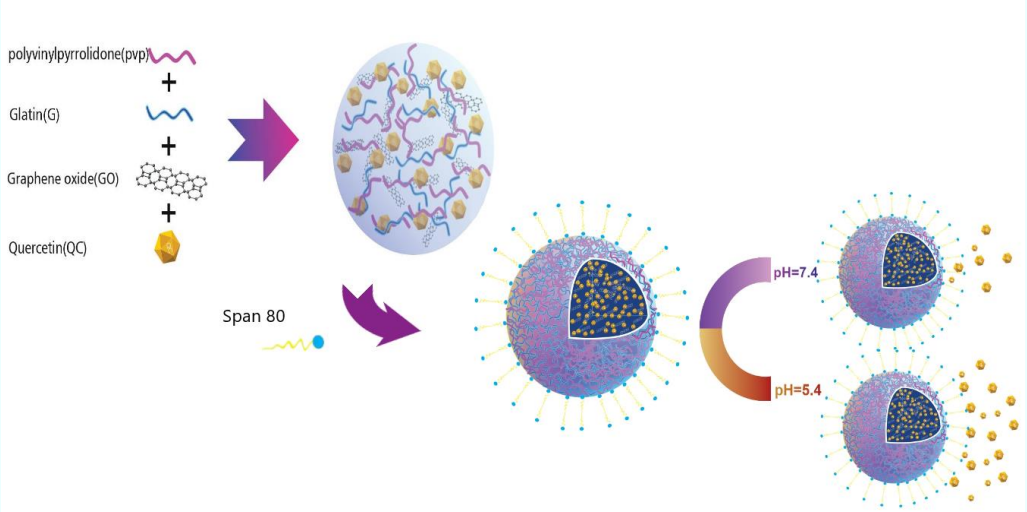
Title: pH-sensitive ameliorated quercetin delivery using graphene oxide nanocarriers coated with potential anticancer gelatin-polyvinylpyrrolidone nanoemulsion with bitter almond oil

Speaker Name: Amin Pirali Najafabadi

Affiliation: Islamic Azad University

Abstract:

The rapid rise of cancer worldwide demonstrates the importance of treatment strategies. In addition to reduce the side effects of conventional treatments, targeted drug delivery systems increase performance and effectiveness. In this research, nanocarriers comprising gelatin (G)-polyvinylpyrrolidone (PVP) coated graphene oxide (GO) were prepared for the first time. The nanocarries were loaded with quercetin (QC) drug and a dual nanoemulsion water/oil/water with bitter almond oil was developed as a membrane around the nanocomposite to control further drug release. XRD, FTIR, FESEM, and DLS analysis confirmed the success of the nanocomposite synthesis and drug loading. The resulting pH-sensitive drug delivery system showed an 87.5% encapsulation efficiency and a 45% drug loading, which are among the highest values reported up to date. The zeta potential of the nanocomposites was about − 40 mV, indicating good stability. The release kinetics of the drug followed the Higuchi model, and the presence of a dual nanoemulsion resulted in better drug entrapping efficiency, drug-controlled release and long-term release. MTT assay and flow cytometry methods revealed a rate of cancer cell death of 53.14%, which was 36.51% in the apoptotic phase. Taking into account the results obtained herein, PVP-G-GO-QC can be considered as a new promising system for cancer treatment.



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Title: Social determinants for the use of complementary and alternative therapies among women during pregnancy, labor and postpartum period in low income countries: a scoping review

Speaker Name: Mabel Kefilwe M. Magowe

Affiliation: University of Botswana

Abstract:

Introduction and objective: Complementary and alternative therapies (CAM) use is reported worldwide, ranging between 36 to 62%. Africa and Asia are leading at 80%. CAM is used for socio-economic reasons, but it can have positive and adverse outcomes on the mother-baby dyad, requiring further research and interventions.

Scope: The purpose and scope of the project was to explore social determinants for the use of CAM among women during pregnancy, labor and the postpartum period, in low resourced countries, to suggest interventions that promote informed use and safety.

Methods used: A scoping review was conducted in Web of Science, Google Scholar, PubMed, and EBACOHOST. Key words used were: “Complementary AND alternative therapies AND Pregnancy AND Labor, AND post-partum AND low resourced settings”. Full text, published between 2019 and 2024, relevant to the topic, were reviewed. The review and screening processes were presented in a PRISMA diagram. The accepted articles were presented in a table and were synthesised to guide discussion and conclusions.

Results: Social determinants of CAM use among the study population have been identified including positive experiences with symptom and side effects management, lack of knowledge about adverse effects, popular culture and low access to conventional medicines.

Discussion: Women use CAM for positive health outcomes because of socio-economic disadvantages, but demonstrate low knowledge of potential negative outcomes such teratogenicity for the fetus, requiring more education and research.

Conclusion: Further research and education to explore social determinants to address the benefits and threats of CAM use, especially teratogenicity and drug interactions.

Title: Collagen silver lipid nanoparticles as matrix and fillers for cosmeceuticals- an invitro and in vivo study

Speaker Name: Kumari Kajal

Affiliation: Birla Institute of Technology

Abstract:

In this context, the formulation and characterization of collagen silver lipid nanoparticles (CSLNs) were studied for their capacity to serve as a novel fillers/matrix material used in cosmeceutical applications. The CSLNs were prepared following a series of studies, such as X-ray diffraction (XRD), field-emission scanning electron microscopy (FESEM) coupled with energy-dispersive X-ray spectroscopy (EDS), Fourier-transform infrared spectroscopy FT-IR; thermogravimetric analysis (TGA); and differential scanning calorimetry (DSC). The studies confirmed the structural integrity of nanoparticles, their cargo and thermal stability.

The biological functionality of CSLNs were studied by carrying in vitro & in vivo studies. The antibacterial effect, hemocompatibility and anti-inflammatory characteristics of these fibres were systematically investigated. The toxicological assays included oral toxicity in mice and aquatic life tests with the fish Danio rerio model. The morphology of the nanoparticles was confirmed using high-resolution transmission electron microscopy (HR-TEM). The report found that CSLNs had strong antimicrobial effects, unmatched hemocompatibility, and low or absent inflammatory reactions, which makes them perfect candidates for cosmeceutical applications. The toxicological evaluations evinced a good safety record without any significant adverse effects in both murine and Danio rerio models. This research reveals the efficient way of CSLNs to the efficacy and safety of dermaceuticals

Title: Effects of leukocyte- and platelet-rich fibrin on diabetic foot ulcers: A retrospective study

Speaker Name: Fen Wang

Affiliation: Tongji Hospital, China

Abstract:

Background: Diabetic foot ulcer (DFU) is one of the most serious complications in diabetes. Leukocyte- and platelet-rich fibrin (L-PRF) is a next generation of autologous platelet-rich plasma. This study is aimed to investigate the clinical effects of L-PRF in diabetic patients in real clinical practice.

Methods: DFU patients who accepted L-PRF treatment and meet the inclusion criteria and exclusion criteria from 2018 to 2019 in Tongji Hospital were enrolled. The clinical features, wound evaluation, treatment of DFU, assessment of therapeutic effectiveness and images of ulcers were retrospectively extracted and analyzed. L-PRF treatment was performed every 7 ± 2 days until the ulcer achieved complete epithelialization or a more than 80% overall percentage volume reduction (PVR). Overall PVR, overall healing rate and weekly healing rate were the main evaluation index.

Results: There are 26 DFU patients enrolled with the ulcer duration 47.0 (35.0, 72.3) days. The severity and infection of ulcers varied with SINBAD score ranging from 2 to 6, Wagner grade ranging from 1 to 4, and PEDIS score ranging from 2 to 4. The initial ulcer volume before L-PRF treatment was 4.94 (1.50,13.83) cm3 and the final ulcer volume was 0.35 (0.03, 1.76) cm3. The median frequency of L-PRF therapy was 3 (2, 5). There were 11 patients who achieved complete epithelialization after the fifth therapy and 19 patients who achieved equal to or more than 80% volume reduction at the seventh week of L-PRF treatment. The overall wound healing rate was 1.47 (0.63, 3.29) cm3/week and the healing rate of the first two weeks were faster than that of the remaining weeks. Concurrent medicines did not change the percentage of complete epithelialization and the healing rate.

Conclusions: Adding L-PRF to SOC significantly improved wound healing in DFU patients independent of ABI index, SINBAD or Wagner grade.

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Title: Modulating mitochondrial quality control mechanism for targeting stemness in Glioblastoma

Speaker Name: Pransu Srivastava

Affiliation: Sanjay Gandhi Post Graduate Institute of Medical Sciences

Abstract:

Glioblastoma multiforme is the most aggressive form of high-grade glioma which exhibits chemotherapeutic resistance and recurrence mainly because of small population of cells commonly referred as glioblastoma initiating cells (GICs). These GICs show high proliferative tendency and resistance to temozolomide (TMZ) therapy even in limiting nutrient conditions. GICs often operate differentially than non-GICs in glioblastoma in terms of metabolism and signaling pathways Mitochondria are central to bioenergetics metabolism, cell survival and apoptosis, although its contribution to glioblastoma is not clear. (i.e. biogenesis, degradation, and dynamics). Therefore, mitochondrial quality control mechanism could be exploited to target GICs population to overcome chemotherapeutic resistance in glioblastoma. In present study, we investigated the mitochondrial quality control mechanisms along with their modulation in GIC enriched spheroids derived from established glioma cell lines. In non-adherent conditioned system, spheroids generated from LN229 and U87MG cells were found to be enriched in populations showing upregulated stemness and resistance to TMZ, with comparison to monolayer counterparts. Furthermore, these enriched population showed disjointed mitochondrial functions; such as elevated superoxide levels, mitochondrial membrane potential and mtDNA content, yet reduced ATP production as well as oxidative stress. This altered functionality was corroborated with increased expression of mitophagy and mitochondrial fission markers (BNIP3 and DRP1 respectively) along with an upregulation in general autophagy (LC3b induction and P62 clearance). This is indicative of altered mitochondrial quality control that supports GICs proliferation and resistance. These mechanisms were jointly targeted by combination of Chloroquine (an autophagy inhibitor) and Mdivi1 (Drp1 inhibitor) along with TMZ. This triple combination showed a significant reduction in GICs viability after 48 hours of treatment. This triple combination also was able to modulate expression levels of stemness and mitochondrial quality control markers which further proved detrimental to survival of GICs. Altogether targeting mitophagy along with dynamics can help overcome glioma therapeutic resistance.

Title: Prevalence of *Pseudomonas spp* in Egyptian dairy products and the efficacy of its control in milk using nanoparticles

Speaker Name: Hamdi Abdelsamei Mohamed

Affiliation: Benha University

Abstract:

Globally, food safety is a critical problem impacting food technology and public health. Milk and dairy products are considered a high-risk category for potential microbial contamination, resulting from processing techniques, livestock and the surrounding environment, all of which can contribute to the contamination. Milk deterioration might occur at any step from the farm to the consumer, even after being thermally heat treated. The milk storage in refrigerators supports the growth of psychrotrophic bacteria, which can thrive below refrigerated temperatures of 4–7 °C and form heat-resistant bacteria. Psychrotrophic bacteria can form hydrolytic enzymes. These enzymes resist high temperatures and cause milk spoilage, leading to economic loss. Pseudomonas spp is a psychrophilic bacterium that promotes the deterioration of most dairy products. It can produce proteases and lipases that can withstand severe thermal treatment and degrade milk proteins and fats, resulting in bitterness, rancidity, and gelation, which has a significant negative impact on the quality of milk and dairy products. So, our study aimed to study the distribution of Pseudomonas spp in raw milk and its associated Egyptian products as in kareish cheese, yogurt and ice cream using specific media and confirmed biochemically and by PCR. Then apply chitosan and selenium nanoparticles at different concentration for control the most common Pseudomonas spp isolated as a recent technology for controlling in milk during cooling storage. Our results declared the highest mean average count was detected in raw milk samples, while the lowest Pseudomonas spp count was in ice cream samples with commonly isolated strain was P. aeruginosa. Chitosan nanoparticles effectively inhibit the growth survival rate of P. aeruginosa, at 50 mg/100 ml milk. Similarly, Selenium nanoparticles exhibited potent antibacterial activity at concentration 0.5 mg/100 ml. we recommend application of nanoparticles in milk after studying the fate of these nanoparticles in human body.

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Title: Spontaneously self-assembling antimicrobial peptides with potent antibiotic and anti-polymicrobial biofilm activity

Speaker Name: Ren Lai

Affiliation: Chinese Academy of Sciences, Kunming

Abstract:

Multidrug-resistant (MDR) bacteria often coexist in polymicrobial biofilms, which exacerbate antibiotic resistance, calling for new antimicrobials. Here, based on motifs frequently presented in antimicrobial peptides (AMPs) and core structures driving AMP self-assembly, we designed AMPs that can spontaneously assemble into microfibrillar structures and are further enhanced by C-terminal PEGylation. These peptides exhibit potent activity with minimum inhibitory concentrations (MICs 0.39-9.4 μM) against many nosocomial and standard reference ESKAPE pathogens and Candida fungi, outperforming many conventional antibiotics. A lead compound, SAP2-PEG, demonstrates robust proteolytic resistance and low propensity for resistance induction. Notably, SAP2-PEG effectively suppresses bacterial quorum sensing, a key system in biofilm formation, thereby eradicating polymicrobial biofilms in Pseudomonas aeruginosa and Staphylococcus aureus co-cultures. In mouse models of polymicrobial biofilm infection, SAP2-PEG shows superior therapeutic efficacy compared to antibiotics, providing promising AMP candidates. The work provides a strategy to engineer AMPs for combating both MDR pathogens and polymicrobial biofilms.

Title: Anomaly detection in Drug Discovery

Speaker Name: Ekin Can Erkuş

Affiliation: Huawei Technologies, Turkey R&D Center

Abstract:

Anomaly detection is an important aspect of drug discovery, as it allows researchers to uncover unexpected patterns and deviations, which can provide useful knowledge about drug safety, effectiveness, and behavior. Techniques designed specifically for time series data are especially useful, as they help overcome the difficulties of analyzing high-dimensional datasets that are common in pharmaceutical research. For example, by using sliding window methods along with ways to measure differences, small and short-term problems in changing datasets can be found. By focusing on smaller parts of the data, these methods can identify unusual patterns those older methods might miss, which is particularly useful in fields like studying how drugs work in the body and how people respond to them. This is important because even tiny changes can give important clues about what is happening inside the body, and even minor anomalies in these contexts may reflect important biological processes. Consequently, time-dependent interactions relevant to drug development can be better understood when such deviations are measured accurately.

Time series analysis is useful for detecting patterns and causal relationships over time, which are important in drug discovery research. It is especially useful in the early stages of drug development, such as predicting side effects, because identifying unusual patterns can provide important insights for decision-making. Recent studies suggest that time series approaches can produce more consistent results and improve the drug discovery process. Furthermore, merging several forms of data or using machine learning models can aid anomaly detection performances even further. Therefore, utilizing time series and anomaly detection approaches in drug discovery not only makes it easier to analyze complex data but also help to build safer and more effective therapies.

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Title: ACE-dependent Alzheimer's disease (AD)

Speaker Name: Sergei M. Danilov

Affiliation: University of Illinois, USA

Abstract:

An analysis of 1200+ existing missense ACE mutations revealed that >400 are predicted to be damaging and led us to hypothesize that heterozygous carriers of these loss-of-function (LoF) ACE mutations (which result in low ACE levels) may be at risk for the development of late-onset Alzheimer's disease (AD) [Danilov, 2024].

The 1st stage of this ACE-dependent AD project is characterization of blood ACE levels, catalytic properties, and conformations (ACE phenotyping) using a wide set of mAbs to ACE that were developed in our lab. We already have performed ACE phenotyping in & gt;200 carriers of 80+ different ACE mutations and 500+ controls [Kryukova, Biomedicines, 2024, PloS One, 2024, unpublished]. Several of the relatively frequent AD-associated ACE mutations (present in at least 2% of the population) are truly damaging and, likely transport- deficient, resulting in plasma ACE levels only ~50% of controls. Some other AD-associated ACE mutations were not associated with a decrease in blood ACE levels, and likely do not affect ACE surface expression. Thus, their mechanism of association with AD is likely different, such as via catalytic changes. However, both these types of ACE mutations may result in reduced degradation of amyloid beta peptide Aβ42, an important component for amyloid deposition, and may pose a risk factor for the development of AD. Therefore, a systematic analysis of blood ACE levels in patients with ACE mutations has the potential to identify individuals at increased risk of late-onset AD.

The 2nd stage of this project will include 1) Cell-based in vitro model (HEK cells transfected with cDNA of different ACE mutations) in order to find transport-deficient ACE mutations, which may be amenable to rescue of impaired trafficking of mutant ACE to the cell surface; 2) medico-genetic analysis of 50-100 families of carriers with the most damaging and transport-deficient ACE mutations. This stage will identify prospective candidates for a future limited clinical trial of preventive or therapeutic interventions to delay the development of ACE-dependent AD.

The 3rd stage of the project could be a limited clinical trial in individuals with several transport-deficient ACE mutations (starting with the most frequent damaging ACE mutation, Y215C) aiming to enhance mutant ACE protein traffic, as we previously demonstrated for the transport-deficient ACE mutation, Q1069R, using a combination of chemical and pharmacological chaperones and proteosome inhibitors [Danilov, PloS One,2010].

Title: Expression Pattern of Drosophila melanogaster Aminopeptidase P (DAP) to understand its physiological function in human

Speaker Name: Suneeta Panicker

Affiliation: Dr. D. Y. Patil Arts, Commerce and Science College

Abstract:

Aminopeptidase P (APP) is a metallopeptidase that cuts N-terminal imido bonds where proline is the penultimate residue. Presence of this enzyme has been shown in many organisms. There are three different isoforms of human APP, coded by separate gene, a (hmAPP), human membrane bound, cytosolic form (hcAPP,) and a mitochondrial form. APP has been related to several diseases such as kidney defects, intellectual disability, side effects of ACE inhibitors, ischemic myocardium, cancer, premature ovarian failure, peptiduria. Activity of the enzyme has been demonstrated in a range of cells inclusive of glia, chromaffin cells, leucocytes and brain cells in culture. A large number of biologically active polypeptides, including hormones, growth factors, neurotransmitters, coagulating proteins, toxins, and cytokines, are potential substrates of hmAPP. This peptide may be useful in designing drugs for the prevention and treatment of cancer, angioedema etc. Thus, APP is of clinical and industrial importance. APP is highly conserved, right from Drosophila to human. Hence, though the mode of action of APP is known, its exact physiological function is yet not known. The study of Drosophila melanogaster APP (DAP) expression pattern was undertaken to get some insights of its physiological function. The wild type expression pattern of DAP protein and RNA was looked in the Drosophila embryos using antibody staining and in situ hybridization techniques respectively. By constructing a transgenic fly DAP gene expression profile was also studied. Data presented here designates DAP functions in the early embryonic and imaginal dics differentiation and development (figure 1A and 1B), suggesting that it may be required for the metabolism of proteins like neuropeptides, and tachykinins. Studying the regulation of expression of APP in Drosophila will be useful to elucidate its functional role to some extent and help the scientific world in using it as a drug target.

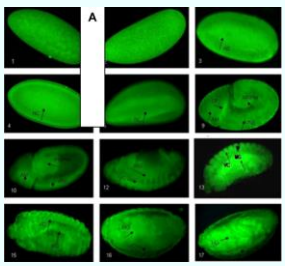

Figure 1A- DAP protein expression pattern in wild type embryos: Lateral view of the embryos depicted with the dorsal surface on the top

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Title: Evaluation and Use of Alternative Materials for the Removal of Hormones, Drugs and Drugs of Abuse in Industrial and Domestic Efluents.

Speaker Name: Daniel T. Lebre

Affiliation: Instituto de Pesquisas Energéticas e Nucleares, Brazil

Abstract:

Currently, consumption and consequently global production of medicines exceed 100,000 tons per year. There is no doubt that these chemical compounds known as drugs benefit thousands of people, as their therapeutic properties act directly against the harm caused by diseases, increasing the quality and life expectancy of human beings. Controversially, pharmaceuticals (including hormones and drugs of abuse), also known as pollutants or emerging contaminants, are commonly found, at relevant and alarming concentration levels, in natural water resources, causing deleterious effects on aquatic life and the ecosystem. These compounds reach water resources through industrial, hospital and domestic effluents, which are not able to remove them completely or simply due to the lack of basic sanitation, in which the urine and feces of human beings secrete them in intact form and/or in the form of its metabolite. Faced with this systemic environmental problem, the main objective of this research work was to evaluate sugarcane bagasse (BCA) as a potential bioadsorbent material for the removal of synthetic hormones: ethinylestradiol; drosperinone and levonorgestrel in industrial effluent. In previously scientific publications, it were found that BCA is an excellent bioadsorbent material for the removal of metals, dyes and some petroleum derivatives in effluents, however, for hormones, pharmaceuticals and drugs of abuse, no evidence was found, which motivated this research. In addition to the fact that Brazil has produced millions of tons of sugar cane every year, generating bagasse as waste. After simple preparation of the BCA, it was properly characterized and the adsorption isotherms were experimentally tested for each synthetic hormone. The linear isotherm, Langmuir and Freundlich models were applied and studied, as well as the parameters that influence the adsorption process (e.g. stirring time, pH, temperature). BCA was successfully applied to remove synthetic hormones in industrial effluent, obtaining an efficiency rate of 98%, compatible with the materials: activated carbon and graphene. As a secondary objective, BCA was used to remove pharmaceuticals, drugs of abuse and hormones from domestic effluent. For lipophilic compounds with lower water solubility, BCA provided the removal efficiency greater than 70%. To sum up this research work focused on innovation and green chemistry was developed with BCA, which is a waste generated in millions of tons in sugarcane plants and can be used for a value purposes other than burning to generate energy and release CO2.

Title: Antimicrobial Potential of *Potentilla indica* (Andrews) Th. Wolf extracts against ESKAPE pathogens and *Candida albicans*: A Step towards combating antimicrobial resistance

Speaker Name: Dimple Guleria

Affiliation: Himachal Pradesh University

Abstract:

Antimicrobial resistance (AMR) is an escalating global health challenge, particularly against pathogens categorized as ESKAPE by the World Health Organization (WHO). This study explores the antimicrobial potential of Potentilla indica (Andrews) Th. Wolf, a wild berry native to the Himalayas, traditionally used in local medicine, against major bacterial and fungal pathogens. The tested microorganisms included Escherichia coli, Staphylococcus aureus, Streptococcus mutans, Streptococcus pneumoniae, Klebsiella pneumoniae, Pseudomonas aeruginosa (ESKAPE pathogens) and Candida albicans. Acetone and methanol extracts of the aerial parts of P. indica were evaluated using the disk diffusion method and minimum inhibitory concentration (MIC) assays. The acetone extract exhibited remarkable antibacterial activity, with the largest zone of inhibition (31.89 ± 0.05 mm) observed against P. aeruginosa. Conversely, the methanol extract showed superior antifungal activity, achieving a significant zone of inhibition (11.90 ± 0.33 mm) against C. albicans. MIC assays further revealed that both extracts displayed the lowest MIC value (39.1 µg/mL) against S. mutans, followed by substantial activity against S. pneumoniae, P. aeruginosa and C. albicans at 1250 µg/mL. These findings highlight the promising antimicrobial properties of P. indica extracts, with the acetone extract showing particular effectiveness against bacterial pathogens and the methanol extract demonstrating efficacy against fungal infections. This study supports the traditional medicinal use of P. indica and underscores its potential as a source for developing novel antimicrobial agents to address the growing threat of AMR.

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Title: Profile Metabolites for Authentication of Chicken Meat Supplied by Different Slaughter Methods of Halal, Non-Halal and Shubha

Speaker Name: Vevi Maritha

Affiliation: Universitas PGRI Madiun, Indonesia

Abstract:

To protect consumers from non-halal and shubha-halal foods, it is essential to authenticate chicken meat based on its slaughtering process. The objective of the present study is to authenticate the halalness of chicken meat based on the slaughter process. Untargeted metabolomics, utilizing UHPLC-HRMS combined with chemometrics, offers a selective and accurate method for verifying the halal status of chicken meat based on the slaughter process. The results of this research identified 28 metabolite profiles, with creatine, carnosine, and 3-methylhistidine being the most prominent metabolites. Principal Component Analysis (PCA) clearly distinguished the metabolite profiles of chicken meat slaughtered using different methods. Additionally, cluster analysis effectively grouped chicken meat based on similarities in metabolite profiles. The correlation network revealed that 21 types of metabolites are interrelated in the halal authentication process. Partial Least Squares Discriminant Analysis (PLS-DA) accurately identified 13 potential biomarkers for halal authentication, including creatine, betaine, 2-amino-1,3,4-octadecanetriol, L-isoleucine, L-phenylalanine, L-histidine, L-glutamic acid, L-glutathione, DL-glutamine, taurine, carnosine, and acetyl-L-carnitine. Overall, untargeted metabolomics combined with UHPLC-HRMS and chemometrics represents a promising method for authenticating the halal status of chicken meat, distinguishing between halal, non-halal, shubha-halal, and mixtures of halal with non-halal or shubha-halal meat.

Title: Knowledge and attitudes towards genomic medicine and pharmacogenomics of medical undergraduate students in Sri Lanka

Speaker Name: Dilini N. Kekulandara

Affiliation: Wayamba University of Sri Lanka

Abstract:

Genomic medicine and pharmacogenomics (PGX) are transformative practices in modern medicine, enabling personalized and efficient patient care. While many countries have integrated these concepts into undergraduate medical curricula to enhance healthcare quality, Sri Lanka is still in the early stages of adopting these advancements. This study aimed to assess the knowledge and attitudes of Sri Lankan medical undergraduates toward genomic medicine and PGX and evaluate the readiness for incorporating genomic insights into the local medical curriculum. A descriptive cross-sectional study was conducted among undergraduate students of the Faculty of Medicine, Wayamba University of Sri Lanka. As a newly established institution, the faculty seeks research-based strategies to refine its curriculum and produce competent graduates. Data were collected through an online questionnaire distributed to all five student batches, with 232 respondents (55% response rate). The findings revealed a generally good level of knowledge on genomic medicine and PGX, with no significant variation across academic years. Students expressed a nuanced range of attitudes, encompassing both positive and negative perspectives. Concerns about data privacy, insurance implications, and the timing of implementation were particularly prominent. The results highlighted the need for curriculum enhancement, recognizing students' baseline knowledge while addressing gaps in understanding and attitudes. Emphasizing ethical, practical, and contextual aspects of genomic medicine and PGX will be critical for advancing healthcare education in a developing country, Sri Lanka and equipping future medical professionals to meet emerging challenges in personalized medicine.

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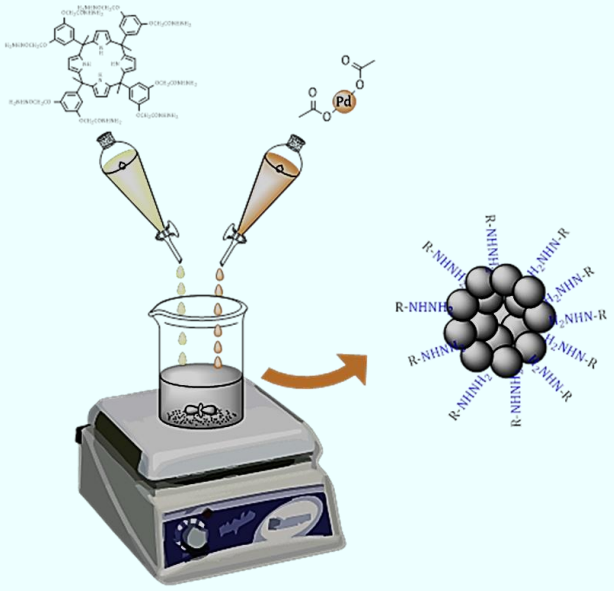
Title: Enhancing Catalytic Performance: Integrating Nano-Palladium with Hetero Calixarenes for Advanced Solutions

Speaker Name: Keyur D. Bhatt

Affiliation: Ganpat University

Abstract:

This study presents an innovative approach to developing high-performance nanocatalysts by integrating mesomodified hydroxycalix[4]pyrrole derivatives (OHCP) with palladium nanoparticles (PdNPs). The resulting OHCP-PdNPs exhibit exceptional catalytic efficiency in C–C coupling reactions, with stability and pH optimization playing crucial roles in their performance. The electron-rich hydrazide functional group and the distinctive four-pyrrole unit structure of OHCP facilitate effective reduction and encapsulation of metal ions, surpassing traditional hydrazine methods. This encapsulation forms a robust, web-like coating around PdNPs, significantly enhancing their stability in aqueous and atmospheric conditions. The encapsulation not only boosts the activity and selectivity of PdNPs but also enables cost-effective production of versatile, stable nanocatalysts. These findings highlight the transformative potential of OHCP-encapsulated PdNPs for sustainable and scalable applications in nanotechnology, green chemistry, and advanced catalytic processes.



Title: Overcoming therapeutic lags by unlocking small molecules interactions- a study on HSP 70 and BCL 2

Speaker Name: Ezhilarasi Sundaram

Affiliation: King George medical university Lucknow, India

Abstract:

Understanding of molecular model of oral carcinogenesis has carried cancer chemotherapy far forward from conventional drug therapies. Small molecule inhibitors has gained acceptance as it has fewer adverse effects and also provides targeted drug therapy. The association of HSP 70 (Heat Shock Protein 70) and BCL 2 (B-cell lymphoma 2) proteins with oral precancer and cancer is already established. However the complex interaction between these two proteins and how they affect each other's expression is still not understood completely. In our study we aimed to correlate the expression of HSP 70 and BCL 2 with different histopathological grades of oral precancer and cancer tissue samples using tissue immunohistochemistry.

Materials and Methods:

Tissue samples were taken from a total of 250 patients (100 OPMDs and 150 OSCCs) and subjected to immunohistochemistry using anti human mouse monoclonal antibody to HSP70 and BCL2. Immunostaining was done and Immunostaining Intensity Distribution (IID) index was calculated.

Results and Discussion:

Immunoreactivity scores for both HSP 70 and BCL 2 were correlated with different grades of dysplasia. However, only HSP 70 had a statistically significant association with increasing grades of dysplasia. On contrary, in OSCC cases we found HSP 70 showed an inverse correlation, with higher expression majorly seen in well differentiated OSCCs. Cancer cells are dependent on aerobic glycolysis for their metabolic needs. With increase in cancer cell population they become glucose deprived. This creates a metabolic stress in the cancer cells and as a rule HSP 70 is expected to be induced in these cells. Overexpression of BCL 2 in cancer cells suppressed the expression of HSP 70 in glucose deprived states.

Conclusion:

Our study unveiled the HSP 70 – BCL 2 interaction and provides insights about how this might affect drug designing and help overcome therapeutic lags.

Title: Performance of Aquatic Plant Bacopa, sp from Bantimurung river South Sulawesi Indonesia

Speaker Name: Media Fitri Isma Nugraha

Affiliation: Research Centre for Pharmaceutical Ingredients and Traditional Medicine- Organisation of Health- National Research and Innovation Agency of Indonesia

Abstract: The genus Bacopa a type of aquatic plant that has been widely used in medicine Ayurvedic medicine. The performance of its bioactive compounds used as an antibacterial agent was observed to control fish diseases. Objective, this study was to reveal the content of antioxidant and antibacterial active compounds of Bacopa sp, from Bantimurung and their effectiveness in controlling the growth of Aeromonas hydrophila, Streptococcus agalactiae, Flavobacterium columnare, Edwardsiella ictaluri, using in vitro methods. Materials and Methods, Bioactive compounds was extracted from Bacopa by employing Ultrasound-Assisted Extraction. Extracts were screened qualitatively for antioxidant activity and then quantified to measure in vitro antioxidant activities using the 2.2 diphenyl 1 picrylhydrazyl DPPH radical scavenging assay and the ferric-reducing antioxidant power FRAP assay. The evaluation of chemical compounds was conducted using GCMS. Antibacterial activity was determined by the paper disc diffusion method and microdilution. Results, extracts were found to contain alkaloids, tannins, flavonoids, saponins, terpenoids, and glycosides. GCMS profiles showed that the extract had 13 identified compounds. Genus Bacopa from Bantimurung herbal extract has strong antioxidant activity with IC50 value50 microgram per mL i.e. 40.37 microgram per mL. While, Bacopa extract inhibited the growth of Aeromonas hydrophila, Streptococcus agalactiae, Flavobacterium columnare bacteria, but not for Edwardsiella ictaluri. Conclusion, The significant potential of secondary metabolites from Bacopa indicates an opportunity as a new potential candidate for aquatic plants that have high antioxidant, antibacterial, and anti-inflammatory activities.

Title: Preparation and Characterization of Amoxicillin- Loaded Polyvinyl Alcohol/Sodium Alginate Nanofibrous Mat: Drug Release Properties, Antibacterial Activity, and Cytotoxicity

Speaker Name: Azize Çerçi

Affiliation: Bursa Uludag University

Abstract: Electrospinning is a widely used nanofiber-producing method that accounts for the stretching of polymer solution by applying a high-voltage electric field. It's highly appreciated since electrospun nanofibers exhibit large surface area, high porosity, and robust mechanical strength similar to human skin. Amoxicillin (AMOX) is a beta-lactam subset of penicillins, which has broad-spectrum antimicrobial activity, bactericidal effect, and high therapeutic index however AMOX has a short half-life and some pharmacokinetic limitations that impede its intestinal uptake. Polyvinyl alcohol (PVA) and sodium alginate (SA) were the main polymers to generate nanofibers since PVA provides excellent biocompatibility and SA is an absorbent for exudative wounds. This study aimed to design a novel amoxicillin-loaded PVSA (PVSA/AMOX) nanofiber and interrogate its performance as an antibiotic-releasing wound dressing. PVSA/AMOX nanofiber was characterized with FTIR, SEM, BET, and mercury porosimetry analyses. Drug release studies have been conducted for glutaraldehyde (GA) crosslinked PVSA/AMOX in case of altered GA concentration and crosslinking time. The antibacterial activity of PVSA/AMOX nanofibers has been studied using disc diffusion assay and bacterial colony counting assay on Gram-positive bacteria (S. aureus ATCC 29213) and Gram-negative bacteria (E. coli ATCC 25922) strains. Cytotoxicity studies have been conducted using human normal keratinocyte cells (HaCaT). The PVSA/AMOX nanofiber drug release profile was compatible with the Korsmeyer-Peppas kinetic model, which defines the drug release as diffusion-controlled and polymer matrix- based erosion. According to antibacterial activity results, PVSA/AMOX nanofiber formed an inhibition zone against S. Aureus greater (23.3 ± 0.6 mm) than E. Coli (11.0 ± 0.2 mm), attributed that gram-negative bacteria have complex outer membrane properties which reduce the permeability of antibiotics. After 48 hours of incubation, PVSA/AMOX nanofiber had no cytotoxic effect on the HaCaT cell line. Cell viability was found %124 for the PVSA/AMOX treated group concluding that our novel PVSA/AMOX nanofiber elevated cell proliferation due to its good biocompatibility.

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Title: Artificial Intelligence enabled Nanosensors for Trace-level Biomarkers Detection

Speaker Name: Ajay Agarwal

Affiliation: Indian Institute of Technology Jodhpur, India

Abstract:

Detecting biomarkers at trace levels is important for many reasons, including early detection of disease which can help in preventing the spread of infectious diseases and reduce the death rate from diseases like cancer; possibilities of personalized medicine as biomarkers can provide individualized information about underlying medical conditions, that can guide treatment decisions and improve patient outcomes; it can help in drugs development as biomarkers can help in identifying the suitable patients for clinical trials and the approval process can speed up; etc. Nanosensors are often used to detect trace-level biomarkers due to their large surface area to volume ratio, which makes them sensitive to chemical compounds, atoms, and single molecules. Nanosensors are categorized by their constituent materials, detection targets, and the signals used to transmit information which include gas-based nanosensors, colorimetric nanosensors, electrochemical sensors, chemo-resistors, piezoelectric sensors, surface enhanced Raman spectroscopy (SERS), etc. The use of nanotechnologies to realize highly sensitive sensors, along with micro-fluidics, are leading to sample-to-answer operations on a chip, suitable for healthcare applications. While detecting trace-level biomarkers, these nano-device encounter a lot of noise from other chemicals in the samples under consideration, which is being taken care by using suitable Artificial Intelligence based algorithms.

Nanotechnologies with micro-fabrication have enabled novel nano-dimensional materials, structures and eventually devices; integrated with AI algorithms-based data analytics are finding several early-diagnostics applications. CNTs, Nano-Gap arrays and Nanowire based bio-chemical sensors are most utilized for such diagnostic applications. Nano-Gap arrays, working on the principle of 'Electro-magnetic enhancement' using micro-Raman spectroscopy is one such technique.

The technology details suitable for the mass realization of the Nano-Gap arrays, for Surface Enhanced Spectroscopy (SERS), along with a few use cases of trace-level early diagnostic applications will be discussed in detail.

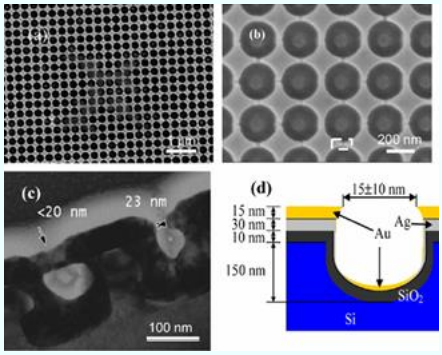

Figure: Nano-gaps in array format, representing SERS nano chip suitable for trace-level molecular/ bio-marker detection.

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Title: Impact of Doxorubicin and Docetaxel on Immune Checkpoint Expression in Colorectal Cancer: Insights into Chemotherapy Resistance Mechanisms

Speaker Name: Mahya Ahmadpour Youshanlui

Affiliation: Tabriz University of Medical Sciences

Abstract: The purpose of this study was to investigate the mechanisms underlying chemotherapy resistance in a colorectal cancer cell line, with a focus on the altered expression of immune checkpoint genes.

Methods: The SW-1116 colorectal cancer cell line was cultured using standard methods. The efficacy of the chemotherapeutic agents docetaxel and doxorubicin was assessed using the MTT assay to determine the IC50 values. Quantitative reverse transcription-polymerase chain reaction (qRT-PCR) was then employed to analyze the expression levels of the immune checkpoint genes PD-L1, CTLA-4, and VISTA after chemotherapy treatment.

Results: The results showed a significant upregulation of VISTA expression ($p<0.0001$) in response to both chemotherapy agents. Similarly, the expression of CTLA-4 ($p<0.0001$) and PD-L1 ($p<0.0001$) displayed notable increases following chemotherapy treatment.

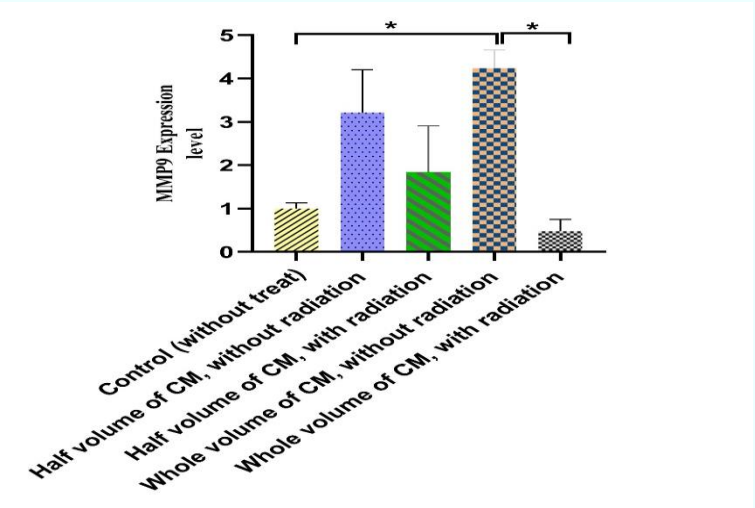
Conclusion: This study demonstrates that chemotherapeutic agents can heighten the expression of immune checkpoint genes in a colorectal cancer cell line. These findings suggest that chemotherapy-induced alterations in immune response pathways may contribute to the development of chemotherapy resistance and tumor recurrence. Further investigation is warranted to elucidate the underlying mechanisms and explore potential therapeutic strategies to overcome this challenge.

Title: An investigation on the effects of culture medium ofcancer-associated fibroblasts exposed to gamma radiation on MMP-9 gene expression in MCF-7 breast cancer cell line

Speaker Name: Aghil Esmaeili-bandboni

Affiliation: Guilan University of Medical Sciences

Abstract: While advancements in breast cancer treatments have led to improved patient outcomes, many still progress to metastatic disease, which is challenging to treat. The failure of certain therapies may be attributed to the fact that most current anti-cancer drugs primarily target cancer cells, disregarding the tumor microenvironment (TME) in which the cancer exists. TME comprises different types of cells, namely, tumor parenchymal cells, stromal cells, epithelial and inflammatory cells, extracellular matrix and messenger molecules, and blood and lymphatic vessels. Of these cell types, stromal cells such as fibroblasts represent the most abundant population within the TME. Additionally, MMP-9 have been extensively researched in breast cancer and are indicators of metastasis. In this study, the intention is to investigate the expression of MMP9 gene in MCF-7 breast cancer cells after exposed to fibroblasts. For this purpose, MCF-7 cell line culture was done and then in different groups, including the group that was exposed to the culture medium of cancer fibroblast cells that received gamma rays and the group that did not received. The desired gene expression was investigated by REAL TIME PCR method. The results showed that the expression of MMP9 gene in MCF-7 cancer cells that were exposed to fibroblast supernatant decreased after fibroblast cells were exposed to gamma rays. Therefore, by affecting the fibroblast cells that are cancer cells in the TME, it is possible to prevent the progress of cancer metastasis.



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Title: The Effectiveness of Mobile-Based Self-Care Education and Counselling on General Health and Quality of Life of Women with Breast Cancer

Speaker Name: Keyhaneh Mohammadi Aref

Affiliation: Babol University of Medical Sciences

Abstract: The self-care program in breast cancer patients is an important and effective factor in controlling and reducing the complications of the disease, which leads to more adherence to treatment and improves the health of patients. Considering the role of smart cell phones in people's lives and their evident capacities for self-care, the purpose of this study is to determine the effect of cell phone-based self-care intervention on the general health and quality of life of women with breast cancer

Methods: The present study was a controlled semi-experimental study conducted on 140 women with breast cancer referred to the Babol and Rasht Breast Cancer Registration Center in the North of Iran who met the criteria for entering the study. The participants were randomly allocated into two groups, control and intervention, and educational intervention sessions in the form of video with text and audio were provided to the clients every week for 6 weeks with telephone follow-up, and sexual counseling sessions with the Plissit model were also provided in the Skyroom was established. Information was collected using demographic information questionnaires, Edmonton symptom questionnaire, general and specific quality of life questionnaires, general health questionnaire (GHQ-12) and feasibility index questionnaire. Data were analyzed using statistical software Stata version 17 and SPSS V26 software.

Results: According to the determination of the average difference between the control and intervention groups by adjusting the intervening factors (age, body mass, occupation, education, marital status, family history of breast cancer) the difference in general health was significant -1.55 ((95% CI: -2.29 to -0.80), P<0.001) but it was not significant in Edmonton symptoms -0.25 ((95% CI: -5.85 to 5.34), P = 0.166). Also, the difference in general quality of life was significant -2.39 ((95% CI: -2.46 to 1.23), P = 0.018) and the difference in specific quality of life was significant -4.31 ((95% CI: -5.68 to -2.93), P<0.001).

Table1– Effects of intervention on public health outcomes during the intervention period

		Intervention	Control		95% CI		P
		mean±standard deviation	mean±standard deviation	Difference*	Lower limit	Upper limit	
General Health	Before	18/843±.48	18/052±.96	-0/61	-2/46	1/23	0/512**
	After	13/042±.78	15/564±.68	-1/55	-2/29	-0/80	<0/001***
	Changes	-5/80±.52	-2/40±.18	-3/40	-4/49	-2/30	<0/001

Conclusion: Mobile phone-based self-care intervention improves the quality of life and general health in women with breast cancer. Therefore, it is recommended that self-care training based on mobile phones be made available to all women with breast cancer.

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Speaker Slots Filling Quickly

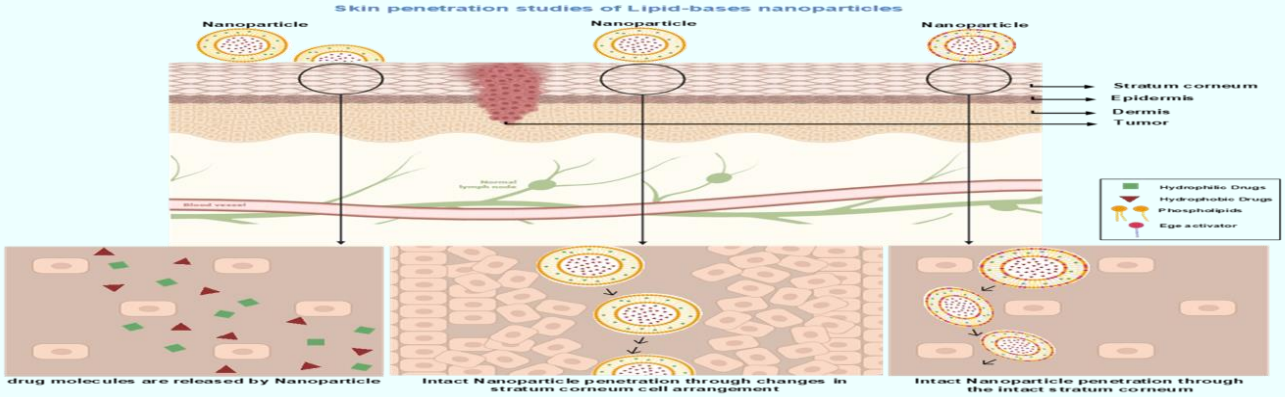
Title: Lipid-based nanoparticles as a promising treatment for the skin cancer

Speaker Name: Parisa Golestani

Affiliation: Islamic Azad University

Abstract:

Skin cancer is increasingly prevalent worldwide, ranking fifth among cancer types. An investigated the potential of eight lipid-based nanoparticles for transdermal drug delivery to treat various types of skin cancer in this Review article. Nanoparticles offer targeted drug delivery, improving bioavailability and minimizing side effects. For example, Liposomes are conventional and fail to penetrate the skin layers and remain on the skin surface, acting as a kind of depot formulation. The presence of ethanol and edge activator in Transfersomes and Transethosomes enhances their flexibility and fluidity and due this kind of elastic nature, vesicles can easily pass through narrow intercellular pathway. The ethanol present in Ethosomes gets intercalated on lipid present in stratum corneum which results in increase in membrane permeability and after fusion with the membrane they successfully deliver the drug inside the cells. The surfactants as essential component of niosomes structure act as permeation enhancers and direct fusion of vesicles with stratum corneum and they can modify the structure of the SC through their surfactant properties, resulting in the layer becoming looser and more permeable. Proniosomes have propensity to attach to the stratum corneum, converted to niosomes after hydration and permeate in skin through stratum corneum that results in increase skin permeation. The modifying agent, glycerol, present in glycerosomes induced hydration of the skin via interaction with the polar groups of the lipids increasing their fluidity and facilitating the diffusion of the nanovesicles. The structural management of cubosome is similar to that of the skin which allows it to be compressed through the pores of the stratum corneum, leading in the deeper penetration of the cubosomes. The invasomes can combine with the lipids of the skin and altered the distribution of SC that loosens the tight lipid junctions. Local treatment of skin cancer with the help of these nanoliposomes can be a good alternative to other skin cancer treatment methods. However, further research and development are necessary to optimize drug delivery systems for enhanced efficacy.



Title: Availability and Affordability of antidiabetic medicines in Herat of Afghanistan in 2023

Speaker Name: Laleh Satarzadeh

Affiliation: Shiraz University of Medical Sciences

Abstract: This study aims to investigate the availability, affordability, and accessibility of antidiabetic medications in Herat, Afghanistan, in 2023.

Methods: Adhering to WHO and HAI guidelines, a systematic survey was utilized to collect data on the pricing, availability, and affordability of commonly prescribed antidiabetic medications. Data collection spanned a month and involved four investigators using a standardized template. Data on the most-sold generic (MSG) and least expensive generic (LPG) options were compiled from pharmacies, and descriptive statistics were employed.

Results: The study reveals a heavy reliance on imported medications, mainly from Pakistan, with limited local production. Availability in pharmacies exhibited notable disparities, with essential medications sometimes lacking consistency. The financial analysis identified affordability challenges, particularly for certain Iranian and Pakistani brands. Notably, Metformin 500 mg emerged as the most consumed medication. Sitagliptin 50 mg had the highest average consumption when considering Pakistani brands, whereas Insulin Regular topped the list for Iranian brands.

Conclusions: The findings emphasize the need for comprehensive strategies to address diabetic patients' challenges in Herat, Afghanistan. Strengthening the pharmaceutical supply chain, bolstering local production, and implementing measures to enhance medication affordability are crucial for improving diabetic care and advancing public health in the region.

Title: *In Silico* Prediction of New Inhibitors for Kirsten Rat Sarcoma G12D Cancer Drug Target Using Machine Learning-Based Virtual Screening, Molecular Docking, and Molecular Dynamic Simulation Approaches

Speaker Name: Chandni Hayat

Affiliation: Abdul Wali Khan University Mardan

Abstract:

Single-point mutations in the Kirsten rat sarcoma (KRAS) viral proto-oncogene are the most common cause of human cancer. In humans, oncogenic KRAS mutations are responsible for about 30% of lung, pancreatic, and colon cancers. One of the predominant mutant KRAS G12D variants is responsible for pancreatic cancer and is an attractive drug target. At the time of writing, no Food and Drug Administration (FDA) approved drugs are available for the KRAS G12D mutant. So, there is a need to develop an effective drug for KRAS G12D. The process of finding new drugs is expensive and time-consuming. On the other hand, in silico drug designing methodologies are cost-effective and less time-consuming. Herein, we employed machine learning algorithms such as K-nearest neighbor (KNN), support vector machine (SVM), and random forest (RF) for the identification of new inhibitors against the KRAS G12D mutant. A total of 82 hits were predicted as active against the KRAS G12D mutant. The active hits were docked into the active site of the KRAS G12D mutant. Furthermore, to evaluate the stability of the compounds with a good docking score, the top two complexes and the standard complex (MRTX-1133) were subjected to 200 ns MD simulation. The top two hits revealed high stability as compared to the standard compound. The binding energy of the top two hits was good as compared to the standard compound. Our identified hits have the potential to inhibit the KRAS G12D mutation and can help combat cancer. To the best of our knowledge, this is the first study in which machine-learning-based virtual screening, molecular docking, and molecular dynamics simulation were carried out for the identification of new promising inhibitors for the KRAS G12D mutant.

PRESENTATION FORUM

KEYNOTE FORUM / MINI-PLENARY SESSIONS

Presentations under Keynote Forum or Mini-Plenary Sessions includes abstracts with remarkable research value selected by the program committee. These significant speeches are delivered by globally recognized honorable speakers and it is open to all registrants.

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In this forum, speakers and experts of the research field gets an opportunity to showcase their noble research work that involves comprehensive research findings. These formal oral presentations include a wide range of talks covering basic research to advanced research findings in accordance to the theme and scientific sessions of the conference.

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POSTER SESSION

This session is particularly introduced to encourage more number of student participation at international conferences, however it is not restricted only to students since it is also available for the participants with language barrier. There are specific guidelines to be followed to prepare the poster. Poster topic should be selected only from relevant scientific sessions with in-depth technical details.

YOUNG INVESTIGATORS FORUM

An exclusive opportunity for students and young investigators to present their research work through a formal oral presentation. Young Investigators Forum provides a global platform for young researchers and scholars to showcase their valuable contribution to the scientific world and to get acknowledged by the global scientific community of experts. It is an excellent opportunity to recognize young scientific assets with promising research ideas. These oral presentations are of shorter time duration with 10-15 minutes of informative and precise presentations in relevant scientific sessions.

EDUCATIONAL WORKSHOPS/RESEARCH WORKSHOPS/ CORPORATE WORKSHOPS/MINI- SYMPOSIA

With an aim of transferring knowledge among the participants, workshops are introduced as a part of international conferences. These interactive and occasionally practical sessions gives an opportunity for participants to engage in detail discussion. Workshops are mostly scheduled for 60 to 90-minutes. It may range from learning about a specific topic relevant to international education, products and research which sometimes involves practical demonstration. It helps in enhancing skills, knowledge and understanding of the research field in depth through interactive discussions.

HIGHLIGHTS OF THE DAY SESSIONS

"Highlights of the Day Sessions" is introduced to discuss and focus a ray upon previous day ORAL ABSTRACT presentations by experts to summarise the key findings. It helps in getting better insights into the various dimensions of the topic.

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This session involves open discussion between the experts and session attendees, it gives enough time for getting answers to specific questions and doubts. It is an opportunity for attendees to increase their professional networking, sometimes also leads to an excellent collaboration opportunity.

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THURSDAY - APRIL 03, 2025

- Combinatorial Chemistry
- Novel Drug DeliverySystems
- Formulations

- Natural Products
- Traditional Medicine
- Drug Repurposing and Drug Repositioning

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- Drugs and Drug Targets
- Drug Discovery, Design and Development
- Pharmacokinetics and Pharmacodynamics

- Computer Aided Drug Design
- Drug Metabolism
- Pharmaceutical Biotechnology

LUNCH BREAK

- Precision Medicine
- Personalized Therapies
- Drug Development and Clinical Trials

- Biomarker Discovery and Development
- Biologics and Biosimilars
- Vaccines and Immunotherapies

COFFEE BREAK

- Steam Cells and Regenerative Medicine
- Drug Safety and Pharmacovigilance
- Pharmacogenomics

- Toxicology
- Rare Diseases
- Receptors as Target for Drug Discovery

CONCURRENT EDUCATIONAL SESSIONS

FRIDAY - APRIL 04, 2025

- Drugs Affecting the Cardiovascular System
- Drugs Affecting the Central Nervous System
- Drugs Affecting Hormonal Systems

- Chemotherapeutic Agents
- Antibacterial Agents
- Antiviral Agents
- Anticancer Agents
- The Opioid Analgesics

GROUP PHOTO | COFFEE BREAK

- Anti-Ulcer Agents
- Non-Steroidal Anti Inflammatory Drugs
- Steroids
- Antibiotics
- Antineoplastic Agents

- Anthelmintics
- Sulphonamides
- Artificial Intelligence and Machine Learning in Drug Discovery and Development

LUNCH BREAK

- Genomics and Proteomics in Drug Discovery and Development

- Gene Therapy and Genome Editing in Treating Genetic Diseases
- Nanotechnology in Drug Delivery and Imaging

COFFEE BREAK

- Virtual and Augmented Reality in Drug Discovery and Development
- Patient Engagement and Patient-Centered Drug Development

- Big Data Analytics in Drug Discovery and Development

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