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Record 1 of 34

Title: Molecular dynamics simulation study of heavy metal ions accumulation between graphene nano-channel under external electric field

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Abstract: Heavy metal ion remediation from water system through accumulation using external electric field is proposed. Here, graphene nano-channel is utilized for heavy metal accumulation under different magnitude of electric fields (1.0 V/& Aring;, 1.5 V/& Aring;, and 2.0 V/& Aring;). Molecular dynamics simulation was carried out in three phases i.e. initiation, accumulation, and cleaning phase. Cadmium, mercury, and lead heavy metal ions were selected and relative position, distance, energy, and radial distribution function were evaluated. The results show that the electrostatic attraction between the positively charged heavy metal ions and the negatively charged graphene nano-channel significantly increases with the increase in the magnitude of the external electric field, consequently enhancing ion accumulation. The interaction of the ions with the graphene nano-channel at the external electric field of 1.5 V/& Aring; was found to be suitable.

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Abstract: Borderline personality disorder (BPD) is a complex personality disorder characterised by immense emotional dysregulation, impulsivity, aggression and substantial interpersonal difficulties. This review begins with examining DSM-5-TR diagnostic clusters for BPD, highlighting the importance of accurate classification. It provides an in-depth analysis of BPD, starting with its epidemiology, diagnostic subtypes, core symptoms, and the challenges these symptoms pose for patients and their support networks. The review explores common co-occurring conditions, such as mood disorders, anxiety disorders, and other personality disorders, which frequently compound the effects of BPD and complicate its management. A detailed examination of BPD's neurobiological underpinnings is presented, focusing on structural and functional alterations in brain, aberrant connectivity, and neurotransmitter dysregulation, particularly within serotonin, dopamine, and glutamate pathways, being vital to understanding the effects of this disorder on impulsivity and emotional instability. Therapeutic strategies for BPD are also reviewed, encompassing psychotherapeutic methods like Dialectical Behavior Therapy (DBT) and other validated therapies, alongside pharmacological treatments that target mood stabilisation, impulsivity, and affective control through antidepressants, antipsychotics, and mood stabilisers. Neuromodulation techniques, such as neurofeedback and transcranial magnetic stimulation (TMS), are discussed for their potential to enhance cognitive and emotional control in BPD. The review closes with future directions, emphasizing the value of integrated, personalised treatment approaches to optimise outcomes for individuals with BPD and reduce the broader social and emotional impact of the disorder.

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Senate Committee on Research and Academic Program (SCRAP, 1974, Document presented to this committee for the start of the Cell for ASTRA in 1974

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Abstract: A number of research institutes sought to address this disconnect in the post-independence development path and the IISc responded with its own research programmes dedicated to the needs of rural India in 1974 with the setting up of the Centre for Application of Science and Technology to Rural Areas (ASTRA, now renamed Centre for Sustainable Technologies (CST). What commenced as a discourse on alternative developmental models with a thrust on appropriate technologies centred around renewable energy and local resources gradually crystallised by the late 1980s into ideas of sustainable development. As its canvas of concerns grew, the ASTRA-CST had to reorient its vision incorporating the larger 'sustainable development goals (SDG) as we understand today. The paper attempts to fathom how certain fields of research and development (R&D) became mainstreamed at this Centre and led to various technology

development efforts. The first phase of activity of ASTRA-CST has not been adequately discussed in literature and this paper attempts to extend and to address that shortcoming. At this time, villages of rural India could best be described as reasonably closed ecosystems with moderate interactions achieving a low-level equilibrium. However, there was very little data about the various material flows, natural and man-made resource cycles, especially that relevant to land productivity, food consumption and its production pattern, water resource and security, health, rural industry, resource transformations and underlying skills, processes and efficiencies, residue management and re-use, environmental impacts, etc. and evolving such a knowledge-base was the key output of the first phase. The second phase involving various 'homegrown' technological and socio-technical interventions including stages of participatory technology development efforts resulted in large scale 'dissemination'. A third phase addressed larger sustainable technologies solutions transgressing boundaries of the rural and urban that had marked the earlier phases. It is heartening to note that in some areas such as biomethanation, water-wastewater reuse, eco-friendly houses, biomass based alternative fuel platforms, rural industrial skilling, participatory technology development, etc. have gradually become policies at the national and global level and ASTRA-CST's contribution is yeoman.

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Abstract: Benzoxazoles and benzimidazoles are a valuable class of heterocyclic compounds and have numerous therapeutic applications. Herein, we present an efficient and facile synthesis of these compounds using a 3D metal-organic framework (MOF), {Mn2(TPA)2(DMF)2}n, referred to as the Mn-TPA MOF (TPAH2 represents terephthalic acid and DMF denotes N,N-dimethylformamide) as a catalyst. The desolvated MOF, Mn-TPADesolv, with its robust nature and manganese open metal sites (OMSs) serves as an effective heterogeneous catalyst. Mn-TPADesolv efficiently facilitates the synthesis of benzoxazole and benzimidazole derivatives via the reaction of o-aminophenol or o-phenylenediamine with various aromatic aldehydes. We recorded high conversions up to 99.9% in both the reactions under optimised conditions within a short reaction time. The catalytic reactions exhibited a remarkably high turnover number (TON) up to 9990, and a turnover frequency (TOF) up to 333 min-1 for various substrates. Notably, Mn-TPADesolv showed excellent catalytic activity for sterically hindered substrates, such as 1-naphthaldehyde and 9-

anthracenecarboxaldehyde, maintaining high TON and TOF values. Furthermore, the recyclability of Mn-TPADesolv revealed that the catalyst could be reused up to 30 cycles with no loss in its structural integrity and catalytic performance. The results obtained in this study demonstrate the excellent catalytic performance of Mn-TPADesolv and emphasize its potential as a scalable, robust, cost-effective catalyst with its broad substrate scope compatibility.

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Abstract: BRAF is a proto oncogene that functions as a key signal transducer in the MAPK-ERK pathway, which regulates cell growth, division, and survival. Mutations in BRAF, particularly the V600E substitution in its kinase domain, are major drivers in melanoma and several other metastatic cancers, including breast, colorectal, NSCLC, and gastrointestinal cancers. In this study, novel inhibitors targeting the BRAF(V600E) mutant using a structure-based drug design approach are identified. Four chemical libraries ChemDiv Kinase, ChemDiv Anticancer, NCI, and ChEMBL Kinase SARfari are screened. Compounds from the ChemDiv Anticancer database show better Glide scores comparable to the FDA-approved BRAF inhibitor Vemurafenib. The compounds P184-1419 and P184-1479 score -12.688 and -12.012 kcal/mol, respectively, versus -14.288 kcal/mol for Vemurafenib. Top hits are further validated using GOLD docking, X-score ranking, and interaction profiling via LigPlot. Molecular dynamics simulations, principal component analysis, and free energy calculations confirm the stability of protein-ligand complexes. Biolayer interferometry assays reveal P184-1419 exhibits stronger binding affinity (KD = 151 mu M) than Vemurafenib (KD = 437 mu M). These findings suggest P184-1419 is a promising lead compound against BRAF(V600E), offering potential for future development of more effective cancer therapies.

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Abstract: center dot The role of PHYTOCHROME INTERACTING FACTOR 3 (PIF3) in thermomorphogenesis, despite being a crucial regulator of photosensory hypocotyl growth in Arabidopsis, remains unknown. center dot Here, we demonstrate PIF3 as a key and novel component of the thermosensory pathway. pif3 mutants show reduced sensitivity to warm temperature-induced hypocotyl elongation, which is more pronounced at higher light intensities. pif3 mutant exhibits moderate impairment in petiole elongation and flowering. By contrast, PIF3 overexpression lines show constitutive thermomorphogenic responses. center dot Whole-genome transcriptome analysis revealed that genes induced by warm temperature are significantly downregulated in the pif3 mutant but are constitutively upregulated in the PIF3 overexpression line. Moreover, PIF3 directly activates PIF4 transcription by binding to the PIF-binding element (PBE-box) in a temperature-dependent manner. center dot Chromatin immunoprecipitation (ChIP) and biochemical data indicate that PIF4 binding to its target genes requires PIF3. The physical interaction between PIF3 and PIF4 is likely required for the optimal expression of downstream genes involved in metabolism and growth. Epistatic and gene regulation analysis further revealed that PIF3 functions in PIF4-dependent and PIF4-independent pathways to regulate gene expression. This study unravels the novel role, and mechanism through which, PIF3 promotes thermomorphogenic growth in Arabidopsis.

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Abstract: Advanced wireless communications demand microwave systems that offer low-loss, narrow linewidth, and large operating frequency range. We have examined the effect of bismuth and gadolinium co-doping in yttrium-iron-garnet (YIG) ferrimagnets through their microstructural, magnetic, and microwave properties for their performance in broad-band high-frequency devices. The GdxBi0.1Y2.9-xFe5O12 (x = 0.0 to 0.3) nanoparticles were prepared using solid-state reaction method. XRD Rietveld-refinements revealed the single-phase YIG structure validating Ia3<overline>d\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$$Ia\overline{3 }d$$\end{document} cubic crystal structure. The saturation magnetization decreased by 32% with increasing Gd doping. Magneto-dynamics key parameters such as gyromagnetic ratio, Gilbert damping factor, and extrinsic linewidth, were evaluated to assess the potential of these materials for use in microwave device applications. Microwave device functionalities were demonstrated from S-to-X-band frequencies using Gdx-Bi0.1YIG samples. The fabricated band-pass filter exhibits large tunability of 140%, large bandwidth of 1.97 GHz, and minimal insertion loss of - 1.17 dB with relatively low bias of 0.25-1.95 kOe. The fabricated phase shifter module demonstrated a large differential phase shift of 300 degrees in the frequency range from 3-10 GHz with Gd substitution. The investigated Gd-YIG-based isolator exhibit isolation over 11 dB at low fields for over the frequency span of 3-10 GHz. We have demonstrated that 0.1 formula unit doped Gd- in YIG shows the best results for microwave devices as compared to other samples.

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Abstract: Breast cancer (BC) is listed as the most prevalent cancer form in women worldwide, with major subtypes classified by hormone receptor (HR) and HER2 status including, HR+/HER2- (similar to 65-70%), HER2+ (similar to 15-20%), Triple-Negative-HR-/HER2- (similar to 10-15%) and rare sybtypes (<5%). Scientific evidence has revealed that PI3K/AKT/mTOR signaling cascade plays an important role in the development and progression of BC, contributing to key cellular processes including cell growth, proliferation, angiogenesis, and metastasis. Dysregulation of the components of this cascade including functional loss of Phosphatase and TENsin homolog (PTEN), PI3K hyperactivation, and gain-of-function of AKT, are frequently observed in BC subtypes, making it a promising target for therapeutic intervention. A myriad of studies have documented the potential of phytochemicals, including curcumin, chrysin, fisetin, genistein, resveratrol and lycopene as modulators of the PI3K/AKT/mTOR axis. These phytochemicals exhibit multifaceted mechanisms of action, including inhibition of key kinases, induction of apoptosis, suppression of angiogenesis, and reversal of resistance to chemotherapy. This review aims to provide a detailed overview about the role of PI3K/AKT/mTOR alteration in BC development and the current research on phytochemicals that modulate the PI3K/AKT/mTOR pathway in BC. We documented the molecular mechanisms through which these compounds exert their effects, their potential synergistic interactions with conventional therapies, and the challenges and prospects for their clinical application. The evidence presented underscores the promise of phytochemicals as novel, less toxic adjuncts to traditional BC therapies, warranting further exploration and development for clinical use.
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Abstract: Pollen presence in the atmosphere, as Primary Biological Aerosol (PBA) fraction, constitutes a significant proportion of aerosol. In recent years, research focusing on the role of pollen grains in the

atmosphere has intensified toward understanding their impacts on environmental processes and human health. Investigation over 15 months, from January 2012 to March 2013, in Jawali, Kangra district of Himachal Pradesh, was undertaken to estimate the abundance and diversity of airborne pollen grains in ambient coarse particulate matter (CPM) sampled using a high-volume PM sampler. The average CPM load of 46.6 mu g m-3 corresponded with an average pollen concentration of 219 pollen grains m-3 during the study. A large diversity of pollen grains in CPM was observed, with 54 different types of pollen grains belonging to 35 plant families, including two gymnosperm families. The major tree genera characterized were Mallotus, Pinus, Eucalyptus, Syzigium, Prosopis, Phyllanthus, Cassia, and Acacia, whereas the shrubs were Dodonaea, Ricinus, and Ephedra. Herbaceous pollen contributed a significant fraction of pollen grains belonging to Poaceae, Asteraceae, Brassicaceae, Cannabaceae, and Urticaceae. A significant number of pollen grains recorded in this investigation have been reported as allergenic in the literature. Most of the pollen grains in CPM belonged to the region's endemic vegetation, suggesting their local origin. The monthly concentration profile of pollen grains displayed significant variation over 15 months. Meteorological parameters, temperature, planetary boundary layer height, and wind speed statistically correlated with CPM. The insignificant correlations with pollen concentration indicated that the sources of CPM and pollen emissions differ. However, pollen showed a weak correlation with wind speed and a negative correlation with relative humidity.
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Abstract: The effects of magnetic field on the atomic spectral properties of plasma embedded Be-like Cr XXI ion have been studied. To accomplish this, we use the relativistic configuration interaction (RCI) technique by incorporating magnetic field and analytical b-potential. Shielding effects on the inter-combination transitions 2s2 1S0 -> 2snp 3P1 and resonance transitions 2s2 1S0 -> 2snp 1P1 (n = 2, 3) of Cr XXI ion are investigated. Blue and red shifts in transition energies are observed for the transitions corresponding to Delta n = 0 and Delta n not equal 0, respectively. We also studied the combined effect of dense plasma and magnetic field on the transition probabilities of magnetic sub levels corresponding to the transition 2s2 1S0 (MJ = 0) -> 2s2p 3P1, 1P1 (MJ = 0, +/- 1) and 2s2 1S0 (MJ = 0) -> 2s3p 3P1, 1P1 (MJ = 0, +/- 1). The present calculated results are in good agreement with the values of NIST database.

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Title: Radiation Pressure-Driven Magneto-Gravitational Instability in Finitely Conducting Strongly Coupled Quantum Plasmas

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Abstract: This paper investigates the radiation pressure-driven linear magneto-gravitational instability in finitely conducting strongly coupled quantum plasma within the framework of the generalized hydrodynamic fluid model. The radiation pressure assists in the dynamic behavior of the plasmas by modifying the dispersion properties of the gravitational instability. Normal mode analysis is applied to the linearized perturbation equations to derive the general dispersion relation. The dispersion relations are discussed in the hydrodynamic and kinetic limits in the transverse and longitudinal propagation modes. The Jeans instability criterion and Jeans length are significantly modified due to radiation pressure, quantum corrections, and strong coupling effects. The viscoelastic compression mode in the kinetic limit has been coupled with quantum diffraction and Alfv & eacute;n mode. It is also observed that the radiation pressure, quantum effects, and viscoelastic parameters suppress the growth rates; thus, these have stabilizing effects on the gravitational instability. The effects of various parameters on the growth rate of the instability are calculated numerically, and the outcomes are represented graphically.

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Abstract: The long-term survival of Mycobacterium tuberculosis (Mtb) requires efficient use of host resources and uninterrupted access to host-derived nutrients. This is done by utilization of a highly flexible and integrated network of metabolic pathways. Phosphoglucomutase A (pgmA) is essential for glycogen biosynthesis, which acts as a nutrient reservoir and is known to modulate carbon flux in various pathogens. We, for the first time, investigated the role of pgmA in Mtb by creating a strain lacking this gene. The absence of pgmA hinders the survival of pathogens under nutrient-limiting and reactivation conditions. Our study shows that the lack of cell membrane-associated glycolipids in Delta pgmA compromises cell wall integrity and increases susceptibility to stress. Interestingly, Delta pgmA exhibits an enhanced growth phenotype on cholesterol compared to the wild type due to low cyclic adenosine monophosphate (cAMP) levels. Differential gene expression and 13C3 carbon dilution analyses indicate that stored carbon as glycogen is crucial for Mtb survival under nutrient-limiting conditions. We demonstrate that pgmA is vital for Mtb growth within the host. This study highlights the critical role of pgmA in metabolic adaptation during nutrient starvation and reactivation and its implication on antibiotic and disease persistence. These insights are crucial for developing novel, shorter, and more effective anti-tuberculosis strategies.IMPORTANCEThis study for the first time investigated the role of metabolic enzyme phosphoglucomutase A (pgmA) in Mycobacterium tuberculosis (Mtb), revealing its crucial functions as a toggle switch between biosynthesis and growth. This work highlights the importance of pgmA in maintaining the metabolic flexibility of Mtb during the nutritional switch. The presence of pgmA is critical for the production of membrane-associated glycolipid, which helps maintain the cell wall integrity under various growth and stress conditions. This adaptability is pivotal for generating starvation-induced antibiotic tolerance in Mtb. In addition to the clinical context, these findings provide a mechanistic foundation for understanding adaptive strategies by Mtb to harsh environments and the development of drug-tolerant bacilli.

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Abstract: N-Carbamoyl putrescine amidase (CPA) is a key enzyme in polyamine synthesis and plays an essential role in cell growth and proliferation in plants and many bacteria. While CPA is absent in humans, its presence in Helicobacter pylori makes it a potential therapeutic target. Despite its biological importance, CPA's structural and functional characteristics are not fully understood. The (-152CWDQW156-) motif in H. pylori CPA is conserved across homologues, where tryptophan residues are critical for oligomerization. This motif forms a short helix near the active site, suggesting a functional role for helix formation. Using computational and solution-based experiments, we show the significance of short-helix formation in CPA function. Unlike the wild-type and the Cys152Ala mutant, which form octamers, the Cys152Pro variant disrupts the helix formation and produces dimers. This indicates that short-helix construction is crucial for producing octamers. Furthermore, we observed that residues Asp154 and Tyr157 interact with His117 within the same monomer. Notably, single Ala mutations of these residues resulted in dimers with significantly reduced catalytic activity despite maintaining helix formation. This finding underscores the importance of the interaction network (Asp154-His117-Tyr157) in stabilizing the helix's orientation and promoting octamerization. We also observed that octamerization enhances protein stability, as evidenced by a 10 degrees increase in T m. Targeting the short helix and its surrounding region, we identified a small-molecule CPA inhibitor that effectively reduced enzymatic activity. These findings reveal a new regulatory mechanism where helix formation and oligomerization are crucial to CPA function, providing a foundation for developing more potent therapeutic inhibitors against H. pylori.

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Author(s): Balkrishna, A (Balkrishna, Acharya); Sinha, S (Sinha, Sandeep); Varshney, A (Varshney, Anurag)

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Abstract: Introduction Ayurvedic medicines with scientifically proven anti-inflammatory, bronchodilator, anti-tussive and anti-microbial activities have an immense potential to be repurposed for the management of obstructive airway symptoms, frequently encountered in patients afflicted with coronavirus disease 2019 (COVID-19). Divya-Swasari-Vati is an Ayurvedic prescription medicine, which contains nine botanical drugs and seven mineral ashes. The individual botanical drugs and minerals present in Divya-Swasari-Vati have been traditionally used for the treatment of upper and lower respiratory tract symptoms, associated with ailments ranging from common cold and cough to chronic asthma and respiratory infections. Divya-Swasari-Vati is enriched with metabolites known to possess pharmacological activity and has demonstrated in-vivo anti-inflammatory effects in a human A549 cell line-xenotransplanted zebrafish model, subsequent to challenge with the spike protein of severe acute respiratory syndrome-coronavirus-2. With an objective to support the preclinical and clinical profile, the non-clinical safety assessment of Divya-Swasari-Vati is highly warranted. Accordingly, in the current study, we report the non-clinical safety of Divya-Swasari-Vati in a repeated-dose, 28-day subacute oral toxicity study, followed by a 14-day recovery period, in Sprague-Dawley rats, under GLP compliance.Methods This toxicological study was conducted according to Organization for Economic Cooperation and Development (OECD) test guideline 407 and in conformance with the OECD principles of Good Laboratory Practice (GLP). Divya-Swasari-Vati was tested at the doses of 100, 300 and 1,000 mg/kg/day, in five males and five female rats of each experimental group.Results In the present study, no mortality or morbidity was observed in any of the test groups. Furthermore, Divya-Swasari-Vati treatment was not associated with any toxicologically relevant outcomes with respect to clinical signs as well as clinical-, gross- and histo-pathological findings, as compared to the vehicle-administered group. Consequently, the No-Observed-Adverse-Effect-Level (NOAEL) of Divya-Swasari-Vati was determined to be 1,000 mg/kg/day, in both male and female rats.Discussion The acceptable safety profile of Divya-Swasari-Vati demonstrated in the present study, provisions for its future non-clinical safety

assessments for longer duration in rodents as well as in higher animals. Additionally, this study also serves as the first step towards the detailed assessment of Divya-Swasari-Vati in clinical settings.

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Title: Achieving a high-strength dissimilar aluminium alloy 6061 and Polypropylene joint by Friction Stir Welding via varying tool rotational and traverse speed

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Abstract: Investigating the robust bonding between dissimilar materials such as aluminium alloys and polymers is vital in welding processes. This research delves into the structural interface and mechanical attributes achieved through aluminium alloy 6061 (AA6061) and Polypropylene (PP) friction stir welding by varying traverse and rotational speeds. A travel speed was varied with a range of 50-80 mm/min, and the tool rotational speed between 1300 and 1900 rpm was investigated to analyse their impact on mechanical properties. The lap joint configuration in which the PP is at the top and AA6061 is at the bottom was chosen from trial experiments. A scanning electron microscope observed that many locations had a tight bond in most interface areas. The average hardness values at the stir zone in the joints at different rotational speeds initially increased up to 1700 rpm due to fine fragmentation and proper distribution of these aluminium chips, and then reduced after rising to 1900 rpm. Evaluation of weld quality encompassed assessments of weld nugget hardness and lap tensile shear strength, elucidating the mechanical interlocking mechanism between AA6061 particles and PP as a critical factor contributing to joint stability. The intersection of aluminium chips and solidified polymer contributes to enhancement in the shear strength due to the phenomenon known as mechanical interlocking. The highest tensile shear strength of 5.4 MPa was observed at a rotational speed of 1700 rpm and a traverse speed of 60 mm/min, signifying optimal process conditions for enhancing mechanical integrity.

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Abstract: Mangrove roots contain metabolites that enhance salt tolerance and support the germination of their propagules under stressful conditions. GC-MS was performed to understand differential responses between roots of two non-salt-secreting mangroves, Kandelia candel (L.) Druce and Rhizophora mucronata Lam. against varying salinity gradients. The analysis revealed abundant organo oxygen compounds, fatty acids, amino acids and peptides, monosaccharides, disaccharides, alcohols and polyols in the germinating roots of these species. After screening, 75 and 61 compounds were identified in K. candel and R. mucronata, respectively. Twenty-one metabolites were commonly found in both plants, including D-pinitol, sucrose, ethanolamine, glycerol, trehalose and palmitic acid. These metabolites increase in concentration following higher salinity treatment. Principal component plotting indicated similarities or differences in their metabolic profiles. For example, the principal components of metabolites in freshwater and salt-treated K. candel root samples differed from those in other salt treatments. However, after 60 days, all treatments exhibited overlapping metabolite profiles. The different treatments applied to R. mucronata propagules were clustered primarily in the positive region of the axis, suggesting similar metabolic responses. The key pathways involved in salt stress responses in K. candel and R. mucronata include alanine, aspartate and glutamate, glutathione, starch, sucrose and galactose metabolism. These findings highlight the metabolic adaptations of K. candel and R. mucronata propagules to salinity gradients during germination, underscoring the complexity and specificity of their responses to salinity.

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Abstract: BackgroundAlzheimer's disease (AD) affects over 55.2 million individuals globally with current treatment modalities only providing symptomatic relief. This highlights the importance of combination therapies which target multiple pathways simultaneously. Donepezil (DNP), an acetylcholinesterase inhibitor, when combined with Quercetin (QCT), a polyhydroxy flavonoid with neuroprotective properties, might alter progression. However, simultaneous estimation of DNP and QCT for concurrent delivery, calls for robust analytical method that can simultaneously estimate both drugs.Research design and methodsA simple, robust, and cost-friendly UHPLC method for simultaneous estimation of DNP and QCT was developed. The analytes were resolved on C18 column (Kromasil C18, 4.6 x 250 mm), with acetonitrile and 0.1% diethyl amine buffer, adjusted to pH 3.5 with glacial acetic acid as mobile phase in ratio 50:50 v/v at 0.6 mL/min, at column oven temperature 40 degrees C in total analysis run time of 10 min.ResultsDNP and QCT were quantified by PDA detector at 268 nm and 370 nm, respectively. The developed method was found to be linear, accurate, precise, specific, and robust as per ICH guidelines.ConclusionThe developed and validated method efficiently quantified DNP and QCT co-loaded inside liposomes estimating their entrapment efficiency, loading efficiency, and in vivo plasma kinetics.

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Abstract: This study investigates the influence of phytic acid on Fe and Zn bioaccessibility and impact of phenolics on free radical scavenging activity in 13 diverse pearl millet (PM) genotypes. Forty-three phenolic compounds were identified using UPLC-(ESI)-QToF-MS. Free (173.01-217.11 mg GAE/100 g), bound (102.97-142.52 mg GAE/100 g), and total phenolic content (286.04-337.63 mg GAE/100 g) varied significantly among genotypes. Phenolic content positively correlated with radical scavenging activity (36.43%-47.56%, DPPH assay). INFOGEST in vitro digestion showed increasing phenolic bioaccessibility from oral (12.58%-23.55%) to gastric (48.4%-72.25%) to intestinal (67.17%-90.26%) phases. Bioaccessibility of Fe (10.55%-14.46%) and Zn (13.48%-19.79%) was negatively correlated with phytic acid (629.02-797.71 mg/100 g) content. WGI 100, with the lowest phytic acid content, had the highest bioaccessibility, whereas Dedha Bajra, with the highest phytic acid content, had the lowest bioaccessibility of Fe and Zn recorded. PM genotypes are rich in phenolics, having high radical scavenging potential. However, higher phytic acid content reduced Fe and Zn bioaccessibility, reinforcing its antinutritional effect on mineral bioavailability.

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Abstract: Background and objective Access to clean drinking water is essential for health and development. Despite global and national initiatives, many regions in India continue to face inadequate water access. This study assesses progress, sociodemographic determinants and geographic disparities in access to drinking water in India, aligning with Sustainable Development Goal (SDG) 6.1.Design This study used secondary data from five rounds of the National Family Health Survey (NFHS-1 to NFHS-5; 1992-2021), nationally representative surveys conducted across India. Logistic regression was employed to examine the association between household sociodemographic characteristics and access to improved drinking water. A Water Access Index (WAI) was constructed using Principal Component Analysis (PCA) based on four indicators: access to improved sources, on-premises availability, 5-minute round-trip access and household water treatment. The scores were normalised to a 0-100 scale.Setting and participants The study used household data from NFHS-1 (88 562 households), NFHS-2 (92 477), NFHS-3 (109 041), NFHS-4 (601 506) and NFHS-5 (636 699), covering all 36 states/union territories in India.Results There has been a notable improvement in access to improved sources, on-premises water and timely availability. Factors such as higher educational attainment, pucca housing and the absence of a below poverty line card were positively associated with better access. Based on WAI scores, 343 districts (49%) were categorised as front runners (65-99%), 142 districts (20%) as performers (50-64%) and 221 districts (31%) as aspirants (0-49%). Only one district (0.1%) achieved universal access. Many districts in West Bengal, Bihar, Odisha, Jharkhand and other states still exhibit low-to-moderate water access.Conclusion While access to improved drinking water has advanced, regional and socioeconomic disparities remain stark. Targeted, multisectoral policies are essential to ensure equitable progress towards SDG 6.1 across all districts and population groups in India.

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Abstract: Cancer continues to pose a significant challenge to global health, resulting in millions of deaths annually despite advancements in treatments like surgery, chemotherapy, and radiotherapy. A key factor complicating successful outcomes is the presence of cancer stem cells (CSCs), which possess distinctive features that facilitate tumor initiation and progression as well as resistance to therapies. These cells are adept at evading conventional treatments and can hinder the effectiveness of immunotherapy, often manipulating the tumor microenvironment to suppress immune responses. This review delves into the complex interplay between CSCs and immune cells, emphasizing their contributions to tumor heterogeneity and therapeutic resistance. By investigating the CSC niche in which these cells thrive and their complex interactions with the immune system, we aim to reveal new therapeutic avenues that could enhance patient outcomes and minimize the risk of recurrence. CSCs are characterized by remarkable self-renewal and plasticity, allowing them to transition between stem-like and differentiated states in response to various stimuli. Their existence within the CSC niche confers immune protection and maintains stem-like properties while promoting immune evasion. Activating key signaling pathways and specific surface markers is crucial in developing CSC traits, pointing to potential strategies for effective tumor eradication. Conventional therapies often fail to eliminate CSCs, which can lead to tumor recurrence. Therefore, innovative immunotherapeutic strategies such as dendritic cell vaccines (DC vaccines), chimeric antigen receptor (CAR) engineered T cells, and immune checkpoint inhibitors (ICIs) are under examination. This review sheds light on CSC's roles across different malignancies, highlighting the necessity for innovative targeted approaches in cancer treatment.

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Abstract: Advances in virtual staining and spatial omics have revolutionized our ability to explore cellular architecture and molecular composition with unprecedented detail. Virtual staining techniques, which rely on computational algorithms to map molecular or structural features, have emerged as powerful tools to visualize cellular components without the need for physical dyes, thereby preserving sample integrity. Similarly, spatial omics enable the mapping of biomolecules across tissue or cell surfaces, providing spatially resolved insights into biological processes. However, traditional dye-based staining methods, while widely used, come with significant limitations. In this context, Raman spectroscopy offers a robust, label-free alternative for probing molecular composition at a high resolution. We present a novel algorithm that reconstructs super-resolved Raman images by extracting spectral patterns from surrounding pixels, enabling detailed, label-free visualization of cellular structures. By employing Raman spectroscopy in conjunction with chemometric tools such as principal component analysis (PCA), multivariate curve resolution-alternating least squares (MCR-ALS), and artificial neural network (ANN), we performed a quantitative analysis of key biomolecular components, including collagen, lipids, glycogen, and nucleic acids, and classify the different cancer cell lines with an accuracy of nearly 99%. This approach not only enabled the identification of distinct molecular fingerprints across the different cancer types but also provided a powerful tool for understanding the biochemical variations that underlie tumor heterogeneity. This innovative combination of virtual staining, spatial omics, and advanced chemometrics highlights the potential for more accurate diagnostics and personalized treatment strategies in oncology.

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Abstract: Cancer is a major global health challenge, with an estimated 19.3 million new cases by 2025, largely due to lifestyle changes, environmental factors, and increased life expectancy. Despite advances in conventional therapies, issues such as drug resistance, systemic toxicity, and relapse continue to hinder long-term survival rates. One underexplored molecular mechanism potentially contributing to cancer progression is the enzyme Human tRNA-dihydrouridine synthase 2 (hDus2). hDus2 plays a pivotal role in tRNA modification by converting uridine residues to dihydrouridine, enhancing tRNA structural flexibility and translational efficiency. Elevated dihydrouridine levels in tRNA have been correlated with cancer progression, highlighting hDus2 as a potential therapeutic target. In this study, we investigated the inhibition of hDus2 as a novel strategy for cancer therapy. Using in silico techniques, we screened a library of FDA-approved drugs against the 3D structure of hDus2. Top candidate compounds identified through virtual screening with the Glide module were further evaluated using molecular dynamics simulations. Parameters such as RMSD, RMSF, Rg, SASA, and PCA were analyzed. Additionally, binding free energy calculations were performed to validate the stability and interaction strength of the hDus2 ligand complexes. Our results identified DB09050, a cephalosporin antibiotic used for treating complicated intra-abdominal infections, and DB00650, a folate analog, as promising hDus2 inhibitors. These findings pave the way for further development of anticancer therapeutics post-experimental validation.

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Abstract: Malaria remains a critical global health issue, particularly in tropical and subtropical regions. Understanding its biology and epidemiology is vital for developing effective prevention and control strategies. Falcipain-2 (FP-2), a cysteine protease in Plasmodium falciparum, the deadliest malaria parasite, is essential for parasite survival in red blood cells, making it an attractive drug target. Inhibiting FP-2 disrupts key metabolic processes, leading to parasite death, offering a promising antimalarial drug development avenue. This study utilized computational approaches to design novel antimalarials. We prepared large fragment libraries, Enamine (similar to 220,174 fragments) and ChemDiv (similar to 18,713 fragments), for virtual screening against FP-2 (PDB ID: 6JW9). Fragments with binding free energies <= -4.0 kcal/mol were selected and evolved into drug-like ligands. SP and XP docking-based screenings prioritized these ligands, refined further using MM-GBSA calculations. Promising ligands underwent 100 ns molecular dynamics simulations to assess conformational changes and complex stability. This study identified two viable inhibitors, T4 and A3, with high affinity, stability, and selectivity towards FP-2 compared to E64.Following computational studies, compound A3 and its ten analogues (KA-series) were synthesized and characterized by using multi-spectroscopic techniques with high purity confirmed by LC-

MS. Biological testing against P. falciparum 3D7 strain revealed KA-5 as the most potent compound with an IC50 value of 3.0 mu M. Future work will involve synthesizing additional analogue series for an extensive structure-activity relationship (SAR) study. Further experimental validation is essential to develop these compounds as effective therapeutic agents for malaria treatment.

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Abstract: Citrus is widely recognized as one of the most extensively cultivated fruit crops globally, particularly in tropical and subtropical regions valued for their economic significance and nutritional benefits. However, their productivity is increasingly threatened by pests and diseases, particularly the citrus nematode Tylenchulus semipenetrans, which causes significant damage to the root systems. This study investigates the nematicidal properties of silver nanoparticles synthesized through green method using Parthenium hysterophorus (Pr-AgNPs) against the second-stage juveniles (J2) of T. semipenetrans. The bioassay results demonstrate that Pr-AgNPs exhibited a maximum mortality of 100% at a concentration of 4 ppm after 6 h of treatment. Both concentration and exposure time had significant effects on mortality of nematodes. Additionally, Pr-AgNPs applied at varying concentration significantly increased the shoot length, root length, shoot weight, root weight and number of leaves of citrus plants. The production of chlorophyll and carotenoid significantly increased in citrus plants treated with 2 ppm and 4 ppm Pr-AgNPs as compared to the control (with nematodes without treatment). According to these findings, Pr-AgNPs are a

promising alternative to conventional chemical nematicides, providing a sustainable solution for managing nematode infestations and improving citrus crop productivity.

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Abstract: Stem cell functions and ageing are deeply interconnected, continually influencing each other in multiple ways. Stem cells play a vital role in organ maintenance, regeneration, and homeostasis, all of which decline over time due to gradual reduction in their self-renewal, differentiation, and growth factor secretion potential. The functional decline is attributed to damaging extrinsic environmental factors and progressively worsening intrinsic genetic and biochemical processes. These ageing-associated deteriorative changes have been extensively documented, paving the way for the discovery of novel biomarkers of ageing for detection, diagnosis, and treatment of age-related diseases. Age-dependent changes in adult stem cells include numerical decline, loss of heterogeneity, and reduced self-renewal and differentiation, leading to a drastic reduction in regenerative potential and thereby driving the ageing process. Conversely, ageing also adversely alters the stem cell niche, disrupting the molecular pathways underlying stem cell homing, self-renewal, differentiation, and growth factor secretion, all of which are critical for tissue repair and regeneration. A holistic understanding of these molecular mechanisms, through empirical research and clinical trials, is essential for designing targeted therapies to modulate ageing and improve health parameters in older individuals.

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Abstract: Lithium metal batteries (LMBs) operating at high cut-off voltages can achieve an energy density exceeding 500 Wh kg-1; however, they often suffer from severe capacity degradation due to electrolyte decomposition. Herein, propylene glycol monomethyl ether acetate (PMA) is introduced as a novel solvent for LMB electrolytes. The unique ether-oxygen functionality in PMA exhibits high steric hindrance, leading to weak lithium-ion coordination, which promotes the formation of contact ion pairs (CIPs) in the electrolyte solvation structure, especially in the presence of dual salts. A Li||LiNi0.8Co0.1Mn0.1O2 (NCM811) battery employing the formulated PMA-based electrolyte demonstrates stable cycling at a high cut-off voltage of 4.5 V for over 100 cycles, retaining 90.1% of its initial capacity even at 60 degrees C. Furthermore, a molecular interfacial model is proposed to elucidate the impact of the designed electrolyte on electrode interfacial behavior and battery performance, providing valuable insights for the development of high-performance LMB electrolytes.

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Abstract: Convective Available Potential Energy (CAPE) is widely considered a good measure of atmospheric convection. Though there is a general consensus among the scientific community about the increasing trend of atmospheric convection in a warming scenario, the tropical region presents an uncertain picture of atmospheric convection as recent studies report disagreement between radiosonde and ERA5-derived CAPE trends. In this study, we attempt to address this uncertainty over the Indian region by considering several other proxies of atmospheric convection, namely surface equivalent potential temperature, outgoing longwave radiation, upper tropospheric carbon monoxide, convective precipitation and lightning in addition to the CAPE trends obtained from radiosonde based observations and ERA5 model-based data sets for the period 2001 to 2024. Our results of radiosonde-reported CAPE from 29 stations spread across the entire India show a significant decreasing trend at 0Z (-30.85 J/kg/year), whereas a slightly increasing trend (0.5 J/kg/year) is observed over these stations in ERA5 CAPE data sets at 0Z. Further, our analysis reveals that the CAPE trend based on radiosonde observations over India is reversed if we compute CAPE following the surface-based approach (i.e., SBCAPE). The disagreement between radiosonde and ERA5 CAPE trends raises questions about the reliability of radiosonde-reported CAPE as a measure of atmospheric convection over India. However, results from all other proxies suggest an increasing trend of atmospheric convection over India. Therefore, we conclude that inferences based solely on radiosonde-reported CAPE may not be sufficient to assess the trends of atmospheric convection over India, and a more holistic approach based on several proxies is needed.

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Abstract: Unregulated release of pharmaceuticals (PhACs) persists in the environment due to their non-biodegradable and highly stable nature. In this study, Ti3+ induced TiO2 nanoparticles (NPs) (7.5 nm average crystallite size) were synthesized through a facile hydrothermal process. Powder X-ray diffraction revealed anatase phase of TiO2 NPs with a band gap of 3.48 eV. The observed bands in Raman spectroscopy, X-ray photoelectron spectroscopy, and electron paramagnetic resonance spectroscopy confirmed the oxygen vacancies and formation of Ti3+ in TiO2 lattice structure. The nanoparticles exhibited proficient photocatalytic degradation of 97% paracetamol (PCM) in 120 min, 95% diclofenac (DCF) in 30 min, and 72% chloramphenicol (CRP) in 120 min. The PCM degradation pathway was analyzed via mass spectroscopy, revealing key steps like coupling, hydroxylation, oxidation, and deacylation. Crucial process parameters (catalyst dose, initial PhAC concentration, pH, and time) were optimized for PCM, DCF, and CRP photocatalytic degradation, with kinetics following the Langmuir-Hinshelwood pseudo-first-order model. Response Surface Methodology-Central Composite Design optimized independent variables, showing higher DCF degradation efficiency at high catalyst doses and an optimal pH of 5.5-7. The role of radical species in the photocatalytic degradation of PhACs was discussed using EDTA-Na2, terephthalic acid, and p-BQ for holes, OH center dot, and O2-center dot radicals, respectively.

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Abstract: A library of forty-eight new capsaicinoids (19a-q, 13, 20a-q, 15, and 22a-l) were prepared and evaluated for their ciprofloxacin activity potentiation effect against a panel of three antibacterial strains of S. aureus1199B, S. aureus1199, and SAK1758. Among the capsaicinoids tested, 20l increased the potency of ciprofloxacin by eight folds at 50 mu g/mL, while exhibiting a minimum effective concentration (MEC) of 12.5 mu g/mL against NorA overexpressing S. aureus 1199B (with four-fold improved potency) whereas capsaicin displayed two folds higher MEC. The kill kinetics curve for the combination at MEC of the lead showed that ciprofloxacin at a sub-inhibitory ratio (0.25 x MIC) was equipotent in effect, to its MIC. Significant decay in ethidium bromide efflux in presence of compound 20l affirmed NorA efflux pump inhibition as the mode of action.

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Abstract: Background In 2022, the World Health Organisation (WHO) announced new cases of the developing Monkeypox Virus (MPXV), a zoonotic orthopoxvirus viral infection that mimics smallpox signs. Despite the ongoing infection, no proper medication is available to completely overcome this infection.Aim The study aims to construct a multi-epitope vaccine targeting Monkeypox Virus (MPXV) membrane glycoprotein to provoke robust immune responses.Objective To construct a potential immuno-dominant epitope vaccine to combat MPXV.Methods The target sequence, sourced from the UAE-to-India travel case, was analyzed to identify potential B-cell and T-cell epitopes (MHC-I and MHC-II). Immunodominant epitopes were selected and fused with beta-defensin-I and PADRE to increase immunogenicity. The vaccine was modeled, docked with TLR3, and subjected to a 500 ns molecular dynamics simulation for stability analysis. Immune responses and bacterial expression were also evaluated.Results The vaccine, comprising 230 amino acids, demonstrated antigenicity (0.6620), non-allergenicity, and broad population coverage. Selected epitopes included 3 B-cells, 4 MHC-I, and 2 MHC-II, ensuring a potent immunodominant profile. Docking with TLR3 revealed a binding affinity of -17.2 kcal/mol, while simulations confirmed their stability. Cloning (pET28a (+)) and immune response analyses showed a strong immunogenic profile, including elevated IgG1, IgM, and antigen levels, supported by a Codon Adaptation Index (CAI) of 1.0.Conclusion The proposed multi-epitope vaccine shows promise against MPXV. However, further in vivo and in vitro investigations are essential to confirm its immune efficacy.

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Abstract: The Open Charge Point Protocol (OCPP) is a widely adopted communication standard that enables vendor-independent communication between charging points and Electric Vehicle (EV) charging station management systems. OCPP has significant cyber risks in terms of weak authentication mechanisms and improper session handling, exposing it to potential EV charging-related security threats. The backward incompatibility of the recent version of OCPP also poses challenges in the seamless adoption of the protocol. This paper introduces a comprehensive cyber defense framework to mitigate the security risks associated with OCPP. Through a detailed analysis of its vulnerabilities, the framework proposes targeted enhancements and mitigation strategies to further strengthen its security. The results demonstrate that the proposed OCPP significantly enhances both security and performance, surpassing its predecessor and current state-of-the-art security solutions for EV charging.

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Abstract: Salinity and drought are major global challenges threatening crop productivity and ecosystem diversity, causing annual losses exceeding US$100 billion. These stresses share a common factor: osmotic stress imposed on plants. While extensive research has explored plant osmotic adjustment mechanisms, the processes underlying osmosensing in plant roots and how this sensing translates into adaptive responses remain poorly understood. This study aims to bridge this gap by examining the structure and function of various putative osmosensors (e.g., histidine kinases, mechanosensitive ion channels, phospholipase enzymes, and receptor-like kinases) across halophytes and glycophytes-two plant groups with contrasting salinity tolerance. We conducted a thorough bioinformatics analysis to explore the molecular evolution and structural diversity of these osmosensors in both plant groups. Our findings reveal that the evolution of putative osmosensors is highly conserved between glycophytes and halophytes, with notable divergence between monocot and dicot species within both groups. While halophytes do not exhibit distinct protein families during their evolutionary process, differences in conserved amino acids between glycophytes and halophytes may significantly influence osmosensing, signaling, and stress adaptation. Importantly, halophytes possess more copies of osmosensor-related genes compared to glycophytes. These findings offer valuable insights for breeding climate-resilient crops, highlighting potential pathways to enhance stress tolerance through genetic improvements.

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Abstract: Clinical isolates of Candida auris show a high prevalence of resistance to Amphotericin B (AmB)-an uncommon trait in most Candida species. Alterations in ergosterol biosynthesis can contribute to acquired AmB resistance in C. auris laboratory strains but are rarely seen in clinical isolates. In this study, we experimentally evolved two drug-susceptible Clade II isolates of C. auris to develop AmB resistance. The evolved strains displayed a four to eight fold increase in MIC50 compared to the parental cells. We analyzed changes in their karyotype, genome, lipidome, and transcriptome associated with this acquired resistance. In one lineage, AOX2 was upregulated, and its deletion reversed the AmB resistance phenotype. The aox2 Delta mutant also failed to evolve AmB resistance under experimental conditions. In the same lineage, restoring the UPC2(S332R) and RTG3(S101T) mutations to the wild-type allele restored AmB susceptibility. In another lineage, the ergosterol and sphingolipid pathways were observed to play a critical role, and upregulation of the ERG genes elevated the total sterol content, while significant downregulation of HSX11 (glucosylceramide synthase) resulted in lower levels of glucosylceramides. To our knowledge, this study is the first to show that AmB resistance in C. auris can be acquired through mechanisms both dependent on or independent of sterol content modulation, highlighting Aox2 and Upc2 as key regulators of amphotericin resistance.

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