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Record 1 of 62

Title: Iterative target updation based boosting ensembles for outlier detection

Author(s): Mukhriya, A (Mukhriya, Akanksha); Kumar, R (Kumar, Rajeev)

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Abstract: In unsupervised settings, the goodness of the alleged outlier set, the target, , is crucial. The entire ensemble design is centered around this target. In this work, we propose an unsupervised outlier ensemble, iBoost, which employs iterative target updation with a boosting-based selection. The proposed iBoost sequentially revises the target by applying multiple selection rounds. We use agreement rates with averages to estimate the errors of detectors by which inaccurate detectors are restricted. Multiple rounds of a boosting-based selection are then conducted, where the target for each round is calculated using the outcome of the previous round. Our modified boosting ensemble, BoostSel+, implements an add-on boosting step for the initial selection and uses weighted aggregation for the target. These weights are derived from detectors' errors. Such continuous reformations lead to a robust target with diverse quality outliers. Experimental results on benchmark datasets suggest that iBoost offers up to 12% improvement in detection performance. It also reveals up to 80% more non-average outliers in its exclusive set to the best competitor.

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Record 2 of 62

Title: Risk of groundwater depletion in Jaipur district, India: a prediction of groundwater for 2028 using artificial neural network

Author(s): Mondal, M (Mondal, Monidip)

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Abstract: The rapidly declining groundwater table calls for risk assessment for future water scarcity conditions in the Jaipur district, a naturally water-scarce region. The study tries to understand the spatio-temporal dynamics of groundwater depletion and predict the groundwater level in 2028 using time-series prediction by an Artificial Neural Network (ANN) of multi-layer perceptron ('mlp') modelling and estimate the projected populations under risk. It has been found that more than 21% of the district will have groundwater access deeper than 60 m.bgl by 2028. With time, groundwater depletion gets more severe in Chomu, Amber, Jaipur, and Sanganer tehsil. Groundwater depletion will intensify in the aeolian landforms of sand sheets and aeolian plains in the western part, along with the built-up areas, which are also densely populated urban centres. Around 58% of the district's total population is estimated to live with groundwater levels below 60 m.bgl in 2028. Analysis of groundwater levels corresponding to different geomorphological and land-use/land-cover facies advocates for groundwater recharge potentials in wetlands, aeolian landforms, flood plains, and pediment-peneplain complexes. Conservation of existing natural water bodies and using them for groundwater recharge can help to replenish the water table. Judicious and regulated groundwater extraction with legally binding policies can lower the groundwater depletion rate in the region.

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Title: Internal waves and Rayleigh-Taylor instability in magnetized compressible strongly coupled dusty plasmas

Author(s): Kumar, D (Kumar, Deepak); Prajapati, RP (Prajapati, Ram Prasad)

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Abstract: This paper investigates the influence of compressibility on the internal wave modes and the density gradient-driven Rayleigh-Taylor (R-T) instability in magnetized strongly coupled dusty plasmas. The dusty magnetohydrodynamic model is formulated for compressible fluids, accounting for the effects of weakly coupled electrons/ions and strongly coupled dust particles under the influence of the gravitational field. The effect of the magnetic field on the dust dynamics has been incorporated through the magnetic force on the electrons and ions in quasineutral dusty plasmas. A dispersion relation of the R-T instability has been derived which has been modified because of the compressibility effect, dust acoustic wave speed and viscoelastic coefficients. The shear Alfv & eacute;n and compressional viscoelastic wave modes become coupled in the dispersion characteristics. The modified R-T instability criterion is derived in terms of the Alfv & eacute;n speed, viscoelastic effects and dust grain parameters. The graphical illustrations show that the growth rate of R-T instability has been suppressed due to compressibility, viscoelastic coefficients and dust acoustic speed. The results are useful to discuss the development of R-T instability in magnetized astrophysical dusty plasmas.

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Title: Does global value chain participation and position lead to innovation in an emerging economy? Industry-level evidence from Indian manufacturing industries

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Source: JOURNAL OF BUSINESS RESEARCH **Volume:** 186 **Article Number:** 114989 **DOI:** 10.1016/j.jbusres.2024.114989 **Early Access Date:** SEP 2024 **Published Date:** 2025 JAN

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Abstract: This study examines the relationship between global value chain (GVC) embeddedness (participation and position) and innovation performance in India using data from the TiVA database for 14 manufacturing industries over the period 2009-2018. To account for the endogeneity issue arising due to reverse causality, the study employs a two-step system GMM. Empirical results show that GVC participation and position both significantly positively affect innovation performance, measured by the number of patent applications filed. However, participation has an inverted U-shaped impact. We contribute to the existing literature by further splitting GVC participation into forward and backward participations and finding that only forward GVC participation significantly impacts an emerging country's innovation performance. These findings suggest that policymakers in emerging countries should prioritize improving GVC position through increased R&D expenditures rather than relying solely on excessive GVC participation for enhancing innovation.

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Abstract: The current research explores the improvements in predictive performance and computational efficiency that machine learning and deep learning methods have made over time. Specifically, the application of transfer learning concepts within Convolutional Neural Networks (CNNs) has proved useful for diagnosing and classifying the various stages of Alzheimer's disease. Using base architectures such as Xception, InceptionResNetV2, DenseNet201, InceptionV3, ResNet50, and MobileNetV2, this study extends these models by adding batch normalization (BN), dropout, and dense layers. These enhancements improve the model's effectiveness and precision in addressing the specified medical issue. The proposed model is rigorously validated and evaluated using publicly available Kaggle MRI Alzheimer's data consisting of 1280 testing images and 5120 patient training images. For comprehensive performance evaluation, precision, recall, F1-score, and accuracy metrics are utilized. The findings indicate that the Xception method is the most promising of those considered. Without employing five K-fold techniques, this model obtains a 99% accuracy and 0.135 loss score. In addition, integrating five K-fold methods enhances the accuracy to 99.68% while decreasing the loss score to 0.120. The research further included the evaluation of the Receiver Operating Characteristic Area Under the Curve (ROC-AUC) for various classes and models. As a result, our model may detect and diagnose Alzheimer's disease quickly and accurately.

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Title: Spatio-temporal deep learning framework for pedestrian intention prediction in urban traffic scenes

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Abstract: Pedestrian intent prediction is an essential task for ensuring the safety of pedestrians and vehicles on the road. This task involves predicting whether a pedestrian intends to cross a road or not based on their behavior and surrounding environment. Previous studies have explored feature-based machine learning and vision-based deep learning models for this task but these methods have limitations in capturing the global spatio-temporal context and fusing different features of data effectively. To address these issues, we propose a novel hybrid framework HSTGCN for pedestrian intent prediction that combines spatio-temporal graph convolutional neural networks (STGCN) and long short-term memory (LSTM) networks. The proposed framework utilizes the strengths of both models by fusing multiple features, including skeleton pose, trajectory, height, orientation, and ego-vehicle speed, to predict their intentions accurately. The framework's performance have been evaluated on the JAAD benchmark dataset and the results show that it outperforms the state-of-the-art methods. The proposed framework has potential applications in developing intelligent transportation systems, autonomous vehicles, and pedestrian safety technologies. The utilization of multiple features can significantly improve the performance of the pedestrian intent prediction task.

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Abstract: The article charts the evolution of Ghar Parivar or Home and Family (1972-mid1980s) and Ghar Bahar or Home and Outside (1979- late 1980s) two early women's programmes, from being classified 'programme for minority' in TV listings to becoming significant counter-public spheres that effectively mounted national discussions from a 'women's perspective'. A historic and contentious Ghar Bahar episode is examined as a media event, including an interview with a session's judge about the unprecedented verdict in a dowry murder case that served as national testimony and led to significant legal reforms. The final section investigates how, despite rising from its marginal position to prime-time programming in the early 1980s, the women's programme was co-opted by the state, which now closely monitored women's issues and appropriated its distinct realist aesthetics to project a progressive image and media autonomy. Given the loss of original episodes, this case study employs textual historicism, relying on interviews, legal rulings, media reports, and a few available fragments of the women's programme to reconstruct the significance of women's shows and women producers in early Indian television.

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Title: Vanillin Mitigates the MPTP-Induced α-Synucleinopathy in a Mouse Model of Parkinson's Disease: Insights into the Involvement of Wnt/β-Catenin Signaling

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Abstract: Background: The abnormal aggregation of alpha-synuclein (alpha-syn) in the substantia nigra pars compacta (SNpc) region of the brain is characteristic of Parkinson's disease (PD), leading to the selective demise of neurons. Modifications in the post-translational processing of alpha-syn, phosphorylation at Ser(129) in particular, are implicated in alpha-syn aggregation and are considered key hallmarks of PD. Furthermore, dysregulated Wnt/beta-catenin signaling, influenced by glycogen synthase kinase-3 beta (GSK-3 beta), is implicated in PD pathogenesis. Inhibition of GSK-3 beta holds promise in promoting neuroprotection by enhancing the Wnt/beta-catenin pathway. Methods: In our previous study utilizing 1-methyl-4-phenylpyridinium (MPP+)-administered differentiated SH-SY5Y cells and a PD mouse model, we explored Vanillin's neuroprotective properties and related mechanisms against neuronal loss induced by MPP+/1-methyl-4-phenyl-1,2,3,6-tetrahydropyridine (MPTP) administration. In the current study, we elucidated the mitigating effects of Vanillin on motor impairments, P-Ser(129)-alpha-syn expression, Wnt/beta-catenin signaling, and autophagic neuron death induced by MPTP in a mouse model of PD by performing motor function tests, western blot analysis and immunostaining. Results: Our results show that Vanillin effectively modulated the motor dysfunctions, GSK-3 beta expression, and activity, activated the Wnt/beta-catenin signaling, and reduced autophagic neuronal demise in the MPTP-lesioned mice, highlighting its neuroprotective effects. Conclusions: These findings underscore the complex interplay between alpha-syn pathology, GSK-3 beta, Wnt/beta-catenin signaling, and autophagic-cell death in PD pathogenesis. Targeting these pathways, particularly with Vanillin, can be a promising therapeutic strategy for restoring dopaminergic (DA-ergic) neuronal homeostasis and slowing the progression of PD. Further research is crucial to resolving existing disputes and translating these discoveries into effective therapeutic interventions for PD patients.

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Title: Multi-functional biotinylated platinum(IV)-SAHA conjugate for tumor-targeted chemotherapy

Author(s): Gupta, A (Gupta, Ajay); Sasmal, PK (Sasmal, Pijus K.)

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Abstract: The development of multi-functional Pt(iv) complexes as chemotherapeutic agents has gained growing attention in medical oncology. However, the design of multi-functional tumor-targeted Pt(iv)

complexes with high hydrolytic stability remains challenging. Herein, we have developed a Pt(iv) prodrug conjugated with vorinostat as a multi-functional cancer therapeutic. In this design, the octahedral Pt(iv) prodrug of a DNA damaging anticancer drug cisplatin is tethered to the cancer cell targeting biotin ligand through one of the axial sites and the other axial site of the Pt(iv) center is attached to the anticancer drug vorinostat (also known as SAHA), a histone deacetylase inhibitor (HDACi) approved by the Food and Drug Administration (FDA) for treatment of cutaneous T-cell lymphoma. The designed biotinylated Pt(iv)-SAHA (Biotin-Pt(iv)-SAHA) conjugate is hydrolytically stable but reduced to Pt(ii) species under intracellularly relevant conditions and concomitantly releases cisplatin and two of its axial ligands such as SAHA and biotin. The anticancer activity of the conjugate is investigated against a panel of cisplatin-sensitive human cancer cells, including cisplatin-resistant cells. Interestingly, the conjugate exhibited significantly higher cytotoxicity than the clinically approved anticancer drug cisplatin and slightly more cytotoxicity than the HDACi SAHA in all the tested cell lines. By combining the Pt(iv) prodrug of cisplatin with SAHA in the conjugate, synergistic cytotoxicity is achieved. The imaging studies revealed that the conjugate is taken up by cancer cells and shows dose-dependent cell death. The studies on our designed multi-pronged conjugate can be further optimized to enhance its efficacy, paving the way for developing a new class of clinically relevant chemotherapeutic agents.

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Author(s): Negi, L (Negi, Lalita); Sethi, T (Sethi, Tapaswini); Das, D (Das, Dinabandhu)

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Abstract: Design of material showing contraction upon heating is highly challenging due to varying mechanism. However, imidazole is found to be a potential molecule that may provide low CTE materials when incorporated in the matrix. Here we have reported thermal expansion property of imidazolium salts of five aliphatic alpha, omega-alkane dicarboxylic acids and three aromatic acids. Either uniaxial or biaxial negative thermal expansion (NTE) has been observed in most of the salts. In some cases, axial zero thermal expansion (ZTE) has been observed. The role of imidazolium moiety for the anomalous thermal expansion behaviour of the salts has been analyzed in this study. The controlled TE behaviour of the salts is attributed to the hydrogen bonding and transverse vibration in all imidazolium salts. Owing to the high transverse vibration observed in imidazolium ion as well as the heavier oxygen atoms of acids in each case, the distance between hydrogen bonded atoms decreases-which provides either low expansion or contraction along one of the principal axes. Thermal expansion is controlled by transverse vibration of atoms in imidazolium moiety, oxygen atoms of carboxylic acids and noncovalent interactions in the crystal structures of organic salts derived from imidazole and carboxylic acids. Either uniaxial or biaxial negative thermal expansion (NTE) has been observed in most of the salts. In some cases, axial zero thermal expansion (ZTE) has been observed. image

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Abstract: The crowded milieu of a biological cell significantly impacts protein aggregation and interactions. Understanding the effects of macromolecular crowding on the aggregation and fibrillation of amyloidogenic proteins is crucial for the treatment of many amyloid-related disorders. Most in vitro studies of protein amyloid formation and its inhibition by small molecules are conducted in dilute buffers, which do not mimic the complexity of the cellular environment. In this study, we used PEGs to simulate macromolecular crowding and examined the inhibitory effects of flavones DHF, baicalein, and luteolin on human lysozyme (HuL) aggregation at pH 2. Naturally occurring flavones have been effective inhibitors of amyloid formation in some proteins. Our findings indicate that while flavones inhibit HuL aggregation and fibrillation in dilute buffer solutions, complete inhibition is observed with a combination of flavones and PEGs, as shown by ThT fluorescence, light scattering, TEM, and AFM studies. The species formed in the presence of PEG 8000 and flavones were less hydrophobic, less toxic, and alpha-helix-rich compared to control samples, which were hydrophobic and beta-sheet-rich, as demonstrated by ANS hydrophobicity, MTT assay, and CD spectroscopy. Fluorescence titration studies of flavones with HuL showed a significant increase in binding constant values under crowding conditions. These findings highlight the importance of macromolecular crowding in modulating protein aggregation and amyloid inhibition. Further studies using disease-causing mutants of HuL and other amyloidogenic proteins are needed to explore the role of macromolecular crowding in small-molecule-mediated modulation and inhibition of protein aggregation and amyloid formation.

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Abstract: In order to meet decarbonisation and net zero goals, the energy transition will play an instrumental role. However, energy transition technologies are raw material intensive and depend on a secure and reliable supply of critical minerals. Over the last few years, the international regime for energy transition and critical minerals have undergone changes. This paper studies the international institutional framework governing critical minerals for energy transition (CMET). There is no single regime that is equipped to address the various facets of CMET. Therefore, the paper describes the existence of regime complex and key features that characterise the regime complex as it unfolds in this new area of study. Since there is a growing interest from institutions from different regimes, there is a great potential for cooperation, mutual learning amongst policy makers and further academic research in the regime complex of CMET.

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Abstract: Conditional regulation is a highly beneficial system for studying the function of essential genes in Plasmodium falciparum and dimerizable Cre recombinase (DiCre) is a recently adapted conditional regulation system suitable for this purpose. In the DiCre system, two inactive fragments of Cre are reconstituted to form a functionally active enzyme in the presence of rapamycin. Different loci have been targeted to generate parasite lines that express the DiCre enzyme. Here, we have used marker-free CRISPR-Cas9 gene editing to integrate the DiCre cassette in a redundant cg6 locus. We have shown the utility of the newly generated triangle cg6DC4 parasites in mediating robust, rapid, and highly specific excision of exogenously encoded gfp sequence. The triangle cg6DC4 parasites are also capable of conditional excision of an endogenous parasite gene, PF3D7_1246000. Conditional deletion of PF3D7_1246000 did not cause any inhibition in the asexual proliferation of the parasites. Furthermore, the health and morphology of the mutant parasites were comparable to that of the control parasites in Giemsa smears. The availability of another stable DiCre parasite strain

competent for conditional excision of target genes will expedite functional characterization and validation of novel drug and vaccine targets against malaria.

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Abstract: International trade can play a catalytic role in economic development and employment enhancement. To understand the employment impact of India's pattern of trade, we use a structural decomposition analysis utilising the World Input - Output Database. Distinguishing between final and intermediate exports from India, we quantify the domestic employment effect during 2000-14. We show that a shift in final exports' composition towards sectors and sub-sectors with lower employment generation potential led to a negative employment effect. However, changes in international production sharing have largely had a positive impact on employment in India. Our structural decomposition analysis is complemented with a panel regression that tracks the employment effect of exports through backward linkages. We find significant differential impacts in India's bilateral trade with middle-income versus high-income countries. While bilateral backward linkages from exports to middle-income countries enhanced employment in India, exports to high-income countries did not yield a positive employment effect.

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Abstract: Candida albicans is an opportunistic fungal pathogen that can switch between yeast and hyphal morphologies depending on the environmental cues it receives. The switch to hyphal form is crucial for the establishment of invasive infections. The hyphal form is also characterized by the cell surface expression of hyphae-specific proteins, many of which are GPI-anchored and important determinants of its virulence. The coordination between hyphal morphogenesis and the expression of GPIanchored proteins is made possible by an interesting cross-talk between GPI biosynthesis and the cAMP-PKA signaling cascade in the fungus; a parallel interaction is not found in its human host. On the other hand, in the nonpathogenic yeast, Saccharomyces cerevisiae, GPI biosynthesis is shut down when filamentation is activated and vice versa. This too is achieved by a cross-talk between GPI biosynthesis and cAMP-PKA signaling. How are diametrically opposite effects obtained from the cross-talk between two reasonably well-conserved pathways present ubiquitously across eukarya? This Review attempts to provide a model to explain these differences. In order to do so, it first provides an overview of the two pathways for the interested reader, highlighting the similarities and differences that are observed in C. albicans versus the well-studied S. cerevisiae model, before going on to explain how the different mechanisms of regulation are effected. While commonalities enable the development of generalized theories, it is hoped that a more nuanced approach, that takes into consideration species-specific differences, will enable organismspecific understanding of these processes and contribute to the development of targeted therapies.

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Abstract: The axial secular frequency in a dual-frequency Paul trap has been evaluated using the modified Lindstedt-Poincare method. The ion motion in the presence of two rapidly oscillating frequencies is transformed to a motion under the influence of an effective potential resulting in a Duffing-like equation with contributions from multipole fields, namely, hexapole, octopole, and decapole fields. The resulting equation is asymmetric, and the secular frequency is different for positive and negative amplitudes of the ion motion. The voltage and frequency ratios have a profound influence on the axial secular frequency. The axial secular frequency increases with an increase in the voltage ratio and decreases with an increase in the frequency ratio. The octopole field has the strongest influence on the axial secular frequency for a given voltage and frequency ratio, whereas hexapole field, the least.

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KeyWords Plus: ION-TRAP; HOMOTOPY PERTURBATION; OSCILLATIONS; SIMULATION

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Author(s): Saha, J (Saha, Jayanti); Hussain, D (Hussain, Dilwar); Debsarma, D (Debsarma, Dhiman)

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Abstract: Objective: Flood is one of the major public health concerns increasing the risk of childhood diarrhea. This study aims to explore the association of floods with diarrhea among under-five children in rural India. Methods: A cross-sectional study was carried out using large-scale nationally representative data from the National Family Health Survey-5. The Central Water Commission reports between the years 2018 and 2020 were used to group all the districts as non-flood-affected districts or flood-affected districts. Bivariate and multivariate logistic regression models were employed to assess the association of floods with childhood diarrhea. Results: The prevalence of diarrhea was higher among children exposed to three consecutive floods during the year 2019-21 than those children not exposed to flood. Children exposed to flood three times between the year 2018-19 to 2020-21 were associated with a 34% higher likelihood of developing diarrhea than those children exposed to flood one or two times. Conclusions: Our study suggests that community health workers should target mothers belonging to the poor wealth quintile, young mothers, and mothers with young infants and more children to receive child health related counseling in flood-prone areas.

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Author(s): Dasgupta, R (Dasgupta, Rajib); Baru, R (Baru, Rama)

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Abstract: The WHO's World Health Day 2024 slogan, "My health, my right," has been unpacked through the lens of an evolving social epidemiological understanding. The operative part of the theme merely reiterates international positions that have been established for a long and is unable to adequately incorporate advances in the understanding of the central role that structural determinants play in the production of ill-health. Given the urgency of addressing Sustainable Development Goal and Universal Health Coverage goals, the reduction of health inequities through the promotion of social justice is as much a governance imperative as moral.

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Author(s): Kumar, N (Kumar, Navneet); Singh, K (Singh, Karan); Lloret, J (Lloret, Jaime)

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Abstract: Wireless Sensor Networks (WSNs) are vital for collecting data from remote environments. Nevertheless, the limited energy resources of sensor nodes render energy-efficient routing a critical concern for the successful operation of WSNs. To address these concerns, clustering, and routing are essential tasks in WSNs; clustering aims to organize sensor nodes into groups or clusters to minimize energy usage and prolong the network's lifespan. On the other hand, routing involves determining the optimum paths for transmitting data from the source nodes to the destination nodes. Nonetheless, it has been established that the current energy-efficient routing problem is an NP-hard, requiring a trade-off between energy and overall network performance. In this paper, we proposed a Hybrid Whale-Ant Optimization Algorithm (WAOA) for energy-efficient routing in WSNs. The proposed WAOA utilizes the Whale Optimization Algorithm (WOA) to find the suitable cluster head in the predefined search space, while the Ant Colony Optimization (ACO) searches the optimal route from the source cluster sensors to the cluster head within its predefined space. Linear programming construction is employed to formulate optimization problems for cluster head selection and search for the optimal route. The performance analysis demonstrates that the proposed WAOA performs better than MOORP, MMABC, and AZEBR by 5.78 %,16.11 %, and 18.52 %, respectively, in terms of network lifetime.

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Title: Organocatalytic enantioselective assembly of dispiro-bisoxindoles with vicinal stereocenters

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Abstract: Notwithstanding the rapid development achieved in enantioselective transformations, accessing contiguous quaternary and tertiary stereocenters ubiquitous in natural products and biologically active compounds has been an important and challenging task for synthetic chemists in modern organic chemistry. Drawing inspiration from the huge significance of spirooxindoles featuring a unique spatial structure and incredible medicinal activities, the search for these fascinating compounds in nature and developing new synthetic routes for installing multiple stereocenters remain core areas for synthetic chemists. This mini-review article demonstrates a transitory overview of the organocatalytic enantioselective strategies developed for assembling broad-spectrum dispiro-bisoxindole scaffolds comprising vicinal quaternary and tertiary stereocenters. While addressing the notable advancement accomplished in this intriguing field, we have also discussed the drawbacks and challenges associated with the reaction findings to support more research.
An enantioselective synthesis of dispiro-bisoxindoles featuring vicinal stereogenic centers using organocatalysis is discussed in this review article.

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Title: Analysing Spatio-temporal Dynamics of Urban Sprawl, Evolving Pattern of Urban Landscape and Driving Forces of Urban Growth: A Case of Varanasi Planning Region, India

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Abstract: Urban sprawl is at the centre of contemporary urban debates and is very often criticised for its negative social and environmental externalities. Building on geo-spatial methodology and field observations, this study sets out to develop a holistic approach to understanding urban sprawl through a particular focus on a rapidly growing metropolitan urban agglomeration of northern India, that is, Varanasi. Following an analysis of principal urban growth modes through landscape expansion index and changing patterns of urban landscape through landscape metrics, this research refers to a geo-spatially grounded logistic regression model in order to shed light on the dynamic impact of multiple growth factors on the trajectory of urban sprawl in the study area. Moreover, in order to address the evolving nature of urban sprawl in Varanasi and its immediate surroundings this study focuses on a temporal span of 20 years, encompassing two consecutive decades of the 21st century (2001-2011 and 2011-2021). The research concludes by paving a platform for an amalgamation of the findings from different geo-spatial metrics as well as by corroborating the principal findings with the propositions of a number of contemporary hypotheses concerning the spatial growth of urbanised territories.

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Abstract: Organic pi-scaffolds are being envisaged for new-age electron- and ion-responsive materials that can accumulate electrons as well as transport proton. However, such systems are extremely rare as electron-deficient scaffolds are unstable in aqueous solution. Here we detail the synthesis of a water-stable core-naphthalenediimide-nitrobenzyl-viologen based tetra-cation, which accumulates up to eight-electrons within an exceptionally narrow potential window of +0.05 V and -1.12 V. The supramolecular interactions and the ensuing ionic framework are tunable based on the three anions, e. g., Cl-, Br- and PF6-, that are investigated in this work. The ionic framework is formed and supported by a range of H-bonds, in which, the nitro benzyl groups act as pillars connecting the 1D water-tapes and the halide anions. The water molecules are hydrogen-bonded with the halide anions and bestow a facile pathway for the proton conduction, with proton conductivity up to 3.19x10-3 S cm-1. In contrast, the ionic assembly formed by the lipophilic PF6- anions do not host the water tapes and consequently the proton conductivity is found to be four orders of magnitude lower. This is a unique example, whereby proton conductivity is realized and is tunable within a highly electron-deficient, eight-electron acceptor, water-stable ionic supramolecular system.
A highly electron-deficient, water-stable, eight-electron acceptor scaffold has been used as a platform to realize proton conduction through ionic self-assembly. In this unique self-assembled material, 1D water tapes are revealed, that undergo hydrogen-bonding with halide anions, thereby generating a pathway for anion-assisted, tunable proton conduction. image

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Title: Medicine Wheel for the Planet: A Journey Towards Personal and Ecological Healing
Author(s): Visvanathan, S (Visvanathan, Susan)
Source: CONSERVATION & SOCIETY **Volume:** 22 **Issue:** 3 **Pages:** 141-142 **DOI:** 10.4103/cs.cs_54_24 **Published Date:** 2024 JUL-SEP
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Title: Correlation between the structural phase transition and magnetic properties of sol-gel synthesized La₂CoFeO₆ nanoparticles

Author(s): Jharwal, S (Jharwal, Swati); Verma, VK (Verma, Vivek kumar); Kumar, A (Kumar, Arvind)

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Abstract: The La2CoFeO6 (LCFO) nanoparticles were synthesized using the sol-gel method and calcined at 600 degrees C, 800 degrees C, and 1000 degrees C. The X-ray diffraction data confirm the successful formation of LCFO nanoparticles. The crystallite size was observed to increase from similar to 13 nm to similar to 26 nm as the calcination temperature rose. Detailed Rietveld analysis revealed the coexistence of both orthorhombic (Pnma: S.G. 62) and rhombohedral (R3c: S.G. 167) phases in the LCFO samples. A two-phase Rietveld refinement demonstrated a structural phase transition (from Pnma to R3c) as the calcination temperature increased. FESEM micrographs exhibited a granular morphology for the LCFO nanoparticles, and the grain size

was observed to increase with the elevated calcination temperature. Magnetization curves illustrated an increase in magnetization with a decrease in crystallite size or a reduction in calcination temperature for LCFO nanoparticles. At higher calcination temperatures, the rhombohedral phase displayed significant antisite disorder, resulting in the disruption of long-range ferromagnetic ordering in the material and a subsequent decrease in maximum magnetization. Copyright (c) 2024 EPLA

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Author(s): Kulriya, PK (Kulriya, Pawan Kumar); Kumar, M (Kumar, Mahesh); Singh, K (Singh, Kedar); Dhaka, RS (Dhaka, Rajendra S.)

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Author(s): Kumar, R (Kumar, Rajiv); Kulshreshtha, D (Kulshreshtha, Diksha); Aggarwal, A (Aggarwal, Ayushi); Asthana, S (Asthana, Somya); Dinda, A (Dinda, Amit); Mukhopadhyay, CK (Mukhopadhyay, Chinmay K.)

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Yadav S, 2024, CYTOKINE, V174, DOI 10.1016/j.cyto.2023.156456

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Abstract: Increased iron level is detected in rat kidney and human urine in diabetic condition and implicated in associated nephropathy. However, the biological cue and mechanism of the iron accumulation remain unclear. Here we reveal that glucose increases iron uptake by promoting transferrin receptor 1 (TFRC) in kidney cells by a translational mechanism but does not alter expression of endosomal iron transporter DMT1. Glucose decreases iron exporter ferroportin (FPN) by a protein degradation mechanism. Hepcidin is known to bind at Cys-326 residue in promoting degradation of human ferroportin. When Cys-326 was mutated to Ser in human-FPNFLAG and expressed in kidney cells, glucose still could degrade FPN-FLAG implicating involvement of hepcidin independent mechanism in glucose induced ferroportin degradation. Chronic hyperglycemia was generated in rats by administering streptozotocin (STZ) with periodic insulin injection to determine the level of iron homeostasis components. Increased TFRC and decreased ferroportin levels were detected in hyperglycemic rat kidney by Western blot and immunohistochemistry analyses. Hepcidin mRNA was not significantly altered in kidney but was marginally decreased in liver. Perls' staining and non-heme iron estimation showed an elevated iron level in hyperglycemic rat kidney. These results suggest that high glucose dysregulates iron transport components resulting iron accumulation in diabetic kidney.

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Abstract: This work reports the systematic variation of linear and nonlinear optical (NLO) properties of ternary boron carbon nitride (BCN) nanosheets with varying carbon concentrations. These nanosheets are synthesized by the thermal substitutional method to modulate the band-gap of BCN nanosheets by varying the hBN and graphene domain ratios which is confirmed through UV-Vis absorption spectroscopy. The third-order optical nonlinearity of nanosheets was explored through the Z-scan technique. With increases in both carbon content and laser power, samples' NLO properties have shifted from saturable absorption to reverse saturable absorption. The enhanced nonlinearity with carbon concentration in BCN samples was responsible for higher photoinduced charge separation time. In UV-Vis driven photoreduction of organic pollutants, BCN nanosheets with a decreased bandgap and an increased charge separation time show higher catalytic efficiency. Therefore, based on the combined effect of many processes, the results revealed that the BCN nanosheets displayed greater potential for photoinduced reduction.

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Abstract: Among the myriad challenges facing humanity, air pollution and climate change emerge as the most formidable existential threats to our future. Ironically, both these are direct fallouts of human activities such as indiscriminate consumption of consumer products/services and burning of fossil fuels. Purchase of consumer goods in 2024 is projected to be in excess of $22.6 trillion worldwide. How these consumers buy, use or dispose consumer goods will profoundly impact all life on the planet. Therefore, it is an imperative to embed

sustainability in every Rupee of consumer spending. Hence a robust digital solution, CarbonShunya, has been developed with the purpose to empower a billion consumers to make sustainable purchase and lifestyle choices. CarbonShunya is India's 1st solution that can measure and mitigate the Greenhouse Gas (GHG) footprint of consumer transactions in real-time. It provides consumers with actionable insights at the point-of-purchase and post-purchase to shape a shift in consumer beliefs, attitudes and behavior. This paper presents the methodology, assumptions and processes which have been adopted to develop the CarbonShunya life-cycle assessment framework and solution in Indian context. It also presents a case study, using the CarbonShunya framework, to measure and mitigate GHG impacts of monthly consumer expenditure on several categories of products/services across various states of India, based on a primary survey of over 174 000 households. The results from the case-study provide actionable insights and conclusions for policymakers and practitioners. CarbonShunya has cross-cutting applications across sectors so as to enable consuming economies to embrace conserving behaviors.

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Abstract: Amyloid beta peptide (A beta) and hyperphosphorylated neuronal tau proteins accumulate in neurofibrillary tangles in Alzheimer's disease (AD), a chronic neurodegenerative illness. Chronic inflammation in the brain, which promotes disease progression, is another feature of the Alzheimer's disease pathogenesis. Approximately 60-70 % of dementia cases are caused by AD. The development of effective therapies for the treatment of AD is urgently needed given the severity of the condition and its rapidly rising prevalence. Cholinesterase inhibitors, beta-amyloid (A-beta), tau inhibitors, and many other medications are currently used as preventive medicine for AD. These medications can temporarily suppress dementia symptoms but cannot halt or reverse the disease's progression. Many international pharmaceutical companies have tried numerous times to develop an amyloid clearing medication based on the amyloid hypothesis, but without success. Therefore, the amyloid theory may not be entirely plausible. This review mainly covers the recent and important reported pharmacophores as the starting point to discuss already known targets like tau, butyrylcholinesterase, amyloid beta, and acetylcholinesterase and covers the literature between years 2019-2024.

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Abstract: To expand the scope of our research and find anticancer drugs with novel structures, heterocyclic derivatives (3a 3n) were designed and synthesized via Suzuki coupling reaction in the presence of Pd(PPh3)(4) [Tetrakis (triphenylphosphine)-palladium(0)] catalyst with good yields. The synthesized heterocyclic analogs were characterized using various spectroscopic techniques like H-1, C-13 NMR, and FT-IR spectroscopy. The cytotoxicity of heterocyclic analogs (3a -3n)) was carried out by MTT assay towards breast cancer cell (MCF-7), and human normal cells (HepG2), analog 3j exhibited excellent activity against an MCF-7 (IC50 = 5 +/- 1.58 mu M) and low toxicity against the HepG2 (IC50 = >80 mu M). Furthermore, the anticancer activity of lead analog against the MCF-7 cancer cell line was confirmed using flow cytometry. Molecular docking study revealed that the derivative fits well at the active site of the target protein epidermal growth factor receptor tyrosine kinase.

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Abstract: Despite extensive research on the sequence-determined self-assembly of both pathogenic and nonpathogenic proteins, the question of how the sequence identity would influence the coassembly or cross-seeding of diverse proteins without distinct sequence similarity remains largely unanswered. Here, we demonstrate that the rapid coaggregation of proteins with negligible sequence similarity is fundamentally governed by preferred heteromeric interactions between their partially unfolded states via the gain of additional charge complementarity and hydrophobic interactions. The partial loss of intramolecular interactions and concurrent gain of non-native intrinsically disordered regions with sticky groups become crucial for both aggressive heteromeric primary nucleation and secondary nucleation events. The results signify the direct relevance of sequence-independent conformational cross-talk between diverse proteins to the foundational events required for the growth of biological multiprotein amyloid deposits.

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Abstract: We study the phase separation kinetics of miktoarm star polymer (MSP) melts/blends with diverse architectures using dissipative particle dynamics simulation. Our study focuses on symmetric and asymmetric miktoarm star polymer (SMSP/AMSP) mixtures based on arm composition and number. For a fixed MSP chain size, the characteristic microphase-separated domains initially show diffusive growth with a growth exponent phi similar to 1/3 for both melts that gradually crossover to saturation at late times. The simulation results demonstrate that the evolution morphology of SMSP melt exhibits perfect dynamic scaling with varying arm numbers; the timescale follows a power-law decay with an exponent theta similar or equal to 1 as the number of arms increases. The structural constraints on AMSP melts cause the domain growth rate to decrease as the number of one type of arms increases while their length remains fixed. This increase in the number of arms for AMSP corresponds to increased off-criticality. The saturation length in AMSP follows a power-law increase with an exponent lambda similar or equal to 2/3 as off-criticality decreases. Additionally, macrophase separation kinetics in SMSP/AMSP blends show a transition from viscous (phi similar to 1) to inertial (phi similar to 2/3) hydrodynamic growth regimes at late times; this exhibits the same dynamical universality class as linear polymer blends, with slight deviations at early stages.

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Abstract: In the recent decade of astrobiological exploration of the Martian surface, there has been a shift from identifying habitable environments to finding markers indicative of biological activity. It requires a prior understanding of the physical and geochemical environment of the setting to decipher whether the conditions were conducive. Generally, quiescent surroundings of lacustrine basins are considered one of the best targets for the preservation of any biological signatures. However, due to logistical limitations, the geochemical information available is mostly restricted to small areas on the surficial level (or in the subsurface in case of layered deposits or impact craters) where sufficient satellite coverage is available and, in some areas, where rovers/landers have been deployed. In this context, terrestrial lacustrine basins offer valuable insights into the environment required for the formation of the minerals observed on the Martian surface. This study was carried

out within Sambhar Lake located in the arid/semiarid climatic zone within the Thar desert. It is a hypersaline playa that has undergone several cycles of desiccation and re-filling, sharing its climate- controlled history with that of several paleolakes on Mars. We conducted physicochemical analysis of the samples collected from the lake and its surrounding area and compared our results with samples from the Curiosity rover (at Gale crater) and to those of the studies carried out in basalt-rich parent settings of Iceland. Our results suggest that Sambhar Lake is a Na-Cl type brine with climate-driven hydrology. The shallow cores and rock samples indicated that the area is rich in evaporites. We propose that even the sites with different parent material may be crucial in understanding the geological evolution of paleolakes on Mars and that Sambhar is a great example to study tectono-geomorphic evolution and the climate-induced transition of a lacustrine basin to a playa. Additionally, the lake is also desirable to study extremophiles and their adaptation to changing environmental variables for future planetary missions, including but not limited to, Mars.

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Abstract: A visible-light-induced C(sp2)-H functionalization of indoles by using Schreiner's thiourea as the organocatalyst has been reported. With the aid of a three-component domino reaction between 2-hydroxybenzaldehydes, cyclic-1,3-diketones, and a variety of indoles, the corresponding densely functionalized xanthene scaffolds were isolated in good to excellent yields. Apart from these, a broad range of other bioactive natural products including kojic acid, lawsone, and 4-hydroxycoumarin were also investigated instead of indoles for the present work. All the molecules participated in the photochemical reaction smoothly and provided the desired xanthenes in synthetically valuable yields. Therefore, the present energy-efficient catalytic strategy was also very successful in executing challenging carbon-sulfur bond formation reactions, demonstrating the synthetic potentiality of the work. Notably, this air-stable, transition metal-free approach with broad functional group tolerability provides an alternative to conventional methods.
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Abstract: In this research, impact of long term solar forcing on stratospheric winter temperature is checked. The 11- year sunspot activity and geomagnetic indices (AE, Kp, Dst) are used as an indicator for solar forcing, as geomagnetic activity indices show good correlation with solar variability. To understand the impact of solar forcing through high latitude, stratospheric winter (November to March) time North Polar Region (60N-90N) temperature anomalies are considered. The findings showed that temperature changes in the stratosphere are significantly correlated with solar activity, as evidenced by a significant positive correlation between the 11-year moving mean of stratospheric (10 hPa) temperature anomalies and sunspot number. Approximately from 1970 to 2000, the North Polar Region saw positive anomalous stratospheric winter temperatures. During the same time, the geomagnetic activity also showed a substantial increase. The year-to-year correlation between stratospheric pole temperature and geomagnetic activity is significant (about 0.5). The Empirical Mode Decomposition analysis reveals a highly significant correlation (around 0.9) between the long-term component of stratospheric winter temperature (IMF-4) and the long-term component of geomagnetic activity (IMF-3 and IMF-4). One of the reasons for the increase in lower stratospheric temperature is an increase in ozone concentration during the same period when geomagnetic activity is higher. Empirical orthogonal function (EOF) and correlation analysis of stratospheric winter temperature with large-scale circulation patterns are also carried out. The spatial correlation is checked for stratospheric winter temperature at North Pole and lower atmospheric levels (250 hPa and 850 hPa) followed by pre-monsoon and monsoon season. This study includes statistical analysis, however, also highlights the necessity of in-depth dynamical analysis to improve our understanding of how solar activity impacts Earth's atmospheric layers, which may be helpful in predicting the weather and climate.

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Abstract: This work investigates the structural, electronic, elastic, and transport properties of the AgSbS2 monolayer, using density functional theory in conjunction with semiclassical Boltzmann transport theory. In this study, we proposed a strategy to enhance the figure of merit (ZT) by optimizing the carrier concentrations. The monolayer of AgSbS2 is found to be both mechanically and thermodynamically stable. The phonon bandstructure and ab-initio molecular dynamics are also used to verify its excellent dynamical and thermal stability. The calculated electronic bandstructure shows a semiconducting nature of AgSbS2 with an indirect band gap of 1.31 eV using the Heyd-Scuderia-Ernzerhof (HSE06) exchange-correlation functional. The investigated monolayer is found to be anisotropic, hence we analyzed its thermoelectric properties at various carrier concentrations along a- and b-directions at 300 K. It attained a high value of Seebeck coefficient of 360 mu VK-1 and 370 mu VK-1 in the a- and b- directions at room temperature, respectively. The low thermal conductivity and high power factor result in an appreciable ZT value. The maximum ZT of AgSbS2 monolayer at an optimized carrier concentration of 2 x 10(19) cm(-3) is found to be 0.54 in the b-direction for the n-type monolayer at 300 K. The present work supports the potential use of AgSbS2 in room-temperature energy harvesting applications.

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Abstract: A visible light-driven photoredox-catalyzed direct C(sp(2))-H functionalization of N-H free indoles with quinoxalinones generated in situ from 2,2-dihydroxy-1H-indene-1,3(2H)-dione and phenylene-1,2-diamines has been reported with the aid of Na-2-Eosin Y as the photocatalyst and the Hunig base as the sacrificial electron and proton donor. The reaction provides easy access to a variety of quaternary-centered C-3 selective indole-substituted tertiary alcohols in good yields. Mechanistic studies demonstrated the realization of photoredox-catalyzed in situ quinoxalinone formation and their proton-coupled single electron reduction to the corresponding ketyl radicals followed by cross-coupling with indoles. The potential applications of the synthesized tertiary alcohols in photoacid-catalyzed carbon-carbon and carbon-sulfur bond-forming reactions feature the key findings of the present work.

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Abstract: Antibiotic resistance has emerged as a global threat, rendering the existing conventional treatment strategies ineffective. In view of this, antimicrobial peptides (AMPs) have proven to be potent alternative therapeutic interventions with a wide range of applications in clinical health. AMPs are small peptides produced

naturally as a part of the innate immune responses against a broad range of bacterial, fungal and viral pathogens. AMPs present a myriad of advantages over traditional antibiotics, including their ability to target multiple sites, reduced susceptibility to resistance development, and high efficacy at low doses. These peptides have demonstrated notable potential in inhibiting microbes resistant to traditional antibiotics, including the notorious ESKAPE pathogens, recognized as the primary culprits behind nosocomial infections. AMPs, with their multifaceted benefits, emerge as promising candidates in the ongoing efforts to combat the escalating challenges posed by antibiotic resistance. This in-depth review provides a detailed discussion on AMPs, encompassing their classification, mechanism of action, and diverse clinical applications. Focus has been laid on combating newly emerging drug-resistant organisms, emphasizing the significance of AMPs in mitigating this pressing challenge. The review also illuminates potential future strategies that may be implemented to improve AMP efficacy, such as structural modifications and using AMPs in combination with antibiotics and matrix-inhibiting compounds.

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Abstract: Metabolic reprogramming and altered cellular energetics have been recently established as an important cancer hallmark. The modulation of glucose metabolism is one of the important characteristic features of metabolic reprogramming in cancer. It contributes to oncogenic progression by supporting the increased biosynthetic and bio-energetic demands of tumor cells. This oncogenic transformation consequently results in elevated expression of glucose transporters in these cells. Moreover, various cancers exhibit abnormal transporter expression patterns compared to normal tissues. Recent investigations have underlined the significance of glucose transporters in regulating cancer cell survival, proliferation, and metastasis. Abnormal regulation of these transporters, which exhibit varying affinities for hexoses, could enable cancer cells to efficiently manage their energy supply, offering a crucial edge for proliferation. Exploiting the upregulated expression of glucose transporters, GLUTs, and Sodium Linked Glucose Transporters (SGLTs), could serve as a novel therapeutic intervention for anti-cancer drug discovery as well as provide a unique targeting approach for drug delivery to specific tumor tissues. This review aims to discussthe previous and emerging research on the expression of various types of glucose transporters in tumor tissues, the role of glucose transport inhibitors as a cancer therapy intervention as well as emerging GLUT/SGLT-mediated drug delivery strategies that can be therapeutically employed to target various cancers.

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Abstract: In many emerging economies with antiquated laws, bribes paid to government officials reduce economic impediments and serve as a device to improve market competition, thereby contributing to the modernization of an economy. In this context, this paper uses a simple two-stage game theoretic model to investigate the effects of the US Foreign Corrupt Practices Act (FCPA) on such economies. We demonstrate, among others, that while an increase in fines under FCPA reduces overall corruption, it leads to a deterioration in the market quality in an emerging economy. In the presence of FCPA, an increase in the US firm's technological advantage unambiguously leads to a decrease in the market quality in an emerging economy.

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Abstract: In this work, the role of non-covalent n -> sigma* intramolecular interactions in bestowing stabilization to exceptionally low-lying LUMO molecules of Naphthalenediimides (NDI) and their radical ions have been investigated utilizing different electronic structure calculation methods at the DFT level of theory and X-ray crystallography. We compared the effect of electron donating groups (EDGs) and electron-withdrawing groups (EWGs), e.g., OMe and F, respectively, at the para-positon of the phenylphosphonium groups integrated at the 2,6-positions of the NDI scaffold on the intramolecular P-O interactions and the evolving electronic effects. The natural bond orbital (NBO) analysis exhibited strong charge transfer from the imide O atoms of the NDI to the phosphorus atom of the phosphonium groups validating a donor-acceptor type of orbital interaction. Atoms in molecule (AIM) analysis also illustrated the strong P-O interaction, as the charge density, rho(r), and the Laplacian of the density del 2 rho(rb) at BCP is within the range of well-known non-covalent interactions. These calculations also revealed long-range electronic communication between the EDGs/EWGs at the phenyl groups and the NDI scaffold.
In this work, role of non-covalent n -> sigma* intramolecular interactions in bestowing stabilization to exceptionally low-lying LUMO molecules of NDIs and their radical ions is investigated.

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Abstract: In this work, we study the effect of Ni-doping on the structural and impedance spectroscopy properties of the polycrystalline YCrO3 ceramic sample. The structural analysis shows all the samples crystallize in an orthorhombic structure with the Pnma space group. The depressed and asymmetric semicircle of complex impedance spectra indicates that the relaxation of charge carriers is of non-Debye type, where the thermally activated charge carriers control it. The temperature dependence of relaxation time and electrical conductivity exhibit an anomaly in the vicinity of diffuse-like relaxor transition temperature (T-C similar to 460 K). The analysis of conductivity data shows hopping-type charge conduction. The analysis further indicates that

while the dc conductivity increases continuously, the activation energy shows a non-monotonous variation with Ni concentration.

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Abstract: Amino-substituted 4H-chromene H-chromene scaffolds, comprising nitrogen and oxygen, have garnered significant attention in modern organic chemistry due to their widespread applications in medicinal chemistry, drug discovery, and material sciences. This study demonstrates the synthesis and investigation of a series of 2-amino-3-cyano-4Hchromenes. The molecular structures of these compounds were established using X-ray diffraction, which revealed their supramolecular features. The fused 4H-chromene molecules crystallise in monoclinic and triclinic crystal systems with space groups P-1, P 2 1 / c, C 2/ c , and P 2 1 / n . These

molecules show interactions like O-H & sdot;& sdot;& sdot;O, & sdot;& sdot;& sdot; O, N-H & sdot;& sdot;& sdot;O, & sdot;& sdot;& sdot; O, N-H & sdot;& sdot;& sdot;N, & sdot;& sdot;& sdot; N, C-H & sdot;& sdot;& sdot;O, & sdot;& sdot;& sdot; O, and C-H & sdot;& sdot;& sdot;N, & sdot;& sdot;& sdot; N, along with the pi-pi - pi stacking and C - H & sdot;& sdot;& sdot; pi arrangements. Hirshfeld surface analysis confirmed the presence of these interactions, and 2D fingerprint plots quantified their contributions. The structural aspects of the compounds, including their optimised molecular geometry and intramolecular hydrogen bonding, were examined using Density Functional Theory (DFT). The constructed structures showed a strong correlation with experimental results. Additionally, the molecular electrostatic potential was studied to understand the energy distribution and chemically reactive regions of the molecules.

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Abstract: This study reports a visible light active Ba/Sc co-doped potassium niobate (KNbO3) ferroelectric material for enhanced photocatalytic applications. Through 5% Ba and Sc co-doping in KNbO3 (i.e., 0.95KNbO(3)-0.05Ba(Nb1/2Sc1/2)O-3), the electronic band gap (E-g) is narrowed down to the visible range of the solar spectrum. The prepared samples are systematically examined by using X-ray diffraction and Raman spectroscopy, which confirms the successful incorporation of Ba and Sc ions into the KNbO3 lattice. Scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS) analysis reveal particle morphology and chemical homogeneity of prepared samples. The UV-vis spectroscopy and ferroelectric PE-loop demonstrate enhanced optical absorption compared to host KNbO3 while retaining ferroelectric behavior. The photoelectrochemical (PEC) measurements under visible light irradiation demonstrate a notable enhancement in the photocurrent for 0.95KNbO(3)-0.05Ba(Nb1/2Sc1/2)O-3 (hereafter denoted by 5KBSNO) compared to undoped KNbO3. Additionally, the 5KBSNO sample displays enhanced RhB dye degradation efficiency, reaching approximate to 50% compared to parent KNbO3 (approximate to 30%) under light irradiation. First-principles density functional theory (DFT) calculations are employed to understand the mechanism responsible for the reduced band gap. This study presents a promising material for developing advanced ferroelectric photocatalysts with tailored band structures for efficient solar energy harvesting for energy conversion and contamination remediation applications.

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Abstract: The locus coeruleus (LC), nucleus tractus solitarius (NTS), and retrotrapezoid nucleus (RTN) are critical chemosensory regions in the brainstem. In the LC, acid-sensing ion channels and proton pumps serve as H+ sensors and facilitate the transition from non-rapid eye movement (NREM) to rapid eye movement (REM) sleep. Interestingly, the potassium inward rectifier (KIR) channels in the LC, NTS, and RTN also act as H+-sensors and are a primary target for improving sleep in obstructive sleep apnea and Rett syndrome patients. However, the role of Kir channels in NREM to REM sleep transition for H+ homeostasis is not known. Male Wistar rats were surgically prepared for chronic sleep-wake recording and drug delivery into the LC, NTS, and RTN. In different animal cohorts, microinjections of the Kir channel inhibitor, barium chloride (BaCl2), at concentrations of 1 mM (low dose) and 2 mM (high dose) in the LC and RTN significantly increased wakefulness and decreased NREM sleep. However, BaCl2 microinjection into the LC notably reduced REM sleep, whereas it didn't change in the RTN-injected group. Interestingly, BaCl2 microinjections into the NTS significantly decreased wakefulness and increased the percent amount of NREM and REM sleep. Additionally, with the infusion of BaCl2 into the NTS, the mean REM sleep episode numbers significantly increased, but the length of the REM sleep episode didn't change. These findings suggest that the Kir channels in the NTS, but not in the LC and RTN, modulate state transition from NREM to REM sleep.

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Abstract: Brassica juncea is a crucial oilseed crop, and its seeds possess high economic value as they are a source of edible oil. In order to understand the role of long non coding RNAs (lncRNAs) in the regulation of seed development, we carried out computational analysis using transcriptome data of developing seeds of two contrasting genotypes of B. juncea, Pusajaikisan (PJK) and Early Heera 2 (EH2). The seeds were sampled at three stages, 15, 30, and 45 days after pollination. We identified 1,539 lncRNAs, of which 809 were differentially expressed. We also carried out extensive characterization and functional analysis of seed lncRNAome. The expression patterns were analysed using k-means clustering, and the targets were analysed using pathway, transcription factor, and GO enrichment, as well as ortholog information. We shortlisted a total of 25 robust lncRNA candidates for seed size, oil content, and seed coat color. We also identified 4 lncRNAs as putative precursors of miRNAs regulating seed development. Moreover, a total of 28 miRNA-lncRNA-mRNA regulatory networks regulating seed traits were identified. We also developed a comprehensive database, (BrassIca juncea database or "BIJ" (https://bij.cuh.ac.in/), which provides seed omics as well as other functional

genomics and genetics data in an easily accessible form. These candidate lncRNAs are suitable for including in crop improvement programs through molecular breeding, as well as for future validations through genome editing. Together, the knowledge of these candidate lncRNAs and availability of BIJ database shall leverage the crop improvement efforts in B. juncea.

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Abstract: Non-small cell lung cancer comprises up to 85% of lung cancer cases and has a poor prognosis. At present, there are still no effective treatments for this illness. Evidence suggests that the prostaglandin [cyclooxygenase-2 (COX-2)] and leukotriene [lipoxygenase-5 (5-LOX)] pathways are involved in lung cancer carcinogenesis. Therefore, novel agents that target COX-2 and 5-LOX may have therapeutic potential. In the present study, we examined the role of asiatic acid (AA), a triterpenoid saponin, in targeting the protein kinases responsible for lung cancer proliferation and mobility. The experimental data revealed that AA inhibited the growth of lung cancer cells (> 50%) and it significantly impeded the proliferation of lung cancer cells by inhibiting COX-2, which results in downregulation of the phosphotidyl inositol-3 kinase/protein kinase B/mammalian target of rapamycin signaling pathway, leading to an induction of cytotoxic autophagy-mediated apoptosis. Mechanistically, the expression of mitogen-activated protein kinase/extracellular signal-regulated kinase, hypoxia-inducible factor-1 and vascular endothelial growth factor is downregulated by AA, thereby reducing cell mobility and invasion. It also shows negative osmotic fragility on healthy human erythrocytes. It is concluded that AA may be a viable therapeutic drug for non-small cell lung cancer treatment, which opens new opportunities for synthesizing analogues.

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Abstract: The socioeconomic prosperity of a region is intricately tied to its infrastructure development, particularly the connectivity provided by highways. Preserving the economic well-being of an area demands meticulous planning and the execution of construction projects with minimal risk. Landslide hazard zonation (LHZ) is a crucial tool for assessing the likelihood of landslide occurrences in specific regions. This study delves into the LHZ of a 171.2 km2 area, focusing on critical causative factors such as slope inclination and aspect, slope mass material, Land Use/Land Cover (LULC), distance from fault lines, roads, and drainage systems. The classification resulted in four distinct zones along the National Highway (NH-109) stretch from Bhowali to Almora. Notably, the moderate-hazard zone encompasses 60.4% of the area, followed by the high-hazard zone at 24.4%, the low-hazard zone at 11.9%, and the very high-hazard zone at 3.3%. To enhance the reliability of the study, 63 previously identified landslide locations were marked based on diverse sources, including field studies and landslide inventory data from the Geological Survey of India (GSI). In the validation process, 12 past landslide occurrences were situated within the very high-hazard zone, 32 in the high-hazard zone, 18 in the moderate-hazard zone, and only one in the low-hazard zone. The receiver operating characteristic (ROC) curve yielded a commendable quality with a % area under the curve (AUC) of 71.2%. In summary, this research underscores the importance of LHZ in assessing and mitigating landslide risks along a stretch of the NH-109 corridor. The findings provide valuable insights for informed decision-making in infrastructure development and risk management, contributing to the sustainable growth and protection of the region's livelihood.
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Abstract: Phototropin (Phot), a blue light-sensing LOV domain protein, mediates blue light responses and is evolutionarily conserved across the green lineage. Klebsormidium nitens, a green terrestrial alga, presents a

valuable opportunity to study adaptive responses from aquatic to land habitat transitions. We determined the crystal structure of Klebsormidium nitens Phot LOV1 domain (KnLOV1) in the dark and engineered different mutations (R60K, Q122N, and D33N) to modulate the lifetime of the photorecovery cycle. We observed unusual, slow recovery kinetics in the wild-type KnLOV1 domain (tau = 41 +/- 3 min) compared to different mutants (R60K: tau = 2.0 +/- 0.1 min, Q122N: tau = 1.7 +/- 0.1 min, D33N: tau = 9.6 +/- 0.1 min). Crystal structures of wild-type KnLOV1 and mutants revealed subtle but critical changes near the protein chromophore that is responsible for modulating protein dark recovery time. Our findings shed light on the unique structural and biochemical characteristics of the newly studied KnLOV1 and its evolutionary importance for phototropin-mediated physiology.

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Abstract: We use Clifford's geometric algebra to extend the Stuart-Landau system to dimensions D > 2 and give an exact solution of the oscillator equations in the general case. At the supercritical Hopf bifurcation marked by a transition from stable fixed-point dynamics to oscillatory motion, the Jacobian matrix evaluated at the fixed point has N = [D/2] pairs of complex conjugate eigenvalues which cross the imaginary axis simultaneously. For odd D there is an additional purely real eigenvalue that does the same. Oscillatory dynamics is asymptotically confined to a hypersphere SD-1 and is characterised by extreme multistability, namely the coexistence of an infinite number of limiting orbits, each of which has the geometry of a torus T-N on which the motion is either periodic or quasiperiodic. We also comment on similar Clifford extensions of other limit cycle oscillator systems and their generalizations.

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Abstract: Lead free perovskite is at the center of the present study due to its multifunctional properties. In the present work, pH (0-5) of the solution during the synthesis of La2CoFeO6 (LCFO) nanoparticles has been varied to study its impact on structural and magnetic properties. X-ray diffraction(XRD) pattern confirms the formation of LCFO nanoparticle with pH variation. Rietveld refinement of the XRD patterns indicates that the LCFO is formed in mixed phase of orthorhombic and rhombohedral structure. The percentage contribution of orthorhombic phase decreases with an increase in the pH value. Morphological studies show the increment in the particle size with pH value (from similar to 16 nm to similar to 32 nm). Structural and morphological investigations indicate that LCFO prepared at pH 0 are highly agglomerated and may have some amorphous phases. Magnetization curves indicate the ferromagnetic response for the LCFO nanoparticles at pH-0. The maximum magnetization (M-S) is found to decrease whereas coercivity (H-C) increases with the increase in pH value. This could be attributed to the structural changes incorporated and presence of anti-site disorder due to the variation of pH. A large exchange bias effect has also been noticed at 60 K for all the LCFO samples.

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Abstract: The present research focuses on the electrical properties of lead-free piezoceramics (0.985-x)(K0.485Na0.485Li0.03)(Nb0.96Sb0.04)O-3-0.015(Bi0.5Na0.5)ZrO3-xSnO(2) (KNNLS-BNZ-xSnO(2), x = 0.003, 0.006, 0.009, 0.012, and 0.015). This study examines the influence of varying SnO2 doping levels on the microstructure and piezoelectric properties of the ceramics. All the ceramics prepared demonstrate pure perovskite structure without any secondary phases. The Rietveld refinement analysis of XRD data reveals the existence of multiphase evolution around room temperature. The tetragonality (c/a) and cell volume of the ceramics tend to rise with an increase in Sn4+ content, potentially leading to improved ferroelectric characteristics. The optimum values obtained were Curie temperature (T-c) = 395 C-o, remnant polarization (P-r) = 21.07 mu C/cm(2), piezoelectric coefficient (d(33))=357 pC/N, piezoelectric voltage constant (g(33)) = 24 x 10(-3) Vm/N, and figure of merit (FOMoff) = 10.34 pm(2)/N, corresponding to the ceramic doped with x = 0.012 SnO2. The findings indicate that an optimal amount of Sn4+ in the host composition KNNLS-BNZ improves piezoelectric properties by constructing an R-O-T phase boundary near room temperature. This study suggests that the ceramic with x = 0.012 SnO2 exhibits a favorably high T-c coupled with an exceptional energy harvesting capability, making it a suitable candidate for energy harvesting applications.

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Abstract: BaFe12O19 (barium ferrite, i.e., BaF) nanoparticles, Co0.5Zn0.5Fe2O4 (cobalt zinc ferrite, i.e, CZF) nanoparticles and their nanocomposite were synthesized for the investigation of electrical, magnetic, dielectric, and electrochemical properties. The X-ray diffraction (XRD) pattern revealed the formation of hexagonal structure for BaF nanoparticles and cubic structure for CZF nanoparticles with crystallite size of 32.44 nm and 31.30 nm, respectively. Whereas, for nanocomposite, the crystallite size obtained is 34.21 nm were shifting of peaks revealed the formation of nanocomposite. The Fourier transform Infrared (FTIR) spectra revealed the presence of metal-oxygen vibrational peaks for all the samples. The dielectric data revealed the increase in dielectric constant of nanocomposite as compared to pristine CZF whereas, loss reduced for nanocomposite significantly. Single semicircle in Nyquist plot for all the samples revealed the contribution of grain resistance in impedance. The hysteresis loop showed the increase in specific saturation magnetization from 16.963 emu/g to 21.305 emu/g for nanocomposite when compared with pristine BaF. Whereas specific remnant magnetization increased to 10.305 emu/g for nanocomposites. The electrochemical properties presented by Cyclic voltammetry showed the presence of cathodic and anodic peaks which revealed the presence of redox reaction in all samples. The specific capacitance calculated for all samples at different scan rate revealed that a

nanocomposite showed highest Cs value 16.43 F/g at 25 mV, whereas it increased to 27.01 F/g, 35.93 F/g and 38.87 F/g with the increase in scan rate to 50 mV, 75 mV and 100 mV, respectively.

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Abstract: The 2019 outbreak of SARS-CoV-2 has caused a major worldwide health crisis with high rates of morbidity and death. Interestingly, it has also been linked to cancer, which begs the issue of whether it plays a role in carcinogenesis. Recent studies have revealed various mechanisms by which SARS-CoV-2 can influence oncogenic pathways, potentially promoting cancer development. The virus encodes several proteins that alter key signaling pathways associated with cancer hallmarks. Unlike classical oncogenic viruses, which transform cells through viral oncogenes or by activating host oncogenes, SARS-CoV-2 appears to promote tumorigenesis by inhibiting tumor suppressor genes and pathways while activating survival, proliferation, and inflammation-associated signaling cascades. Bioinformatic analyses and experimental studies have identified numerous interactions between SARS-CoV-2 proteins and cellular components involved in cancer-related processes. This review explores the intricate relationship between SARS-CoV-2 infection and cancer, focusing on the regulation of key hallmarks driving initiation, promotion and progression of cancer by viral proteins. By elucidating the underlying mechanisms driving cellular transformation, the potential of SARS-CoV-2 as an oncovirus is highlighted. Comprehending these interplays is essential to enhance our understanding of COVID-19 and cancer biology and further formulating strategies to alleviate SARS-CoV-2 influence on cancer

consequences.Graphical AbstractSchematic representation of SARS-CoV-2 associated alterations contributing to various hallmarks of cancer. PI3K/ AKT/mTOR: Phosphoinositide 3-kinase/Protein Kinase B/ Mammalian Target of Rapamycin; TGF-beta, Transforming Growth Factor-beta; VEGF, Vascular Endothelial Growth Factor; JNK, Jun N-terminal Kinase; HDAC, Histone Deacetylase; DNMT, DNA Methyltransferase; HIF-1 alpha: Hypoxia-Inducible Factor 1-alpha; pRB, Retinoblastoma Protein. This image was created using BioRender software.

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Title: Polydatin inhibits histone deacetylase 1 and shows an anti-angiogenic action in head and neck squamous cell carcinoma

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Abstract: Polydatin, a natural derivative of resveratrol, has shown many anticancer properties. However, the underlying mechanisms of its anticancer properties including its effect on the epigenetic landscape are not well understood. Here, we explored the effect of polydatin on histone deacetylase 1 (HDAC1) activity. We used in silico approaches to assess the possible binding of polydatin to the active site pockets of HDAC1 and in vitro approaches to test the potential effects of the interaction on its enzymatic activity. As compared to SAHA, an approved drug, the polydatin showed stronger and stable binding to the HDAC1. The binding energy, conformational changes, formation of extra hydrogen bonding, and other interactions within and outside the active site all favour largely stable and strong polydatin binding to the enzyme. Further, the ADME and toxicity prediction values are encouraging for the evaluation of polydatin as a drug. The laboratory leg of the study substantiated that the polydatin binding was strong and stable enough to inhibit HDAC1 activity in UMS-CC-22B cells as demonstrated by an increase in H3K9 acetylation. In addition, polydatin treated cells showed attenuated proliferation. The in vitro tube formation and migration by HUVEC and UM-SCC-22B cells were inhibited by polydatin. The decreased tube formation due to HDAC1 inhibition is possibly due to up-regulation of the anti-angiogenic gene - TSP1 in UM-SCC-22B cells. As compared to SAHA, more promising results were shown both in its computational calculations and on the cell physiology features. Stronger and stable binding, more anti-proliferative and anti-angiogenic potential were observed with respect to polydatin. Further, the cell death was more pronounced with SAHA treatment. Therefore, polydatin might be a better anticancer drug and can have a potential to replace SAHA in combinational therapeutic regimen.

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Abstract: Presently, the distinct charge transport and interface interaction of the S-scheme heterojunction has garnered significant interest. Herein, a S-scheme-based charge transportation Mo-doped Bi2WO6/WO3/Biochar heterojunction was synthesized in situ using a coprecipitation technique to improve methylene blue adsorption and photocatalytic reactive oxygen species production. The doped Mo altered the band gap of Bi2WO6 to increase light absorption, which can facilitate electron-hole separation and transfer. Likewise, the S-scheme band structure improved sunlight utilization, enhanced the reduction and oxidation power of photogenerated electrons, and boosted charge carrier separation and transfer. Thus, due to the synergetic impact of doping and the S scheme band structure, the photocatalysts efficiently eliminated Methylene blue up to 87.5 % in 30 min of photoirradiation. Fabricated heterojunction Mo-Bi2WO6/WO3/Biochar photocatalyst have highest Kapp values 0.02816 min- 1 while Mo-Bi2WO6/WO3, Mo-Bi2WO6, Bi2WO6, and WO3 photocatalysts have 0.02816, 0.02273, 0.01527, 0.00643, and 0.00735 min- 1, respectively which was 4.38 times greater than pristine Bi2WO6. The study offers a novel perspective for the in-situ production of S-scheme heterojunction with doping to remove different types of contaminants.

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Abstract: Antimicrobial resistance (AMR) poses a critical threat to global public health, necessitating the development of novel strategies. AMR occurs when bacteria, viruses, fungi, and parasites evolve to resist antimicrobial drugs, making infections difficult to treat and increasing the risk of disease spread, severe illness, and death. Over 70% of infection-causing microorganisms are estimated to be resistant to one or several antimicrobial drugs. AMR mechanisms include efflux pumps, target modifications (e.g., mutations in penicillin-binding proteins (PBPs), ribosomal subunits, or DNA gyrase), drug hydrolysis by enzymes (e.g., beta-lactamase), and membrane alterations that reduce the antibiotic's binding affinity and entry. Microbes also resist antimicrobials through peptidoglycan precursor modification, ribosomal subunit methylation, and alterations in metabolic enzymes. Rapid development of new strategies is essential to curb the spread of AMR and microbial infections. Nanomedicines, with their small size and unique physicochemical properties, offer a promising solution by overcoming drug resistance mechanisms such as reduced drug uptake, increased efflux, biofilm formation, and intracellular bacterial persistence. They enhance the therapeutic efficacy of antimicrobial agents, reduce toxicity, and tackle microbial resistance effectively. Various nanomaterials, including polymeric-based, lipid-based, metal nanoparticles, carbohydrate-derived, nucleic acid-based, and hydrogels, provide efficient solutions for AMR. This review addresses the epidemiology of microbial resistance, outlines key resistance mechanisms, and explores how nanomedicines overcome these barriers. In conclusion, nanomaterials represent a versatile and powerful approach to combating the current antimicrobial crisis.
Antimicrobial mechanism of nanomaterials to combat AMR.

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Abstract: Drones also called Unmanned Aerial Vehicles (UAVs) have become more prominent in several applications such as package delivery, real-time object detection, tracking, traffic monitoring, security surveillance systems, and many others. Asa key member of IoT, the group of Radio Frequency IDentification (RFID) technologies is referred to as Automatic Identification and Data Capturing (AIDC). In particular, RFID technology is becoming a contactless and wireless technique used to automatically identify and track the tagged objects via radio frequency signals. It also has drawn a lot of attention among researchers, scientists, industries, and practitioners due to its broad range of real-world applications in various fields. However, RFID systems face two key concerns related to security and privacy, where an adversary performs eavesdropping, tampering, modification, and even interception of the secret information of the RFID tags, which may cause forgery and privacy problems. In contrast to security and privacy, RFID tags have very limited computational power capability. To deal with these issues, this paper puts forward an RFID-based Lightweight and Provably Secure Authentication Protocol (LPSAP) for Unmanned Aerial Vehicle Systems. The proposed protocol uses secure Physically Unclonable Functions (PUFs), Elliptic-Curve Cryptography (ECC), secure one-way hash, bitwise XOR, and concatenation operations. We use Ouafi and Phan's formal security model for analyzing security and privacy features such as traceability and mutual authentication. The rigorous informal analysis is carried out which ensures that our proposed protocol achieves various security and privacy features as well as resists various known security attacks. The performance analysis demonstrates that our proposed protocol outperforms

other existing protocols. In addition, Scyther and Automated Validation of Internet Security Protocols and Applications (AVISPA) tool simulation results demonstrates that there is no security attack possible within bounds. Therefore, our proposed LPSAP protocol achieves an acceptable high level of security with the least computational, communication, and storage costs on passive RFID tags.

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Abstract: In an era where global biodiversity hotspots are under unprecedented threat, understanding the intricate balance between land use land cover (LULC) changes and their implications on ecosystem services value (ESV) becomes paramount. The region of Jammu and Kashmir, with its distinctive ecological importance, is well known for these challenges and opportunities. This region embodies various conservation reserves and national parks, and one of the most ecologically rich is called Kishtwar High Altitude National Park. It is often considered an example of biodiversity richness in the Indian subcontinent, as it protects a myriad of species and provides essential ecosystem services. However, despite its significance, it faces pressures from both peripheral human activities, such as seasonal grazing by nomadic communities and broader climatic changes. This study aims to investigate the complex relationship between these LULC shifts and their consequent effects on the park's ESV. We used the cellular automata (CA)-Markov model to simulate the LULC for the future. Using the LULC from 1992 to 2020 and projecting for 2030, 2040, and 2050, we employed the global value coefficient method to understand the ESV contributions of different LULC types. Our results revealed a 7.43% increase in ESV from 1992 to 2020, largely due to the increase of forests and waterbodies. In contrast, our projections for

2020 to 2050 intimate a 7.55% decline in ESV, even amidst anticipated grassland expansion. These results highlight the role of forests in securing resilient ecosystem services. These findings shall help offer informed conservation strategies, that are relevant both regionally and globally.

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Abstract: Chemical insecticides (organophosphates and pyrethroids) in the form of IRS (Indoor Residual Sprays) and LLINs (Long Lasting Insecticidal Nets) are the cornerstone for vector control, globally. However, their incessant use has resulted in widespread development of resistance in mosquito vectors, warranting continuous monitoring and investigation of the underlying mechanisms of resistance. Here, we identified a previously uncharacterized- Cub and Sushi Domain containing Insecticide Resistance (CSDIR) protein and generated evidence for its role in mediating insecticide resistance in the Anopheles stephensi. A strong binding affinity of the CSDIR protein towards different classes of insecticide molecules-malathion (K-D 6.43 mu M) and deltamethrin (K-D 46.7 mu M) were demonstrated using MD simulation studies and Surface Plasmon Resonance (SPR) experiments. Further, the recombinant CSDIR913-1190 protein exhibited potent esterase-like activity (alpha-naphthyl acetate (alpha-NA)- 1.356 +/- 0.262 mM/min/mg and beta-naphthyl acetate (beta -NA)- 1.777 +/- 0.220 mM/min/mg). Interestingly, dsRNA-mediated gene silencing of the CSDIR transcripts caused >60% mortality in resistant An. stephensi upon 1-h exposure to deltamethrin and malathion insecticides, compared to the control group. A significant reduction in the esterase-like activity was also observed against alpha-NA (p = 0.004) and beta-NA (p = 0.025) in CSDIR silenced mosquitoes compared to the control group. Using computational analysis and experimental data, our results provided significant evidence of the involvement of the CSDIR protein in mediating insecticide resistance in Anopheles mosquitoes. Thereby making the CSDIR protein, a novel candidate for exploration of novel insecticide molecules. These data would also be helpful in further understanding the development of metabolic resistance by the Anopheles vector.

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Abstract: Hazardous heavy metal (HM) pollution constitutes a pervasive global challenge, posing substantial risks to ecosystems and human health. The exigency for expeditious detection, meticulous monitoring, and

efficacious remediation of HM within ecosystems is indisputable. Soil contamination, stemming from a myriad of anthropogenic activities, emerges as a principal conduit for HM ingress into the food chain. Traditional soil remediation modalities for HM elimination, while effective are labor-intensive, susceptible to secondary contamination, and exhibit limited efficacy in regions characterized by low metal toxicity. In response to these exigencies, the ecofriendly paradigm of bioremediation has garnered prominence as a financially judicious and sustainable remedial strategy. This approach entails the utilization of hyperaccumulators, Genetically Modified Microorganisms (GMM), and advantageous microbes. The current review offers a comprehensive elucidation of cutting-edge phyto/microbe-based bioremediation techniques, with a specific emphasis on their amalgamation with nanotechnology. Accentuating their pivotal role in advancing sustainable agricultural practices, the review meticulously dissects the synergistic interplay between plants and microbes, underscoring their adeptness in HM remediation sans secondary contamination. Moreover, the review scrutinizes the challenges intrinsic to implementing bioremediation-nanotechnology interface techniques and propounds innovative resolutions. These discernments proffer auspicious trajectories for the future of agriculture. Through the environmentally conscientious marvels of phyto/microbe bioremediation, an optimistic outlook emerges for environmental preservation and the cultivation of a sustainable, salubrious planet via the conduit of cleaner agricultural production.

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