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Record 1 of 31

Title: Network-Based Integrative Analysis to Identify Key Genes and Corresponding Reporter Biomolecules for Triple-Negative Breast Cancer

Author(s): Singh, P (Singh, Pooja); Chaturvedi, R (Chaturvedi, Rupesh); Somvanshi, P (Somvanshi, Pallavi)

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Abstract: BackgroundThe malignant neoplasm of the TNBC is the leading cause of death among Indian women. Recent studies identified the global burden of TNBC affecting approximately more than 40 percent of all BC cases in women worldwide. The absence of expression of receptors such as ER, PR, and HER2 characterizes TNBC.ObjectivesDue to the lack of specific targets, standard treatment options for TNBC are limited. This integrative study aims to identify key genes and provide insights into the underlying molecular mechanisms of TNBC, which can potentially lead to the development of more effective therapeutic strategies.Material and MethodologyThis study integrates PPI and WGCNA analysis of TNBC-related datasets (GSE52194 and GSE58135) to identify key genes. Subsequently, downstream analysis is conducted to explore potential therapeutic targets for TNBC.ResultsThe present study renders the potential 13 key genes (PLCG2, CXCL10, CDK1, STAT1, IL6, PLK1, CCNB1, AURKA, NDC80, EGFR, 1L1B, FN1, BUB1B), along with their associated 6 TFs and 20 miRNAs, as reporter biomolecules around which the most significant changes occur. There were some miRNAs hsa-mir-449b-5p, hsa-let-7b-5p, hsa-mir-26a-5p, hsa-mir-155-5p, hsa-mir-24-

3p, hsa-mir-212-3p, hsa-mir-21-5p, hsa-mir-210-3p and hsa-mir-20a-5p whose association with other cancers and other BC subtypes have been reported but their association with TNBC need to be explored. Further, enrichment and cumulative survival analysis support the disease association of identified key genes with TNBC.ConclusionThis integrative analysis could be regarded for experimental inspection as it provides the platform for future researchers in drug designing and biomarker discovery for TNBC diagnosis and treatment.

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Author(s): Jangu, N (Jangu, Nupur); Raza, Z (Raza, Zahid)

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Abstract: Integration of fog and cloud has become increasingly important in the age of IoT, where everything is connected to the Internet. The cloud-only models face many challenges when serving the requests from IoT devices due to several factors such as latency, network congestion, data privacy, and security. Despite the popularity and numerous advantages of hybrid models, task scheduling is still an unsolvable multiobjective optimization problem. This research uses an improved bioinspired jellyfish search algorithm to solve the nonlinear np-hard task scheduling optimization problem. The work proposes a multiobjective improved jellyfish search (MOIJS) framework using a multiobjective adaptation function to minimize the make-span, cost, and power consumption that benefit customers and providers by considering the expenses associated with execution and power consumption. The performance of MOIJS is evaluated by comparing it with the discrete nondominated sorting genetic algorithm II using a MATLAB simulator. The experimental outcomes demonstrate the proposed work's efficacy in reducing the make-span, cost, and energy in cloud-fog environments in different batches of tasks.

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Author(s): Dixit, V (Dixit, Vimal); Rajkumar, K (Rajkumar, Krishnan)

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Abstract: Breast cancer continues to be a major worldwide health issue, requiring advanced predictive models for better healthcare outcomes and early detection. This research presents the novel quantum-enhanced neural network (QENN), a hybrid classical-quantum approach that integrates a classical neural network with a quantum feature map and a parameterized quantum circuit to enhance breast cancer classification performance. The QENN model is applied to both the wisconsin (diagnostic) breast cancer dataset (WBCD) and the SEER breast cancer dataset (SBCD). For the WBCD, QENN was able to deliver high-performance comparable to classical machine learning models and state-of-the-art research work, thus demonstrating the capability to extract complex patterns in biomedical datasets. For the SBCD, a dataset with class imbalance and high number of categorical features, QENN performed reasonably compared to classical machine learning models, after application of several preprocessing steps. However, it demonstrated a comparably high AUC-ROC score, which has been proven to be one of the most reliable metrics for imbalanced datasets. The study demonstrates the potential of QENN in biomedical applications, showing strong performance on balanced and well-processed datasets while maintaining comparable effectiveness on datasets with moderate class imbalance and high cardinality categorical features by leveraging quantum principles for distinct data representation and class separability.

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Abstract: The Partition of British India (1947) marks a crucial chapter in South Asian history. Scholarship, particularly from West Bengal, India, reveals that dominant narratives have largely ignored caste-based differences in the experiences of displacement and rehabilitation, creating homogenized national memories. Official narratives often portrayed Partition as a necessary cost of independence, with refugees being blamed for their own plight. In response, upper(ed)-caste male refugees constructed a counter-narrative of victimhood and struggle, asserting their rights to citizenship. This narrative, coupled with rising communist influence, positioned refugees as the new proletariat in Leftist politics, erasing distinctions of caste, class, and gender. State policies on refugee rehabilitation, however, were often caste-blind or actively discriminatory, further marginalizing lowered-caste refugees. This paper explores these dynamics through an ethnographic study in Asansol, West Bengal. The lowered-caste migrants, relocated to Asansol to serve as cheap labour for industrial development, faced ongoing hardship, exacerbated by industrial closures and labour informalization. Women from these families, excluded from formal labour, were forced into devalued, caste-based work, a pattern that has persisted across generations. The structures of caste, then, have rendered lowered-caste refugee families as marginalized 'quasi-citizens.' Unlike upper(ed)-caste refugees, they have struggled to overcome the consequences of Partition and become integrated as 'successful' citizens; in a context where the degree of citizenship has been increasingly defined as being inversely proportional to one's economic dependence on the government and directly proportional to one's performance of 'caste-moral respectability'. But, in a teleological fashion, their insufficient capacity to display adequate citizenship has only reinforced their de-valuation as labourers.

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Abstract: 'The theories propounded by the Aryanists and Dravidianists are utterly groundless and mere dreams of very learned men, and perhaps even more imaginative than learned'. -John Crawford 1861 1 'The theory is a perversion of scientific investigation. It is not allowed to evolve out of facts. On the contrary, the theory is preconceived, and facts are selected to prove it. The theory of the Aryan race is just an assumption and no more'. -B. R. Ambedkar 2The Rgveda eulogises Divodasa and Sudas as the great Arya kings and recounts several times the heroic battle fought by the chief deity Indra against Vr.tra to protect Dasadya. The hymns describe Vr.tra not only as an Arya but also as a Dasa and a Dasyu. The Rgveda equally demonises certain Aryas and Dasas as the enemies of yag & ntilde;a. Several sages identify the opponents of the yag & ntilde;a form of worship as their own brothers-sajatan and jamim, and friend-s & aacute;kha. This article attempts to explore these contradictions and the validity of the argument that the fair-skinned Aryans subjugated the dark-skinned Dasas and Dasyus. It also analyses the representation of colour and its importance in the Rgveda and factors in the writings of Herodotus. It looks at the complex relationship among Aryas, Asuras, Dasas and

Dasyus before and after Dasaraj & ntilde;a-the Battle of Ten Kings. It traces the reason for their migration to the Gangetic plains. It examines the interpretations of British Sanskrit scholars like William Jones and R. T. H. Griffith and Orientalists like H. T. Colebrooke, James Prinsep, H. T. Prinsep, H. H. Wilson, Max Mueller and others. It also brings B. G. Tilak and B. R. Ambedkar's perspectives into the debate.

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Abstract: Elevated temperature stress limits the growth, metabolism and productivity of medicinal plants. However, the response of Withania somnifera (L.) Dunal (Ashwagandha) which has diverse therapeutic properties, to elevated temperature stress remains unexplored. This study investigated the effects of elevated temperature stress exposure on the phytochemical content and antioxidant activity of Ashwagandha four varieties namely: Vallabh 01, Vallabh 02, Pratap, and Chetak, across leaf, stem, root, and fruit parts. The selected varieties were exposed to ambient temperature (10.4 +/- 2.6 to 31.6 +/- 5.9 degrees C) and elevated temperature (ET) levels (13.5 +/- 3.5 to 34.3 +/- 5.6 degrees C) in net house and control environment facility chamber, respectively from November 2021 to April 2022. Fruiting stage samples of different parts of all varieties from both treatments were analysed for total phytochemical content, total flavonoid content (TFC) and

antioxidant activity. The results revealed the variable response of varieties and their parts to ET stress. ET stress enhanced the cumulative (root + stem + leaf + fruit) phytochemical content of Vallabh 02, Pratap and Chetak by 112.9%, 15.2%, and 84.9%, respectively, and suppressed in the Vallabh 01 (3.6%). TFC and antioxidant activity were significantly ($p < 0.05$) higher under ET stress in all the varieties in the following order Pratap > Chetak > Vallabh 01 > Vallabh 02. The findings indicate that ET stress exposure significantly alters as well as enhances Ashwagandha varieties' total phytochemical content and antioxidant activity. Among the four varieties, Pratap is the most tolerant to ET stress. This study indicates that climate change associated ET levels up to 2 degrees C may enhance therapeutic potential of Ashwagandha varieties through synthesis of novel and unique phytochemicals. Novel knowledge of ET levels exposure to favour the production of specific phytochemicals can aid in optimizing the cultivation of medicinal plants for higher yields of desired medicinal compounds.

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Abstract: India is experiencing a rising incidence of cancer with a high mortality rate at a younger age. With high catastrophic healthcare expenditures and inadequate social security, it is imperative to investigate the health-seeking behaviour and corresponding economic burden on cancer-affected households. Using a nationally representative database, we use the matching methods to analyse healthcare utilization, healthcare expenditure, and financial distress of cancer-affected households. We find that the cancer-affected households report a longer hospital stay, more surgery, medicine uptake, and diagnostic tests per member compared to non-cancer households. The out-of-pocket healthcare expenditure borne by the affected households are significantly higher and mostly inflated through inpatient care. Further, we find some adverse spill-over effect in terms of lower per-member inpatient and outpatient visits and lower healthcare expenditure for non-cancer members of affected households when they are afflicted with any diseases. The catastrophic expenditures inflict income loss and distress financing to the cancer affected households. Further, we find per-member work force participation and non-medical consumption expenditures significantly low. We also observe heterogeneous effect in terms of lower inpatient visits, lower medicine uptake, lower capability to pay for treatment, and significantly higher borrowing and selling off assets among various cancer affected socioeconomically disadvantaged groups.

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Author(s): Yadav, K (Yadav, Kanchana); Das, T (Das, Trishala); Lynn, AM (Lynn, Andrew M.)

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Abstract: DNA damage is a key factor in many human disorders, including cancer, chronic inflammation, and early aging. Genes involved in DNA damage repair (DDR) not only maintain genomic stability but also contribute to immune responses by regulating the expression of antimicrobial peptides and ligands that activate immune receptors. Various components of the DNA damage response (DDR), including DNA damage sensors, transducer kinases, and effector proteins, are capable of activating diverse immunological signaling pathways. While DDR gene mutations are common in cancers, their effects on immune characteristics are not well understood. We investigated how mutations in DDR genes influence the expression of immune regulatory genes, including immune stimulators, inhibitors, and genes related to the major histocompatibility complex (MHC) pathway. Using gene expression data from The Cancer Genome Atlas (TCGA) and mutation data from cBioPortal, we analyzed 264 DDR-related genes and 66 immune regulatory genes. These genes were clustered and categorized using Metascape, an integrative bioinformatics tool that applies enrichment-based analysis to group functionally related genes into clusters. The clustered genes were further validated through a literature review and the GeneCards database. We scored the change in immune regulatory gene expression in response to DDR gene mutations to identify differentially expressed immune stimulators, inhibitors, and MHC-related genes. Our analysis revealed positive and negative correlations between DDR gene mutations and the

expression of immune modulators. These findings could help guide future cancer treatments based on biomarkers and immunotherapy strategies.

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Abstract: In the semiconductor industry there is constant demand to improve critical performance parameter of transistor including lowering of power requirement. Tunnel FET has emerged as one of the most favourable candidate for the next generation transistor for extremely low power requirements in mixed signal circuits. These tunnels FET have an edge in terms of power requirements but major challenges still persist including low ON current, high OFF current, low ION/IOFF ratio and high Ambipolar current for digital applications. In this paper, the investigation and exploration is on our unique embedded gate where gate is embedded into the channel from top and bottom, resulting in three different types of Embedded Double Gate TFET (EDG-TFET) structures for the very first time for extremly low-power applications. We introduced and studied for the first time EDG-TFET structure with Dual Material in the first type (DM), Dual dielectric in the second type (DD), and drain dielectric pocket in the third type (DP) in EDGTFET. It was possible to obtain promising result in terms of ON current with DMEDG-TFET structure with maximum ON current value of 1.1 x 10-3 A mu m-1. It was also possible to obtain promising result in terms of OFF current in all the above mention configuration where OFF current reaches minimum value of 10-19 A mu m-1. This study has helped to achieve an improvement in Ambipolarity behaviour in EDGTFET configuration where DP structure shows minimum

ambipolar current of value 1.1 x 10-20 A mu m-1. All the above DC parameter may be good for digital logic application. While EDGTFET having DM structure shows most promising results for RF/Analog applications. Lastly, we compared a unique embeded double gate with other non-embedded TFET structures for analog and digital applications.

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Author(s): Singh, MK (Singh, Manoj Kumar); Chand, S (Chand, Satish); Kumar, D (Kumar, Devender)

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Abstract: In automated diagnostics and biomedical research, accurate cell nuclei segmentation is essential, but it is still challenging because of differences in cell size, complicated backgrounds, and overlapping nuclei. We introduce DenseSegNet, an advanced deep learning (DL) framework meant to solve these problems by raising segmentation accuracy and resilience. DenseSegNet improves feature extraction and multi-scale fusion using dense separable blocks, a Spatial-Channel Attention Residual Block (SCARB), and a Bidirectional Feature Pyramid Network (BiFPN). Beginning with a convolutional encoder that effectively extracts hierarchical features using dense separable blocks, the network moves. By amplifying pertinent information, and so, reducing noise, the SCARB module enhances spatial and channel-wise feature representations. As such, the BiFPN guarantees efficient semantic representation at several feature levels by supporting bidirectional multi-

scale feature refining. High-resolution segmentation maps are produced in the decoder phase by feature concatenation of obtained elements and upsampling. DenseSegNet is assessed against a benchmark-the 2018 Data Science Bowl (DSB) dataset. We investigated several optimizers and loss functions to assess the architecture and learn its strength and adaptability fully. With a dice coefficient of 93.8%, an Intersection over Union (IoU) of 88.2%, a precision of 96.7%, and a recall of 91.8%, the results highlight the beneficial segmentation ability of DenseSegNet.

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Abstract: This study explores the synthesis and characterization of europium-doped silver selenide (Eu-Ag2Se) nanoparticles along with their application in electrochemical studies. The nanoparticles are synthesized via a hydrothermal method using silver, selenide and europium as precursors in the environment of octylamine solution. Comprehensive structural, morphological, and functional analyses are performed using X-ray diffraction (XRD), field-effect scanning electron microscopy (FESEM), high-resolution transmission electron microscopy (HRTEM), and Fourier transform infrared spectroscopy (FTIR). Electrochemical performance i.e., in supercapacitors and glucose sensors, is assessed through electrochemical experiments like cyclic voltammetry (CV), galvanostatic charge-discharge (GCD), chronoamperometry (CA) and electrochemical impedance spectroscopy (EIS). It has been observed that Europium doping significantly enhanced the specific capacitance, achieving 337.8 F g-1 at a current density of 0.14 A g-1, with an energy density of 8.4 W h kg-1 and a power density of 29.9 W kg-1. Additionally, the materials exhibited excellent cyclic stability, retaining 93% of their initial capacitance after 6000 cycles. Similarly, the sensitivity of the Eu-Ag2Se nanoparticles is calculated as 0.52 mu A mu M-1cm-2 in the linear range having good stability, selectivity and reproducibility.

These results highlight the potential of Eu-Ag2Se nanoparticles as a promising candidate for next-generation energy storage systems and glucose sensing applications.

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Abstract: Graphitic carbon nitrides are unique it-conjugated polymers, now known for their physiochemical stability, earth-abundance in nature, visible-light-driven, electron-hole pair conduction leading to photocatalysis, and environmentally benign materials. This review summarizes recent and emerging concepts in heterogeneous catalysis employing carbon nitrides and their fabricated materials towards heterocyclic syntheses.

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Abstract: The wave modes and linear Jeans instability in the ultra-relativistic degenerate strongly coupled quantum plasma have been studied using the quantum hydrodynamic fluid description considering the influence of radiation pressure, Ohmic diffusivity and uniform rotation. The modified equation of state is considered in the fluid model, which includes the effects of radiation pressure of weakly coupled, degenerate, and ultra-relativistic electrons and non-degenerate strongly coupled ions. The general dispersion relation is analytically derived using the normal mode analysis and examined in the transverse and longitudinal modes of propagation in hydrodynamic and kinetic limits. The Jeans instability criterion depends upon the characteristic wave speed of the system modified due to radiation pressure, electron degeneracy pressure, and ion gas pressure. For an infinitely conducting fluid, the Alfv én speed is observed to intervene in the instability condition and modify the critical Jeans wavenumber in transverse propagation. The graphical illustrations show that the growth rate of Jeans instability in the kinetic limit is significantly reduced due to the prominent role of radiation pressure, compressional viscoelastic effects, electron degeneracy pressure, fluid rotation, and quantum corrections. The dispersion properties of wave modes and linear instabilities are analyzed in various limiting cases of interest. The present theoretical results have been applied to understand the gravitational collapse of white dwarfs, and it is observed that perturbations of wavelength larger than the Jeans length lambda J similar or equal to 1.7x105km\documentclass[12pt]{minimal} \usepackage{amsmath} \usepackage{wasysym} \usepackage{amsfonts} \usepackage{amssymb} \usepackage{amsbsy} \usepackage{mathrsfs} \usepackage{upgreek} \setlength{\oddsidemargin}{-69pt} \begin{document}$${\lambda _{\text{J}}} \simeq 1.7 \times {10<^>5}\;{\text{km}}$$\end{document} make white dwarfs gravitationally unstable.

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Abstract: Estimating criteria pollutants is crucial due to their continuous increase and impact on respiratory health. To mitigate the impact of air pollution on human health, it is essential to understand the concentration of air pollutants at specific locations. This study aims to evaluate the variation, estimate the levels of criteria pollutants, and assess their potential health risks in the vicinity of a coal mine complex and a thermal power plant situated in an eastern coastal state of India. The pre-existing hot spot regions-Talcher (T) and Brajrajnagar (B)-which host many coal-fired power plants and clusters of coal-mining blocks in the coastal state of Odisha, are considered. Talcher consistently shows higher levels of particulate matter (PM10), nitrogen dioxide (NO2), and sulfur dioxide (SO2), reflecting a greater industrial impact. Brajrajnagar, while also impacted, exhibits comparatively lower pollutant concentrations. The observed seasonal trends highlight the necessity for targeted mitigation strategies to address pollution levels and associated health risks in these regions. Novel machine learning (ML) models, including independent component regression (ICR), ElasticNet (ENET), and boosted tree (BT), are applied to estimate criteria pollutants. Statistical analyses highlight BT as the superior model, outperforming ENET and ICR in pollutant estimation, particularly in Talcher. Taylor plots and statistical evaluations further validate the BT model's robustness in air pollutant estimation. Additionally, the study assesses the associated health risks posed to nearby populations of Talcher and Brajrajnagar. The analysis highlights significant spatial disparities in pollution levels, with Talcher consistently recording higher concentrations of PM10, NO2, and SO2 and poorer air quality index (AQI) than Brajrajnagar. Talcher also shows greater health risks, with pollutant exposure linked up to 6% higher risks for PM10, 5% for NO2, and up to 3% for SO2. The health risk-based air quality index (HAQI) reveals an underestimation of health risks by the current AQI, emphasizing the need for improved metrics to address the impacts of multi-pollutant exposure.

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Abstract: Electroactive polymer-based composites have made significant strides in advancing societal applications, though their multifunctional potential remains an active area of research. This study explores the potential of poly(vinylidene fluoride)- CoFe2O4 (PVDF-CFO) nanocomposites for applications in energy harvesting, microwave absorption, and airflow detection by incorporating CFO nanoparticles at varying concentrations (0-20 wt%). The optimized 10 wt% CFO nanocomposite exhibited remarkable properties, including high beta-phase content, polarization, and breakdown strength (164 kV/cm). P-E loop measurements confirmed an excellent mechanical energy conversion efficiency of 89%. The piezoelectric nanogenerator (PENG) fabricated using the 10 wt% PVDF-CFO nanocomposite produced an output voltage of approximately 10 V across a 10 M Omega load under gentle fist tapping, achieving a power density of 3.0 mu W/cm2 and charging a capacitor to 0.45 V in 14 s. Furthermore, microwave absorption studies revealed enhanced absorption properties for 10 wt% PVDF-CFO nanocomposite, with reflection losses (S11-parameter) of -21.5 dB and -17 dB in the K-band, compared to -20.4 dB in the X-band for neat PVDF. Additionally, the device demonstrated high sensitivity to airflow, converting mechanical stress into electrical signals. These findings demonstrate the multifunctionality of PVDF-CFO nanocomposites and their potential applications in energy harvesting, environmental monitoring, microwave absorption, and antennas.

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Title: Neurogrit Gold Attenuates 6-OHDA-Induced Dopaminergic Neurodegeneration in Parkinson's Model of Caenorhabditis elegans by Reducing α-Synuclein Accumulation and Pink/Pdr-1 Driven Mitochondrial Dysfunction

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Abstract: Introduction Parkinson's disease (PD) is a neurodegenerative disorder majorly associated with movement and behavioral disturbances. Pathologically, the loss of dopaminergic (DA) neurons triggered by the deposition of alpha-synuclein (SNCA) leads to the decrease in dopamine levels affecting motor and cognitive functions of the brain. Current pharmacotherapy for PD only addresses its symptoms but is not able to halt its progression. Traditional medicines are being increasingly used for the treatment of neurodegenerative disorders. Aim The present study investigated the effects of Neurogrit Gold (NG), a herbo-mineral prescription medicine, on a Parkinson's model of Caenorhabditis elegans. Methods Chemical characterization of NG was performed on HPLC and GC-MS/MS platforms. Evaluation of NG was done in the neurotoxicant 6-OHDA-induced N2, BZ555, and NL5901 strains of C. elegans. Results It was observed that NG treatment did not hamper the lifespan, survival, and progeny development of C. elegans strains. The worms treated with NG were able to resist the deleterious effects of 6-OHDA on survival, progeny development, body bends, and chemotaxis in N2 and DA neuron degeneration in BZ555 worms. In NL5901 worms, NG treatment reduced SNCA aggregation,

restored lipid content, as well as improved body bends, chemotaxis, and food uptake. Gene expression studies on 6-OHDA exposed and NG-treated N2 worms suggest that the neuroprotective effects of NG stem from its ability to regulate genes involved in mitochondrial autophagy (pink-1, pdr-1); dopamine synthesis (cat-2); redox (sod-3) and protein folding homeostasis (hsf-1, hsp-12.3). Conclusion Neurogrit Gold has robust neuroprotective effects, making it a suitable treatment option against etiologies of Parkinson's disease.

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Abstract: Even after several attempts, very few therapeutics have been successfully translated clinically for mitigating neurodegeneration. The major obstacle to effective treatment is the highly restrictive blood-brain barrier, which impedes the free access of antigens and therapeutics to the brain parenchyma, thereby limiting their therapeutic efficacy. Addressing this challenge, we have devised a biologically inspired nanoformulation using a neural cell membrane and ceria nanoparticles (NM@MCN-MM) for antioxidant activity and neuroprotection. The mesoporous ceria nanoparticle was optimized and fabricated using a soft template method and subsequently encapsulated within Neuro-2a (N2a) cell membranes. Given that mitochondrial dysfunction, increased oxidative stress, and calcium imbalance are common hallmarks of various neurodegenerative diseases, NM@MCN-MM has demonstrated promising results in addressing these pathological characteristics. Additionally, the formulation exhibits enhanced systemic circulation with natural brain-homing properties and reduced immunogenicity, which collectively improve the brain-targeting efficiency of the developed carrier and facilitate BBB permeation, as estimated through LC-MS/MS and optical live imaging using indocyanine green as a fluorescent probe. The significant findings of the developed biomimetic formulation against common hallmarks of neurodegenerative diseases, retaining the biomimetic catalytic activity of nanoceria upon an increase in size, suggest its potential in wider applications for mitigating other neurodegenerative diseases.

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Abstract: Highly dipolar molecules are crucial in areas of optics, energy, etc. However, their effective design, synthesis, and purification remain a challenge. Herein, we report the synthesis of highly dipolar zwitterions by successive ArSN reactions via C-C and C-N bond formation to pivot donor and acceptor at the NDI core. The

zwitterions reveal a large nonlinear optical response, excited-state dipole moments up to 47 D, which is one of the largest observed in arylene diimides.

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Zou YK, 2023, J ELECTRON MATER, V52, P2852, DOI 10.1007/s11664-023-10250-y

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Abstract: In this paper, an ultra-wideband (UWB) terahertz Metamaterial Perfect Absorber (MPA) based on the phase change feature of vanadium dioxide (VO2) is proposed. The proposed absorber consists of two square loops of vanadium dioxide (VO2), silicon dioxide (SiO2) as the dielectric substrate and a layer of gold (Au) acting as the ground. Phase transition material VO2 changes the conductivity (conductivity is changed from 200 to 2 x 105 S m-1, concerning temperature 300 K to 341 K) by several orders of magnitude at temperatures above 340 K by shifting from an insulating to a metallic state. The absorption of this suggested absorber can be adjusted from 4% to 100% within the conductivity range of 200 to 2 x 105 S m-1, which corresponds to temperatures between 300 K and 341 K. In the 2.2-6.8 THz range, with a bandwidth of up to 4.6 THz, more than 80% absorption is observed. The absorber design we proposed is polarization insensitive, simple and easily integrable. There are numerous uses for the suggested absorber in communication-related futuristic devices.

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Abstract: Staphylococcus aureus (S. aureus) is a deadly, gram-positive bacterium causing life-threatening diseases such as fatal pneumonia, sepsis, and severe skin infections highlighting the need for urgent medical intervention. Metal-organic frameworks (MOFs), a novel class of porous materials have recently shown promising antibacterial action against various pathogens possibly due to the slow release of metal ions when dissolved in aqueous media. The current work focuses on exploring the antibacterial potential of Fe-MOF against S. aureus. The assay results substantiate the antibacterial action of Fe BDC MOF in an aqueous environment against S. aureus. Furthermore, a combination of Fe BDC MOF and antibiotic gentamicin exhibits a remarkable enhancement in antimicrobial efficacy with a 34 mm zone of inhibition in antibacterial action, demonstrating a synergistic effect between the two compounds against the pathogen. This work paves the way for the development of novel combination drug therapies against S. aureus and other deadly pathogens. To further advance the antibacterial research this study adopts a combination drug therapy approach, screening Fe BDC MOF with gentamicin to combat the growth of S. aureus.

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Title: Measuring the effect of hydrological insecurity on landscape and ecological condition of floodplain wetland (Jul, 10.1007/s10668-024-05248-3, 2024)

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Author(s): Giri, S (Giri, Soma); Tiwari, AK (Tiwari, Ashwani Kumar); Mahato, MK (Mahato, Mukesh Kumar); Singh, AK (Singh, Abhay Kumar)

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Abstract: Groundwater resources in mica mining areas of Jharkhand are vital for local communities, agriculture, and domestic utilization. The study investigates the major ion chemistry of groundwater in the mica

mining regions, focusing on key physicochemical parameters such as pH, electrical conductivity (EC), total dissolved solids (TDS), and concentrations of major cations (Ca-2(+), Mg-2(+), Na+, K+) and anions (HCO3-, Cl-, SO42-, NO3-, F-). Groundwater samples from the study area were collected before the monsoon season, during the monsoon season, and after the monsoon season. The hydro-chemical analysis reveals that groundwater in the mica mining zones exhibits elevated levels of dissolved ions, with NO3-, F-, Ca-2(+), Mg-2(+) and total hardness exceeding permissible limits set by Bureau of Indian Standards (BIS) for drinking purposes at some locations. Water Quality Index (WQI) assessments suggest that a significant proportion of groundwater samples fall into the "good" to "very good" category for drinking and about 29% of the samples fall under the "poor" category. The groundwater was generally suitable for irrigational use with exception of a few due to high salinity. The principal component analysis revealed rock weathering as a dominant source of ions along with anthropogenic sources like mining and agriculture contributing minorly to the ionic load. The predominant hydro-chemical facies identified were Ca-Mg-HCO3 and Ca-Mg-Cl-SO4 types. Both carbonate and silicate weathering play an important role in the geochemical signature of the groundwater in the area. The study implicates the potential health impacts of using the groundwater as drinking water without treatment at a few locations owing to high fluoride, nitrate and dissolved solids. The study also highlights the need for sustainable water management practices and regular monitoring of groundwater quality to mitigate the anthropogenic impacts on groundwater resources.

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Author(s): Mekap, S (Mekap, Smrutiranjan); Kumar, B (Kumar, Birendra); Ananthram, KS (Ananthram, K. S.); Tarafder, K (Tarafder, Kartick); Ghosh, S (Ghosh, Subhasis); Roy, A (Roy, Anushree)

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Abstract: This paper discusses the coupling between spin-wave-mediated magnetic interactions and lattice degrees of freedom in bilayer La1.4Sr1.6Mn2O7 (BL-LSMO-0.3). The thermal evolution of the Raman shift, as obtained from micro-Raman spectroscopic measurements over a wide temperature range, reveals the evolution of phonon dynamics while the system undergoes a balance between double and superexchange spin-spin interactions through spin-wave modulation in different magnetic phases. The evolution of relative magnetoelastic coupling strengths for nearest-neighbor ferromagnetic and next-nearest-neighbor antiferromagnetic superexchange interactions in the high-temperature canted antiferromagnetic phases are estimated. We have also demonstrated the existence of orbital ordering and its correlation with spin-phonon dynamics in the canted antiferromagnetic phases of BL-LSMO-0.3 from the detailed analysis of the high-wave-number orbiton-related phonon modes. Our study further reveals the absence of charge ordering in the

compound. The complex coupling of lattice distortion, orbital ordering, the nearest- and next-nearest-neighbor spin-spin interactions in determining the canted spin states of the system is discussed.

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Abstract: Heterostructure construction is a strategic approach to boost electrode performance for high-efficiency supercapacitors. Herein, a coreshell heterostructure of MnMoO4 @1T-MoS2 was synthesized and evaluated in both symmetric and asymmetric configurations. The heterojunction between these materials generates a built-in electric field, which significantly enhances conductivity and accelerates charge transport. In addition, the core-shell structure reduces the volume expansion and restacking of nanoflakes, providing high stability and active sites. Density Functional Theory (DFT) calculations were carried out to explore the theoretical properties of MnMoO4@MoS2, revealing a strong built-in electric field of 1.072 V & Aring;-1 and a remarkably high quantum capacitance (CQ) of 387.06 mu F cm(-2) at -1 V. The MnMoO4@MoS2 SSC exhibits a specific capacitance (C_sp) of 319 F g-1 at a current density of 1 A g-1 with a cyclic stability 87.9% after 10000 cycles. Furthermore, it delivers a high Ed of 46 Wh/kg with a Pd of approximate to 653 W kg-1. Meanwhile, the asymmetric capacitor shows a high of C_spof approximate to 173 F g-1, with a high Ed of approximate to 51 Wh kg-1 and a Pd of approximate to 720 W kg-1. The findings indicate that this composite material possesses significant promise as an electrode material for energy storage applications.

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Abstract: This study initiates the development of Ru1, a metalloantibiotic derived from p-cymene, which delivers dual functionality. Our approach begins with the design and synthesis of half-sandwich ruthenium complexes, Ru1-Ru11. By varying the structure of the ancillary ligand, the biological activities of eleven ruthenium complexes against five bacterial strains were explored. Most active, Ru1 (4 mu g mL-1) and Ru 11 (1 mu g mL-1) was solicited for further study. To assess the safety of these compounds, hemolytic activity and cytotoxicity were evaluated against human red blood cells (RBCs) and the HEK cell line, respectively. Based on these results, Ru1 was selected for further investigation. Ru1 exhibited significant efficacy against MRSA (methicillin-resistant S. aureus) and VRSA (vancomycin-resistant S. aureus). Additionally, Ru1 exhibited strong DNA-binding affinity (Kb = 1.73*105 M-1 and 1.6 *105 M-1). Molecular docking studies further highlighted Ru1's potent interaction with the active sites of key bacterial proteins, including S. aureus MurB, topoisomerase II DNA gyrase, and 1BNA, with binding energies of -12.05 kcal/mol, -6.30 kcal/mol and -7.77 kcal/mol, respectively. Furthermore, Ru1 showed high photoacoustic signal intensity at 902 nm in MSOT imaging, underscoring its potential as a dual-function therapeutic and diagnostic (theragnostic) agent.

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Abstract: BackgroundMicronutrient deficiency is a global public health concern, especially among the adolescents of developing countries including India. Folate, an essential B-vitamin plays an indispensable role in various physiological processes throughout life. This is a cross-sectional study to determine prevalence of folate insufficiency among North-Indian school-going adolescents of various socio-economic backgrounds.MethodsA total of 3129 healthy school-going adolescents from North India were selected for the study and circulatory folate levels were measured using an electrochemiluminescence assay. Relationship of circulatory folate with various biochemical and anthropometric parameters were evaluated. Genetic determinants of folate levels in the study population were explored via both genome-wide and exome-wide association studies.ResultsOur results indicate higher prevalence (41%) of folate insufficiency in urban adolescents attending government-funded schools, with distinct relationship of folate levels, biochemical parameters, and anthropometric traits with varied socioeconomic strata. Girls exhibited a higher percentage of folate insufficiency than their male contemporaries. Results from genome-wide association study indicate significant associations of MYO1B (p = 5.13 x 10-7), CDH9 (p = 5.36 x 10-7), and PANK3 (p = 6.66 x 10-7) genes with folate levels in adolescents. Single variant analysis from exome-wide association analysis reaffirms the association of a previously reported variant in MTHFR gene (rs1801133; p = 1.87 x 10-6) along with identification of novel missense variants in KRT7 (rs2608009; p = 2.16 x 10-6 and rs6580870; p = 9.49 x 10-6) and AK9 (rs1406957; p = 4.76 x 10-6) genes.ConclusionsOur study highlights the importance of large-scale studies on prevalence of folate insufficiency and nutrigenomic regulation of folate levels in Indian population. Implementing multifaceted measures including food fortification, dietary diversification and health education in adolescents is crucial to combat folate deficiency in developing nations like India.

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Abstract: We compare tropospheric column nitrogen dioxide (NO2) in the United Kingdom Chemistry and Aerosol (UKCA) model version 11.0 with satellite measurements from NASA's Earth Observing System (EOS) Aura satellite Ozone Monitoring Instrument (OMI) to investigate the seasonality and trends of tropospheric NO2 over south and east Asia (S and E Asia). UKCA is the atmospheric composition component of the UK Earth System Model (UKESM). UKCA was run with nudged meteorology, producing hourly output over S and E Asia for 2005-2015. OMI averaging kernels have been applied to the model hourly data sampled at Aura's

local overpass time of 13:45 LT +/- 15 min to allow for consistent model-data comparison. Background UKCA and OMI tropospheric column NO2 typically ranges between 0x1015 and 2x1015 molec.cm-2. Diurnal cycles and vertical profiles of the tropospheric NO2 column in UKCA show that the daily minimum tropospheric column NO2 occurs around the satellite overpass time. UKCA captures the seasonality but overestimates NO2 by a factor of similar to 2.5, especially during winter over eastern China and north India, at times and locations with high aerosol loadings. Heterogeneous chemistry is represented in the version of UKCA used here as uptake of N2O5 on internally generated sulfate aerosol. However, aerosol surface area may be underestimated in polluted locations, contributing to overestimation of NO2. In addition, the model may underestimate emissions of volatile organic compounds (VOCs) and associated peroxy acetyl nitrate (PAN) formation, leading to insufficient long-range transport of oxidised nitrogen and also contributing to overestimation of NO2 over polluted regions and underestimation over remote regions. Quantifying and understanding discrepancies in modelled NO2 warrant further investigation as they propagate into modelling of multiple environmental issues.

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Abstract: Antipathogenic strategies are radical vectors in symptomatic treatment and averting morbidity of high-risk contagious contributing to the complex paradigm of one health management. This study investigates the physicochemical attributes and antimicrobial activities in synergy with the photocatalytic efficacy of biogenic silver nanoparticles (AgNPs). Biogenic AgNPs were engineered using an economical and eco-friendly route employing the Lemongrass's essential oil as a multifunctional reducing, capping, stabilizing, and doping agent. Structural and morphological outcomes reveal the formation of crystalline spherical AgNPs with a size of 7 to 30 nm. Fabricated AgNPs exhibited broadband antibacterial (against Bacillus subtilis and Escherichia coli) potencies comparable to state-of-the-art antipathogenic drugs utilized for treating infectious disorders. Besides, engineered biogenic AgNPs demonstrated excellent photocatalytic degradation effectiveness of roughly 96.63% towards methylene blue (MB) in Sunlight for 2 h without the use of an external reducing agent. Moreover, the biogenic AgNPs open new windows to tackle the prominent issues of antimicrobial resistance and greener dye removal causative to sustainable water health management. Based on the exceptional results, imperative from a biocompatible, non-toxic, eco-friendly, and economic perspective, such essential oil -mediated AgNPs are novel nanoplatforms for broadband one health applications.

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Abstract: Malaria elimination faces challenges from drug resistance, stemming from mutations within the parasite's genetic makeup. Genetic adaptations in key erythrocyte proteins offer malaria protection in endemic regions. Emulating nature's approach, and implementing methodologies to render indispensable host proteins inactive, holds the potential to reshape antimalarial therapy. This study delves into the functional implication of the single-span membrane protein Kell ectodomain, which shares consensus sequence with the zinc endopeptidase family, possesses extracellular enzyme activity crucial for parasite invasion into host erythrocytes. Through generating Kell-null erythrocytes from an erythroid progenitor, BEL-A, we demonstrate the indispensable nature of Kell activity in P. falciparum invasion. Additionally, thiorphan, a metallo-endopeptidase inhibitor, which specifically inhibits Kell activity, inhibited Plasmodium infection at nanomolar concentrations. Interestingly, individuals in malaria-endemic regions exhibit low Kell expression and activity, indicating a plausible Plasmodium-induced evolutionary pressure. Both thiorphan and its prodrug racecadotril, demonstrated potent antimalarial activity in vivo, highlighting Kell's protease role in invasion and proposing thiorphan as a promising host-oriented antimalarial therapeutic.

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