Web of Science™

JNU publications for the month of January 2025

Record 1 of 59

Title: Re-induction based mining for high utility item-sets

Author(s): Mathur, PS (Mathur, Pushp S.); Chand, S (Chand, Satish)

Source: APPLIED INTELLIGENCE **Volume:** 55 **Issue:** 1 **Article Number:** 75 **DOI:** 10.1007/s10489-024-05855-7 **Published Date:** 2025 JAN

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 1

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Cited Reference Count: 34

Abstract: The High Utility Itemset mining (HUIM) is an important research area in the field of data mining and knowledge discovery. HUIM aims to discover the high utility patterns from a given database, based on a utility threshold value, where the utility is a user-defined objective function. The existing HUIM algorithms fail to consider the actual behaviour of the occurrence of patterns in database. They consider all the patterns having the same utility value to be of equal importance. However, this may not always be the case, since some patterns may occur in localized clusters in the database while others can have a more uniform sequence of occurrence. The Frequent Itemset Mining (FIM) approaches also fail to address this problem since they are based on a support framework that considers only the frequency of occurrence of an itemset in the database. To address this research gap, this study introduces a novel concept of maintaining a count value of the itemsets, called re-induction count, in order to keep track of the relative occurrence of items in the database. A novel algorithm, named Ri-Miner, is proposed to mine itemsets based on both a minimum utility threshold and their re-induction count. The experimental results show that Ri-Miner outperforms existing methods by achieving a 15% improvement in execution time and a 10% reduction in memory usage. The proposed method can be useful in various applications that require capturing the underlying occurrence behaviour of the patterns the database, like market-basket analysis, healthcare, web stream analytics, etc.

Accession Number: WOS:001369346400001

Language: English

Document Type: Article

Author Keywords: Datasets; Data mining; Knowledge discovery; Utility mining; Pattern recognition

KeyWords Plus: EFFICIENT ALGORITHMS

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Publisher: SPRINGER

Publisher Address: VAN GODEWIJCKSTRAAT 30, 3311 GZ DORDRECHT, NETHERLANDS
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Research Areas: Computer Science
IDS Number: O2F2Z
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eISSN: 1573-7497
29-char Source Abbrev.: APPL INTELL
ISO Source Abbrev.: Appl. Intell.
Source Item Page Count: 17
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Record 2 of 59

Title: Deep diversities and widening chasms of inequality

Author(s): Ali, A (Ali, Amir)

Source: ETHNIC AND RACIAL STUDIES **DOI:** 10.1080/01419870.2025.2451374 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 18
Times Cited in Web of Science Core Collection: 0
Total Times Cited: 0
Usage Count (Last 180 days): 0
Usage Count (Since 2013): 0
Cited Reference Count: 9

Abstract: This article assesses the arguments of the authors in terms of the challenge that diversity poses to polities. Appreciating the comparative, contextual and iterative method of the authors that entwines the normative and the empirical, this article suggests that the arguments of the book may be weakened by an overlooking of how diversity fares in the face of widening material inequalities and the workings of the neoliberal market. This article questions the use of the term "governance" of diversity and suggests that it inadvertently suggests a technocratic and managerial approach to diversity on account of the neoliberal underpinnings of the term. Finally, it welcomes the case for religion as public good that the authors make but suggests that this can only flourish with an accompaniment of public goods such as health, housing and education, publicly provisioned by the exchequer for all citizens and not subject to commoditization for individual consumers.

Accession Number: WOS:001401766700001
Language: English
Document Type: Article; Early Access
Author Keywords: Diversity; multiculturalism; secularism; governance; groups; public good

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29-char Source Abbrev.: ETHNIC RACIAL STUD
ISO Source Abbrev.: Ethn. Racial Stud.
Source Item Page Count: 8
Output Date: 2025-03-04

Record 3 of 59
Title: Being rooted yet open: Cultural plurality and cross-cultural conversations
Author(s): Mahajan, G (Mahajan, Gurpreet)
Source: ETHNICITIES **Volume:** 25 **Issue:** 1 **Pages:** 155-162 **DOI:** 10.1177/14687968241306894 **Early Access Date:** JAN 2025 **Published Date:** 2025 FEB
Times Cited in Web of Science Core Collection: 0
Total Times Cited: 0
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Usage Count (Since 2013): 0
Cited Reference Count: 14
Accession Number: WOS:001390117300001
Language: English
Document Type: Review
Author Keywords: Multiculturalism; cultural plurality; cross-cultural conversations; dialogue; Bhikhu Parekh
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Publisher Address: 1 OLIVERS YARD, 55 CITY ROAD, LONDON EC1Y 1SP, ENGLAND
Web of Science Index: Social Science Citation Index (SSCI)
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29-char Source Abbrev.: ETHNICITIES
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Record 4 of 59

Title: Eradication of Antibiotic-Resistant Gram-Positive Bacteria and Biofilms by Rationally Designed AIE-Active Iridium(III) Complexes Derived from Cyclometalating 2-Phenylquinoline and Ancillary Bipyridyl Ligands

Author(s): Gautam, A (Gautam, Aryan); Sasmal, PK (Sasmal, Pijus K.)

Source: INORGANIC CHEMISTRY **Volume:** 64 **Issue:** 6 **Pages:** 2905-2918 **DOI:** 10.1021/acs.inorgchem.4c05064 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 31

Abstract: Antibiotic resistance caused by Gram-positive bacteria is a growing global human health threat. Selective discrimination and eradication of Gram-positive bacteria and their biofilms is challenging. Therapeutic strategies with multiple modes of action are urgently needed to address the increase in Gram-positive bacteria-resistant nosocomial infections. In this work, we have presented rationally designed aggregation-induced emission (AIE)-active cationic cyclometalated iridium(III) complexes derived from 2-phenylquinoline and 2,2 '-bipyridine ligands for Gram-positive antibacterial studies. The AIE properties of these complexes were exploited for selective discrimination between Gram-positive and Gram-negative bacteria. These complexes displayed good antimicrobial activity against critical Gram-positive ESKAPE pathogens with minimum inhibitory concentrations in the low micromolar range but were inactive against Gram-negative pathogens. Importantly, the complexes can inhibit biofilm formation and eradicate bacteria from mature biofilms, which are major causes of persistent infections and antibiotic resistance and are more difficult to eliminate. In addition, these complexes showed low hemolytic activity against mammalian cells and a high therapeutic index, indicating good selectivity. Interestingly, the complexes kill bacteria through a variety of modes of mechanism, including ROS generation, cell membrane disruption, and depolarization and the loss of bacterial membrane integrity. These findings offer opportunities for designing metal AIEgens to treat Gram-positive bacterial infections effectively.

Accession Number: WOS:001411234500001

PubMed ID: 39887057

Language: English

Document Type: Article

KeyWords Plus: INDUCED EMISSION CHARACTERISTICS; STAPHYLOCOCCUS-AUREUS; AGGREGATION; PROBE; DISCRIMINATION; BLOOD

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Research Areas: Chemistry
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Output Date: 2025-03-04

Record 5 of 59

Title: Effect of Divalent Cations on Polarity and Hydration at the Lipid/Water Interface Probed by 4-Aminophthalimide-Based Dyes

Author(s): Alam, P (Alam, Parvez); Kumar, P (Kumar, Pramod); Sahu, H (Sahu, Harsh); Sardana, D (Sardana, Deepika); Kundu, P (Kundu, Pronab); Chand, AK (Chand, Ajay Kumar); Sen, S (Sen, Sobhan)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 129 **Issue:** 3 **Pages:** 930-941 **DOI:** 10.1021/acs.jpcb.4c05404 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 10

Abstract: The ion binding to the lipid/water interface can substantially influence the structural, functional, and dynamic properties of the cell membrane. Despite extensive research on ion-lipid interactions, the specific effects of ion binding on the polarity and hydration at the lipid/water interface remain poorly understood. This study explores the influence of three biologically relevant divalent cations-Mg2+, Ca2+, and Zn2+-on the depth-dependent interfacial polarity and hydration of zwitterionic DPPC lipid in its gel phase at room temperature. To measure these depth-dependent properties, we use a series of solvatochromic fluorescent probes synthesized based on 4-aminophthalimide with varying alkyl chain lengths (4AP-Cn; n = 5, 7, and 9). Employing steady-state fluorescence experiments and all-atom molecular dynamics (MD) simulations, we quantify changes in interfacial polarity and hydration induced by the cations binding to the lipid/water interface. Our results reveal that Zn2+ induces a significant blue shift in the fluorescence spectra

of all 4AP-Cn dyes, indicating a marked decrease in local polarity (E-T(N) <= 0.05) at the lipid/water interface compared to Mg2+ and Ca2+, which results in a higher polarity (E-T(N) >= 0.2). The depth-dependent fluorescence spectra of dyes at the interface in the presence of Mg2+ and Ca2+ remain similar to those in the absence of cations, with only a minor red shift observed for Mg2+, implying a slight hydration effect. MD simulations show that cations primarily bind to the headgroup and glycerol regions of lipid. Simulations also reveal that Zn2+ causes substantial dehydration at the lipid/water interface, as detected by the 4AP-Cn dyes, while Mg2+ and Ca2+ have less pronounced effects, with only slight hydration induced by Mg2+. This study highlights the distinct positional effects of cations probed by 4AP-Cn probes at the lipid-water interface, underscoring the potential of 4AP-Cn dyes for monitoring depth-dependent changes in membrane properties induced by external agents or environmental conditions.

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PubMed ID: 39791376

Language: English

Document Type: Article

KeyWords Plus: METAL-IONS; CALCIUM-IONS; LIPID-BILAYERS; PHASE-BEHAVIOR; CA2+ IONS; DYNAMICS; LOCATION; GEL; GRAMICIDIN; MEMBRANES

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Output Date: 2025-03-04

Record 6 of 59

Title: Exogenous Treatment of Caffeic Acid and Methylglyoxal Synergistically Enhances Anticancer Effect in Prostate Cancer via Inhibition of Glyoxalase-1

Author(s): Anjaly, K (Anjaly, Km); Tiku, AB (Tiku, Ashu Bhan)

Source: PROSTATE **Volume:** 85 **Issue:** 5 **Pages:** 463-470 **DOI:** 10.1002/pros.24849 **Early Access Date:** JAN 2025 **Published Date:** 2025 APR

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 0

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Cited Reference Count: 21

Abstract: BackgroundCaffeic acid (CA), a dietary compound, has been studied for its potential impact on inhibiting prostate cancer (PCa) growth. PCa is often associated with heightened expression of glyoxalase-1 (Glo-1), making it a target for potential therapeutic interventions. CA's mechanisms in suppressing Glo-1 expression and its effects on PCa cell proliferation are areas of interest for understanding its potential as an anticancer agent.MethodsCellular viability and proliferation were evaluated through MTT and clonogenic assays. The expression levels of particular proteins were assessed using western blot analysis and immunocytochemistry.ResultsResults indicated significant reduction in PCa cell proliferation by CA, accompanied by induction of DNA double-strand breaks, leading to apoptotic cell death through decreased pro-caspases expression. Additionally, CA was found to inhibit Glo-1 expression. To enhance CA's anticancer effect, a novel approach was taken by combining it with methylglyoxal (MG). Exogenous MG treatment, a glycolysis by-product and glyoxalase enzyme substrate, exhibited dose and time-dependent toxicity in PCa cells when combined with CA. This combination treatment showed heightened toxicity against PCa cells, attributed to CA's inhibition of Glo-1 expression and the nontoxic doses of exogenous MG. Consequently, increased levels of endogenous MG were observed, leading to apoptosis and suggesting a promising strategy for targeting glyoxalase oncogenic signaling pathways in PCa with minimal adverse effects.ConclusionThe study highlights the potential of CA as a therapeutic agent for inhibiting PCa growth through multiple mechanisms, including the induction of apoptotic cell death and inhibition of Glo-1 expression. Combining CA with MG enhances its anticancer effects, offering a promising strategy for targeting glyoxalase oncogenic pathways in PCa.

Accession Number: WOS:001388993500001

PubMed ID: 39748483

Language: English

Document Type: Article

Author Keywords: caffeic acid; glyoxalase-1; methylglyoxal

KeyWords Plus: BREAST-CANCER; MECHANISM; CELLS; PROLIFERATION; APOPTOSIS; ELICITS

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Web of Science Index: Science Citation Index Expanded (SCI-EXPANDED)

Web of Science Categories: Endocrinology & Metabolism; Urology & Nephrology

Research Areas: Endocrinology & Metabolism; Urology & Nephrology

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Source Item Page Count: 8

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Output Date: 2025-03-04

Record 7 of 59

Title: Groundwater Quality and Its Suitability in the Semi-Arid River Basin in India: An Analysis of Hydrogeochemical Processes Using Multivariate Statistics

Author(s): Yadav, P (Yadav, Pooja); Sreekesh, S (Sreekesh, S.); Nandimandalam, JR (Nandimandalam, Janardhana Raju)

Source: ENVIRONMENTAL MODELING & ASSESSMENT **DOI:** 10.1007/s10666-024-10017-7 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 27

Abstract: A groundwater quality assessment has been conducted to determine the suitability of the groundwater for various purposes. In June 2021, groundwater samples were obtained from 65 locations in the Mendha river basin, Rajasthan, India, and then analysed for a range of chemical parameters. About 30% and 43% of the samples exhibit higher TDS and fluoride values than the permissible limits. Approximately 83% of the samples had very hard water, with a total hardness (TH) above 300 mg/l. The trend of major cations is in the order of Na+ > Mg2+ > Ca2+ > K+, and major anions are in the order of Cl- > HCO3- > F- > NO3- > SO42-. The analysis of ionic ratio plots reveals that silicate weathering is the predominant geochemical activity in the study area. Statistical analysis shows that both natural and anthropogenic activities contributed to ionic enrichment in the groundwater. According to the water quality index, most of the study area has good to poor quality for drinking purposes. In the irrigation indices, the sodium absorption ratio (SAR) is mostly suitable, but sodium percentage (SP) suggests that over one-third of the samples pose sodium-related risks to soil health. Kelly's index (KI) reveals that most of the samples are classified as suitable. Permeability index (PI) and magnesium hazard (MH) indicate that a significant percentage of water samples categorized as unsuitable for irrigation could degrade soil permeability and structure in the long term. The basin exhibits a high salinity and low to very high alkali hazards. One-third of the basin's groundwater is classified as unfit for drinking and irrigation, emphasizing the necessity of regular monitoring and effective management strategies to mitigate hydrogeochemical contamination.

Accession Number: WOS:001406586900001

Language: English

Document Type: Article; Early Access

Author Keywords: Drinking and irrigation suitability; Groundwater quality indices; Hydrogeochemistry; Rock-water interaction; Spatial modelling; Statistical analysis

KeyWords Plus: HUMAN HEALTH-RISK; DRINKING-WATER QUALITY; PRATAPGARH DISTRICT; INDEX; GEOCHEMISTRY; PURPOSES; FLUORIDE; CONTAMINATION; IRRIGATION; MECHANISMS

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Web of Science Categories: Environmental Sciences
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ISO Source Abbrev.: Environ. Model. Assess.
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Record 8 of 59

Title: Analyzing the functions of Translationally controlled tumor protein2 during growth, development and autophagy of Dictyostelium discoideum

Author(s): Choudhary, C (Choudhary, Chanchal); Jain, B (Jain, Bhavya); Saran, S (Saran, Shweta)

Source: EXPERIMENTAL CELL RESEARCH **Volume:** 445 **Issue:** 1 **Article Number:** 114400 **DOI:** 10.1016/j.yexcr.2024.114400 **Early Access Date:** JAN 2025 **Published Date:** 2025 FEB 1
Times Cited in Web of Science Core Collection: 0
Total Times Cited: 0
Usage Count (Last 180 days): 0
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Cited Reference Count: 30

Abstract: Translationally controlled tumor protein (TCTP) is a well conserved and ubiquitously expressed multifunctional protein found in many organisms and is involved in many pathophysiological processes like cell proliferation, differentiation, development and cell death. The role of TCTP in anti-apoptosis and cancer metastasis makes it a promising candidate for cancer therapy. Dictyostelium discoideum, a protist, has two isoforms (TCTP1 and TCTP2, now referred to as TPT1 and TPT2) of which we have earlier elucidated TPT1. Here, we analyzed the role of TPT2 in this organism. tpt2 transcript was present throughout growth and development and is localized in the prestalk/ stalk regions of multicellular structures developed. tpt2 gene was disrupted with a BSR cassette using a double homologous recombination method. Disruption of tpt2 gene (tpt2-) exhibit reduced cell proliferation and nutrient-uptake. Additionally, development in tpt2- was delayed by 2 h, formed small-sized aggregates that developed into stalky fruiting bodies with reduced spore viability. In contrast, overexpressed tpt2 (tpt2OE) showed increased cell proliferation and development, formed large-size aggregates that developed into spory fruiting bodies with increased spore viability. TPT2 regulates prestalk/prespore ratio and cell-type differentiation as abrogation of tpt2 gene resulted in altered localization of cell-type markers and an inclination towards the prestalk/stalk pathway while tpt2OE showed a prespore/spore biasness when mixed with wild-type cells. Deletion of either tpt1 or tpt2 gene showed increased autophagic flux indicating their involvement in negative regulation of autophagy. This study provides insights into the intricate involvement of TCTP in cellular dynamics and development of D. discoideum.

Accession Number: WOS:001411360900001

PubMed ID: 39753197

Language: English

Document Type: Article

Author Keywords: Dictyostelium; TCTP; Cell differentiation; Cell-type patterning; Autophagy; Cell proliferation

KeyWords Plus: TCTP; EXPRESSION; REVERSION; REVEALS; CELLS

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IDS Number: U4F0L

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Record 9 of 59

Title: Efficient synthesis of coumarin based triazole linked O-glycoconjugates as new bio-active glycohybrids

Author(s): Sharma, S (Sharma, Sunil); Sagar, R (Sagar, Ram)

Source: CARBOHYDRATE RESEARCH **Volume:** 550 **Article Number:** 109395 **DOI:** 10.1016/j.carres.2025.109395 **Early Access Date:** JAN 2025 **Published Date:** 2025 APR

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

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Usage Count (Since 2013): 0

Cited Reference Count: 39

Abstract: Glycohybrids are biologically significant molecules with variety of biological functions and are found as structural motifs in numerous natural products. Here, we report the synthesis of various new coumarin-based O-glycoconjugates as glycohybrids that are chirally enriched and bridged by 1,2,3-triazoles ring system. The1,2,3-triazoles bridging was done via CuAAC click-chemistry. Click chemistry offers several advantages, including high chemo- and regioselectivity, mild reaction conditions, easy purification, and compatibility with multiple functional groups. Two series of O-glycoconjugates as new glycohybrids were designed and efficiently synthesized in very good isolated yields, using D-glucose, D-galactose, D-mannose, D-arabinose, 3,4,6-tri-O-acetyl-D-glucal, 3,4,6-tri-O-acetyl-D-galactal and 3,4-di-O- acetyl-D-arabinal derived 1-O-propargylated glycosides, reacting with various 4-azidocoumarins under click-chemistry reaction conditions. The prepared new coumarin-based O-glycoconjugates as glycohybrids were found to possess anticancer activity against MCF-7 breast cancer cell lines at micromolar concentration.

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PubMed ID: 39864121

Language: English

Document Type: Article

KeyWords Plus: BIOLOGICAL-ACTIVITY; CLICK CHEMISTRY; BIOISOSTERISM; DERIVATIVES; INHIBITORS; GLYCOSIDES; ANALOGS; CANCER

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Output Date: 2025-03-04

Record 10 of 59

Title: Glycals as Chiral Synthons in Organic Synthesis of Privileged Molecular Scaffolds

Author(s): Yadav, Y (Yadav, Yogesh); Sagar, R (Sagar, Ram)

Source: CHEMISTRY-AN ASIAN JOURNAL **DOI:** 10.1002/asia.202401773 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 23
Times Cited in Web of Science Core Collection: 0
Total Times Cited: 0
Usage Count (Last 180 days): 2
Usage Count (Since 2013): 2
Cited Reference Count: 114

Abstract: Chirality is a vital characteristic of molecules and crucial for biological functioning. Glycals are unsaturated chiral sugars that contain an enolic double bond within the ring structure and they introduce the chirality in the molecular scaffolds. Since their discovery and synthesis by Fischer and Zach in 1913, they have been used as a flexible chiral synthon for synthesising natural products and biologically significant molecules. An important area of study in organic synthesis involves functionalizing glycals, with particular emphasis on creating novel molecular scaffolds with a common backbone using various topologies. This review discusses recent advancements in synthesizing chiral molecules, emphasizing the innovative use of glycals as chiral synthons, and covers literature from 2020 to the present.

Accession Number: WOS:001402664700001
PubMed ID: 39745137
Language: English
Document Type: Review; Early Access

Author Keywords: Glycals; Chiral synthons; Carbohydrate; 2,3-dideoxy unsaturated sugars; Ferrier rearrangment; Organic synthesis

KeyWords Plus: STEREOSELECTIVE-SYNTHESIS; C-GLYCOSIDES; COMPREHENSIVE STRATEGIES; GLYCOSYLATION; REARRANGEMENT; EVOLUTION

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Publisher: WILEY-V C H VERLAG GMBH

Publisher Address: POSTFACH 101161, 69451 WEINHEIM, GERMANY

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Record 11 of 59

Title: Gene expression profiling to uncover prognostic and therapeutic targets in colon cancer, combined with docking and dynamics studies to discover potent anticancer inhibitor

Author(s): Kashif, M (Kashif, Mohammad)

Source: COMPUTATIONAL BIOLOGY AND CHEMISTRY **Volume:** 115 **Article Number:** 108349 **DOI:** 10.1016/j.compbiolchem.2025.108349 **Early Access Date:** JAN 2025 **Published Date:** 2025 APR

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 3

Usage Count (Since 2013): 3

Cited Reference Count: 73

Abstract: Drug resistance poses a major obstacle to the efficient treatment of colorectal cancer (CRC), which is one of the cancers that kill people most often in the United States. Advanced colorectal cancer patients frequently pass away from the illness, even with advancements in chemotherapy and targeted therapies. Developing new biomarkers and therapeutic targets is essential to enhancing prognosis and therapy effectiveness. My goal in this study was to use bioinformatics analysis of microarray data to find possible biomarkers and treatment targets for colorectal cancer. Using an ArrayExpress database, I examined a dataset on colon cancer to find genes that were differentially expressed (DEGs) in tumor versus healthy tissues. Integration of advanced bioinformatics tools provided robust insights into the identification and analysis of EGFR as a key player. STRING and Cytoscape enabled the construction and visualization of protein-protein interaction networks, highlighting EGFR as a hub gene due to its centrality and interaction profile. Functional enrichment analysis through DAVID revealed EGFR's involvement in critical biological pathways, as identified in GO and KEGG analyses. This underscores the power of combining computational tools to uncover significant biomarkers like EGFR. Autodock Vina screening of the NCI diversity dataset identified two potential EGFR inhibitors, ZINC13597410 and ZINC04896472. MD simulation data revealed that ZINC04896472 could be potential anticancer inhibitor. These findings serve as a basis for the creation of novel therapeutic approaches that target EGFR and other discovered pathways in CRC. The suggested strategy may improve the efficacy of CRC therapy and advance personalized medicine.

Accession Number: WOS:001401804600001

PubMed ID: 39813876

Language: English

Document Type: Article

Author Keywords: Colon cancer; ArrayExpress; EGFR; Hub genes; Differentially expressed genes; Autodock vina; MD simulation

KeyWords Plus: DRUG-RESISTANCE; MECHANISMS; IDENTIFICATION; STRATEGIES; MODELS

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Research Areas: Life Sciences & Biomedicine - Other Topics; Computer Science

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Output Date: 2025-03-04

Record 12 of 59

Title: WRGAT-PTBERT: weighted relational graph attention network over post-trained BERT for aspect based sentiment analysis

Author(s): Verma, S (Verma, Sharad); Kumar, A (Kumar, Ashish); Sharan, A (Sharan, Aditi)

Source: APPLIED INTELLIGENCE **Volume:** 55 **Issue:** 2 **Article Number:** 181 **DOI:** 10.1007/s10489-024-06011-x **Published Date:** 2025 JAN

Times Cited in Web of Science Core Collection: 1

Total Times Cited: 1

Usage Count (Last 180 days): 5

Usage Count (Since 2013): 5

Cited Reference Count: 43

Abstract: Aspect-based sentiment analysis (ABSA) focused on forecasting the sentiment orientation of a given aspect target within the input. Existing methods employ neural networks and attention mechanisms to encode input and discern aspect-context relationships. Bidirectional Encoder Representation from Transformer(BERT) has become the standard contextual encoding method in the textual domain. Researchers have ventured into utilizing graph attention networks(GAT) to incorporate syntactic information into the task, yielding cutting-edge results. However, current approaches overlook the potential advantages of considering word dependency relations. This work proposes a hybrid model combining contextual information obtained from a post-trained BERT with syntactic information from a relational GAT (RGAT) for the ABSA task. Our approach leverages dependency relation information effectively to improve ABSA performance in terms of accuracy and F1-score, as demonstrated through experiments on SemEval-14 Restaurant and Laptop, MAMS, and ACL-14 Twitter datasets.

Accession Number: WOS:001379761300003

Language: English

Document Type: Article

Author Keywords: Aspect-based sentiment analysis; Graph neural networks; Post-trained BERT; Attention

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Web of Science Categories: Computer Science, Artificial Intelligence

Research Areas: Computer Science

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Source Item Page Count: 11

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Record 13 of 59

Title: Physics-Based Machine Learning to Predict Hydration Free Energies for Small Molecules with a Minimal Number of Descriptors: Interpretable and Accurate

Author(s): Yadav, AK (Yadav, Ajeet Kumar); Prakash, MV (Prakash, Marvin V.); Bandyopadhyay, P (Bandyopadhyay, Pradipta)

Source: JOURNAL OF PHYSICAL CHEMISTRY B **Volume:** 129 **Issue:** 5 **Pages:** 1640-1647 **DOI:** 10.1021/acs.jpcb.4c07090 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 22

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 0

Usage Count (Since 2013): 0

Cited Reference Count: 50

Abstract: Hydration free energy (HFE) of molecules is a fundamental property having importance throughout chemistry and biology. Calculation of the HFE can be challenging and expensive with classical molecular dynamics simulation-based approaches. Machine learning (ML) models are increasingly being used to predict HFE. Although the accuracy of ML models for data sets for small molecules is impressive, these models suffer from lack of interpretability. In this work, we have developed a physics-based ML model with only six descriptors, which is both accurate and fully interpretable, and applied it to a database for small molecule HFE, FreeSolv. We evaluated the electrostatic energy by an approximate closed form of the Generalized Born (GB) model and polar surface area. In addition, we have log P and hydrogen bond acceptor and donors as descriptors along with the number of rotatable bonds. We have used different ML models, such as random forest and extreme gradient boosting. The best result from these models has a mean absolute error of only 0.74 kcal/mol. The main power of this model is that the descriptors have clear physical meaning, and it was found that the descriptor describing the electrostatics and the polar surface area, followed by the hydrogen bond donors and acceptors, are the most important factors for the calculation of hydration free energy.

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PubMed ID: 39841935

Language: English

Document Type: Article

KeyWords Plus: SOLVATION FREE-ENERGIES; EFFICIENT GENERATION; AM1-BCC MODEL; SOLVENT; EXPLICIT

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Publisher: AMER CHEMICAL SOC

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DST	

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Output Date: 2025-03-04

Record 14 of 59

Title: Polyoxometalate-naphthalenediimide supramolecular hybrid materials

Author(s): Mishra, NK (Mishra, Neeraj Kumar); Supriya, S (Supriya, Sabbani)

Source: JOURNAL OF MOLECULAR STRUCTURE **Volume:** 1329 **Article Number:** 141386 **DOI:** 10.1016/j.molstruc.2025.141386 **Early Access Date:** JAN 2025 **Published Date:** 2025 MAY 5

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 2

Usage Count (Since 2013): 2

Cited Reference Count: 56

Abstract: We report the synthesis and characterization of three organic-inorganic hybrid compounds [C18H9N8O4]2[HPW12O40]center dot 6(CH3)2NOH (1), [C24H14N4O4][HPMo12O40]center dot 2(CH3)2NH center dot 4C3H7NO (2) and [C24H14N4O4][H2PMoVMoVI11O40]center dot 2(CH3)2NH center dot 4C3H7NO (3) consisting of Keggin polyoxoanion and protonated naphthalenediimide (NDI) cation. Compounds 1, 2 , and 3 are prepared by protonation of NDI molecules using H2SO4 acid. The single crystals of compounds 1 and 2 are obtained by ether diffusion into respective dimethylformamide (DMF) reaction mixtures. Interestingly, compound 2 exhibits reversible photochromism on irradiation with sunlight. The pale green color single crystals of compound 2 on irradiation with sunlight are converted to blue color compound 3 . The blue color crystals of compound 3 are transformed back to green color on standing in dark at room temperature. The dark blue color of compound 3 results due to reduction of Keggin anion. The compounds 1, 2 and 3 are characterized by various spectroscopic techniques and unambiguously by single crystal X-ray diffraction studies. In compounds 1, 2 and 3 , the naphthalenediimide cation and polyoxometalate (POM) anion are held together by electrostatic interactions resulting in supramolecular networks in the respective crystal structures.

Accession Number: WOS:001405853200001

Language: English

Document Type: Article

Author Keywords: Polyoxometalates; Naphthalenediimide; Photochromism; Supramolecular interactions; Emission studies

KeyWords Plus: CHARGE-TRANSFER; ELECTRON-TRANSFER; FRAMEWORKS; DESIGN; DRUG

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Output Date: 2025-03-04

Record 15 of 59

Title: Large electrocaloric effect in BiScO₃ doped K_{0.5}Na_{0.5} NbO₃ ceramics

Author(s): Lodhi, IA (Lodhi, Ishtiaq Ahmed); Kumar, R (Kumar, Raju); Tyagi, UP (Tyagi, Udai Prakash); Singh, S (Singh, Satyendra)

Source: JOURNAL OF MATERIALS SCIENCE-MATERIALS IN ELECTRONICS **Volume:** 36 **Issue:** 1 **Article Number:** 14 **DOI:** 10.1007/s10854-024-14049-3 **Published Date:** 2025 JAN

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 5

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Cited Reference Count: 48

Abstract: Exploring an electrocaloric (EC) material with a large electrocaloric effect (ECE) value is of high interest and importance to realize a solid-state cooling solution. We have investigated the electrocaloric performance and energy storage density in lead-free (1-x) K0.5Na0.5NbO3-xBiScO(3) (KNN-xBS) ferroelectric ceramics. The KNN-xBS (x = 0.01, 0.02, 0.03, and 0.10) ceramics were synthesized by the typical solid-state route and ECE was examined by an indirect method based on Maxwell's relations. The maximum value of ECE has obtained 0.61 K at 428 K for 60 kV/cm applied field, and the recoverable energy density has 0.57 J/cm(3) for x = 0.01 ceramics. The obtained positive ECE has a larger value among different lead-free ceramics. The BiScO3 doped K0.5Na0.5NbO3 ceramics have presented enormous potential in solid-state cooling technology for a cleaner environment.

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Language: English

Document Type: Article

KeyWords Plus: COEXISTENCE

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Research Areas: Engineering; Materials Science; Physics

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Record 16 of 59

Title: Colossal enhancement in ionic conductivity of La2Mo2O9 thin films: Role of lattice strain and oxygen vacancy

Author(s): Patel, A (Patel, Avinash); Patel, RK (Patel, Roshan Kumar); Rahman, AGA (Rahman, A. G. A.); Pramanik, AK (Pramanik, A. K.); Singh, S (Singh, Satyendra); Nath, C (Nath, Chandrani)

Source: JOURNAL OF PHYSICS AND CHEMISTRY OF SOLIDS **Volume:** 199 **Article Number:** 112550 **DOI:** 10.1016/j.jpcs.2025.112550 **Early Access Date:** JAN 2025 **Published Date:** 2025 APR

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 0

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Cited Reference Count: 56

Abstract: Search for high oxygen-ion conducting electrolyte forms a crucial step towards lowering the operating temperature of conventional solid oxide fuel cell. Here, we report an investigation of conductivity in polycrystalline films of Er and W codoped La1.8Er0.2W0.3Mo1.7O9 (WEr0.2), deposited on four different substrates Si(111), SrTiO3(100), LaAlO3(100) and MgO(100) with different growth orientation and lattice parameters. While all the films show an increase of conductivity by several orders compared to its bulk counterpart, a magnificent increase of about six orders (13 S/cm @ 375 degrees C) has been observed in films on Si substrate. Films with SrTiO3 and LaAlO3 substrate further show steep rise in conductivity around 450 degrees C, mimicking the undoped bulk La2Mo2O9 which is triggered by

structural phase transition. This large modification of conductivity is believed to be induced by interfacial strain and consequent oxygen vacancy that increases from MgO to Si substrate due to their difference in lattice parameters and growth orientation. The oxygen vacancy concentration calculated using Nernst-Einstein analysis of frequency dependent impedance data further supports an increasing oxygen vacancies in film on Si substrate. The present results show an effective way of tuning conductivity through substrate strain which would hopefully have considerable effect on much sought low temperature operation of fuel cell.

Accession Number: WOS:001398131300001

Language: English

Document Type: Article

Author Keywords: Solid oxide fuel cell; Ionic conductivity; Thin film; Interfacial strain; Oxides

KeyWords Plus: ELECTRICAL-PROPERTIES; TRANSPORT-PROPERTIES; ACTIVATION-ENERGY; OXIDE; ELECTROLYTES; SUPERLATTICES; RELAXATION; GROWTH; DEFECT; CEO2

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Record 17 of 59

Title: Intergenerational transitions in age at menarche: insights from Chandauli district, Uttar Pradesh, India

Author(s): Sumedha (Sumedha); Singh, S (Singh, Suman); Pathak, PK (Pathak, Praveen Kumar)

Source: BMC WOMENS HEALTH **Volume:** 25 **Issue:** 1 **Article Number:** 9 **DOI:** 10.1186/s12905-024-03462-9 **Published Date:** 2025 JAN 7

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 0

Usage Count (Since 2013): 0

Cited Reference Count: 55

Abstract: Background Menarche, a milestone in a woman's reproductive journey, is influenced by various factors such as lifestyle and dietary habits. Recent studies have corroborated this claim and prompted further investigation. This study explores the connection between menarche timing with lifestyle and dietary habits among three generations of women from the Sakaldiha block of Chandauli district and presents valuable insights into the role of diet and lifestyle in this crucial reproductive event. Methods The study is based on primary data collected using multistage stratified random sampling. A comparative analysis of the mean age at menarche across independent variables has been conducted using the one-way analysis of variance (ANOVA) technique. Additionally, a multiple regression model has been developed to investigate the association between menarcheal age and various dietary, lifestyle and socio-economic factors among 400 respondents. Results The average age of menarche for respondents was 14.29 years (95% CI: 14.12, 14.45), which has decreased by 1.66 years from 14.89 years (95% CI: 14.63, 15.15) in women over 40 years of age to 13.23 years (95% CI: 12.97, 13.49) in the < 20 years age group. The study additionally found that dietary and lifestyle factors had an impact on the age of menarche, with those who regularly consumed junk food, occasionally ate meat/fish or eggs, completely avoided curd or buttermilk and engaged in non-resting leisure activities experiencing an earlier onset of menarche. Conclusion The study shows that diet and lifestyle affect age at menarche, with current generations experiencing an earlier onset of menstruation. The effect of socioeconomic status remains inconclusive.

Accession Number: WOS:001392931300003

PubMed ID: 39773444

Language: English

Document Type: Article

Author Keywords: Menarche; Diet; Lifestyle; Age; Decline

KeyWords Plus: REPRODUCTIVE HEALTH; PUBERTY; WOMEN

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Record 18 of 59

Title: In-vitro assay studies and molecular docking of functionalized chitosan decorated vanadium pentoxide nano-agents as an antidiabetic drug

Author(s): Bansal, S (Bansal, Smriti); Tomer, A (Tomer, Archana); Singh, A (Singh, Anu); Tyagi, N (Tyagi, Nipanshi); Kushwaha, HR (Kushwaha, Hemant Ritturaj); Jain, P (Jain, Purnima)

Source: INTERNATIONAL JOURNAL OF BIOLOGICAL MACROMOLECULES **Volume:** 298 **Article Number:** 139986 **DOI:** 10.1016/j.ijbiomac.2025.139986 **Early Access Date:** JAN 2025 **Published Date:** 2025 APR

Times Cited in Web of Science Core Collection: 0

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Abstract: This study aims to enhance the antidiabetic potential of Vanadium pentoxide (V2O5) by synthesizing chitosanbased nanoparticles (NPs). Chitosan and its derivatives were used to fabricate V2O5 NPs, ensuring enhanced antioxidant and antidiabetic activity. Surface topography was analyzed using atomic force microscopy (AFM), revealing bioactive sites on the NPs with improved electron-transfer capability, as confirmed by cyclic voltammetry (CV). Furthermore, NPs were exploited for their possible antioxidant and antidiabetic potency by using different in-vitro assays. Among the fabricated NPs, chitosan-salicylaldehyde decorated V2O5 NPs (CHVD2) exhibited highest antidiabetic activity with 72.69 +/- 0.76 % inhibition against alpha-amylase, 69.15 +/- 0.58 % inhibition against alpha-glucosidase, and glycemic diffusion retardation index (GDRI) of 60.33 +/- 0.47 %. Importantly, CHVD2 did not inhibit the growth of Bifidobacterium bacteria, as shown by disc-diffusion assay and exhibit least cytotoxicity among all NPs as tested on HacaT cell line. Molecular docking studies revealed strong binding interactions between CHVD2 and the target enzymes, alpha-amylase, and alpha-glucosidase supporting its inhibitory potential. This work demonstrates the promising enhanced antidiabetic and antioxidant properties of chitosancoated V2O5 NPs.

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Document Type: Article

Author Keywords: Nano-V 2 O 5; Antidiabetic; Chitosan

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Record 19 of 59

Title: Elucidating the binding specificity of interactive compounds targeting ATP-binding cassette subfamily G member 2 (ABCG2)

Author(s): Kumar, P (Kumar, Pawan); Kumari, I (Kumari, Indu); Prasad, R (Prasad, Rajendra); Ray, S (Ray, Shashikant); Banerjee, A (Banerjee, Atanu); Prakash, A (Prakash, Amresh)

Source: MOLECULAR DIVERSITY **DOI:** 10.1007/s11030-024-11078-2 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 9

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Cited Reference Count: 49

Abstract: The ATP-binding cassette transporter superfamily plays a pivotal role in cellular detoxification and drug efflux. ATP-binding cassette subfamily G member 2 (ABCG2) referred to as the Breast cancer resistance protein has emerged as a key member involved in multidrug resistance displayed by cancer cells. Understanding the molecular basis of substrate and inhibitor recognition, and binding within the transmembrane domain of ABCG2 is crucial for the development of effective therapeutic strategies. Herein, utilizing state-of-the-art molecular docking algorithms and molecular dynamic (MD) simulations, molecular binding of substrates and inhibitors with ABCG2 are defined, distinctly. We performed extensive virtual screening of Drugbank to identify the potential candidates, and MD simulations of docked complexes were carried out in POPC lipid bilayer. Further, the binding affinities of compounds were estimated by free binding energy employing MM-GBSA. To gain deeper insight into the binding affinities and molecular characteristics contributing to inhibitory potential of certain substrates, we included some well-known inhibitors, like Imatinib, Tariquidar, and Ko 143, in our analysis. Docking results show three compounds, Docetaxel > Tariquidar > Tezacaftor having the highest binding affinities (<= 12.00 kcal/mol) for ABCG2. Remarkably, MM-GBSA results suggest the most stable binding of Tariquidar with ABCG2 as compared to the other inhibitors. Furthermore, our results suggested that Docetaxel, Ozanimod, Pitavastatin, and Tezacaftor have the strongest affinity for the drug-binding site(s) of ABCG2. These results provide valuable insights into the key residues that may govern substrate/inhibitor recognition, shedding light on the molecular determinants influencing substrate specificity, transport kinetics, and ABCG2-mediated drug efflux.
[GRAPHICS]

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PubMed ID: 39786520

Language: English

Document Type: Article; Early Access

Author Keywords: ABC transporter; Multidrug resistance; Molecular docking; MD simulations; Tariquidar; ABCG2/BCRP; Substrate; Inhibitor; POPC

KeyWords Plus: PROTEIN; RESISTANCE; INHIBITOR; TRANSPORTER; BCRP/ABCG2; IMATINIB

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Record 20 of 59

Title: Complex p53 dynamics regulated by miR-125b in cellular responses to reactive oxidative stress and DNA damage

Author(s): Malik, MZ (Malik, Md Zubbair); Dashti, M (Dashti, Mohammed); Jangid, A (Jangid, Amit); Channanath, A (Channanath, Arshad); John, SE (John, Sumi Elsa); Singh, RKB (Singh, R. K. Brojen); Al-Mulla, F (Al-Mulla, Fahd); Thanaraj, TA (Thanaraj, Thangavel Alphonse)

Source: BRIEFINGS IN BIOINFORMATICS **Volume:** 26 **Issue:** 1 **Article Number:** bbae706 **DOI:** 10.1093/bib/bbae706 **Published Date:** 2025 JAN 16

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Abstract: In response to distinct cellular stresses, the p53 exhibits distinct dynamics. These p53 dynamics subsequently control cell fate. However, different stresses can generate the same p53 dynamics with different cell fate outcomes, suggesting that the integration of dynamic information from other pathways is important for cell fate regulation. The interactions between miRNA-125b, p53, and reactive oxygen species (ROS) are significant in the context of cellular stress responses and apoptosis. However, the regulating mechanism of miR-125b with p53 is not fully studied. The dynamics of p53 and its response to the miR-125b regulation are still open questions. In the present study, we try to answer some of these fundamental questions based on basic model built from available experimental reports. The miR-125b-p53 regulatory network is modeled using a set of 11 molecular species variables. The biochemical network of miR-125b-p53, described by 22 reaction channels, is represented by coupled ordinary differential equations (ODEs) using the mass action law of chemical kinetics. These ODEs are solved numerically using the standard fourth-order Runge-Kutta method to analyze the dynamical behavior of the system. The biochemical network model we designed is based on both experimental and theoretical reported data. The p53 dynamics driven by miR-125b exhibit five distinct dynamical states: first and second stable states, first and second dynamical states, and a sustained oscillation state. These different p53 dynamical states may correspond to various cellular conditions. If the stress induced by miR-125b is weak, the system will be weakly activated, favoring a return to normal functioning. However, if the stress is significantly strong, the

system will move to an active state. To sustain this active state, which is far from equilibrium with little scope for returning to normal conditions, the system may transition to an apoptotic state by crossing through other intermediate states, as it is unlikely to regain normal functioning. The p53 dynamical states show a multifractal nature, contributed by both short- and long-range correlations. The networks illustrated from these dynamical states follow hierarchical scale-free features, exhibiting an assortative nature with an absence of the centrality-lethality rule. Furthermore, the active dynamical state is generally closer to hierarchical characteristics and is self-organized. Our research study reveals that significant activity of miR-125b on the p53 regulatory network and its dynamics can only be observed when the system is slightly activated by ROS. However, this process does not necessarily require the direct study of ROS activity. These findings elucidate the mechanisms by which cells integrate signaling pathways with distinct temporal activity patterns to encode stress specificity and direct diverse cell fate decisions.

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Author Keywords: cell stress responses; dynamics; miR-125b; p53; ROS; cellular state

KeyWords Plus: PANCREATIC BETA-CELLS; P53-MDM2 FEEDBACK LOOP; TUMOR-SUPPRESSOR; G(1) ARREST; APOPTOSIS; MDM2; METABOLISM; CANCER; ARF; ACTIVATION

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Record 21 of 59

Title: LDL2 and PAO5 genes are essential for systemic acquired resistance in Arabidopsis thaliana

Author(s): Saxena, S (Saxena, Shobhita); Roy, S (Roy, Shweta); Ahmad, MN (Ahmad, Mir Nasir); Nandi, AK (Nandi, Ashis Kumar)

Source: PHYSIOLOGIA PLANTARUM **Volume:** 177 **Issue:** 1 **Article Number:** e70102 **DOI:** 10.1111/ppl.70102 **Published Date:** 2025 JAN

Times Cited in Web of Science Core Collection: 0

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Usage Count (Last 180 days): 1

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Cited Reference Count: 57

Abstract: A partly infected plant becomes more resistant to subsequent infections by developing systemic acquired resistance (SAR). Primary infected tissues produce signals that travel to systemic tissues for SAR-associated priming of defense-related genes. The mechanism through which mobile signals contribute to long-lasting infection memory is mostly unknown. RSI1/FLD, a putative histone demethylase, is required for developing SAR. Here, we report that two other FLD homologs, LSD1-LIKE2 (LDL2) and POLYAMINE OXIDASE 5 (PAO5), are required for SAR development. The mutants of LDL2 and PAO5 are not defective in local resistance but are specifically impaired for SAR. The mutants are defective in salicylic acid accumulation and priming of defence-related genes such as PR1, FMO1, and SnRK2.8. LDL2 and PAO5 are expressed in systemic tissues upon SAR induction by pathogens or SAR mobile signal azelaic acid. The ldl2 and pao5 mutants generate SAR mobile signals like wild-type (WT) plants but fail to respond to the signal at the systemic leaves. Both LDL2 and PAO5 proteins contain polyamine oxidase (PAO) domains, suggesting their involvement in polyamine metabolism. Exogenous applications of polyamines such as spermine and spermidine activate SAR in WT and rescue SAR defects of ldl2 and pao5 plants. Inhibition of polyamine biosynthetic gene arginine decarboxylase blocks SAR development. Results altogether demonstrate specific non-redundant roles of LDL2 and PAO5 in SAR development with their possible involvement in polyamine metabolism.

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Document Type: Article

KeyWords Plus: FLOWERING-LOCUS-D; PATHOGEN DEFENSE; PIPECOLIC ACID; IMMUNITY; PROMOTE; PLANTS; DECARBOXYLASE; DEMETHYLATION; EXPRESSION; BACTERIAL

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Record 22 of 59

Title: A brief study of the effects of magnesium divalent ions on the Dickerson DNA sequence at varying molar concentrations

Author(s): Sharma, A (Sharma, Angad); Mishra, RK (Mishra, Rakesh Kumar)

Source: EUROPEAN PHYSICAL JOURNAL PLUS **Volume:** 140 **Issue:** 1 **Article Number:** 60 **DOI:** 10.1140/epjp/s13360-025-06000-0 **Published Date:** 2025 JAN 22
Times Cited in Web of Science Core Collection: 0
Total Times Cited: 0
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Cited Reference Count: 63

Abstract: The interaction of nucleic acids with metallic ions is crucial for DNA function. Mg2+ can bond directly or indirectly via water. We explored Mg2+ interaction with Dickerson DNA at varying Mg2+ concentrations with fixed NaCl concentration. Analysing the correlation function, we mapped Mg2+ density around DNA regions. We found that the Mg2+ interaction decreased with rising Mg2+ concentrations. Mg2+ also displayed a higher affinity for the Phosphate group over grooves. We explored the variation of stacking parameters by varying Mg2+ concentrations, indicating slight structural changes which have not been explored yet. Our study reflects that the Mg2+ concentrations had almost minimal impact on Dickerson-DNA structure, instead stabilizing it.

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Language: English
Document Type: Article

KeyWords Plus: MOLECULAR-DYNAMICS SIMULATIONS; BASE-STACKING; METAL-IONS; B-DNA; GROOVE BINDING; MG2+ IONS; ALGORITHM; NUCLEOTIDES; STABILITY; COMPLEXES

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Record 23 of 59

Title: Surface energy balance changes impact on hydrometeorological variables over Indus-Ganga-Brahmaputra

Author(s): Yadav, M (Yadav, Mohit); Sharma, A (Sharma, Aka); Maharana, P (Maharana, P.); Mal, S (Mal, S.); Dimri, AP (Dimri, A. P.)

Source: THEORETICAL AND APPLIED CLIMATOLOGY **Volume:** 156 **Issue:** 1 **Article Number:** 11 **DOI:** 10.1007/s00704-024-05241-w **Published Date:** 2025 JAN

Times Cited in Web of Science Core Collection: 0

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Usage Count (Last 180 days): 2

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Abstract: Over the past decades, the estimation of changes in climate and energy mass balance of Earth's surface has become crucial. The Himalayas, in the South Asian region, are highly vulnerable to precipitation and hydrological/hydrometeorological balance/change. It will significantly affect freshwater availability and the associated sectors of these habitats. The understanding of these changes in hydrological balance for water resource management; identifying the water-sensitive areas; etc. over three major Himalayan river basins, Indus-Ganga-Brahmaputra (IGB), are considered. The geomorphological features, seasonal variability, topographic and geographical differences, landuse/landcover heterogeneity, etc. are distinctly different among them. These in conjugate interaction with above atmosphere induce different feedback mechanisms and processes. Precipitation, turbulent fluxes, evaporation, potential evaporation etc., are considered to assess surface energy balance and different thermodynamical processes. Nonparametric Mann-Kendall method for trend analysis, while the Pettit test for change point detection is employed over data period of 1950-2020. Based on the change point year 1981, the difference in mean precipitation between the periods 1982-2020 and 1950-1981 shows a decreased during monsoon and post-monsoon over GRB and BRB. Interestingly, the change years of potential evaporation and evaporation are highly correlated with monsoon in BRB while the same is weak for GRB. It shows the impact of land use type of the two basins where BRB has more forest cover than of GRB. A lead-lag relationship between the Bowen ratio and different hydrometeorology variables is seen. Present results on changes are important and will be useful for planning and policy for societal benefit viz., better water resource management, potential impacts due to climate change, etc. This study helps policymakers in better understanding of the changing precipitation pattern which will help in formulation of new policies for agriculture and sustainable use of water resources.

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Language: English

Document Type: Article

Author Keywords: Bowen ratio; Change point; Turbulent fluxes; Energy balance; IGB

KeyWords Plus: CLIMATE-CHANGE; SUMMER MONSOON; RIVER-BASINS; RAINFALL; TRENDS; BUDGET; RATIO; HYDROLOGY; HIMALAYA; EVAPOTRANSPIRATION

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Record 24 of 59

Title: Anti-furfurative comparison of Kesh Kanti-Herbal Shampoos and synthetic shampoos against Malassezia furfur for dandruff management

Author(s): Balkrishna, A (Balkrishna, Acharya); Ngpoore, NK (Ngpoore, Nem Kumar); Jonwal, H (Jonwal, Harshita); Lochab, S (Lochab, Savita); Varshney, A (Varshney, Anurag)

Source: AMB EXPRESS **Volume:** 15 **Issue:** 1 **Article Number:** 8 **DOI:** 10.1186/s13568-024-01818-w **Published Date:** 2025 JAN 13

Times Cited in Web of Science Core Collection: 0

Total Times Cited: 0

Usage Count (Last 180 days): 0

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Cited Reference Count: 28

Abstract: Malassezia furfur is the primary etiological agent of dandruff (Pityriasis capitis). Although herbal shampoos are preferred for their natural, mild ingredients over synthetic counterparts, they are often perceived as less effective in managing flaky scalp conditions or furfuration causing dandruff. The study compares the antifungal efficacy of herbal and synthetic shampoos against M. furfur. Seven shampoos including herbal (HS_Adv, HS_M&P, HS_Aloe), synthetic (SYN_01, SYN_02, SYN_03) and an antifungal shampoo containing ketoconazole (KETO) were employed in the study. Experiments were designed to stimulate real-world conditions, utilizing disc-diffusion assay, 3-minute shampoo contact at mild dilutions (1% and 5%), recurrent 3-minute shampoo contact every 24 h with intermittent recovery. Both disc diffusion and 3-minute shampoo contact demonstrated that all shampoos were effectively inhibiting the viability of M. furfur. However, a single 3-minute shampoo contact followed by a prolonged recovery of 72 h revealed SYN_01 and KETO with maximal antifungal action. In contrast, herbal shampoos were as effective as synthetic options when M. furfur was subjected to 3-minute shampoo contact every 24 h with intermittent recovery. Comprehensive ingredient analysis revealed the robust antifungal activity in SYN_01 was probably because of the presence of various surfactants, allergens and a potent synthetic antifungal agent, Piroctone olamine. This study experimentally demonstrates that herbal shampoos are as effective as synthetic options in managing M. furfur-induced dandruff when applied consistently. The findings highlight the importance of regular scalp cleansing for dandruff management and provide valuable insights into the antifungal potential of both herbal and synthetic formulations.

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Language: English

Document Type: Article

KeyWords Plus: PACHYDERMATIS; SULFATE

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Record 25 of 59

Title: Magneto-transport properties of NiCoCrFePd high entropy alloy films

Author(s): Hussain, A (Hussain, Abid); Khan, SA (Khan, S. A.); Kumari, A (Kumari, Anju); Meena, RC (Meena, R. C.); Kedia, SK (Kedia, Sanjay K.); Khandelwal, D (Khandelwal, Deeksha); Kulriya, PK (Kulriya, P. K.)

Source: MATERIALS TODAY PHYSICS **Volume:** 51 **Article Number:** 101644 **DOI:** 10.1016/j.mtphys.2024.101644 **Early Access Date:** JAN 2025 **Published Date:** 2025 FEB

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Abstract: This study aims to develop for the first time thin films of NiCoCrFePd high entropy alloy (HEA) to investigate the structural, magnetic, and transport properties for potential room temperature spin gapless semiconducting (SGS) applications. The as grown films were subjected to different annealing temperatures ranging from 400 degrees C to 600 degrees C to investigate the role of thermal generation of charge carriers and its effect on the (SGS) properties. The temperature dependent X-ray diffraction unveils structural stability down to 30 K with no phase transformations, however improvement in the crystallinity was observed with the increase in the annealing temperature. Rutherford backscattering spectroscopy shows depth dependent uniformity in the elemental distribution. Additionally, the magneto-transport studies revealed ferromagnetic behavior with a magnetic saturation values ranging from 165 emu/cm3 to 375 emu/cm3 and the Curie temperatures in the range of 263 K to 507 K. Further, the resistivity measurements confirmed a semiconducting behavior, with negative magnetoresistance corresponding to all the annealed samples. A two-channel conduction mechanism is used to explain the transport behaviour with one gapless and another gapped channel with activation energies ranging from 216.47 f 3.63 meV to 86.85 f 0.93 meV for different annealed samples. The observation of small anomalous Hall conductivity ranging from 25.2 Scm-1 to 66.7 Scm-1 and vanishing thermoelectric power lying in the range 3.11 mu V/K to 4.11 mu V/K confirms the SGS behavior with hole-dominant charge carriers. Thus, evidently the annealing temperature can be used to tune the spin transport properties by altering energy band gaps and density of states near the Fermi energy (epsilon F).

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Language: English

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Author Keywords: High entropy alloy; e -beam evaporation; Thin film; Structural stability; Transport properties; Spin gapless semiconductors

KeyWords Plus: MAGNETIC-ANISOTROPY; TRANSPORT

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Record 26 of 59

Title: Novel Dipeptide Inhibitors of PfPNP: In-Silico Identification of Promising New Antimalarials

Author(s): Devi, K (Devi, Kanika); Chandra, A (Chandra, Anshuman); Chaudhuri, S (Chaudhuri, Susmita); Goel, VK (Goel, Vijay Kumar)

Source: CHEMISTRY & BIODIVERSITY **Volume:** 22 **Issue:** 1 **Article Number:** e202401668 **DOI:** 10.1002/cbdv.202401668 **Published Date:** 2025 JAN

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Abstract: Malaria, an infectious disease caused by Plasmodium falciparum, is becoming increasingly difficult to treat due to the emergence of drug-resistant strains. Recent studies have proposed purine nucleoside phosphorylase from P. falciparum (PfPNP) as a potential target for malaria treatment. In the present study, we designed a virtual library of 400 dipeptides to discover novel anti-malarial peptide inhibitors. A structure-based molecular docking method was employed to virtually screen the designed library against the wild-type structure of PfPNP (PDB: 5ZNC). The best four (Phe-Arg, Arg-His, Trp-Arg and Tyr-Arg) dipeptides, which were then investigated for their binding potential against PfPNP using Molecular Dynamics simulation studies. Parameters such as RMSD, RMSF, Rg, and SASA were analyzed to understand the structural changes, energetics, and overall behavior of PfPNP-dipeptide complexes. The PfPNP demonstrated significant stability upon binding with each of the identified dipeptides with Delta G of over -168kcal/mol. Additionally, DFT and ADME predictions indicated that the electronic structure, energetics, and pharmacokinetic properties of Phe-Arg, Arg-His, Trp-Arg and Tyr-Arg were favourable for drug development. Our comprehensive computational investigation has identified these four dipeptides as promising candidates. These designed and selected dipeptides may further be modified using peptidomimetic and medicinal chemistry tools to develop a novel class of promising antimalarials.

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Record 27 of 59

Title: Analysis of the interaction of influenza a virus nucleoprotein with host cell nucleolin

Author(s): Mishra, S (Mishra, Shruti); Pandey, A (Pandey, Achyut); Verma, J (Verma, Jyoti); Rajala, MS (Rajala, Maitreyi S.)

Source: ARCHIVES OF VIROLOGY **Volume:** 170 **Issue:** 1 **Article Number:** 1 **DOI:** 10.1007/s00705-024-06189-y **Published Date:** 2025 JAN

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Abstract: Targeting interactions between a virus and a host protein is one of the important approaches to developing antiviral therapies. We previously identified host nucleolin as a novel interacting partner of the influenza A virus nucleoprotein, and it was demonstrated that this interaction restricts virus replication. In the current study, we examined the interaction of nucleolin with the viral nucleoprotein at the domain and amino acid levels using in vitro and in silico approaches. Both approaches demonstrated a direct and specific interaction between these two proteins. Furthermore, it was observed that previous pandemic strains of influenza A virus had specific amino acid residues in their nucleoproteins that were predicted to be critical for interaction with nucleolin. This preliminary analysis provides insights into the binding process, which could be explored for developing antiviral strategies.

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Author Keywords: Nucleoprotein; Nucleolin; Molecular docking; Protein domains; Amino acid residues; Pandemic strains

KeyWords Plus: SEQUENCE; BINDING; PROTEIN

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Record 28 of 59

Title: Anti-ulcerogenic activity of the marine-pearl derived medicine mukta Pishti in Rat model of pylorus ligation-induced peptic ulcer

Author(s): Balkrishna, A (Balkrishna, Acharya); Sinha, S (Sinha, Sandeep); Shukla, S (Shukla, Sunil); Bhattacharya, K (Bhattacharya, Kunal); Varshney, A (Varshney, Anurag)

Source: JOURNAL OF ETHNOPHARMACOLOGY **Volume:** 342 **Article Number:** 119378 **DOI:** 10.1016/j.jep.2025.119378 **Early Access Date:** JAN 2025 **Published Date:** 2025 FEB 27

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Abstract: Ethnopharmacological relevance: Mukta Pishti (MKP) is a traditional Ayurvedic medicine described in classical textbook 'Rasatarangini' and synthesized from marine pearls following classical methodology. MKP is used as therapeutic medicine against hyperacidity, irritable bowel syndrome, and gastric ulcers. Aim of the study: Here, we explored the therapeutic properties of MKP in alleviating peptic ulcer in male Wistar rat model of pylorus ligation. Methods: Physicochemical properties of MKP were explored using scanning electron microscope, electron dispersive X-ray, dynamic light scattering, and Fourier-transform-infrared (FTIR)-spectroscopy analysis. Animals were orally treated twice daily with dosages of MKP, over a period of 15 days. The animals underwent 6 h pylorus ligation for the induction of peptic ulcers and analyzed for biochemical changes in gastric content, gross and histopathological changes in the stomach region. Results: Physicochemical analysis showed 0.1-30 mu m particles size for MKP, with elemental composition of oxygen, calcium, silica, carbon, phosphorus, and sodium. FTIR-spectroscopy indicated presence of aragonite crystals in MKP with capability of physically binding to gastric mucin molecules. Additionally, MKP treatment modulated gastric pH in simulated digestion model but did not affect the overall gastric content and total/free acidity levels in the in vivo pylorus ligation model. However, MKP treatment in rats significantly reduced ulcer index in stomach region and protected it against epithelial damages, hemorrhages and edema induced by pylorus ligation. Conclusion: MKP alleviated peptic ulcer induced by pylorus ligation in the male Wistar rats. Further research is warranted to elucidate the precise mode of action and long-term safety of Mukta Pishti.

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Author Keywords: Mukta pishti; Ayurveda; Anti-ulcerogenic activity; Pylorus ligation; Peptic ulcer

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Record 29 of 59

Title: Frequency and temperature dependent impedance studies: Impact of cobalt substitution on Ni-Zn ferrites for high frequency applications

Author(s): Jangra, S (Jangra, Shivani); Thakur, P (Thakur, Preeti); Singh, S (Singh, Satyendra); Thakur, A (Thakur, Atul)

Source: INORGANIC CHEMISTRY COMMUNICATIONS **Volume:** 174 **Article Number:** 113948 **DOI:** 10.1016/j.inoche.2025.113948 **Early Access Date:** JAN 2025 **Published Date:** 2025 APR **Part:** 1

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Abstract: Frequency and temperature dependent impedance studies along with the structural characteristics of Co-doped Ni-Zn ferrite of the composition Ni 0.5 Zn 0.5-x Co x Fe 2 O 4 (x = 0 to 0.5) synthesized via co-precipitation method are examined in this work. X-ray Diffraction (XRD) confirmed a cubic spinel phase with decreasing lattice constants from 8.221 & Aring; to 8.185 & Aring; as cobalt replaced zinc. The crystallite size averaged to 22.78 nm, and Williamson-Hall analysis showed lattice strain values between 1.46 x 10-3 and 3.79 x 10-3. Raman spectra provided insights into the cation distribution, confirming the presence of active vibrational modes (A1g, Eh, and T2g). The dielectric relaxation and conductivity mechanisms were studied using complex impedance spectroscopy as a function of composition, temperature and frequency. Nyquist plots indicate the presence of multiple relaxation processes. Also, the obtained semicircle arc from these Nyquist or Cole-Cole plot confirms the contribution of grain and grain boundaries in the conduction process. The resistivity decreases significantly as a function of Cobalt concentration, with the sample x = 0.5, exhibiting the lowest resistivity with a value of approximately 600 Omega.m at high frequencies. Variation of dielectric loss tangent is studied in the frequency range 10 kHz to 120 MHz. The low dielectric loss values at high frequencies make Ni-Zn ferrite suitable for application in high-frequency devices like inductors, transformers, and electromagnetic equipment.

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Record 30 of 59

Title: Eugenol attenuates aluminium-induced neurotoxicity in rats by inhibiting the activation of STAT3 and NF-?B

Author(s): Prakash, C (Prakash, Chandra); Tyagi, J (Tyagi, Jyoti); Singh, KV (Singh, Kumari Vandana); Kumar, G (Kumar, Gautam); Sharma, D (Sharma, Deepak)

Source: METABOLIC BRAIN DISEASE **Volume:** 40 **Issue:** 1 **Article Number:** 87 **DOI:** 10.1007/s11011-024-01526-1 **Published Date:** 2025 JAN 6

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Abstract: Aluminium is a common metallic toxicant that easily penetrates the brain and exerts severe pathological effects e.g., oxidative stress, inflammation and neurodegeneration. Eugenol is a natural phenolic compound possessing numerous therapeutic properties including antioxidant, anti-inflammatory and neuroprotective. The compound has also been reported to interfere with important transcription factors like STAT3 and NF-& kcy;B. Thus, the present study intended to explore the therapeutic potential of eugenol in aluminium neurotoxicity. Rats were administered AlCl3 (100 mg/kg b. wt., orally) and eugenol (200 mg/kg b. wt., orally) alone or in combination for 45 days. The results revealed that AlCl3 administration increases acetylcholinesterase (AChE) activity, lipid peroxidation (LPO), and protein oxidation (PO) along with decreasing superoxide dismutase (SOD) and catalase (CAT) activities, and glutathione (GSH) content in the cortex and hippocampus regions of the brain. Moreover, AlCl3 induces neuronal loss and astroglial activation in both brain areas. The study further revealed that AlCl3 also increases the expression of transcription factors STAT3 and NF-& kcy;B in neurons and astrocytes of the

cortex and hippocampus. However, co-administration of eugenol with AlCl3 restored the enzymatic activities of AChE, SOD and CAT, and GSH content, and rescued the cortex and hippocampus from LPO, PO, neuronal loss and astroglial activation. Furthermore, the study reported that eugenol reverses the expression pattern of STAT3 and NF-& kcy;B in AlCl3-intoxicated rats. In conclusion, the study suggests that eugenol ameliorates oxidative stress, neuronal loss and reactive astrogliosis in aluminium-induced neurotoxicity by inhibiting signalling molecules, STAT3 and NF-& kcy;B.

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Record 31 of 59

Title: Identification of novel inhibitors from Rubus ellipticus as anti-leishmanial agents targeting DDX3-DEAD box RNA helicase of Leishmania donovani

Author(s): Gouri, V (Gouri, Vinita); Roy, G (Roy, Gargi); Kanojia, A (Kanojia, Akanksha); Singh, S (Singh, Sumeet); Muthuswami, R (Muthuswami, Rohini); Samant, M (Samant, Mukesh)

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Abstract: Visceral leishmaniasis (VL), caused by Leishmania donovani, remains challenging to treat due to severe side effects and increasing drug resistance associated with current chemotherapies. Our study investigates the anti-leishmanial potential of Rubus ellipticus from Uttarakhand, India, with extracts prepared from leaves and stems using ethanol and hexane. Advanced GC-MS analysis identified over 100 bioactive compounds, which were screened using molecular docking to assess their binding to LdHEL-67, a DDX3-DEAD box RNA helicase of L. donovani. Our results spotlighted nine major compounds with high binding energy, which were then further analyzed for ADMET properties and toxicity predictions, demonstrating their promising pharmacokinetic profiles. Among these, clionasterol emerged as the standout compound, displaying superior results in all in silico analyses compared to Amphotericin B (the control). Notably, clionasterol was present in significant proportions across all the mentioned extracts. Subsequent treatment with these extracts led to a remarkable reduction in the intracellular amastigote and axenic amastigote, and promastigote forms of L. donovani and non-toxic to THP-1-derived macrophages. Moreover, the extracts induced apoptotic effects, as evidenced by the fragmentation of parasitic genomic DNA. This study marks a significant leap in developing herbal-based, target-specific inhibitors against VL. Hence, our findings highlight the immense potential of R. ellipticus as a natural treatment for VL.

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Author Keywords: Phytocompounds; DDX3-DEAD box RNA helicase; Molecular docking; Cytotoxicity; Anti-leishmanial activity; Clionasterol; Visceral leishmaniasis

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Record 32 of 59

Title: Microstructure characteristics and crystallographic orientation in dissimilar friction stir welding

Author(s): Kumar, KK (Kumar, Kethavath Kranthi); Srinivasnaik, M (Srinivasnaik, Mukuloth); Ramavath, G (Ramavath, Ganapati); Sangmesh (Sangmesh, Adepu); Kumar, A (Kumar, Adepu)

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Abstract: This study examines the microstructural properties such as grain structure, grain boundary misorientation, and crystallographic texture of friction stir welding (FSW) joints under two cooling media (air and water cooling). The microstructural evolution of FSW joints was characterized using light and electron microscopy techniques. Specifically in electron microscopy, inverse pole figure maps, pole figures, and orientation distribution functions were evaluated for both conditions of FSW joints using Electron Back Scattered Diffraction (EBSD). The water-cooling FSW (WCFSW) joint exhibited the smallest grain sizes at the stir zone (SZ) location compared to the corresponding condition in the air-cooling FSW (ACFSW) joint. EBSD analysis revealed that grain size in the SZ was about 7.6 mu m in the ACFSW joint and further refined to 3.2 mu m in the WCFSW joint. The misorientation angle distribution of water cooling conditions generated high-angle grain boundaries. The main texture components observed in the FSW samples were Brass [{110} < 112>] and Goss [{110} < 001>]. Additionally, Orientation Distribution Function (ODF) analysis found a higher texture intensity in water-cooled joints than in air-cooled joints. The WCFSW joint also had higher ultimate tensile strength values and a faster strain hardening rate. This is because the grains were smaller, more dislocations were created, and suitable texture components and intensity were favorable.

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Document Type: Article; Early Access

Author Keywords: Friction stir welding; microstructural characteristics; crystallographic texture; pole figure; and orientation distribution function

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Record 33 of 59

Title: OsLdh7 Overexpression in Rice Confers Submergence Tolerance by Regulating Key Metabolic Pathways: Anaerobic Glycolysis, Ethanolic Fermentation and Amino Acid Metabolism

Author(s): Chatterjee, Y (Chatterjee, Yajnaseni); Tomar, S (Tomar, Surabhi); Mishra, M (Mishra, Manjari); Pareek, A (Pareek, Ashwani); Singla-Pareek, SL (Singla-Pareek, Sneh Lata)

Source: PLANT CELL AND ENVIRONMENT **DOI:** 10.1111/pce.15358 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 9

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Abstract: Lactate dehydrogenase plays a key role in alleviating hypoxia during prolonged submergence. To explore the function of the OsLdh7 gene in enhancing submergence tolerance, we overexpressed this gene in rice (Oryza sativa cv. IR64) and subjected the transgenic lines to complete inundation. The overexpression lines showed enhanced viability, chlorophyll content and photosystem II (PSII) efficiency compared to wild-type (WT) plants under stress and recovery conditions. Additionally, these lines exhibited better starch accumulation and reduced reactive oxygen species (ROS) accumulation. Protein-protein interaction studies revealed that OsLdh7 interacts with OsLos2, OsPdc2, OsAlaAT2 and OsAsp2. Under submergence, enhanced enzyme activities of OsLdh7, OsAsp2 and OsAdh1 led to higher NAD(+) levels, sustaining anaerobic glycolytic flux and increasing pyruvate, a critical carbon source for amino acid metabolism as well as anaerobic fermentation pathways. Elevated l-lactate levels resulted in increased activity of OsPdc2, which eventually led to enhanced ethanol production. The overexpression lines also accumulated higher levels of aspartate, glutamate and alanine, crucial for ROS reduction and energy production during recovery. These findings suggest that OsLdh7 overexpression confers tolerance to submergence stress by regulating the important metabolic pathways- anaerobic glycolysis, ethanolic fermentation and amino acid metabolism in rice.

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Author Keywords: glycolytic flux; hypoxia; L-lactate; lactate dehydrogenase; ROS

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Record 34 of 59

Title: Comparative analysis of electromechanical performance of morphotropic phase boundary (MPB) based normal ferroelectric and non-MPB based relaxor ferroelectric perovskites

Author(s): Shankar, U (Shankar, Uma); Kumar, N (Kumar, Naveen); Ji, GP (Ji, Gopal); Singh, MK (Singh, Manvandra Kumar)

Source: MATERIALS TODAY COMMUNICATIONS **Volume:** 42 **Article Number:** 111283 **DOI:** 10.1016/j.mtcomm.2024.111283 **Published Date:** 2025 JAN

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Abstract: In the present work, we demonstrate that one can obtain comparable properties in composition far from Morphotropic phase boundary (MPB) by tuning the correlation length of polar-structural ordering in single phase relaxor ferroelectric perovskite. We examined this idea by a comparative structure-property analysis of a ferroelectric system (1-x) PbTiO3-(x)BiScO3 (PT-BS) (d(33) similar to 500 pC/N at MPB) and a non-MPB (1-x)PbTiO3-(x)Bi(Ni1/2Hf1/2)O-3 (PT-BNH) system (d(33) similar to 425 pC/N at pseudo-MPB). Structural analysis of x-ray powder diffraction (XRPD) data of MPB (x = 0.3725) composition of (1-x) PbTiO3-(x)BiScO3 (PT-BS) shows tetragonal + rhombohedral/monoclinic phase co-existence and there is a increment in tetragonal structural phase fraction at the cost of rhombohedral phase after poling, resulting in large piezoelectric property. On the other hand XRPD data of pseudo-MPB (x = 0.39) composition of (1-x)PbTiO3-(x)Bi(Ni1/2Hf1/2)O-3 (PT-BNH) shows cubic like (CL) + tetragonal phase co-existence and tetragonal structural phase fraction increases at the cost of co-existing cubic like phase upon poling, giving rise to the piezoelectric property comparable to that of MPB PT-BS. Raman spectra and x-ray pair distribution analysis show cubic like phase, which is the manifestation of miniaturized domains with tetragonal symmetry and its correlation length increases upon poling. Our analysis suggests that increased polar-structure heterogeneity at the non-MPB composition can result in large piezoelectric response and requirement of a MPB composition is not a necessary criterion to obtain enhanced electromechanical property.

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Record 35 of 59

Title: Molecular Design, Synthesis and Anti-cancer Activity of Novel Pyrazolo [3,4-b]pyridine-based Glycohybrid Molecules

Author(s): Verma, N (Verma, Neetu); Tiwari, G (Tiwari, Ghanshyam); Khanna, A (Khanna, Ashish); Mishra, VK (Mishra, Vinay Kumar); Yadav, Y (Yadav, Yogesh); Malviya, M (Malviya, Manisha); Sagar, R (Sagar, Ram)

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Abstract: Molecular hybridization is an emerging strategy in medicinal chemistry for designing new bioactive molecules that link pharmacophores covalently and shows synergistic enhanced properties. Herein, we have developed pyrazolo[3,4-b]pyridine-based new glycohybrids considering the Warburg effect. A microwave-assisted, copper-catalyzed efficient synthesis of new triazole-linked glycohybrids based on pyrazolo[3,4-b]pyridines scaffold was achieved successfully in high yields with inherent stereochemical diversity from D-glucose, D-galactose, and D-mannose. The twenty-three distinct new glycohybrids, incorporating various electron-donating and electron-withdrawing groups with stereochemical diversities, were prepared using developed synthetic protocol. This efficient synthesis significantly reduced reaction time and furnished products with high isolated yields, showcasing its potential for glycohybrids synthesis. In-vitro study revealed that among the synthesized glycohybrids, compound 8e emerged as a potential compound against MDA-MB231 (SI > 31) and MCF-7 (SI > 434) with an IC50 value of 19.58 mu M and 1.42 mu M respectively. The molecular docking study predicts the binding interaction of the chemical probe with the target protein HCK. The enzyme inhibition assay revealed that compound 8e is having strong inhibitory potency against HCK enzyme. This article highlights the synthetic utility of this strategy and the potential applications of these newly designed and prepared glycohybrids.

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Record 36 of 59

Title: A 0.5-5 Gb/s Wide Range, 160 fJ/Pulse Fully Integrated 13th-Order CMOS IR-UWB Transmitter for Wireless Capsule Endoscopy Systems

Author(s): Akuri, NG (Akuri, Naga Ganesh); Kumar, K (Kumar, Kunal); Kumar, S (Kumar, Sandeep); Nikhil, KS (Nikhil, K. S.); Song, H (Song, Hanjung)

Source: INTERNATIONAL JOURNAL OF CIRCUIT THEORY AND APPLICATIONS **DOI:** 10.1002/cta.4379 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 5

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Abstract: This paper proposes a novel technique based fully integrated 13th-order derivative CMOS impulse-radio ultrawideband (IR-UWB) transmitter with wide range of adaptive data rates for wireless capsule endoscopy systems (WCE). The proposed IR-UWB transmitter involves BPSK modulator-integrated RF power amplifier (PA) approach for WCE in first time as per author's best knowledge. The CMOS BPSK modulator with resonator technique generates 13th-order Modulated Gaussian pulse without the pulse generator. It has a peak-to-peak value of 25 mV and PSD level of -72.60 dBm/MHz, data rate variability from 500 Mbps to 5 Gbps. The BPSK modulator with resonator is designed by time constant analysis in first time. In addition, a proposed CMOS PA is designed using four stacked transistors, which achieves a high output power as well as high efficiency for entire frequency band of operation from 3 to 16 GHz and wide impedance matching. The PA achieved an excellent gain of 16.55 dB with gain ripple of 0.25 dB only. Moreover, the PA achieved the saturated output power of 18.2 to 19.3 dBm with OP1dB of 15.96 to 16.72 dBm across entire bandwidth. Without violating FCC guidelines, PA strengths both peak-to-peak values, and PSD level of BPSK modulated signal to 80 mV and -46.42 dBm/MHz. An IR-UWB transmitter has been implemented and fabricated using 65-nm CMOS Process, which consumes of only 160 fJ/pulse for generating Gaussian pulses order ranging from third-order to more than 13th-order at various data rates.

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Author Keywords: binary phase shift keying (BPSK); complementary metal oxide semiconductor (CMOS); impulse radio ultrawideband (IR-UWB); power amplifier (PA); power spectral density (PSD); ultrawide band (UWB)

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Record 37 of 59

Title: Model-based fed-batch cultivation of Viola odorata plant cells exhibiting antimalarial and anticancer activity

Author(s): Babu, R (Babu, R.); Veeramani, M (Veeramani, Manokaran); Aadinath, W (Aadinath, Wallepure); Muthuvijayan, V (Muthuvijayan, Vignesh); Singh, S (Singh, Shailja); Srivastava, S (Srivastava, Smita)

Source: FRONTIERS IN BIOENGINEERING AND BIOTECHNOLOGY **Volume:** 13 **Article Number:** 1528570 **DOI:** 10.3389/fbioe.2025.1528570 **Published Date:** 2025 JAN 29

Abstract: Introduction Viola odorata is a medicinal plant used in the indigenous systems of medicine in India, to treat respiratory tract disorders. V. odorata natural plant source is limited in availability. Bioprocess principles can be applied to develop sustainable methods for the commercial production of high-quality V. odorata plant biomass.Methods To this effect, the in vitro culture conditions of V. odorata were rationally optimized to increase the biomass production up to 21.7 +/- 0.8 g DW L-1 in 12 days in shake flasks. In the current study, a modified stirred tank reactor and a balloon-type bubble column reactor were used to improve the biomass production at the batch reactor level. Sufficient nutrient feeding strategies were developed using first principle-based mathematical modelling to overcome substrate inhibition and achieve higher cell

density in the reactor. In addition, bioreactor-cultivated biomass extracts (aqueous/alcoholic) were tested for various bioactivities like hemolytic, cytotoxic, anti-inflammatory, and antiplasmodial.Results Experimental validation of the fed-batch model-predicted strategy resulted in a two-fold enhancement in biomass production (32.2 g DW L-1) at the bioreactor level. Biomass extracts showed no hemolytic activity up to 4 mg mL-1 concentrations. Further, the stirred tank cultivated biomass extract displayed cytotoxicity against Caco2 - colon carcinoma cell lines, exhibiting an IC50 of 1.5 +/- 0.1 mg mL-1. In vitro experiments also indicated the anti-inflammatory property in the bioreactor cultivated plant biomass extracts. As a new application, the biomass extracts also demonstrated up to 80% inhibition of malarial parasite growth in vitro. Additionally, when administered alongside artesunate (1.8 mg kg-1d-1), the plant extracts (400 mg kg-1d-1) effectively controlled parasite growth in vivo.Discussion It is to be noted that a first report on fed-batch cultivation of V. odorata cell suspension culture in lab-scale bioreactors and on the antiplasmodial activity of the V. odorata plant extracts. Overall, the bioactive potential of the in vitro-generated plant biomass extracts is similar to that in the natural plant biomass extracts.

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Publisher Address: AVENUE DU TRIBUNAL FEDERAL 34, LAUSANNE, CH-1015, SWITZERLAND

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Research Areas: Biotechnology & Applied Microbiology; Engineering

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Open Access: gold

Output Date: 2025-03-04

Record 38 of 59

Title: Preclinical model of Mycobacteroides abscessus lung disease by nose-only exposure of mice to bacterial powder aerosol

Author(s): Verma, K (Verma, Khushboo); Garg, T (Garg, Tanu); Singh, S (Singh, Shriya); Deivreddy, VSR (Deivreddy, Venkata Siva Reddy); Raman, SK (Raman, Sunil K.); Bharti, R (Bharti, Reena); Sofi, HS (Sofi, Hasham Shafi); Singh, K (Singh, Kavita); Shaik, M (Shaik, Mehazabeen); Dasgupta, A (Dasgupta, Arunava); Mugale, MN (Mugale, Madhav N.); Misra, A (Misra, Amit)

Source: TUBERCULOSIS **Volume:** 151 **Article Number:** 102606 **DOI:** 10.1016/j.tube.2025.102606 **Early Access Date:** JAN 2025 **Published Date:** 2025 MAR

Times Cited in Web of Science Core Collection: 0

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Usage Count (Last 180 days): 0

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Cited Reference Count: 13

Abstract: The limitations of existing mouse models of lung infection with Mycobacteroides abscessus impede drug discovery and development. In contrast to current animal models that introduce NTM intravenously or by intranasal/intra-tracheal instillation or via bronchoscopy-guided insufflation, we developed a dry powder inhalation (DPI) of M. abscessus ATCC 19977 that generated paucibacillary lung infection and histopathology in immunocompetent mice. Swiss outbred mice receiving similar to 1000 (3-log) colony forming units (CFU) of M. abscessus/gram lung tissue via the DPI administered by nose-only inhalation for 90 s showed peak bacterial burden of similar to 3.35-log CFU/g in the lungs after 28 days. This was maintained at similar to 2-log/g from Day 35 through 56 in the lungs, but not in the spleen. Histopathology indicated increasing severity of inflammation, fibrosis and lung consolidation. Bacteria were rarely recovered from spleen, and histopathological examination indicated partial resolution in the spleen between Days 49-56. The DPI, prepared by freeze-drying log-phase liquid culture with cryoprotectants was formulated to possess aerosol characteristics suitable for alveolar deposition. Aerosol exposure to inoculum mimics natural airborne infection. Non-invasive aerosol infection is convenient, inexpensive, does not require special equipment or extensive training and mitigates stress to animals, but biosafety level 3 containment is recommended to mitigate risk to experimenters.

Accession Number: WOS:001406620200001

PubMed ID: 39823776

Language: English

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Author Keywords: Animal model; Non-invasive; Pulmonary delivery; Alveolar deposition; Aerogenic infection; Mycobacterium; Non-tubercular mycobacteria

KeyWords Plus: INHALABLE MICROPARTICLES

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Publisher: CHURCHILL LIVINGSTONE

Publisher Address: JOURNAL PRODUCTION DEPT, ROBERT STEVENSON HOUSE, 1-3 BAXTERS PLACE, LEITH WALK, EDINBURGH EH1 3AF, MIDLOTHIAN, SCOTLAND

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Output Date: 2025-03-04

Record 39 of 59

Title: Dopamine degrades ferritin by chaperone-mediated autophagy to elevate mitochondrial iron level in astroglial cells

Author(s): Dev, S (Dev, Som); Asthana, S (Asthana, Somya); Singh, P (Singh, Pratibha); Seth, P (Seth, Pankaj); Banerjee, C (Banerjee, Chayanika); Mukhopadhyay, CK (Mukhopadhyay, Chinmay K.)

Source: FREE RADICAL BIOLOGY AND MEDICINE **Volume:** 229 **Pages:** 39-57 **DOI:** 10.1016/j.freeradbiomed.2025.01.021 **Early Access Date:** JAN 2025 **Published Date:** 2025 MAR 1

Times Cited in Web of Science Core Collection: 0

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Abstract: Iron accumulation and mitochondrial dysfunction in astroglia are reported in Parkinson's disease (PD). Astroglia control iron availability in neurons in which dopamine (DA) synthesis is affected in PD. Despite their intimate relationship the role of DA in astroglial iron homeostasis is limited. Here we show that DA degrades iron storage protein ferritin in astroglial cells involving lysosomal proteolysis. Lysosomal ferritinophagy is mainly associated with macroautophagy; however, we revealed the involvement of chaperone-mediated autophagy (CMA) in DA- induced ferritin degradation. In CMA, cytosolic proteins containing a specific pentapeptide motif bind with HSC70 to be transported to lysosome mediated by LAMP2A. We identified the conserved pentapeptide motif in ferritin-H (Ft-H), mutations of which resulted loss of its interaction with HSC70. Pharmacological inhibitors of HSC70 or LAMP2/2A knockdown blocks DA-induced Ft-H degradation. DA also induces cytosolic cargo NCOA4 for ferritinophagy. We further reveal that DA promotes cathepsin B to lysis ferritin within the lysosome. Inhibitor of cathepsin B, knocking down of LAMP2, or HSC70 inhibitor attenuate DA-induced elevated mitochondrial iron level. Our results establish a direct role of DA on astroglial iron homeostasis and novel involvement of CMA in ferritin degradation in response to a biological stimulus. These results also may help in better understanding iron dyshomeostasis and mitochondrial dysfunction reported in PD.

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Author Keywords: Dopamine; Astroglia; Ferritin; Chaperone-mediated autophagy; NCOA4; Cathepsin B; Mitochondrial iron

KeyWords Plus: HEAVY-CHAIN; DEGRADATION; HOMEOSTASIS; MOBILIZATION; PARKINSONS; RELEASE; DISEASE; STORAGE; GENES; BRAIN

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Output Date: 2025-03-04

Record 40 of 59

Title: On investigation of complexity in extracellular matrix-induced cancer dynamics under deterministic and stochastic framework

Author(s): Upadhyay, RK (Upadhyay, Ranjit Kumar); Barman, AK (Barman, Amit Kumar); Das, P (Das, Parthasakha); Panda, B (Panda, Binay)

Source: NONLINEAR DYNAMICS **DOI:** 10.1007/s11071-024-10836-z **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 17

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Abstract: Cancer attracts significant attention nowadays due to its rising global incidence, the complexity of its biological mechanisms, and the challenges it presents in treatment and prevention. In this context, a mathematical model provides a powerful tool for understanding this critical aspect of cancer biology. This paper introduces a novel, comprehensive mathematical model that looks into the intricate interactions between cancer cells, immune cells, cytokines, and the extracellular matrix. We derive biologically feasible equilibria and examine both local and global stability. Using Sotomayor's theorem, the occurrence of saddle-node bifurcation is established, and the Hopf bifurcation is thoroughly analyzed. We investigate codimension-2 bifurcations, such as the Bogdanov-Takens bifurcation, using normal form theory and the center manifold theorem. Furthermore, an uncertainty analysis utilizing Latin hypercube sampling is performed to evaluate the influence of parameter uncertainties on tumor growth, which is then followed by a sensitivity analysis. The model incorporates multiplicative white noise terms into the deterministic system to construct a stochastic framework. Then we identify the sufficient conditions for mean persistence and extinction for every variable. Finally, numerical simulations are conducted by adjusting the parameters to confirm the analytical findings, providing new perspectives on controlling tumor behavior.

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Language: English

Document Type: Article; Early Access

Author Keywords: Cancer; Extracellular matrix (ECM); Bogdanov-Takens bifurcation; Codimension-2 bifurcations; Stochastic model; Extinction

KeyWords Plus: IMMUNE-SYSTEM; TUMOR; MODEL; PD-1; BIFURCATION; STABILITY; STIFFNESS; INVASION

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Publisher: SPRINGER

Publisher Address: VAN GODEWIJCKSTRAAT 30, 3311 GZ DORDRECHT, NETHERLANDS

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Web of Science Categories: Engineering, Mechanical; Mechanics

Research Areas: Engineering; Mechanics

IDS Number: S6S0L

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Output Date: 2025-03-04

Title: Advancements in graphene-based nanostructured conducting polymer hybrid composite electrodes for high-performance supercapacitors

Author(s): Singh, P (Singh, Paramjit); Singh, A (Singh, Avtar); Saini, R (Saini, Rashmi); Deepika (Deepika); Kulriya, P (Kulriya, Pawan); Kumar, R (Kumar, Rajesh)

Source: JOURNAL OF POWER SOURCES **Volume:** 630 **Article Number:** 236176 **DOI:** 10.1016/j.jpowsour.2025.236176 **Early Access Date:** JAN 2025 **Published Date:** 2025 FEB 28

Abstract: This comprehensive review provides a detailed analysis of carbon-based conducting polymer (CP) composites synthesized using advanced methodologies like in situ chemical polymerization and electrochemical polymerization, aimed at producing porous nanostructures with superior specific capacitance, exceptional cyclic stability and robust mechanical attributes. These composite materials, integrating carbon elements such as graphene (GP) and CPs, exhibit enhanced performance capabilities through meticulous control over nucleation and growth processes. CPs modulate their microstructural and morphological features, facilitating electrolyte diffusion within the electrode material, accelerating ion transport and boosting supercapacitive efficacy. The review explores the development of GP-based CP nanostructures, emphasizing the importance of controlling interlayer it-it interactions, binder effects, and electrolyte composition to improve supercapacitor performance. It discusses strategies to address CP limitations in supercapacitors, such as low capacitance and inferior cyclic stability, through improved synthesis and better GP-CP integration. The review also covers the potential applications of these composites in flexible electronics, wearable devices, and energy storage, along with advancements in scalable production, environmental impact, and future research directions to enhance supercapacitor efficiency.

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Language: English

Document Type: Review

Author Keywords: Supercapacitor; Graphene oxide; Polyaniline; Polypyrrole; Nanocomposites

KeyWords Plus: WALLED CARBON NANOTUBE; SOLID-STATE SUPERCAPACITORS; ONE-POT SYNTHESIS; ENERGY-STORAGE; ELECTROCHEMICAL PROPERTIES; OXIDE COMPOSITE; OXIDE/POLYPYRROLE COMPOSITE; TERNARY COMPOSITE; STAINLESS-STEEL; GREEN SYNTHESIS

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Publisher Address: RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS

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Research Areas: Chemistry; Electrochemistry; Energy & Fuels; Materials Science

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Output Date: 2025-03-04

Record 42 of 59

Title: Optical tuning of polymer functionalized zinc oxide quantum dots as a selective probe for the detection of antibiotics

Author(s): Verma, AK (Verma, Awadhesh Kumar); Lakshmi, GBVS (Lakshmi, G. B. V. S.); Dhiman, TK (Dhiman, Tarun Kumar); Hashmi, SZH (Hashmi, S. Z. H.); Kumar, A (Kumar, Anil); Solanki, PR (Solanki, Pratima R.)

Source: SCIENTIFIC REPORTS **Volume:** 15 **Issue:** 1 **Article Number:** 1648 **DOI:** 10.1038/s41598-024-62827-0 **Published Date:** 2025 JAN 10

Cited Reference Count: 59

Abstract: Excess consumption of antibiotics leads to antibiotic resistance that hinders the control and cure of microbial diseases. Therefore, it is crucial to monitor the antibiotic levels in the environment. In this proposed research work, an optical nano-sensor was devised that can sense the ultra-low concentration of antibiotics, in samples like tap water using fluorescent zinc oxide quantum dots (ZnO QDs) based nano-sensor. For this, different polymers (polyvinylalcohol-PVA and polyvinylpyrrolidine-PVP) capped florescent ZnO QDs were synthesized using a modified sol-gel technique. These were used as fluorescent probes to monitor the presence of antibiotics. The optical characterizations of synthesized QDs were performed using UV-visible absorption and fluorescence spectroscopic methods while structural characteristics were analyzed by using Raman spectroscopy and X-ray diffraction spectroscopy. The formation of capped QDs was confirmed by Fourier transform infrared spectroscopy (FTIR). Charge on the synthesized QDs was obtained with the help of ZETA potential. Here ten different antibiotics were checked, Ciprofloxacin and Moxifloxacin have shown excellent sensing and specificity with PVA-ZnO QDs and PVP-ZnO QDs with LOD of 1.4 nM and 0.8 nM, and sensitivity of 36.17 units/mM and 19.33 units/mM respectively. This study also inferred the tuning of the ZnO QDs properties and specificity towards the different antibiotics can be achieved by capping QDs with different polymers.

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Author Keywords: Ciprofloxacin; Moxifloxacin; Antibiotic resistance; Optical Sensing; Quantum Dots

KeyWords Plus: ZNO; FLUORESCENCE; ANTIBACTERIAL; EXTRACTION; BIOSENSOR

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Author	Web of Science ResearcherID	ORCID Number
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Dhiman, Tarun Kumar	AAQ-3961-2021	0000-0003-0006-7267

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Record 43 of 59

Title: The Layer Oxide Cathode Exhibits Optimal Capacitance Cooperative Effects in Capacitor Batteries

Author(s): Luo, ZH (Luo, Zhenhao); Li, JT (Li, Jintao); Zhang, ST (Zhang, Songtong); Chen, XF (Chen, Xuefang); Kumar, P (Kumar, Pushpendra); Wang, J (Wang, Jing); Zhu, XY (Zhu, Xiayu); Meng, WJ (Meng, Wenjie); Qiu, JY (Qiu, Jingyi); Ming, H (Ming, Hai)

Source: ACS APPLIED ENERGY MATERIALS **Volume:** 8 **Issue:** 2 **Pages:** 1292-1307 **DOI:** 10.1021/acsaem.4c02750 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 3

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Total Times Cited: 0

Usage Count (Last 180 days): 3

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Cited Reference Count: 55

Abstract: Capacitor batteries utilizing a dual-energy storage mechanism demonstrate enhanced energy and power densities. These batteries typically incorporate hybrid electrodes, formed by combining cathode materials with nanocarbon or other supercapacitor materials. However, the capacitance-cooperative effect of nanocarbons remain complex due to the intricate surface and interfacial interactions between the electrode and electrolyte, particularly in cathodes operating at high voltages, which accelerate the decomposition or reconstruction of chemical-electrochemical interface films. In this study, a series of hybrid electrodes composed of various nanostructured carbons and different cathode materials, such as olivine, spinel, and Na x MO2-layered oxides, are evaluated to assess their capacitance-cooperative effect on electrochemical performance. The results reveal that graphene-based nanocarbons are the optimal additives due to their high stability (up to similar to 5.0 V), conductivity, and large specific surface area. Additionally, a mass ratio of around 8-10% graphene is identified as the optimal additive concentration for nearly all cathodes. Most notably, the niobium-doped Na x MO2-layered oxide cathode demonstrates an energy density of approximately 420 Wh kg-1 at a power density of 16 kW kg-1, attributed to its internal capacitance effect. These findings are supported by both physicochemical characterizations and theoretical calculations. This work aims to establish guidelines for designing batteries that exhibit both excellent energy and power characteristics, which are essential for extreme operating conditions and environments.

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Language: English

Document Type: Article

Author Keywords: capacitor battery; hybrid electrode; capacitanceeffect carbon; graphene; layer oxide cathode

KeyWords Plus: LI-ION; CYCLING STABILITY; ACTIVATED CARBON; LIMN2O4 CATHODE; ENERGY-DENSITY; LICOO2 CATHODE; HIGH-POWER; LITHIUM; PERFORMANCE; GRAPHENE

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Research Areas: Chemistry; Energy & Fuels; Materials Science

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Record 44 of 59

Title: Sterile sector impacting the correlations and degeneracies among mixing parameters at the Deep Underground Neutrino Experiment

Author(s): Parveen, S (Parveen, Sabila); Masud, M (Masud, Mehedi); Bishai, M (Bishai, Mary); Mehta, P (Mehta, Poonam)

Source: JOURNAL OF HIGH ENERGY PHYSICS **Issue:** 1 **Article Number:** 139 **DOI:** 10.1007/JHEP01(2025)139 **Published Date:** 2025 JAN 28

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Abstract: We investigate the physics potential of the upcoming Deep Underground Neutrino Experiment (DUNE) in probing active-sterile mixing. We present analytic expressions for relevant oscillation probabilities for three active and one sterile neutrino of eV-scale mass and highlight essential parameters impacting the oscillation signals at DUNE. We then explore the space of sterile parameters as well as study their correlations among themselves and with parameters appearing in the standard framework (delta 13 and theta 23). We perform a combined fit for the near and far detector at DUNE using GLoBES. We consider alternative beam tune (low energy and medium energy) and runtime combinations for constraining the sterile parameter space. We show that charged current and neutral current interactions over the near and far detector at DUNE allow for an improved sensitivity for a wide range of sterile neutrino mass splittings.

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Author Keywords: Neutrino Mixing; Non-Standard Neutrino Properties; Sterile or Heavy Neutrinos

KeyWords Plus: OSCILLATION EXPERIMENTS; SIMULATION; SEARCH

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Record 45 of 59

Title: Beam dynamics design and optimization of a standalone radio frequency quadrupole accelerator for swift heavy ions

Author(s): Koyickal, SV (Koyickal, Sruthy Varma); Kumar, S (Kumar, Sarvesh); Jakhar, N (Jakhar, Niketan); Thakur, C (Thakur, Chandan); Yogesh (Yogesh, Manish K.); Kashyap, MK (Kashyap, Manish K.); Lombardi, A (Lombardi, Alessandra)

Source: PHYSICA SCRIPTA **Volume:** 100 **Issue:** 1 **Article Number:** 015312 **DOI:** 10.1088/1402-4896/ad9e37 **Published Date:** 2025 JAN 1

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Abstract: A standalone high energy, 352 MHz radio frequency quadrupole (RFQ) design is presented, resulting into targeted energy gain of 1.8 MeV/u with a beam current of 1 mA for mass to charge (A/q) ratio <= 4. It avoids many separate stages of transverse and longitudinal matching of beams compared to a standard RFQ + DTL accelerator combination due to automatic adiabatic bunching, focusing and acceleration of the beam and thus prevent many beam diagnostic and vacuum components. It is compact (only 4.63 meters) comparatively to other accelerator of equivalent energy gain and operation is quite easy in terms of beam tuning. The beam dynamics and vane designs are presented in details using PARMTEQ and Poisson/Superfish code. Such an accelerator promises to be a good candidate for establishing compact and more efficient nuclear physics research facilities compared to electrostatic Pelletron accelerators.

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Language: English

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Author Keywords: radio frequency quadrupole; beam optics; emittance; ion beams; nuclear Physics

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Record 46 of 59

Title: Interaction studies unveil potential binding sites on bovine serum albumin for gut metabolite trimethylamine n-oxide (TMAO)

Author(s): Verma, AK (Verma, Awadhesh Kumar); Gulati, P (Gulati, Payal); Lakshmi, GBVS (Lakshmi, Gbvs); Mohan, A (Mohan, Anand); Sharma, NR (Sharma, Neeta Raj); Solanki, PR (Solanki, Pratima R.); Kumar, A (Kumar, Anil)

Source: BMC CHEMISTRY **Volume:** 19 **Issue:** 1 **Article Number:** 22 **DOI:** 10.1186/s13065-024-01375-0 **Published Date:** 2025 JAN 21

Times Cited in Web of Science Core Collection: 0

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Cited Reference Count: 60

Abstract: Trimethylamine-N-oxide (TMAO) is gut microbiota-derived metabolite, plays a critical role in human health and diseases such as metabolic, cardiovascular, colorectal cancer and, neurological disorders. Binding interactions between TMAO and serum albumins are crucial to understand the impact of TMAO on disease mechanisms. However, detailed insights into the interaction mechanisms, preferred binding locations, and conformational changes in BSA upon binding TMAO are still unclear. TMAO interacts with serum albumin in human body and thus, a model study of interaction for TMAO-BSA conjugate is presented in support of it. Decrease in absorbance intensity of protein upon interaction with metabolites reveals conjugate formation, while fluorescence spectroscopy indicate static quenching. Contact angle measurements further reveal the hydrophilic nature of the TMAO-BSA complex, while CD and FTIR support conformational changes in BSA upon binding but structure remain intact. Computational studies, such as molecular docking, molecular dynamics simulation and, MM/GBSA, confirm a stable complex with a binding energy of - 3.6 kcal/mol. These findings provide a foundation for understanding the pharmacodynamics and pharmacokinetics of TMAO and may aid in developing strategies for treating diseases, such as chronic kidney disease and neurological disorder where TMAO-serum albumins interaction are implicated.

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PubMed ID: 39838440

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Author Keywords: TMAO; Bovine serum albumin (BSA); In silico; DFT; Docking; Spectroscopy; Molecular dynamics simulation; Mmgbsa

KeyWords Plus: IN-VIVO; FLUORESCENCE; FLAVONOIDS; PROTEINS; STRESS; PH

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Record 47 of 59

Title: Global impact of vitamin D deficiency and innovative biosensing technologies

Author(s): Chauhan, D (Chauhan, Deepika); Yadav, AK (Yadav, Amit K.); Bhatia, D (Bhatia, Dhiraj); Solanki, PR (Solanki, Pratima R.)

Source: CHEMICAL ENGINEERING JOURNAL **Volume:** 506 **Article Number:** 159790 **DOI:** 10.1016/j.cej.2025.159790 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 15

Times Cited in Web of Science Core Collection: 0

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Abstract: Vitamin D (VD) is of interest to an internist, pediatricians, physicians, orthopediacian, pathologists, endocrinologists, nutritionists, ecologists, geneticists, and others for almost a century due to its wide range of etiologies, clinical, biochemical, and pathological manifestations. VD insufficiency is a widespread problem that is often overlooked and not properly addressed as a dietary deficit worldwide. Nevertheless, traditional diagnostic techniques have limitations such as expensive costs, time-consuming procedures, and a substantial need for human resources. This emphasizes the necessity for intelligent, rapid, and on-site methods for diagnosis. Nanoenabled smart biosensors supported by artificial intelligence (AI) offer a promising solution for rapid point-ofcare (POC) detection of VD. These advanced biosensors provide real-time, sensitive, and portable diagnostic capabilities. In this account of the literature, we want to present an update on VD recommendations and the current scientific knowledge about the role of VD in human health. We present a critical and detailed review on the growing risk of VD deficiency and its health importance, recommended intake, analytical methods of detection and future aspects. This review also thoroughly examines different kinds of optical and electrochemical nanobiosensor for VD diagnosis. By using the unique characteristics of nano-enabled intelligent biosensors, such as fast outcomes, heightened sensitivity, mobility, and compatibility with Internet-of-Things (IoT) technologies, it is feasible to bring about a significant transformation in the diagnosis of VD. In addition, nanomaterial-based biosensors allow for on-site monitoring and personalized monitoring, greatly cutting down on turnaround time and removing the requirement for human resources for sample transportation and preservation. Adopting these cutting-edge diagnostic technologies is expected to increase the ability of the global healthcare system to fight VD insufficiency and protect one's health.

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Language: English

Document Type: Review

Author Keywords: Vitamin D; 25-hydroxyvitamin D; Biosensors; Point-of-care devices; Analytical methods

KeyWords Plus: TANDEM MASS-SPECTROMETRY; D-BINDING PROTEIN; 25-HYDROXYVITAMIN D; ELECTROCHEMICAL IMMUNOSENSOR; OPTICAL BIOSENSOR; GRAPHENE OXIDE; SERUM; CARE; RISK; SENSOR

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Record 48 of 59

Title: Vesicular mechanisms of drug resistance in apicomplexan parasites

Author(s): Haldar, K (Haldar, Kasturi); Bhattacharjee, S (Bhattacharjee, Souvik)

Source: MICROBIOLOGY AND MOLECULAR BIOLOGY REVIEWS **DOI:** 10.1128/mmbr.00010-24 **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 24
Times Cited in Web of Science Core Collection: 0
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Abstract: Vesicular mechanisms of drug resistance are known to exist across prokaryotes and eukaryotes. Vesicles are sacs that form when a lipid bilayer 'bends' to engulf and isolate contents from the cytoplasm or extracellular environment. They have a wide range of functions, including vehicles of communication within and across cells, trafficking of protein intermediates to their rightful organellar destinations, and carriers of substrates destined for autophagy. This review will provide an in-depth understanding of vesicular mechanisms of apicomplexan parasites, Plasmodium and Toxoplasma (that respectively cause malaria and toxoplasmosis). It will integrate mechanistic and evolutionarily insights gained from these and other pathogenic eukaryotes to develop a new model for plasmodial resistance to artemisinins, a class of drugs that have been the backbone of modern campaigns to eliminate malaria worldwide. We also discuss extracellular vesicles that present major vesicular mechanisms of drug resistance in parasite protozoa (that apicomplexans are part of). Finally, we provide a broader context of clinical drug resistance mechanisms of Plasmodium, Toxoplasma, as well as Cryptosporidium and Babesia, that are prominent members of the phyla, causative agents of cryptosporidiosis and babesiosis and significant for human and animal health.

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Author Keywords: artemisinin; drug resistance mechanisms; apicomplexan parasites; vesicular trafficking

KeyWords Plus: PLASMODIUM-FALCIPARUM; ARTEMISININ RESISTANCE; PARASITOPHOROUS VACUOLE; TOXOPLASMA-GONDII; QINGHAOSU ARTEMISININ; ANTIMALARIAL-DRUG; MALARIA; CELL; MEMBRANE; PROTEIN

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Record 49 of 59

Title: Plasmodium falciparum raf kinase inhibitor is a lipid binding protein that interacts with and regulates the activity of PfCDPK1, an essential plant-like kinase required for red blood cell invasion

Author(s): Sharma, M (Sharma, Manish); Krishnan, D (Krishnan, Deepak); Singh, A (Singh, Ayushi); Negi, P (Negi, Pooja); Rani, K (Rani, Komal); Revikumar, A (Revikumar, Amjesh); Munde, M (Munde, Manoj); Bansal, A (Bansal, Abhisheka)

Source: BIOCHEMICAL AND BIOPHYSICAL RESEARCH COMMUNICATIONS **Volume:** 749 **Article Number:** 151350 **DOI:** 10.1016/j.bbrc.2025.151350 **Early Access Date:** JAN 2025 **Published Date:** 2025 FEB 16

Abstract: Raf Kinase Inhibitor Protein (RKIP) is an important regulator of the MAPK signaling pathway in multicellular eukaryotes. Plasmodium falciparum RKIP (PfRKIP) is a putative phosphatidylethanolamine binding protein (PEBP) that shares limited similarity with Homo sapiens RKIP (HsRKIP). Interestingly, critical components of the MAPK pathway are not expressed in malaria parasites and the physiological function of PfRKIP remains unknown. PfRKIP is expressed throughout the asexual schizogony with maximum expression in late schizonts. Interestingly, PfRKIP and HsRKIP show pH-dependent differential interaction profiles with various lipids. At physiological pH, PfRKIP shows interaction with phosphatidic acid and lipids containing phosphorylated phosphatidylinositol group; however, HsRKIP shows no interaction under the same conditions. Mutation of conserved residues in the PEBP domain of PfRKIP decreases its interaction with PtdIns(3)P. Additionally, in silico docking and mutagenesis studies identified a unique IKK motif within the PEBP domain of PfRKIP that is important for its interaction with the lipids. Using ELISA, we demonstrate the interaction of PfRKIP with PfCDPK1. Importantly, we establish the interaction of PfRKIP and PfCDPK1 within the parasites using immunofluorescence assay and proximity biotinylation technique. Furthermore, our results suggest that PfRKIP regulates the kinase activity of PfCDPK1. In the presence of its substrate, PfCDPK1 hyper-phosphorylates PfRKIP which leads to its dissociation from PfCDPK1. Dissociation of PfRKIP allows PfCDPK1 to trans-phosphorylate its substrates. The molecular mechanism of interaction between PfRKIP and PfCDPK1 may be explored further to identify novel anti-malarial compounds.

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Record 50 of 59

Title: Rapid metabolic fingerprinting meets machine learning models to identify authenticity and detect adulteration of essential oils with vegetable oils: Mentha and Ocimum study

Author(s): Ratnasekhar, CH (Ratnasekhar, C. H.); Khan, S (Khan, Samreen); Rai, AK (Rai, Abhishek Kumar); Mishra, H (Mishra, Himanshu); Verma, AK (Verma, Anoop Kumar); Lal, RK (Lal, Raj Kishore); Kumar, TMA (Kumar, T. M. Ananda); Elliott, CT (Elliott, Christopher T.)

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Abstract: Essential oils (EOs) are gaining popularity due to their potent antibacterial properties, as well as their applications in food preservation and flavor enhancement, offering growth opportunities for the food industry. However, their widespread use as food preservatives is limited by authenticity challenges, primarily stemming from adulteration with cheaper oils. This study investigated a rapid, cost-effective, and non-destructive method for assessing the authenticity of widely used Mentha and Ocimum EOs. The proposed approach integrates Fourier transform near-infrared (FT-NIR) spectroscopy with machine learning to enable rapid metabolic fingerprinting of EOs. Four Mentha species and three Ocimum species were analysed, and the system was tested on market samples adulterated with vegetable oils. The approach achieved exceptional performance, with Q2, R2, and accuracy exceeding 0.98, alongside specificity and sensitivity greater than 98 %. These findings demonstrated that FT-NIR, combined with machine learning, offers a highly efficient solution for addressing authenticity and adulteration issues in EOs.

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Author Keywords: Rapid metabolic fingerprinting; Essential oils; FT-NIR; Authenticity; Machine learning models

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Record 51 of 59

Title: Electrolyte exchange experiment in batteries: Failure analysis and prospect q

Author(s): Guo, XL (Guo, Xiaoliang); Xie, HL (Xie, Hongliang); Ma, Z (Ma, Zheng); Kumar, P (Kumar, Pushpendra); Zhang, ZX (Zhang, Zixu); Wang, YQ (Wang, Yuqi); Chen, YH (Chen, Yinghua); Liang, HH (Liang, Honghong); Wang, J (Wang, Jia); Li, Q (Li, Qian); Ming, J (Ming, Jun)

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Abstract: The solid electrolyte interphase (SEI) layer, formed on the electrode through electrolyte decomposition, has garnered significant attention over the past several decades. Numerous characterization studies have shown that the SEI enhances the stability of both the electrolyte and electrode, particularly by mitigating the well-known cation-solvent co-intercalation in graphite electrodes in lithium-ion batteries. However, recent electrolyte exchange experiments have revealed that variations in electrolyte solvation structure and the resulting desolvation behaviors play a more dominant role than the SEI in influencing electrolyte and electrode stability, which in turn critically impacts battery performance. In addition to contributing to the ongoing debate, electrolyte exchange experiments have proven to be a valuable tool for analyzing failures in electrolytes, electrodes, and batteries. This review highlights the application of electrolyte exchange experiments across various metal-ion batteries, incorporating diverse combinations of electrolytes and electrodes. It examines the influence of electrolyte solvation structures and desolvation behaviors on the stability of both electrolytes and electrodes. The aim is to enhance the methodology of

electrolyte exchange experiments to deepen the understanding of the molecular interactions among metal ions, anions, and solvents within the electrolyte. This approach complements existing insights into SEI effects, providing a more thorough and accurate framework for battery failure analysis.

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Document Type: Review

Author Keywords: Batteries; Electrolyte; Exchange experiment; Failure analysis; De-solvation process

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Record 52 of 59

Title: Electrolyte Solvent-Ion Configuration Deciphering Lithium Plating/Stripping Chemistry for High-Performance Lithium Metal Battery

Author(s): Li, Q (Li, Qian); Liu, G (Liu, Gang); Chen, YH (Chen, Yinghua); Wang, J (Wang, Jia); Kumar, P (Kumar, Pushpendra); Xie, HL (Xie, Hongliang); Wahyudi, W (Wahyudi, Wandi); Yu, H (Yu, Hao); Wang, ZX (Wang, Zexu); Ma, Z (Ma, Zheng); Ming, J (Ming, Jun)

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Abstract: Electrolyte engineering plays a critical role in tuning lithium plating/stripping behaviors, thereby enabling safer operation of lithium metal anodes in lithium metal batteries (LMBs). However, understanding how electrolyte microstructures influence the lithium plating/stripping process at the molecular level remains a significant challenge. Herein, using a commonly employed ether-based electrolyte as a model, the role of each electrolyte component is elucidated and a relationship between electrolyte behavior and the lithium plating/stripping process is established by investigating the effects of electrolyte compositions, including solvents, salts, and additives. The variations in Li+ deposition kinetics are not only analyzed by characterizing the lithium deposition overpotential and exchange current density but it is also identified that the intermolecular interactions are the previously unexplored cause of these variations by 2D nuclear overhauser effect spectroscopy (NOESY). An interfacial model is developed to explain how solvent interactions, distinct roles of anions, and critical effects of additives influence Li+ desolvation kinetics and the thermodynamic stability of desolvation clusters during lithium plating/stripping process. This model clarifies how these configurations of solvents and ions are related to the macroscopic properties of lithium plating/stripping chemistry. These findings contribute to more uniform and controllable lithium deposition, providing valuable insights for designing advanced electrolyte systems for LMBs.

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Document Type: Article; Early Access

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KeyWords Plus: INTERFACIAL MODEL; SULFUR BATTERIES; ANTIMONY ANODE; LI IONS; NUCLEATION; SOLVATION; ADDITIVES; GROWTH; ELECTRODEPOSITS; STABILITY

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Record 53 of 59

Title: Biotic Stress Alleviation in Plant Using Rhizobacteria: An Overview of Mechanism of Action, Antimicrobial Compounds Production, (Nano) Formulations and Employment Methods

Author(s): Rana, A (Rana, Anuj); Rani, A (Rani, Annu); Nayana, KR (Nayana, K. R.); Deswal, S (Deswal, Sumit); Singh, AP (Singh, Arvind Pratap); Rana, S (Rana, Sravendra); Chahar, M (Chahar, Madhvi); Singh, N (Singh, Namita); Dhaka, RK (Dhaka, Rahul Kumar)

Source: INDIAN JOURNAL OF MICROBIOLOGY **DOI:** 10.1007/s12088-024-01429-w **Early Access Date:** JAN 2025 **Published Date:** 2025 JAN 3

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Cited Reference Count: 162

Abstract: The biotic stress induced by phytopathogens causes a significant loss to several crops in terms of yield and quality. Biotic stress may disrupt phenotypic characteristics and alter metabolic pathways in plants. Sustainable approaches like the employment of rhizobacteria control phytopathogens and diseases thereof through production of antimicrobial compounds and boosting plant defense systems. Rhizobacteria protect plants through mechanisms such as competition for food and niche to pathogens, production of antibiotics, induced systemic resistance and stimulation of antioxidant enzymes in plants helping them to mitigate pathogen-induced oxidative stress. This review concisely presents ample studies on the role of rhizobacteria in controlling phytopathogens including their mechanism of action, pathogenesis responsive metabolic pathways and regulatory genes. There are commercially available biocontrol agents for a variety of crops and more need to be developed based on host specificity and agro climatic conditions. This review further highlights the approaches for rhizobacterial formulation development and employment methods followed by future prospects to reduce the dependence on agrochemicals to ensure food security and quality using an eco-friendly sustainable approach. Encapsulated formulation of bacteria with nanomaterial is an innovative technological approach for enhanced efficacy and controlled delivery of active chemicals leading to suppression of plant disease severity more effectively versus bare bacteria to achieve improved plant health and food security.

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Document Type: Review; Early Access

Author Keywords: Biotic stress; Biocontrol; Plant pathogens; Rhizobacteria; Biopesticides; Induced systemic resistance (ISR); Nano-formulation

KeyWords Plus: GROWTH-PROMOTING RHIZOBACTERIA; INDUCED SYSTEMIC RESISTANCE; BIOLOGICAL-CONTROL; BIOCONTROL AGENTS; RHIZOME ROT; PSEUDOMONAS; DISEASE; INOCULATION; BACTERIA; PATHOGENS

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Record 54 of 59

Title: Investigation of MoS₂-hydrogen interaction using in-situ X-ray diffraction studies

Author(s): Kumar, R (Kumar, Ramesh); Chourasia, NK (Chourasia, Nitesh K.); Kulriya, PK (Kulriya, Pawan K.); Kumar, M (Kumar, Mahesh); Singh, V (Singh, Vinod)

Source: APPLIED PHYSICS A-MATERIALS SCIENCE & PROCESSING **Volume:** 131 **Issue:** 1 **Article Number:** 14 **DOI:** 10.1007/s00339-024-08143-w **Published Date:** 2025 JAN

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Abstract: The present manuscript examines the significant effects of hydrogen (H-2) exposure on the structural properties of molybdenum disulfide (MoS2) thin films through in-situ X-ray diffraction (XRD) analysis. Molybdenum (Mo) thin films were initially deposited using the electron beam (e-beam) deposition method and subsequently sulfurized via chemical vapor deposition (CVD) to obtain MoS2 thin films. The quality of the MoS2 films was optimized by varying the thickness of the Mo layer, sulfurization temperature, and the temperature of the Mo film. It was determined that crystalline MoS2 thin films with an optimal thickness of 20 nm can be achieved through sulfurization at 220 degrees C, while maintaining the Mo thin film at 600 degrees C. Pressure-dependent hydrogenation of the MoS2 thin films, as investigated by in-situ XRD, reveals an increase in crystallite size accompanied by a decrease in the relative intensity of the diffraction peaks with rising hydrogen pressure. Furthermore, a microstrain of approximately 6.3% is induced in the MoS2 films upon exposure to 1% and 10% hydrogen. Notably, the MoS2 thin films remain predominantly stable up to a hydrogen pressure of 400 mbar; however, they undergo abrupt transformations and become entirely amorphous when the hydrogen gas pressure is subsequently elevated to 800 mbar. These observations of hydrogen-induced crystalline-amorphous phase transformation in MoS2 not only enhance the understanding of the interactions between MoS2 and hydrogen but also have critical implications for the application of MoS2 thin films in various devices.

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Document Type: Article

Author Keywords: Hydrogenation; MoS2; In-situ XRD; Phase transformation

KeyWords Plus: HYDROGEN STORAGE; MOS2; ADSORPTION

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Record 55 of 59

Title: Impedance spectroscopic study on nanocrystalline Ce_{0.75}Zr_{0.25}O₂ ceramics

Author(s): Kumari, S (Kumari, Sushama); Sharma, SK (Sharma, S. K.); Meena, R (Meena, Ramcharan); Goel, VK (Goel, Vijay Kumar); Bugalia, S (Bugalia, Swati)

Source: BULLETIN OF MATERIALS SCIENCE **Volume:** 48 **Issue:** 1 **Article Number:** 17 **DOI:** 10.1007/s12034-024-03387-x **Published Date:** 2025 JAN 11

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Abstract: The effect of the grain size on the dielectric properties and electrical conductivity was studied for single-phase solid solution of the ZrO2-CeO2 system with 75% CeO2 . The bi-ceramic composition of ZrO2-CeO2 as Ce0.75Zr0.25O2 was prepared through a solid-state reaction to synthesize single-phasic material followed by high-energy ball milling to make finer particle size. Structural properties were confirmed through advanced analytical techniques such as XRD and Raman spectroscopy. SEM confirmed large porosity with a grain size of 204 +/- 3 nm, which is larger than the crystallite size of 22.64 +/- 8.6 nm calculated from the XRD analysis for Ce0.75Zr0.25O2. The dielectric measurements were performed as a function of temperature by impedance spectroscopy. The relative dielectric constant decreases on increasing frequency for all temperatures, which validates the polar nature of nanocrystallineCe(0.75)Zr(0.25)O(2) ceramic. In addition, temperature-dependent enhancement in epsilon(r) is more pronounced in low-frequency regions due to low-frequency dielectric dispersion phenomena. The dielectric loss also increases with increasing temperature over the frequency region from 100 Hz to 2 MHz. The electrical conductivity of nanocrystalline Ce0.75Zr0.25O2 was found to be smaller than the micron-sized sample of Ce0.75Zr0.25O2. The present study revealed the crucial role of grain size in tuning the dielectric properties of Ce0.75Zr0.25O2 along with ac conductivity.

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Document Type: Article

Author Keywords: Nanocrystalline; Ce0.75Zr0.25O2; fuel cell; MOSFET; X-ray diffraction; dielectric properties

KeyWords Plus: MICROWAVE DIELECTRIC-PROPERTIES; ELECTRICAL-PROPERTIES; IONIC-CONDUCTIVITY; SCATTERING; TEXTURE; OXIDE; CEO2

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Record 56 of 59

Title: Addressing tropical cyclone risks: stratified for wellbeing and global policy coordination

Author(s): Ramachandran, AK (Ramachandran, Aswathi Kadarala); Panneer, S (Panneer, Sigamani); Rice, L (Rice, Louis); Rathnayake, U (Rathnayake, Upaka); Kantamaneni, K (Kantamaneni, Komali)

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Abstract: Tropical cyclones are one of nature's most catastrophic occurrences, causing significant humanitarian crises, economic losses, and human fatalities, particularly in coastal regions. This paper explores the diverse challenges, such as health, inequality, and developmental issues caused by tropical cyclones. Accordingly, a structured literature review methodology was devised that focuses on inclusion and exclusion criteria using publications between 1994 and 2023 by including key search words. This review of published evidence from electronic bibliographic databases underscores the substantial effects of tropical cyclones on physical, mental and socio-economic well-being of the population. The disastrous situation caused by cyclones is exacerbated by inequalities in gender, education, livelihoods, economics, disabilities, and displacement. Exclusion of affected people from developmental programmes and inadequate policy formulation further compound the challenge of safeguarding the deprived. The paper highlights the crucial role of community participation in improving environmental governance and reducing disaster risk. It addresses adaptation strategies aimed at tackling vulnerabilities, aligning them with the Sustainable Development Goals (SDGs). Specifically, it focuses on SDG 3 (good health and well-being), SDG 9 (Industry, innovation, and infrastructure, which emphasizes building resilient infrastructure), and SDG 13 (Climate action). The review shows that there is limited empirical evidence available, and most of the articles identified were published after 2010, indicating growing academic interest in empirical studies on tropical cyclones. Nevertheless, further research is required to comprehend how tropical cyclones affect the lives of people living in coastal regions to enhance risk reduction management and develop resilient adaptation strategies.

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Author Keywords: Tropical cyclones; Developmental challenges; Humanitarian crisis; Sustainable development goals; Resilience; Disaster risk reduction; Global governance

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Title: Au-based core-shell nanoparticles for wastewater treatment and hydrogen production: An insight

Author(s): Verma, R (Verma, R.); Aljohani, K (Aljohani, Khalid); Aljohani, BS (Aljohani, Bassam S.); Chauhan, A (Chauhan, A.); Kumar, P (Kumar, Pradeep); Singh, S (Singh, S.); Thakur, P (Thakur, Pankaj); Pallavi, P (Pallavi, Pragya)

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Abstract: Core-shell nanoparticles (CSNPs) represent a fascinating category of nanostructured materials that have recently attracted considerable interest owing to their remarkable properties and the extensive array of applications across various domains, such as catalysis, biology, materials chemistry, and sensor technology. Gold (Au)-based CSNPs have garnered considerable attention from the scientific community due to their unique chemical, electrical, physical, and optical properties. The potential applications of these nanoparticles extend to the biomedical sector, particularly in cancer treatment, pharmaceutical delivery, imaging techniques for oncology, Hydrogen generation and water purification processes. The size and morphology of Au-based core-shell nanoparticles comprehensively decides their photocatalytic activity in water purification and Hydrogen Generation. Moreover, presence of Au imparts the LSPR (Local Surface Plasmon Resonance) effect which is responsible for improve efficacy. The Au-based CSNPs showed the dye degradation efficacy around 98 % in 12 min for Au-Pd CSNPs. Further, Fe3O4/PDA/Au CSNPs showed

98.16 % efficiency in 360 min with 0.0812 min-1against tetracycline (TC). Thus, this review gives a thorough look at a topic, starting with how gold-based core-shell nanoparticles are made and ending with how they can be used to break down dyes, find and remove heavy metals, break down antibiotics, and to produce hydrogen.

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Title: Perspective-Metal Halide Perovskites-based Sensing Technologies: Recent Updates and Future Directions

Author(s): Gupta, K (Gupta, Khushboo); Kumar, M (Kumar, Manish); Singh, DV (Singh, Dharm Veer); Chaudhary, V (Chaudhary, Vishal); Kumar, A (Kumar, Arvind); Dwivedi, DK (Dwivedi, D. K.); Kumar, S (Kumar, Santosh); Kumar, R (Kumar, Rajesh); Thakur, OP (Thakur, O. P.); Sharma, S (Sharma, Subhash)

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Abstract: Recently, metal-halide perovskites (MHPs) have become an epicenter of research because of their outstanding optoelectronic properties. MHPs have not only proved to be the best materials for sensing applications due to their unique optical and electronic properties along with easy fabrication, they also display good sensing ability, including ultrahigh sensitivities, rapid response rate, and outstanding selectivity. To keep the research community informed, we critically focused on the recent updates in the MHPs-based sensor, followed by highlighting the synthesis route and their potential while addressing important challenges and future outlooks and unlocking their capabilities in sensing technologies. Focused analysis on metal-halide perovskites based sensing technologyHighlighting the synthesis routesAddressing important challenges and future outlooksUnlocking the metal-halide perovskites capabilities in sensing technologies

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Title: Weak coupling of observed surface PM_{2.5} in Delhi-NCR with rice crop residue burning in Punjab and Haryana

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Abstract: Air pollution impacts on human health are of serious concern in northern India, and over the Delhi National Capital Region (NCR) in particular. The Kharif crop residue burning (CRB) is often blamed for degradation of Delhi-NCR's seasonal air quality. However, the concentration of fine particulate matter (PM2.5) remained stable in Delhi, while the fire detection counts (FDCs) from satellites over Punjab and Haryana declined by 50% or more during 2015-2023. We measured PM2.5, carbon monoxide (CO) and related parameters over Delhi-NCR, Haryana and Punjab from a network of 30 low-cost sensors (CUPI-Gs) in a selected period (September-November) of 2022 and 2023. Measured PM2.5 showed lower concentration in 2023 compared to 2022 at Punjab and Haryana sites, in compliance with FDC reductions. Using the CUPI-G measurements, airmass trajectories, particle dispersion and chemical-transport model simulations, we show that the CRB emissions over Punjab contributed only a meagre similar to 14% to the overall PM2.5 over Delhi-NCR during October-November 2022. This indicates that there exists only a very weak coupling between PM2.5 mass over Delhi-NCR and the CRB over Punjab, highlighting the effectiveness of the Graded Response Action Plan (GRAP) in controlling air pollution in the region.

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