

### Record 1 of 29

**Title:** Evaluating non-western disturbances winter precipitation over the western Himalayas

**Author(s):** Pooja (Pooja, A. P.); Dimri, AP (Dimri, A. P.)

**Source:** CLIMATE DYNAMICS **DOI:** 10.1007/s00382-024-07431-8 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 13

**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:** 25

**Abstract:** Western Himalayas (WH) receives precipitation through eastward propagating synoptic weather systems, Western Disturbances (WDs), embedded in large scale subtropical westerly jet (SWJ) during Northern Hemispheric boreal winter (December, January and February; DJF). In the recent decade, WDs have undergone certain changes in their characteristic's viz., decreased associated precipitation, no significant changes in the WDs frequency and intensity, etc. However, Non-WDs days and associated precipitation gained its importance as it contributes similar to 20% of winter precipitation over WH. In this study, structure, dynamics and moisture availability associated with changing WDs and Non-WDs precipitating days are analyzed. Robust statistical methods and Theil-Sen slope on ERA5 data during 1987-2020 is considered to comprehend why active WDs' (Non-WDs) precipitation frequency is declining (notably increasing). Interestingly, it is as well found that all the WDs do not precipitate and there are Non-WDs days when precipitation occur. It shows declining trend in WD precipitation and the increasing importance of Non-WDs. The findings show formation of 'Omega shape' flow - where high pressure is locked between two low pressure systems - over Indian subcontinent during Non-WDs days. Such dynamical wind col formation ('Omega shape') from lower (850Hpa) to upper (200 hPa) troposphere provides conducive situation for enhanced moisture incursion from Bay of Bengal (BoB) towards and over the WH during Non-WDs days leading to precipitation. This new finding needs to be looked from sustaining and replenishment of glaciers; agriculture; socioeconomic benefits during winters and needs to be addressed.

**Accession Number:** WOS:001312258800001

**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** Non-WDs days; Winter precipitation; Western disturbances; Omega shape flow; infinity shape formation; Secondary WDs

**KeyWords Plus:** CLIMATE-CHANGE; RESOLUTION

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**Publisher:** SPRINGER

**Publisher Address:** ONE NEW YORK PLAZA, SUITE 4600, NEW YORK, NY, UNITED STATES

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

**Web of Science Categories:** Meteorology & Atmospheric Sciences

**Research Areas:** Meteorology & Atmospheric Sciences

**IDS Number:** F8L2F

**ISSN:** 0930-7575

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**29-char Source Abbrev.:** CLIM DYNAM

**ISO Source Abbrev.:** Clim. Dyn.

**Source Item Page Count:** 13

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The authors are thankful to the European Centre for Medium-Range Weather Forecasts (ECMWF) for reanalysis data. This work is supported by the Indian Institute of Geomagnetism (IIG), Department of Science and Technology, India.

**Output Date:** 2024-10-01

**Record 2 of 29**

**Title:** Federated learning based multi-head attention framework for medical image classification

**Author(s):** Firdaus, N (Firdaus, Naima); Raza, Z (Raza, Zahid)

**Source:** CONCURRENCY AND COMPUTATION-PRACTICE & EXPERIENCE **DOI:** 10.1002/cpe.8280 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 13

**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:** 51

**Abstract:** In this study, we propose a novel Federated Learning Based Multi-Head Attention (FBMA) framework for image classification problems considering the Independent and Identically Distributed (IID) and Non-Independent and Identically Distributed (Non-IID) medical data. The FBMA architecture integrates FL principles with the Multi-Head Attention mechanism, optimizing the model performance and ensuring privacy. Using Multi-Head Attention, the FBMA framework allows the model to selectively focus on important regions of the image for feature extraction, and using FL, FBMA leverages decentralized medical institutions to facilitate collaborative model training while maintaining data privacy. Through rigorous experimentation on medical image datasets: MedMNIST Dataset, MedicalMNIST Dataset, and LC25000 Dataset, each partitioned into Non-IID data distribution, the proposed FBMA framework exhibits high-performance metrics. The results highlight the efficacy of our proposed FBMA framework, indicating its potential for real-world applications where image classification demands both high accuracy and data privacy.

**Accession Number:** WOS:001310795800001

**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** convolutional neural network; deep learning; federated learning; medical image classification; multi-head attention mechanism

**KeyWords Plus:** ACCURACY; MODELS

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Firdaus, Naima		0000-0002-4067-2448

**Publisher:** WILEY

**Publisher Address:** 111 RIVER ST, HOBOKEN 07030-5774, NJ USA

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

**Web of Science Categories:** Computer Science, Software Engineering; Computer Science, Theory & Methods

**Research Areas:** Computer Science

**IDS Number:** F6G9Z

**ISSN:** 1532-0626

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**29-char Source Abbrev.:** CONCURR COMP-PRACT E

**ISO Source Abbrev.:** Concurr. Comput.-Pract. Exp.

**Source Item Page Count:** 28

**Output Date:** 2024-10-01

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### Record 3 of 29

**Title:** House of the People: Parliament and the Making of Indian Democracy

**Author(s):** Jha, S (Jha, Shefali)

**Source:** INDIAN ECONOMIC AND SOCIAL HISTORY REVIEW **DOI:**

10.1177/00194646241281184 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 21

**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:** 0

**Abstract:** Ronojoy Sen, House of the People: Parliament and the Making of Indian Democracy (Cambridge: Cambridge University Press, 2022), 311 pp.

**Accession Number:** WOS:001318372800001

**Language:** English

**Document Type:** Book Review; Early Access

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**Publisher:** SAGE PUBLICATIONS INDIA PVT LTD

**Publisher Address:** B-1-I-1 MOHAN CO-OPERATIVE INDUSTRIAL AREA, MATHURA RD, POST BAG NO 7, NEW DELHI 110 044, INDIA

**Web of Science Index:** Social Science Citation Index (SSCI); Arts & Humanities Citation Index (A&HCI)

**Web of Science Categories:** History

**Research Areas:** History

**IDS Number:** G7K1R

**ISSN:** 0019-4646

**eISSN:** 0973-0893

**29-char Source Abbrev.:** INDIAN ECON SOC HIST

**ISO Source Abbrev.:** Indian Econ. Soc. Hist. Rev.

**Source Item Page Count:** 3

**Output Date:** 2024-10-01

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#### **Record 4 of 29**

**Title:** Prediction of Ca<sup>2+</sup> Binding Site in Proteins With a Fast and Accurate Method Based on Statistical Mechanics and Analysis of Crystal Structures

**Author(s):** Basit, A (Basit, Abdul); Choudhury, D (Choudhury, Devapriya); Bandyopadhyay, P (Bandyopadhyay, Pradipta)

**Source:** PROTEINS-STRUCTURE FUNCTION AND BIOINFORMATICS **DOI:** 10.1002/prot.26743 **Early**

**Access Date:** SEP 2024 **Published Date:** 2024 SEP 11

**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:** 97

**Abstract:** Predicting the precise locations of metal binding sites within metalloproteins is a crucial challenge in biophysics. A fast, accurate, and interpretable computational prediction method can complement the experimental studies. In the current work, we have developed a method to predict the location of Ca<sup>2+</sup> ions in calcium-binding proteins using a physics-based method with an all-atom description of the proteins, which is substantially faster than the molecular dynamics simulation-based methods with accuracy as good as data-driven approaches. Our methodology uses the three-dimensional reference interaction site model (3D-RISM), a statistical mechanical theory, to calculate Ca<sup>2+</sup> ion density around protein structures, and the locations of the Ca<sup>2+</sup> ions are obtained from the density. We have taken previously used datasets to assess the efficacy of our method as compared to previous works. Our accuracy is 88%, comparable with the FEATURE program, one of the well-known data-driven methods. Moreover, our method is physical, and the reasons for failures can be ascertained in most cases. We have thoroughly examined the failed cases using different structural and crystallographic measures, such as B-factor, R-factor, electron density map, and geometry at the binding site. It has been found that x-ray structures have issues in many of the failed cases, such as geometric irregularities and dubious assignment of ion positions. Our algorithm, along with the checks for structural accuracy, is a major step in predicting calcium ion positions in metalloproteins.

**Accession Number:** WOS:001310070500001

**PubMed ID:** 39258438

**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** 3D-RISM; calcium ion prediction in proteins; improved curation of structures; statistical mechanics; validation with x-ray structures

**KeyWords Plus:** CA2+-BINDING SITES; ION-BINDING; METAL; CALCIUM; VALIDATION; PARAMETERS; DENSITY; NMR; CRYSTALLOGRAPHY; METALLOPROTEIN

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**Publisher:** WILEY  
**Publisher Address:** 111 RIVER ST, HOBOKEN 07030-5774, NJ USA  
**Web of Science Index:** Science Citation Index Expanded (SCI-EXPANDED)  
**Web of Science Categories:** Biochemistry & Molecular Biology; Biophysics  
**Research Areas:** Biochemistry & Molecular Biology; Biophysics  
**IDS Number:** F5F3L  
**ISSN:** 0887-3585  
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**29-char Source Abbrev.:** PROTEINS  
**ISO Source Abbrev.:** Proteins  
**Source Item Page Count:** 16  
**Funding:**

Funding Agency	Grant Number
Science and Engineering Research Board	BT/PR45865/BID/7/1016/2023
Department of Biotechnology (DBT) grant	BT/PR/40251/BITS/137/11/2021
DBT	
Jawaharlal Nehru University	MTR/2021/000365
MATRICS grant from SERB	

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**Output Date:** 2024-10-01

**Record 5 of 29**

**Title:** Determinants of livelihood vulnerability to climate change among the agrarian community: Empirical evidence from the coastal region of Indian Sundarban Biosphere Reserve  
**Author(s):** Das, S (Das, Shibu)  
**Source:** REGIONAL STUDIES IN MARINE SCIENCE **Volume:** 78 **Article Number:** 103777 **DOI:** 10.1016/j.rsma.2024.103777 **Early Access Date:** SEP 2024 **Published Date:** 2024 DEC 15  
**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:** 66

**Abstract:** The impacts of climate change on the livelihood of agrarian households on the coast of the Indian Sundaraban Biosphere Reserve have not been addressed. Thus, it is important to identify the underlying factors for livelihood vulnerability in this region and know how climate change-related events and socio-economic conditions affect them. This work aimed to measure six major domains of livelihood vulnerability, such as overall livelihood loss, livestock loss, crop and crop area loss, fishing area loss, housing loss, and income loss. I selected the ordered probit regression and focus group discussion approaches. Results revealed that the significant determinant factors of livelihood vulnerability were early warning system, education, land holding size, social group, type of house, occupation, distance to the local market and health centre, membership of self-help group, agreement with summer temperature increased, cyclone increased, flood increased, drought in Kharif season increased. In this region, several agrarian households have taken some adaptation measures such

as changing crop varieties, crop diversification, converting agriculture to fishery, and saline tolerant varieties. This approach is adaptable and can be put into practice on different levels, not just in other parts of India but also in diverse developing countries.

**Accession Number:** WOS:001311559600001

**Language:** English

**Document Type:** Article

**Author Keywords:** Agrarian community; Climate change; Coastal region of Indian Sundarban Biosphere Reserve; Determinant factors; Livelihood vulnerability; Mixed method approach; Mixed method approach

**KeyWords Plus:** HOUSEHOLD VULNERABILITY; IMPACT; HAZARDS; LEVEL; MODEL

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**Publisher:** ELSEVIER

**Publisher Address:** RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS

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

**Web of Science Categories:** Ecology; Marine & Freshwater Biology

**Research Areas:** Environmental Sciences & Ecology; Marine & Freshwater Biology

**IDS Number:** F7K3I

**ISSN:** 2352-4855

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**Source Item Page Count:** 19

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## Record 6 of 29

**Title:** Switching from positive to negative thermal expansion in a tetrayne-diol compound

**Author(s):** Sethi, T (Sethi, Tapaswini); Das, D (Das, Dinabandhu)

**Source:** CRYSTENGCOMM **Volume:** 26 **Issue:** 37 **Pages:** 5133-5137 **DOI:** 10.1039/d4ce00703d **Early**

**Access Date:** SEP 2024 **Published Date:** 2024 SEP 23

**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:** 65

**Abstract:** Switching from positive (PTE) to negative thermal expansion (NTE) in a molecular crystal is a rare phenomenon. Here we report the switching of PTE to NTE in 1,1'-(octa-1,3,5,7-tetrayne-1,8-diyl)dicyclopentanol (1) along the crystallographic a-axis. Small PTE has been observed from 100 K to 200 K due to zigzag packing arrangement and then the large transverse vibration overpowers the PTE resulting in NTE after 200 K.

Switching from positive to negative thermal expansion has been observed in 1,1'-(octa-1,3,5,7-tetrayne-1,8-diyl)dicyclopentanol due to a certain packing pattern and transverse vibration of atoms.

**Accession Number:** WOS:001308700200001

**Language:** English

**Document Type:** Article

**KeyWords Plus:** COLOSSAL; ZERO

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**Corresponding Address:** Das, D (corresponding author), Jawaharlal Nehru Univ, Sch Phys Sci, New Delhi 110067, India.

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**Publisher:** ROYAL SOC CHEMISTRY

**Publisher Address:** THOMAS GRAHAM HOUSE, SCIENCE PARK, MILTON RD, CAMBRIDGE CB4 0WF, CAMBS, ENGLAND

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

**Web of Science Categories:** Chemistry, Multidisciplinary; Crystallography

**Research Areas:** Chemistry; Crystallography

**IDS Number:** G6B9M

**eISSN:** 1466-8033

**29-char Source Abbrev.:** CRYSTENGCOMM

**ISO Source Abbrev.:** Crystengcomm

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DST	

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## Record 7 of 29

**Title:** Cosmopolitan elites: Indian diplomats and the social hierarchies of global order

**Author(s):** Guha, P (Guha, Pausali)

**Source:** INTERNATIONAL AFFAIRS **Volume:** 100 **Issue:** 5 **Pages:** 2282-2283 **DOI:** 10.1093/ia/iiae188 **Published Date:** 2024 SEP 9

**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:** 0

**Accession Number:** WOS:001315125500001

**Language:** English

**Document Type:** Book Review

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**Publisher:** OXFORD UNIV PRESS

**Publisher Address:** GREAT CLARENDON ST, OXFORD OX2 6DP, ENGLAND

**Web of Science Index:** Social Science Citation Index (SSCI)

**Web of Science Categories:** International Relations

**Research Areas:** International Relations

**IDS Number:** G2Q0F

**ISSN:** 0020-5850

**eISSN:** 1468-2346

**29-char Source Abbrev.:** INT AFF

**ISO Source Abbrev.:** Int. Aff.

**Source Item Page Count:** 2

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**Record 8 of 29**

**Title:** An enhanced localization algorithm for 3D wireless sensor networks using group learning optimization

**Author(s):** Niranjana, M (Niranjana, Maheshwari); Sinha, A (Sinha, Adwitiya); Singh, B (Singh, Buddha)

**Source:** SADHANA-ACADEMY PROCEEDINGS IN ENGINEERING SCIENCES **Volume:** 49 **Issue:** 3 **Article Number:** 248 **DOI:** 10.1007/s12046-024-02588-8 **Published Date:** 2024 SEP 3

**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:** 34

**Abstract:** Localization in sensor communication is considered one of the most foundational concepts that facilitates targeted monitoring, optimized deployment, and real-time navigation. The localization algorithms have several applications, including asset tracking, environmental monitoring, industrial automation, and other location-based services. This drives the need for continually refining and enhancing localization techniques for three-dimensional sensor networks. The DV-Hop is a widely used localization technique owing to its lesser range requirements, easy to implement, and suitable for large-scale network of sensors. In this research, we have proposed an enhanced group learning optimization-based three-dimensional DV-Hop algorithm, termed as GL-3DDVHop. The proposed method overcomes the limitations of the original variant of DV-Hop and extended it to three-dimensional environment. In the proposed approach, the communication ring partitioning-based location aware node selection approach is developed to calculate the hopsize of location aware node. The correction factor for hopsize refinement is also added to obtain the corrected distances between location unaware node and location aware nodes in terms of the modified hopsize and hop count. Finally, group learning optimization technique is used to estimate the position coordinates of location unaware nodes. According to our experimentation conducted for 3D wireless sensor network, the localization accuracy of GL-3DDVHop surpassed its existing counterparts, namely 3DDV-Hop and PSO-3DDVHop techniques by 9% and 3%, respectively.

**Accession Number:** WOS:001304016600001

**Language:** English

**Document Type:** Article

**Author Keywords:** Wireless sensor network; Localization; Hop-size correction; Group learning optimization; DV-hop localization

**KeyWords Plus:** PARTICLE SWARM OPTIMIZATION; RANGE-FREE LOCALIZATION

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**Publisher:** SPRINGER INDIA

**Publisher Address:** 7TH FLOOR, VIJAYA BUILDING, 17, BARAKHAMBHA ROAD, NEW DELHI, 110 001, INDIA

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

**Web of Science Categories:** Engineering, Multidisciplinary

**Research Areas:** Engineering

**IDS Number:** E6I3K

**ISSN:** 0256-2499

**eISSN:** 0973-7677

**29-char Source Abbrev.:** SADHANA-ACAD P ENG S

**ISO Source Abbrev.:** Sadhana-Acad. Proc. Eng. Sci.

**Source Item Page Count:** 16

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## **Record 9 of 29**

**Title:** Deciphering Sino-Indian blue mining competencies in the Indo-Pacific

**Author(s):** Yadav, D (Yadav, Dhanwati)

**Source:** MARINE POLICY **Volume:** 170 **Article Number:** 106378 **DOI:** 10.1016/j.marpol.2024.106378 **Early Access Date:** SEP 2024 **Published Date:** 2024 DEC

**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:** 71

**Abstract:** Minerals beneath the sea are posited to have a ripple effect on the country's economy. An incessant rush to ocean mining by nations has launched a costly battle for minerals never preceded. China, in the race has emerged a prospective performer after charging the global electronic market direly fed by critical minerals. The imported rare earth by China is of special significance here in prolonging its strategic monopoly over the supply of minerals and rare earth derivatives to the world. India, another pioneer investor with a promising economy, is also increasingly scrambling to mine the deep sea for its mineral satiety and to overcome its longstanding dependency on Beijing. China's ascending control in the international rare earth market has also had a strategic impact on other countries, who are hunting for an alternative to China's sway. India, with its developing capabilities in undersea mining and partnered manufacturing of high-end products could settle their quest at large. Its advances in seabed mining are also eulogized by the ISA (director). The paper, given this backdrop probes into certain aspects vital to uncover the competencies of India and China in securing their multi-layered blue mining goals. This may immensely interest the world economies that inexorably have a bearing of the globalized supply chain of minerals and propose for resource-based geopolitics.

**Accession Number:** WOS:001309910200001

**Language:** English

**Document Type:** Article

**Author Keywords:** Seabed mining; Strategic; India; China; ISA; Critical minerals

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**Publisher:** ELSEVIER SCI LTD  
**Publisher Address:** 125 London Wall, London, ENGLAND  
**Web of Science Index:** Social Science Citation Index (SSCI)  
**Web of Science Categories:** Environmental Studies; International Relations  
**Research Areas:** Environmental Sciences & Ecology; International Relations  
**IDS Number:** F4Z3B  
**ISSN:** 0308-597X  
**eISSN:** 1872-9460  
**29-char Source Abbrev.:** MAR POLICY  
**ISO Source Abbrev.:** Mar. Pol.  
**Source Item Page Count:** 9  
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## **Record 10 of 29**

**Title:** PerR: A Peroxide Sensor Eliciting Metal Ion-dependent Regulation in Various Bacteria  
**Author(s):** Kandari, D (Kandari, Divya); Joshi, H (Joshi, Hemant)  
**Source:** MOLECULAR BIOTECHNOLOGY **DOI:** 10.1007/s12033-024-01266-8 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 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:** 59

**Abstract:** Bacteria have to thrive in difficult conditions wherein their competitors generate partially reduced forms of oxygen, like hydrogen peroxide and superoxides. These oxidative stress molecules can also arise from within via the autoxidation of redox enzymes. To adapt to such conditions, bacteria express detox enzymes as well as repair proteins. Transcription factors regulate these defenses, and PerR is one of them. PerR is a Fur family transcriptional regulator that senses peroxide stress. Metal-bound PerR (either Mn<sup>2+</sup> or Fe<sup>2+</sup>) can repress transcription of its regulon, but only the Fe<sup>2+</sup>-bound form of PerR can sense H<sub>2</sub>O<sub>2</sub>. This review describes different aspects of PerR and its varied roles, specifically in bacterial pathogens. Despite having roles beyond sensing peroxides, it is an underrated regulator that needs to be explored more deeply in pathogens.

**Accession Number:** WOS:001315053900001

**PubMed ID:** 39294512

**Language:** English

**Document Type:** Review; Early Access

**Author Keywords:** Oxidative stress; Pathogenic bacteria; Metalloregulator; Virulence; Transcription factor

**KeyWords Plus:** OXIDATIVE STRESS RESISTANCE; BACILLUS-SUBTILIS; HYDROGEN-PEROXIDE; CRYSTAL-STRUCTURE; IRON; VIRULENCE; FUR; REGULON; MANGANESE; CATALASE

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**Publisher:** SPRINGER NATURE

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

**Web of Science Categories:** Biochemistry & Molecular Biology; Biotechnology & Applied Microbiology

**Research Areas:** Biochemistry & Molecular Biology; Biotechnology & Applied Microbiology

**IDS Number:** G2N3D

**ISSN:** 1073-6085

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**29-char Source Abbrev.:** MOL BIOTECHNOL

**ISO Source Abbrev.:** Mol. Biotechnol.

**Source Item Page Count:** 12

**Output Date:** 2024-10-01

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## Record 11 of 29

**Title:** Surface-directed dynamics in living liquid crystals

**Author(s):** Vats, A (Vats, Aditya); Banerjee, V (Banerjee, Varsha); Puri, S (Puri, Sanjay)

**Source:** PHYSICAL REVIEW E **Volume:** 110 **Issue:** 3 **Article Number:** 034701 **DOI:** 10.1103/PhysRevE.110.034701 **Published Date:** 2024 SEP 3

**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:** 63

**Abstract:** We study living liquid crystals (LLCs), which are an amalgam of nematic liquid crystals (LCs) and active matter (AM). These LLCs are placed in contact with surfaces which impose planar/homeotropic boundary conditions on the director field of the LC and the polarization field of the AM. The interplay of LC-AM interactions and the surface-directed conditions yield controlled pattern dynamics in the LLC, which has important technological implications. We discuss two representative examples of this pattern dynamics.

**Accession Number:** WOS:001309864400006

**Language:** English

**Document Type:** Article

**KeyWords Plus:** BACTERIA; DEFECTS

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**Publisher:** AMER PHYSICAL SOC

**Publisher Address:** ONE PHYSICS ELLIPSE, COLLEGE PK, MD 20740-3844 USA

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**Research Areas:** Physics

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Open Access: Green Submitted  
Output Date: 2024-10-01

Record 12 of 29

**Title:** Design and Simulation of Circular Dielectric Resonator Antenna and Investigation of Structure, Microstructure, and Dielectric Properties of Mn-Modified  $\text{Sr}_{2-x}\text{SnO}_4$

**Author(s):** Kumar, U (Kumar, Upendra); Yadav, V (Yadav, Vedika); Kumar, R (Kumar, Raj); Singh, P (Singh, Pinki)

**Source:** PHYSICA STATUS SOLIDI A-APPLICATIONS AND MATERIALS SCIENCE **DOI:** 10.1002/pssa.202400523 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 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:** 46

**Abstract:** Samples with compositions of  $\text{Sr}_2\text{Sn}_{1-x}\text{Mn}_x\text{O}_4$  (SSM) with  $0 \leq x \leq 0.10$  are prepared by conventional ceramic route via heat treatment at 1350 degrees C. Phase and crystal structure analysis is studied using X-ray diffraction and Rietveld refinement to confirm the crystallization of samples in the tetragonal structure under space group  $I4/mmm$ . The size-strain plot method is employed to identify the role of Mn on crystallite size/microstrain/dislocation density. The scanning electron microscope and energy-dispersive X-ray spectroscopy analysis confirm a significant change in the grain size and compositional homogeneity of all samples with Mn-doping. Dielectric properties of samples are explained in terms of interfacial and orientation polarization of dipoles  $\text{Sn}-\text{Sn}^{4+}(2+)''-\text{V}-\text{O} \cdot \cdot \cdot \cdot 2\text{Mn}(2\text{Mn}^{3+})(2+)'\text{-VO} \cdot \cdot \cdot \cdot$  Modulus studies show the exclusion of electrode contribution from the electrical properties. The single-segment circular dielectric resonator antenna is designed with the help of experimental dielectric parameters and showed two major resonant frequencies at 3.6 and 6.7 GHz. The reduction in the S11 parameter and -10 dB reflection coefficient bandwidth with Mn-doping observed due to overlapping of the E-field line suggests the application in patch array antenna for radar and satellite communication applications. This study also enables to explore  $\text{Sr}_2\text{SnO}_4$ -based Ruddlesden Popper oxide for antenna and mm-wave communication applications.

**Accession Number:** WOS:001318491900001  
**Language:** English  
**Document Type:** Article; Early Access

**Author Keywords:** arrhenius transport; dielectric resonator antenna; nyquist plot; rietveld refinement; ruddlesden popper oxide

**KeyWords Plus:** MICROWAVE; CERAMICS

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**Publisher:** WILEY-V C H VERLAG GMBH

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

**Web of Science Categories:** Materials Science, Multidisciplinary; Physics, Applied; Physics, Condensed Matter

**Research Areas:** Materials Science; Physics

**IDS Number:** G7O7K

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**Output Date:** 2024-10-01

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## Record 13 of 29

**Title:** Blockchain and Quantum Machine Learning Driven Energy Trading for Electric Vehicles

**Author(s):** Kashyap, PK (Kashyap, Pankaj Kumar); Dohare, U (Dohare, Upasana); Kumar, M (Kumar, Manoj); Kumar, S (Kumar, Sushil)

**Source:** AD HOC NETWORKS **Volume:** 165 **Article Number:** 103632 **DOI:**

10.1016/j.adhoc.2024.103632 **Early Access Date:** SEP 2024 **Published Date:** 2024 DEC 1

**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:** 53

**Abstract:** With the steep growth of Electric Vehicles (EV's), the consequent demand of energy for charging puts significant load to powergrids. Renewable Energy Sources enabled microgrids can alleviate the problem of energy demand and trade the energy locally in Peer-to-Peer (P2P) manner, where seller (microgrid) and buyer

(EV's) "meet" to trade electricity directly on agreed term without any intermediary. However, a foolproof system required for audit and verification of transaction record between seller and buyer to address privacy and security in untrusted and opaque local energy trading market (LETM). Centralized public blockchain enabled system (for audit the transaction records and storage) based on conventional learning models faces mainly two issues in the LETM. (a) if, centralize system runs out of energy and tear down then whole energy trading plunges treated as single point of failure (b) Conventional learning models fail to converge optimal point in case of large state and action space (large number of EV's and their energy demand). The primary objective of this paper to provide secure system for LETM, 1) Distributed nature of Consortium Blockchain used that solve the problem of single point of failure to audit and storage of transaction and profile info of microgrids and EV's. 2) Quantum based Reinforcement Learning (QRL) easily handles the large number of EV's energy supply and demand for smoothly run LETM. In this context, this paper presents Blockchain and Quantum Machine Learning driven energy trading model for EVs (B-MET). A utility maximization problem formulated as Markov Decision Process (MDP) and their solution provided by using QRL focusing on join optimization of selling price, loan amount and quantity of shared energy. MDP is a mathematical framework used to model decision-making in situations where outcomes are partly random and partly under the control of a decision-maker, i.e., the future state depends only on the current state and action, not on the sequence of events that preceded it. QRL method combines quantum theory with traditional RL. It is inspire by the principles of state superposition and quantum parallelism. Convergence analysis and performance results attest that B-MET convergences faster, maximizes the utility with lower confirmation delay in P2P energy trading as compare to state of the art techniques.

**Accession Number:** WOS:001306919500001

**Language:** English

**Document Type:** Article

**Author Keywords:** Blockchain; Electric Vehicles; Quantum Reinforcement Learning; Energy Trading; Smart Contract

**KeyWords Plus:** REINFORCEMENT; COORDINATION; MANAGEMENT

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**Publisher:** ELSEVIER

**Publisher Address:** RADARWEG 29, 1043 NX AMSTERDAM, NETHERLANDS

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**Research Areas:** Computer Science; Telecommunications

**IDS Number:** F0P2M

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**29-char Source Abbrev.:** AD HOC NETW

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**Source Item Page Count:** 18

**Record 14 of 29**

**Title:** Full body sensillar diversity of pumpkin fruit fly, *Bactrocera tau* (Walker) (Diptera: Tephritidae)

**Author(s):** Rana, A (Rana, Alka); Sharma, D (Sharma, Dixit); Thakur, H (Thakur, Himanshu); Thakur, P (Thakur, Pankaj); Kumar, S (Kumar, Sunil)

**Source:** ZOOMORPHOLOGY **DOI:** 10.1007/s00435-024-00680-5 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 11

**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:** 66

**Abstract:** The pumpkin fruit fly, *Bactrocera tau* (Walker) (Diptera: Tephritidae) is one of the most serious insect pests of fruits, vegetables and nuts over the world due to its polyphagous nature and high reproductive rate. To gain insight into their sensory system, the external morphology, typology, density, and distribution of sensilla on full bodies of both adult male and female *B. tau* were observed using a scanning electron microscope. The observed sensilla showed organ as well as sex specific differences. Seven previously described sensilla (two non-olfactory, five olfactory with 17 subtypes) and a new sensillum named as "branched sensilla" (two subtypes) were identified and observed on the different body parts. Olfactory sensilla named as sensilla trichodea and sensilla basiconica were reported on the compound eyes for the first time. Majority of the olfactory sensilla were reported on the head appendages. The presence of species-specific as well as sex-specific branched sensilla in females showed different typology patterns of sensilla. The potential roles of observed sensilla were hypothesized through comparative analysis with prior research. The current findings can provide a reference for understanding the diversity of various olfactory and non-olfactory sensilla in *B. tau* as well as sex-specific morphological differences and functions of various body parts; thereby, aiding in the development of precise methods for regulating and managing insect behaviour.

**Accession Number:** WOS:001309916200001

**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** Sensilla; Olfaction; *Bactrocera tau*; Morphology; SEM

**KeyWords Plus:** ANTENNAL SENSILLA; MAXILLARY PALP; FINE-STRUCTURE; COLEOPTERA; MORPHOLOGY

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[Thakur, Pankaj] Jawaharlal Nehru Univ, Dept Nanosci, New Delhi 110067, India.

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Author	Web of Science ResearcherID	ORCID Number
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**Publisher:** SPRINGER

**Publisher Address:** ONE NEW YORK PLAZA, SUITE 4600, NEW YORK, NY, UNITED STATES

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**Research Areas:** Anatomy & Morphology; Zoology

**IDS Number:** F4Z5I

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**Output Date:** 2024-10-01

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## Record 15 of 29

**Title:** THF induces apoptosis by downregulating initiation, promotion, and progression phase biomarkers in skin and lung carcinoma

**Author(s):** Raza, W (Raza, Waseem); Meena, A (Meena, Abha); Luqman, S (Luqman, Suaib)

**Source:** JOURNAL OF BIOCHEMICAL AND MOLECULAR TOXICOLOGY **Volume:** 38 **Issue:** 9 **Article Number:** e23838 **DOI:** 10.1002/jbt.23838 **Published Date:** 2024 SEP

**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:** 80

**Abstract:** 3,5,7-Trihydroxy-2-phenylchromen-4-one (THF) possesses a diverse range of pharmacological activities. Evidence suggests that THF exerts anticancer activity by distinct mechanisms of action. This study explores the anticancer potential of THF in human lung (A549) and skin (A431) cancer cells by employing different antiproliferative assays. 3-(4,5-Dimethylthiazol-2-yl)-2,5-diphenyltetrazolium bromide, neutral red uptake, sulphorhodamine B, and cell motility assays were used to confirm the anticancer potential of THF. Cell target-based and quantitative reverse transcription polymerase chain reaction (qRT-PCR) assays were used to explore the effect of THF on the initiation, promotion and progression phase biomarkers of carcinogenesis. THF suppresses the activity of lipoxygenase-5 up to similar to 40% in both A549 and A431 cells and up to similar to 50% hyaluronidase activity in A549 cells. qRT-PCR assay reveals that THF inhibits the activity of phosphatidylinositol-3 kinase/protein kinase B/mammalian target of rapamycin in both cell lines, which is responsible for the initiation of cancer. It also arrests the G2/M phase of the cell cycle in A431 cells and increases the sub-diploid population in both A549 and A431 cell lines which leads to cell death. Annexin V-FITC assay confirmed that THF induces apoptosis and necrosis in A431 and A549 cell lines. Further investigation revealed that THF not only enhances reactive oxygen species production but also modulates mitochondrial membrane potential in both cell lines. It significantly inhibits S-180 tumour formation at 5 and 10 mg/kg bw, i.p. dose. An acute skin toxicity study on mice showed that erythema and edema scores are within the acceptable range, besides acceptable drug-likeness properties and non-toxic effects on human erythrocytes. Conclusively, THF showed potent anticancer activity on skin and lung carcinoma cell lines, suppressed the level of the biomarkers and inhibited tumour growth in mice.

**Accession Number:** WOS:001308113000001



**PubMed ID:** 39243196

**Language:** English

**Document Type:** Article

**Author Keywords:** apoptosis; cell-cycle; Hyaluronidase; necrosis; S-180; THF

**KeyWords Plus:** HEPATOCELLULAR-CARCINOMA; GALANGIN SUPPRESSES; CANCER-CELLS; INHIBITION; PROLIFERATION; ANTICANCER; PATHWAY; GROWTH; ASSAY; TUMOR

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Meena, Abha	AAE-2270-2022	
MEENA, ABHA		0000-0002-1014-1486
Luqman, Suaib		0000-0001-6568-8107

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**Research Areas:** Biochemistry & Molecular Biology; Toxicology

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SERB, New Delhi, India	

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**Output Date:** 2024-10-01

**Title:** Activation of Induced Systemic Resistance in Cotton Plants Against *Fusarium* and *Macrophomina* by Microbial Antagonists

**Author(s):** Poria, V (Poria, Vikram); Jhiltia, P (Jhiltia, Prakriti); Kumar, S (Kumar, Sandeep); Rana, A (Rana, Anuj); Pranaw, K (Pranaw, Kumar); Singh, S (Singh, Surender)

**Source:** JOURNAL OF PLANT GROWTH REGULATION **DOI:** 10.1007/s00344-024-11495-5 **Early**

**Access Date:** SEP 2024 **Published Date:** 2024 SEP 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:** 120

**Abstract:** The use of microbial antagonists (MAs) against phytopathogens is a cost-effective, environmentally sustainable strategy that successfully enhances crop yield. In this study, we evaluated the in-planta efficacy of multistress-tolerant MAs isolated previously from the cotton rhizosphere showing high antagonistic activity against *Macrophomina phaseolina* and *Fusarium oxysporum*. During pathogenicity testing, *M. phaseolina* was found more aggressive compared to *F. oxysporum* as indicated by disease area percentage on cotton seeds but the use of MAs lowered the seed mortality rate (0-20%) in the pot experiment compared to pathogen control (47-60%) indicating their high antagonistic potential. The mode of antagonism was investigated by identifying antifungal metabolites and volatile organic compounds secreted by these agents using HPLC-MS and GC-MS coupled with SPME fiber, respectively, which revealed compounds like iturins, surfactins, mixirins, fengycins, undecanone, involved in the activation of induced systemic resistance (ISR) along with the antifungal activity. The increased levels of two defense enzymes, polyphenol oxidase [110-180% increase over absolute control (IOC)] and phenylalanine ammonia-lyase (22-58% IOC), and three antioxidant enzymes, catalase (36-98% IOC), peroxidase (44-71% IOC), and superoxide dismutase (72-145% IOC) in MA-treated plants confirmed the activation of ISR against both pathogens. The proline, total phenolic, and glycine betaine contents also increased in the MAs-treated plants, whereas a decreased malondialdehyde content was observed. These results indicate that these MAs are reliable and sustainable options for enhancing crop growth and that their bioformulations can be used to control fungal pathogens and help plants endure biotic and abiotic stresses.

**Accession Number:** WOS:001318539500001

**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** Biocontrol; Induced systemic resistance; Iturins; Phytopathogens; Root rot; Surfactins

**KeyWords Plus:** ANTIFUNGAL ACTIVITY; IN-VITRO; BACILLUS-AMYLOLIQUEFACIENS; CYCLIC LIPOPEPTIDES; ANALOGS; STREPTOMYCETES; IDENTIFICATION; INHIBITION; BIOCONTROL; PEPTIDES

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**Publisher:** SPRINGER

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**Web of Science Categories:** Plant Sciences

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**IDS Number:** G7Q5R

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**Output Date:** 2024-10-01

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## Record 17 of 29

**Title:** Phytochemicals and Nanotechnology: A Powerful Combination against Breast Cancer

**Author(s):** Shafi, S (Shafi, Sadat); Ahmed, F (Ahmed, Faraha); Waheed, A (Waheed, Ayesha); Ahmad, SS (Ahmad, Syed Sufiyan); Khan, S (Khan, Sana); Khan, MA (Khan, Mohammad Ahmed); Pottoo, FH (Pottoo, Faheem Hyder); Rabbani, SA (Rabbani, Syed Arman); Singh, S (Singh, Shailja); Najmi, A (Najmi, Abul Kalam)

**Source:** MINI-REVIEWS IN MEDICINAL CHEMISTRY **DOI:**

10.2174/0113895575297312240903055926 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 13

**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:** 175

**Abstract:** Considerable advancements have been made in breast cancer therapeutics in the past few decades. However, the advent of chemo-resistance and adverse drug reactions coupled with tumor metastasis and recurrence posed a serious threat to combat this lethal disease. Novel anti-cancer agents, as well as new therapeutic strategies, are needed to complement conventional breast cancer therapies. The quest for developing novel anti-cancer drugs caused an upsurge in exploring and harnessing natural compounds, especially phytochemicals. Various research groups have explored and documented the anti-cancer potential of wide variety of phytochemical groups including flavonoids (curcumin, kaempferol, myricetin, quercetin, naringenin, apigenin, genistein epigallocatechin gallate), stilbenes (resveratrol), carotenoids (crocin, lycopene, lutein), and anthraquinone (Emodin). However, low chemical stability, poor water solubility, and short systemic half-life impede their clinical utility. The implication of nano-technological approaches to decode the pharmacokinetic challenges associated with phytochemical usage, as well as selective drug targeting, have markedly enhanced the pre-clinical anti-cancer activity, thus aiding in their clinical translation. This review documented the recent advances in utilizing phytochemicals for breast cancer prevention and lipid-based nanotechnological approaches for circumventing their pharmacokinetic concerns to enhance their systemic availability, cytotoxicity, and targeted delivery against breast cancer alone as well as in combination with conventional therapeutic agents.

**Accession Number:** WOS:001315933900001

**PubMed ID:** 39279694

**Language:** English

**Document Type:** Review; Early Access

**Author Keywords:** Breast cancer; phytochemicals; flavonoids; lipid nano-carriers; liposomes; lipid nanocapsules

**KeyWords Plus:** SOLID LIPID NANOPARTICLES; FATTY-ACID SYNTHASE; DRUG-DELIVERY; FORMULATION OPTIMIZATION; ALPHA EXPRESSION; DOWN-REGULATION; CELL-GROWTH; STEM-CELLS; 3 SUBTYPES; CURCUMIN

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**Record 18 of 29**

**Title:** Structural insights into polyethylene terephthalate (PET)-degrading archaeal lipase enzyme: An *in silico* approach

**Author(s):** Puri, P (Puri, Prathana); Pandey, K (Pandey, Kamini); Khuman, AB (Khuman, Aniruddha Bhai); Kumar, S (Kumar, Shubham); Mehtab, S (Mehtab, Sameena); Chaudhary, B (Chaudhary, Bhupendra); Singhal, B (Singhal, Barkha)

**Source:** BIOREMEDIATION JOURNAL **DOI:** 10.1080/10889868.2024.2404880 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 14

**Times Cited in Web of Science Core Collection:** 0

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**Abstract:** Biodegradation of plastic is the most eco-friendly degradation process conferred by various microbial enzymes, especially the lipase enzymes. The lipase enzymes depict a broad substrate range, high regio/stereoselectivity, and stability in organic solvents. However, enhancing the catalytic activity of lipases for industrial production remains a challenge, predominantly due to the need for their extensive mechanistic characterization. Here, we employed a multidisciplinary approach to illustrate the comprehensive physiochemical and mechanical properties of 102 lipase sequences from six different groups of plastic-degrading microorganisms. Molecular docking-based evaluation of the binding efficiencies of selected lipases with the most common plastic polymers- polyurethane (PUR) and polyethylene terephthalate (PET), revealed that the archaeal lipase had the lowest binding energy of -7.1 kcal/mol with PET. Remarkably, the molecular dynamic simulation studies (up to 100 ns) and very low RMSD (0.3 nm) and RMSF (0.25 nm) values further ascertained the stability of archaeal lipase after binding with PET polymer. Further, a 2.19 nm radius of gyration (Rg) within 100 ns simulation time, binding free energy  $\Delta G(\text{TOTAL})$  with -24.36 kcal/mol and entropy factor  $-T \Delta S$  7.65 kcal/mol also indicated strong binding of archaeal lipase with PET polymer. The mechanistic exploration of archaeal lipase yielded valuable insights into its effective binding with PET polymer, paving the way for future lipase enzyme engineering and harnessing its industrial potential for plastic biodegradation.

**Accession Number:** WOS:001317545300001

**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** Biodegradation; environmental sustainability; lipase; molecular docking; PET; plastic

**KeyWords Plus:** MOLECULAR-DYNAMICS SIMULATIONS; MICROBIAL LIPASES; PROTEIN; FEATURES; WEB

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**Output Date:** 2024-10-01

**Record 19 of 29**

**Title:** Gut microbiota derived short-chain fatty acids in physiology and pathology: An update

**Author(s):** Archana (Archana, Abhijeet Kumar); Gupta, AK (Gupta, Abhijeet Kumar); Noumani, A (Noumani, Ashab); Panday, DK (Panday, Dharmendra Kumar); Zaidi, F (Zaidi, Fareen); Sahu, GK (Sahu, Gaurav Kumar); Joshi, G (Joshi, Gunjan); Yadav, M (Yadav, Manisha); Borah, SJ (Borah, Shikha Jyoti); Susmitha, V (Susmitha, Vanne); Mohan, A (Mohan, Anand); Kumar, A (Kumar, Anil); Solanki, PR (Solanki, Pratima R.)

**Source:** CELL BIOCHEMISTRY AND FUNCTION **Volume:** 42 **Issue:** 7 **Article Number:** e4108 **DOI:** 10.1002/cbf.4108 **Published Date:** 2024 SEP

**Times Cited in Web of Science Core Collection:** 0

**Total Times Cited:** 0

**Usage Count (Last 180 days):** 3

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**Cited Reference Count:** 205

**Abstract:** Short-chain fatty acids (SCFAs) are essential molecules produced by gut bacteria that fuel intestinal cells and may also influence overall health. An imbalance of SCFAs can result in various acute and chronic diseases, including diabetes, obesity and colorectal cancer (CRC). This review delves into the multifaceted roles of SCFAs, including a brief discussion on their source and various gut-residing bacteria. Primary techniques used for detection of SCFAs, including gas chromatography, high-performance gas chromatography, nuclear magnetic resonance and capillary electrophoresis are also discussed through this article. This review study also compiles various synthesis pathways of SCFAs from diverse substrates such as sugar, acetone, ethanol and amino acids. The different pathways through which SCFAs enter cells for immune response regulation are also highlighted. A major emphasis is the discussion on diseases associated with SCFA dysregulation, such as anaemia, brain development, CRC, depression, obesity and diabetes. This includes exploring the relationship between SCFA levels across ethnicities and their connection with blood pressure and CRC. In conclusion, this review highlights the critical role of SCFAs in maintaining gut health and their implications in various diseases, emphasizing the need for further research on SCFA detection, synthesis and their potential as diagnostic biomarkers. Future studies of SCFAs will pave the way for the development of novel diagnostic tools and therapeutic strategies for optimizing gut health and preventing diseases associated with SCFA dysregulation. Understanding the role of short-chain fatty acids (SCFAs) is crucial because they are fundamental to maintaining colonic health and overall bodily function. Imbalances in SCFAs are linked to serious conditions like diabetes, obesity and colorectal cancer, making it essential to explore their regulation and impact.

Additionally, studying the variations in SCFA levels across different ethnicities can provide insights into disease susceptibility and health disparities. Furthermore, advancing detection methods and developing sensors for SCFAs could revolutionize diagnostics, allowing for earlier and more precise intervention in metabolic and gut-related diseases. Thus, this review addresses significant gaps in knowledge and technology that could lead to better health outcomes.

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**Language:** English

**Document Type:** Review

**Author Keywords:** diseases; gut microbiota; metabolites; sensors; short-chain fatty acids

**KeyWords Plus:** GAS CHROMATOGRAPHY/MASS SPECTROMETRY; PERFORMANCE LIQUID-CHROMATOGRAPHY; BUTYRATE-PRODUCING BACTERIA; WOOD-LJUNGDAHL PATHWAY; HUMAN FECES; REACTOR MICROBIOMES; AMINO-ACIDS; CAPILLARY-ELECTROPHORESIS; CLOSTRIDIUM-KLUYVERI; MEGASPHAERA-ELSDENII

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## **Record 20 of 29**

**Title:** Re-inventing traditional aluminum-based adjuvants: Insight into a century of advancements

**Author(s):** Gogoi, H (Gogoi, Himanshu); Mani, R (Mani, Rajesh); Bhatnagar, R (Bhatnagar, Rakesh)

**Source:** INTERNATIONAL REVIEWS OF IMMUNOLOGY **DOI:** 10.1080/08830185.2024.2404095 **Early**

**Access Date:** SEP 2024 **Published Date:** 2024 SEP 17

**Times Cited in Web of Science Core Collection:** 0

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**Usage Count (Since 2013):** 0

**Cited Reference Count:** 144

**Abstract:** Aluminum salt-based adjuvants like alum, alhydrogel and Adju-Phos are by far the most favored clinically approved vaccine adjuvants. They have demonstrated excellent safety profile and currently used in vaccines against diphtheria, tetanus, pertussis, hepatitis B, anthrax etc. These vaccinations cause minimal side effects like local inflammation at the injection site. Aluminum salt-based adjuvants primarily stimulate CD4+ T cells and B cell mediated Th2 immune response leading to generate a robust antibody response. In this review article, we have compiled the role of physio-chemical role of the two commonly used aluminum salt-based adjuvants alhydrogel and Adju-Phos, and the effect of surface properties, buffer composition, and adjuvant dosage on the immune response. After being studied for almost a century, researchers have come up with various mechanism by which these aluminum adjuvants activate the immune system. Firstly, we have covered the initial works of Glenny and his "repository effect" which paved the work for his successors to explore the involvement of cytokines, chemokines, recruitment of innate immune cells, enhanced antigen uptake by antigen presenting cells, and formation of NLRP3 inflammasome complex in mediating the immune response. It has been reported that aluminum adjuvants activate multiple immunological pathways which synergistically activates the immune system. We later discuss the recent developments in nanotechnology-based preparations of next generation aluminum based adjuvants which has enabled precise size control and morphology of the traditional aluminum adjuvants thereby manipulating the immune response as per our desire. Aluminum salt adjuvants like alum, aluminum hydroxide gel, and aluminum phosphate have been regularly used in vaccine formulations to potentiate the immune response. Despite being discovered nearly a century ago by Alexander Glenny, the cellular and molecular mechanism behind the working of these adjuvants is still elusive. In this article, we review the advances made in understanding the mechanism of action of these adjuvants. Firstly, we cover the "repository theory" put forward by Glenny, and gradually review the role of innate and adaptive immune cells, immune complexes, and different immunological pathways in aluminum adjuvant orchestrated immune response. We also take a dig into the role of physio-chemical parameters like surface properties, buffer composition and adjuvant dosage of aluminum adjuvants in eliciting an immune response. Finally, we discuss the advances made by nano-preparations of aluminum adjuvants and their diverse physio-chemical properties as well as hypothesize their probable mechanism of action.

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**PubMed ID:** 39310923

**Language:** English

**Document Type:** Review; Early Access

**Author Keywords:** Adju-Phos; adjuvant; alhydrogel; antigen presenting cells; cytokines; depot effect; inflammasome complex; nanotechnology; vaccine

**KeyWords Plus:** HEPATITIS-B-VACCINE; RECOMBINANT PROTECTIVE ANTIGEN; HYDROXIDE NANOPARTICLES SHOW; DENDRITIC CELL-POPULATIONS; IMMUNE-RESPONSE; MACROPHAGIC



MYOFASCIITIS; PARTICLE-SIZE; INFLAMMATORY RESPONSE; ANTIBODY-PRODUCTION;  
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## Record 21 of 29

**Title:** Overexpression of CBK1 or deletion of SSD1 confers fludioxonil resistance in yeast by suppressing Hog1 activation

**Author(s):** Kundu, D (Kundu, Debasree); Martoliya, Y (Martoliya, Yogita); Sharma, A (Sharma, Anupam); Sasan, SP (Sasan, Soorya Partap); Wasi, M (Wasi, Mohd); Prasad, R (Prasad, Rajendra); Mondal, AK (Mondal, Alok K.)

**Source:** GENE **Volume:** 933 **Article Number:** 148905 **DOI:** 10.1016/j.gene.2024.148905 **Early Access**

**Date:** SEP 2024 **Published Date:** 2025 JAN 15

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**Cited Reference Count:** 46

**Abstract:** Group III hybrid histidine kinases (HHK3) are known molecular targets of the widely used fungicidal agent fludioxonil which indirectly converts these kinases to a phosphatase form that causes constitutive activation of Hog1 MAPK. To better understand the fungicidal effect of fludioxonil we have screened *S. cerevisiae* haploid deletion collection for fludioxonil resistant mutant and identified Ssd1 as a critical factor for this. Deletion of SSD1 not only promoted resistance to fludioxonil but also abrogated Hog1 activation and other cellular damages caused by fludioxonil. Our results showed that fludioxonil perturbed the localization of Cbk1 kinase, an essential protein in yeast, at the bud neck triggering the accumulation of Ssd1 in P-bodies. As a result, localized synthesis of Ssd1 bound mRNA encoding cell wall proteins at the polarized

growth site was impaired which created a sustained cell wall stress causing constitutive activation of Hog1. Our data, for the first time, clearly indicated the role of Cbk1 upstream of Hog1 and provided a novel paradigm in the mechanism of action of fludioxonil.

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**PubMed ID:** 39218413

**Language:** English

**Document Type:** Article

**KeyWords Plus:** HYBRID HISTIDINE KINASES; POLARIZED GROWTH; SACCHAROMYCES; FAMILY; VIRULENCE; GENE; MORPHOGENESIS; LOCALIZATION; SENSITIVITY; RESPONSES

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**Title:** Ensuring Sustainable Agricultural Practices: Treated Wastewater Quality and Its Impact on Groundwater for Irrigation in Oman

**Author(s):** Al-Shali, M (Al-Shali, Mohammed); Al-Farsi, K (Al-Farsi, Kutaila); Al-Rashdi, Y (Al-Rashdi, Yarub); Abdullahi, I (Abdullahi, Ibrahim); Mahato, S (Mahato, Susanta); Al-Busaidi, A (Al-Busaidi, Ahmed); Meena, U (Meena, Usha); Meena, R (Meena, Ramovatar)

**Source:** WATER AIR AND SOIL POLLUTION **Volume:** 235 **Issue:** 9 **Article Number:** 556 **DOI:** 10.1007/s11270-024-07285-0 **Published Date:** 2024 SEP

**Times Cited in Web of Science Core Collection:** 0

**Total Times Cited:** 0

**Usage Count (Last 180 days):** 4

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**Abstract:** The utilization of treated wastewater (TWW) for agricultural irrigation can enhance soil properties and fertility for better crop growth. However, toxic chemicals in TWW, if exceeding permissible limits, pose environmental and health risks. This study aims to evaluate the quality of treated wastewater (TWW) and groundwater used for irrigation in alfalfa and date palm fields, focusing on specific ion toxicity, salinity, heavy metal concentrations, and other water quality parameters. Water samples were collected from four plantation sites in the Ibra and Alqabil provinces during the summer and winter seasons of 2020 and 2021. The samples were analyzed for electrical conductivity (EC), pH, total dissolved solids (TDS), carbonate, bicarbonate, and the presence of arsenic (As), cadmium (Cd), cobalt (Co), boron (B), lead (Pb), nickel (Ni), copper (Cu), iron (Fe), zinc (Zn), manganese (Mn), and chromium (Cr). The findings reveal that both TWW and groundwater in the sampled sites exhibited salinity levels detrimental to sensitive crops. Trace element concentrations generally adhered to permissible limits as defined by FAO and Oman standards, except for boron, which exceeded allowable limits by up to 40% in groundwater when compared to the control site. Notably, cobalt (Co), arsenic (As), and cadmium (Cd) were undetectable in all water samples. Additionally, groundwater samples taken in close proximity to sewage treatment plants (STPs) displayed a 37% increase in EC, TDS, and heavy metal concentrations. This suggests that groundwater, like TWW, may contain undesirable salts and heavy metals that could compromise water quality. This research underscores the importance of monitoring and assessing the quality of both treated wastewater and groundwater used for irrigation. While these water sources hold potential benefits for agriculture, they also carry the risk of negatively impacting soil and crop health due to salinity and the presence of certain contaminants. This study provides critical insights into the safe use of TWW and groundwater in agricultural practices, highlighting areas for improvement in water treatment and management strategies to ensure sustainable agricultural productivity.

**Accession Number:** WOS:001276250200003

**Language:** English

**Document Type:** Article

**Author Keywords:** Physicochemical assessment; Environmental sustainability; Human health risks; Heavy metal contamination; Water quality analysis

**KeyWords Plus:** POLLUTION

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**Research Areas:** Environmental Sciences & Ecology; Meteorology & Atmospheric Sciences; Water Resources

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**Record 23 of 29**

**Title:** Temporal Gene Expression Profiles From Pollination to Seed Maturity in Sorghum Provide Core Candidates for Engineering Seed Traits

**Author(s):** Jain, R (Jain, Rubi); Dhaka, N (Dhaka, Namrata); Krishnan, K (Krishnan, Kushagra); Yadav, G (Yadav, Garima); Priyam, P (Priyam, Prachi); Sharma, MK (Sharma, Manoj Kumar); Sharma, RA (Sharma, Rita A.)

**Source:** PLANT CELL AND ENVIRONMENT **DOI:** 10.1111/pce.15134 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 9

**Times Cited in Web of Science Core Collection:** 0

**Total Times Cited:** 0

**Usage Count (Last 180 days):** 1

**Usage Count (Since 2013):** 1

**Cited Reference Count:** 238

**Abstract:** Sorghum (*Sorghum bicolor* (L.) Moench) is a highly nutritional multipurpose millet crop. However, the genetic and molecular regulatory mechanisms governing sorghum grain development and the associated agronomic traits remain unexplored. In this study, we performed a comprehensive transcriptomic analysis of pistils collected 1-2 days before pollination, and developing seeds collected -2, 10, 20 and 30 days after pollination of *S. bicolor* variety M35-1. Out of 31 337 genes expressed in these stages, 12 804 were differentially expressed in the consecutive stages of seed development. These exhibited 10 dominant expression patterns correlated with the distinct pathways and gene functions. Functional analysis, based on the pathway mapping, transcription factor enrichment and orthology, delineated the key patterns associated with pollination, fertilization, early seed development, grain filling and seed maturation. Furthermore, colocalization with previously reported quantitative trait loci (QTLs) for grain weight/size revealed 48 differentially expressed genes mapping to these QTL regions. Comprehensive literature mining integrated with QTL mapping and expression data shortlisted 25, 17 and 8 core candidates for engineering grain size, starch and protein content, respectively.

We report transcriptomic analysis of pistils before pollination and four temporal stages of seed development in sorghum. Based on expression patterns, orthology, pathway and QTL information, candidate genes have been shortlisted to engineer seed weight/size, starch content and protein digestibility.

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**PubMed ID:** 39248611

**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** grain filling; seed development; seed size; seed storage proteins; sorghum; starch content; transcriptome

**KeyWords Plus:** ADP-GLUCOSE PYROPHOSPHORYLASE; ENDOSPERM-SPECIFIC GENE; IMPROVES GRAIN-SIZE; RICE DWARF MUTANT; TRANSCRIPTION FACTOR; PLANT ARCHITECTURE; TARGETED MUTAGENESIS; CELL-PROLIFERATION; NATURAL VARIATION; ORGAN SIZE

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Science and Engineering Research Board (SERB)	IFA17-LSP90
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Indo-German Science & Technology Centre (IGSTC)	
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## Record 24 of 29

**Title:** FPGA Implementation of an Effective Image Enhancement Algorithm Based on a Novel Daubechies Wavelet Filter Bank

**Author(s):** Islam, MT (Islam, Md Tarikul); Samantaray, AK (Samantaray, Aswini Kumar); Gorre, P (Gorre, Pradeep); Jatoth, DN (Jatoth, Deepak Naik); Kumar, S (Kumar, Sandeep); Al-Shidaifat, A (Al-Shidaifat, Alaaddin); Song, HJ (Song, Hanjung)

**Source:** CIRCUITS SYSTEMS AND SIGNAL PROCESSING **DOI:** 10.1007/s00034-024-02842-8 **Early**

**Access Date:** SEP 2024 **Published Date:** 2024 SEP 19

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**Abstract:** The primary issues in producing natural images are low contrast and poor quality. A novel Daubechies wavelet transform technique is proposed for image enhancement which is implemented in field-programmable gate array (FPGA). The new Daubechies-2 (tap-4) wavelet filter bank splits the image into high-pass subband image and low-pass subband image. These subbands are enhanced parallelly using FPGA architectures of adaptive thresholding and top-hat transform. High-pass subband images are improved by employing FPGA architecture of adaptive thresholding technique. The FPGA architecture of morphology-based top-hat transform is used to improve low-pass subband images. The FPGA architecture of newly designed Daubechies-2 wavelet, adaptive thresholding and morphology based top-hat transform, are implemented in FPGA using Xilinx Kintex-7 board. The hardware usage of the proposed technique is compared with that of existing techniques. In addition, PSNR and RMSE are used to assess the extent to which the suggested method performs. Experiments revealed that this technique is excellent at both enhancing an image's details and effectively preserving its edge features with using less hardware.

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**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** Image enhancement; Adaptive thresholding; Top-Hat transform; Daubechies wavelet; Peak signal to noise ratio

**KeyWords Plus:** DESIGN

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**Record 25 of 29**

**Title:** Evaluation of Land Use Land Cover Changes in Response to Land Surface Temperature With Satellite Indices and Remote Sensing Data

**Author(s):** Zhao, Q (Zhao, Qun); Haseeb, M (Haseeb, Muhammad); Wang, XY (Wang, Xinyao); Zheng, XT (Zheng, Xiangtian); Tahir, Z (Tahir, Zainab); Ghafoor, S (Ghafoor, Sundas); Mubbin, M (Mubbin, Muhammad); Kumar, RP (Kumar, Ram Pravesh); Purohit, S (Purohit, Sanju); Soufan, W (Soufan, Walid); Almutairi, KF (Almutairi, Khalid F.)

**Source:** RANGELAND ECOLOGY & MANAGEMENT **Volume:** 96 **Pages:** 183-196 **DOI:** 10.1016/j.rama.2024.07.003 **Published Date:** 2024 SEP

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**Abstract:** Land use and land cover (LULC) changes are known as the main factors causing soil degradation, which presents considerable obstacles to maintaining soil quality and the resilience of ecosystems. Human activities substantially impact LULC changes, particularly in areas experiencing rapid development. The objective of this study is to assess the changes in LULC, land surface temperature (LST), Normalized Differentiate Vegetation Index (NDVI), and Normalized Differentiate Built-up Index (NDBI) in Kasur District from 1991 to 2021. The study analyzed five major LULC classes: Water bodies, Urban areas, barren land, forest Cover, and vegetated areas. Our analysis revealed that the Urban area of Kasur expanded by around 16.27%. The vegetation cover experienced a slight decline of just 1%, while water bodies declined by 0.26%. Forest cover experienced a decrease of about 0.54%, and bare land decreased significantly by 14.4%. The imagery classification achieved an overall accuracy of 88% to 92%. The highest NDVI value was observed in 1991 ( + 0.89), while the lowest was in 2021 ( + 0.56). Similarly, the highest NDBI recorded was + 0.83 in 2021, while the lowest was + 0.65 in 1991. The linear regression analysis revealed a strong negative association between the NDVI and NDBI. LST results exhibited a 0.55 degrees C increase between the years 1991 and 2021. The study's findings align with the Sustainable Development Goals (SDGs), particularly SDG-15, which aims to protect, restore, and promote sustainable use of terrestrial ecosystems, sustain- ably manage forests, combat desertification, and halt land degradation and biodiversity loss. (c) 2024 The Society for Range Management. Published by Elsevier Inc. All rights are reserved, including those for text and data mining, AI training, and similar technologies.

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**Language:** English

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**Author Keywords:** Soil degradation; Climate change; Geospatial techniques; Pakistan

**KeyWords Plus:** USE/COVER CHANGE; GIS; CLASSIFICATION; URBANIZATION; CYCLES; WATER; CITY; LST

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**Record 26 of 29**

**Title:** Statistical Estimation of Uniaxial Compressive Strength in Geotechnical Projects Using Regression Analysis: A Comparative Study

**Author(s):** Verma, RK (Verma, Rahul Kumar); Singh, R (Singh, Rajesh); Kumar, V (Kumar, Vijay); Singh, TN (Singh, T. N.); Umrao, RK (Umrao, Ravi Kumar); Mishra, P (Mishra, Pranshu); Sharma, P (Sharma, Prateek)

**Source:** INTERNATIONAL JOURNAL OF GEOMECHANICS **Volume:** 24 **Issue:** 9 **Article Number:** 05024009 **DOI:** 10.1061/IJGNALGMENG-9384 **Published Date:** 2024 SEP 1

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**Cited Reference Count:** 42

**Abstract:** The present study focuses on the estimation of uniaxial compressive strength (UCS) in geotechnical projects. UCS is a crucial parameter in designing such projects, and traditional methods of measurement outlined by standards are often time-consuming and cumbersome. Additionally, obtaining standard core samples is always a challenging task in fractured or discontinuous rock masses. To overcome these limitations, alternative techniques such as simple regression (SR), multivariable regression (MVR), and artificial intelligence (AI) have been utilized to estimate UCS based on easily derived geotechnical parameters. While SR and MVR provide simple equations that can be used without the need for complex calculations, AI techniques offer the potential for higher prediction accuracy. However, AI models often require more complex solutions due to their intricate algorithms and computational processes. This makes AI less practical for ongoing geotechnical projects in which simple and quick estimations are often preferred. In this study, both the SR and the MVR models were employed to estimate the UCS using the Schmidt hammer rebound number (RN),

density ( $\rho$ ), porosity ( $\phi$ ), and point load index ( $Is_{50}$ ) as input parameters. Various SR and MVR models were tested, and the best-performing models were selected based on performance indices such as the normalized root mean square error (NRMSE), relative root mean square error (RRMSE), variance accounted for (VAF), efficiency (E), and correlation coefficient (R<sup>2</sup>). Furthermore, this study proposes a new performance index (PI<sub>mod</sub>) to evaluate the predictive capabilities of the models. This index likely incorporates additional criteria or metrics beyond the aforementioned traditional performance indices. Overall, the equations derived from the regression models in this study offer a simpler and more practical approach for geotechnical practitioners to quickly assess UCS in any given area, providing a useful tool for their work.

**Accession Number:** WOS:001272356000022

**Language:** English

**Document Type:** Article

**Author Keywords:** Uniaxial compressive strength (UCS); Multivariable regression; Simple regression; Performance indices; Geotechnical stability

**KeyWords Plus:** SCHMIDT HAMMER; FUZZY MODEL; PREDICTION; HARDNESS; MODULUS; TESTS

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## Record 27 of 29

**Title:** Inhibition of PERK-mediated unfolded protein response acts as a switch for reversal of residual senescence and as senolytic therapy in glioblastoma

**Author(s):** Ketkar, M (Ketkar, Madhura); Desai, S (Desai, Sanket); Rana, P (Rana, Pranav); Thorat, R (Thorat, Rahul); Epari, S (Epari, Sridhar); Dutt, A (Dutt, Amit); Dutt, S (Dutt, Shilpee)

**Source:** NEURO-ONCOLOGY **DOI:** 10.1093/neuonc/noae134 **Early Access Date:** SEP 2024 **Published Date:** 2024 SEP 3

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**Usage Count (Last 180 days):** 1

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**Abstract:** Background Glioblastoma due to recurrence is clinically challenging with 10-15 months overall survival. Previously we showed that therapy-induced senescence (TIS) in glioblastoma reverses causing recurrence. Here, we aim to delineate the TIS reversal mechanism for potential therapeutic intervention to prevent glioblastoma (GBM) recurrence. Methods Residual senescent (RS) and end of residual senescence (ERS) cells were captured from GBM patient-derived primary-cultures and cell lines mimicking clinical scenarios. RNA-sequencing, transcript/protein validations, knock-down/inhibitor studies, ChIP RT-PCR, biochemical assays, and IHCs were performed for the mechanistics of TIS reversal. In vivo validations were conducted in GBM orthotopic mouse model. Results Transcriptome analysis showed co-expression of endoplasmic reticulum (ER) stress-unfolded protein response (UPR) and senescence-associated secretory phenotype (SASP) with TIS induction and reversal. Robust SASP production and secretion by RS cells could induce senescence, Reactive oxygen specis (ROS), DNA damage, and ER stress in paracrine fashion independent of radiation. Neutralization of most significantly enriched cytokine from RS-secretome IL1 beta, suppressed SASP, and delayed senescence reversal. Mechanistically, with SASP and massive protein accumulation in ER, RS cells displayed stressed ER morphology, upregulated ER stress markers, and PERK pathway activation via pelf2 alpha-ATF4-CHOP which was spontaneously resolved in ERS. ChIP RT-PCR showed CHOP occupancy at CXCL8/IL8, CDKN1A/p21, and BCL2L1/BCLXL aiding survival. PERK knockdown/inhibition with GSK2606414 in combination with radiation led to sustained ER stress and senescence without SASP. PERKi in RS functioned as senolytic via apoptosis and prevented recurrence in vitro and in vivo ameliorating overall survival. Conclusion We demonstrate that PERK-mediated UPR regulates senescence reversal and its inhibition can be exploited as a potential seno-therapeutic option in glioblastoma. Graphical Abstract

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**Language:** English

**Document Type:** Article; Early Access

**Author Keywords:** ER stress; glioblastoma; PERK; TIS reversal; unfolded protein response

**KeyWords Plus:** ENDOPLASMIC-RETICULUM; CELLULAR SENESCENCE; TUMOR PROGRESSION; CANCER-CELLS; DNA-DAMAGE; GROWTH; REGULATOR; PHENOTYPE; ESCAPE; STRESS

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**Title:** Thermally activated damage recovery in ion-irradiated  $\text{Gd}_{2-x}\text{Ti}_x\text{Zr}_y\text{O}_7$  pyrochlore

**Author(s):** Singh, Y (Singh, Yogendar); Kumar, A (Kumar, Ajay); Kumar, V (Kumar, Vivek); Chattaraj, A (Chattaraj, Ananya); Pandey, KK (Pandey, Krishan K.); Kulriya, PK (Kulriya, Pawan Kumar)

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**Abstract:** Ionizing events having a wide variety of radiation-induced effects can radically affect the kinetics of defect production or structural transformation in the pyrochlore structured oxides ( $\text{A}_2\text{B}_2\text{O}_7$ ). Therefore, a thorough understanding of the kinetics associated with cation ordering and disordering is required for various technological applications. The structural responses of  $\text{Gd}_{2-x}\text{Ti}_x\text{Zr}_y\text{O}_7$  ( $y = 0.4, 1.2, 1.6$ ) pyrochlore series irradiated by 120 MeV  $\text{Au}^{9+}$  ions were investigated using in situ synchrotron x-ray diffraction (SR-XRD), micro-Raman spectroscopy, and scanning electron microscopy (SEM). Each pyrochlore composition irradiated at the highest fluence, where structural modifications occur, was subsequently isochronally annealed from room temperature to 1000 degrees C. The SR-XRD results indicate that Ti-rich composition ( $y = 0.4$ ) retains its pre-irradiated pyrochlore structure ( $\text{Fd}\overline{3}\text{m}$ ) at 1000 degrees C. In contrast, Zr-rich compositions exhibit recrystallization to an intermediate defect-fluorite phase ( $\text{Fm}\overline{3}\text{m}$ ) above 500 degrees C, and the pre-irradiated pyrochlore superstructure does not recover even on annealing at 1000 degrees C. These results reveal that recrystallization temperature strongly depends on the accumulated radiation damage, generally described with the cationic radius ratio ( $r(\text{A})/r(\text{B})$ ). Thus, investigation of the thermal annealing behavior of irradiated pyrochlores helps better understanding the general mechanisms of radiation damage and recovery of pyrochlores, which is important for their use in nuclear applications.

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**Author Keywords:** pyrochlore; radiation damage; recrystallization; synchrotron diffraction

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## Record 29 of 29

**Title:** Computational investigation of novel synthetic analogs of C-1' $\beta$  substituted remdesivir against RNA-dependent RNA-polymerase of SARS-CoV-2

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**Abstract:** Remdesivir, a C-nucleotide prodrug binds to the viral RNA-dependent-RNA polymerase ( RdRp ) and inhibits the viral replication by terminating RNA transcription prematurely. It is reported in literature that interaction between the C-1'(-CN (- CN moiety of Remdesivir (RDV) RDV ) and the Ser861 residue in RdRp enzyme, causes a delayed chain termination during the RNA replication process and is one of the important aspect of its mechanism of action. In the pursuance of increasing the biological activity of RDV and enhancing

the SAR studies, against RNA viruses, we have designed its fourteen C1' (substituted analogs, 10 - 23 bearing 4/5-membered heterocyclic rings. The docking and 100 ns molecular dynamics (MD) simulations of 10-23-23 to the RdRp protein (PDB ID: 7L1F) revealed important interactions between 2',3'-diol, oxo group of phosphoramidate, nitrogen residues of heterocyclic rings of synthetic molecules with Arg555, Arg553, Ser759, Cys622, Asn691, Asp623 amino acid residues of protein. The docking score of 2-ethylbutyl ((S) (((2R,3S,4R,5R)-5-(4-aminopyrrolo[2,1-f][1,2,4]triazin-7-yl)-3,4-dihydroxy-5-(1H-1,2,3-triazol-4-yl)tetrahydrofuran-2-yl)methoxy)(phenoxy)phosphoryl)-L-alaninate, 11 was found to be higher than RDV among 14 new compounds i.e. -5.20 kcal/mol. Out of 3 compounds, 10, 12 and 13 submitted for MD simulations and Molecular Mechanics Poisson-Boltzmann Surface Area (MMPBSA) analysis, trifluoro-oxadiazole derivative, 13 showed higher binding energy as compared to Remdesivir. The predicted ADMET properties of 14 compounds showed their potential for being drug candidates. The present study suggests that substitution at the C1' (position by 4/5-membered rings plays an important role in the interactions between nucleoside/tide and target protein.

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