SCHOLARLY PUBLICATIONS
School of Biotechnology
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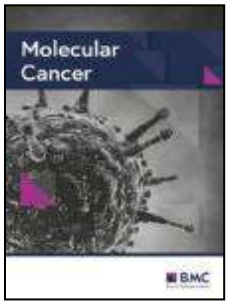
Journal Name: Molecular Cancer **IF: 33.9**

Title: Epithelial-to-mesenchymal transition (EMT) and cancer metastasis: the status quo of methods and experimental models 2025

Author: Allgayer H.; Mahapatra S.; Mishra B.; Swain B.; Saha S.; Khanra S.; Kumari K.; Panda V.K.; Malhotra D.; Patil N.S.; Leupold J.H.; Kundu G.C.

Details: Volume 24, Issue 1, December 2025, Article number 167

Abstract: Epithelial-to-mesenchymal transition (EMT) is a crucial cellular process for embryogenesis, wound healing, and cancer progression. It involves a shift in cell interactions, leading to the detachment of epithelial cells and activation of gene programs promoting a mesenchymal state. EMT plays a significant role in cancer metastasis triggering tumor initiation and stemness, and activates metastatic cascades resulting in resistance to therapy. Moreover, reversal of EMT contributes to the formation of metastatic lesions. Metastasis still needs to be better understood functionally in its major but complex steps of migration, invasion, intravasation, dissemination, which contributes to the establishment of minimal residual disease (MRD), extravasation, and successful seeding and growth of metastatic lesions at microenvironmentally heterogeneous sites. Therefore, the current review article intends to present, and discuss comprehensively, the status quo of experimental models able to investigate EMT and metastasis in vitro and in vivo, for researchers planning to enter the field. We emphasize various methods to understand EMT function and the major steps of metastasis, including diverse migration, invasion and matrix degradation assays, microfluidics, 3D co-culture models, spheroids, organoids, or latest spatial and imaging methods to analyze complex compartments. In vivo models such as the chorionallantoic membrane (CAM) assay, cell line-derived and patient-derived xenografts, syngeneic, genetically modified, and humanized mice, are presented as a promising arsenal of tools to analyze intravasation, site specific metastasis, and treatment response.



URL: https://molecular-cancer.biomedcentral.com/articles/10.1186/s12943-025-02338-2

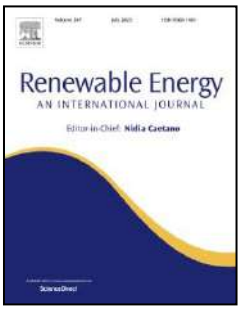
Journal Name: Renewable Energy **IF: 9.0**

Title: Biodiesel synthesis from Ricinus communis and Pongamia pinnata oil blends by injecting superheated methanol â€“ isopropanol mixtures: Optimization through CCD and ANN approaches

Author: Karmakar B.; Chakrabortty S.; Kumar R.; Halder G.

Details: Volume 249, 15 August 2025, 123223

Abstract: In the current study, blends of castor and karanja oils were subjected to uncatalysed alcoholysis with superheated mixtures of 2-propanol and methanol for their rapid conversion into fuel-grade esters. Optimizable ranges identified from batch studies for 6 parameters: alcohol preheat temperature, castor oil to karanja oil ratio, initial oil mass, methanol to 2-propanol ratio, reaction temperature and retention duration were fed into a spherical central composite design (CCD-S, used for identifying process conditions for optimal biodiesel yield. It was noted that a maximum biodiesel yield of 98.79 % could be obtained when 650g castor and karanja oil blend at a ratio of 2:1 was charged into the reactor. The alcohols at a ratio of 3:5 for methanol: 2-proanol had to be pre-heated to 140 °C to achieve desired energy, reactivity and flow. The reaction provided best results when allowed to occur at 260 °C for a duration of 8 min. The experimentally obtained data were verified for reliability through ANOVA studies and ANN was used to validate the data as well as develop a model capable of predicting output accurately, with a 6-10-1 algorithm giving an R^2 of 0.987, indicating high reliability.



URL:https://www.sciencedirect.com/science/article/pii/S0960148125008857?via%3Dihub

SCHOLARLY PUBLICATIONS
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Journal Name: Journal of Environmental Management **IF: 8.4**

Title: Algae-based nanoparticles for enhancing sustainable applications in integrated food-water ecosystem

Author: Nayak S.; Behera B.; Newmei K.; S. M.S.; Kumar V.; Lalnunmawii E.; Senthil Kumar N.; Das B.; Rathinavel L.

Details: Volume 392, September 2025

Abstract: Over the past decade with the ever-increasing population growth, the concurrent demands for food and water have risen, thus significantly affecting sustainability. Recently, biogenic nanoparticles produced from algal biomass inherently rich in secondary metabolites have garnered huge attention to sort the complexities related to food-water nexus. This critical review aims to explore recent advancements in the synthesis, characterization, and functional properties of algae-based nanoparticles (ANPs), highlighting their role in supporting sustainable solutions across the food and water sectors. Interactions of ANPs with various components present in water and soil are discussed to comprehend the potential challenges and seek solutions for improving their real-time applicability. Further, the underlying mechanisms have been correlated with potential applications linked to environmental bioremediation, agricultural applications and food supply chain management. The morphology and physicochemical characteristics of ANPs depend on the algae type, procedure used, and other factors such as the concentration of algal extract and metal, incubation time, temperature, and pH levels. ANPs depending on their surface and functional properties have been reported to have a higher remediation efficiency for heavy metals, dyes, and nutrients from wastewater. High antimicrobial and antioxidant activity also makes them a good candidate for active food packaging to extend shelf-life. Challenges in scalability, stability, and environmental risk are also elaboratively discussed. Overall, this review provides a foundational framework for future interdisciplinary research aimed at optimizing algae-based nanotechnologies for sustainable development

URL: https://www.sciencedirect.com/science/article/abs/pii/S0301479725027537?via%3Dihub

SCHOLARLY PUBLICATIONS
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Journal Name: Biomass and Bioenergy **IF: 5.8**

Title: Fermentation of sugarcane bagasse for production of value-added phenolic compounds using potential bacterial strains: A comparative analysis

Author: Pattnaik B.; Preeti; Gupta D.; Deb D.; Selvaraj M.; Assiri M.A.; Mohapatra S.R.; Sahoo H.P.; Tapas S.; Sarangi P.K.

Details: Volume 202, November 2025

Abstract: The present study investigates the potential of bacterial strains, viz., Pseudomonas fragi, Lactobacillus plantarum, and Lactobacillus acidophilus, for the production of phenolic compounds from sugarcane bagasse (SCB). The important bio-transformed phenolic products isolated from the medium were ferulic acid (FA), vanillin and vanillic acid (VA), whose identification and quantification were done by high-performance thin-layer chromatography. Carbohydrate concentration from the de-starched bagasse was also assessed and compared with that of the original (control) bagasse. Results revealed that the utmost FA yield per kg of SCB was 275 mg from Lactobacillus acidophilus, 225 mg from Pseudomonas fragi on the 9th day, and 212 mg from Lactobacillus plantarum on the 12th day of incubation. Likewise, the peak vanillin and VA quantified per ml of fermented extract were 16 mg on 9th and 12th day of incubation, respectively, for Lactobacillus plantarum, 14 mg of vanillin and 13 mg of VA on 9th day for Pseudomonas fragi. However, in Lactobacillus acidophilus 15 mg of Vanillin and 18 mg of VA was recorded on 12th day of incubation. To compare enzymatic efficiency and structural integrity among ferulic acid esterases (FAEs), a 3D structural model was constructed. We first time demonstrated that the lid domain's structural integrity enhances enzyme efficiency which has been expressed in terms of yield. An ∼18 % higher yield of primary phenolic compound was obtained for L. acidophilus with compact FAE lid domain compared to PsfFAE. This finding highlights the metabolic potential of these strains for phenolics production and their relevance in biotransformation processes.

URL: https://www.sciencedirect.com/science/article/abs/pii/S0961953425005720?via%3Dihub

SCHOLARLY PUBLICATIONS
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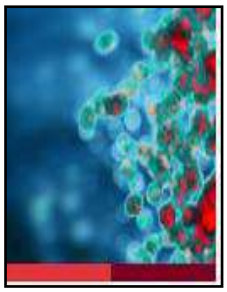
Journal Name: Frontiers in Immunology **IF: 5.7**

Title: Designing a potent multivalent epitope vaccine candidate against Orientia tsutsugamushi via reverse vaccinology technique - bioinformatics and immunoinformatic approach

Author: Panda S.; Swain S.K.; Sahu B.P.; Mahapatra S.R.; Dey J.; Sarangi R.; Ranade A.V.; Mishra N.

Details: Volume 16, 2025, Article number 1513245

Abstract: Scrub typhus is a life-threatening, undifferentiated febrile illness caused by a gram-negative bacterium, Orientia tsutsugamushi. The bacterial strain is a global health concern that should be considered. Despite several years of effort for the development of an effective immunogenic vaccine, no successful licensed vaccine is available. The aim of the study is to construct an epitope response using a reverse vaccinology approach. The TSA56 and ScaA proteins combined can be the most promising subunit vaccine candidates against O. tsutsugamushi. B-cell, CTL, and HTL epitopes were predicted, and subsequently, all the epitopes were linked by KK, AAY, and GPGPG linkers, respectively, along with an adjuvant at the N-terminal region. Furthermore, molecular docking and MD simulations were performed that exhibited a higher affinity towards TLR-2. A total of 16 linear B-cells, 6 CTL, and 2 HTL epitopes were identified and validated. The final vaccine construct showed high antigenicity, stability, and solubility. Molecular docking and MD simulations indicated strong binding interactions with TLR-2 and a stable vaccine-receptor complex. The expression of the vaccine in pET28a (+) vector was successfully implemented via in silico cloning as well as significant results from immune simulation demonstrated the efficacy of the vaccine in the immune cell interaction during the innate and adaptive immune responses immune simulation. In conclusion, the outcome suggested that the newly developed vaccine will be a promising candidate for controlling and providing definitive preventive measures against scrub typhus if further investigation is conducted experimentally.



URL:https://www.frontiersin.org/journals/immunology/articles/10.3389/fimmu.2025.1513245/full

SCHOLARLY PUBLICATIONS
School of Biotechnology
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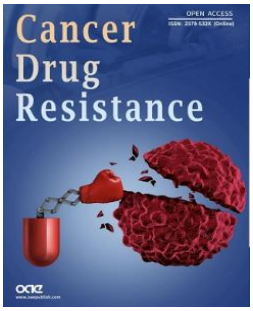
Journal Name: Cancer Drug Resistance **IF: 5.2**

Title: Decoding breast cancer treatment resistance through genetic, epigenetic, and immune-regulatory mechanisms: from molecular insights to translational perspectives

Author: Saha, S; Mahapatra, S; Khanra, S; Mishra, B; Swain, B; Malhotra, D; Saha, S; Panda, VK; Kumari, K; Jena, S; Thakur, S; Singh, PK; Kundu, GC

Details: July, 2025

Abstract: Breast cancer continues to be the primary cause of cancer-related deaths among women globally, with increased rates of incidence and mortality, highlighting the critical need for effective treatment strategies. Recent developments have introduced a variety of treatment options that address the molecular diversity of breast cancer; nonetheless, drug resistance remains a significant barrier to achieving favorable results. This review explains the crucial role of genetic and epigenetic changes in contributing to therapeutic resistance, in addition to other factors such as increased drug efflux, enhanced DNA repair, evasion of senescence, tumor heterogeneity, the tumor microenvironment (TME), and epithelial-to-mesenchymal transition (EMT). At the same time, epigenetic modifications-like DNA methylation, alterations to histones, and dysregulation of non-coding RNAs-reprogram gene expression, supporting adaptive resistance mechanisms. These molecular abnormalities contribute to the plasticity of tumors, allowing cancer cells to evade therapeutic approaches. This review consolidates recent discoveries regarding how these genetic and epigenetic modifications affect treatment responses and resistance in breast cancer, highlighting their interaction with disease advancement. By pinpointing new drug targets, including immunotherapeutic strategies, this article seeks to shed light on the molecular underpinnings of chemoresistance, aiding in the refinement of existing treatment protocols. A more profound understanding of these mechanisms offers the potential for developing precision therapies to overcome resistance, reduce relapse rates, and improve clinical outcomes for breast cancer patients.



URL: https://www.oaepublish.com/articles/cdr.2025.69

SCHOLARLY PUBLICATIONS
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Journal Name: Cancer Gene Therapy **IF: 5.0**

Title: Engineered L-asparaginase variants with enhanced therapeutic properties to improve treatment of childhood acute lymphatic leukemia

Author: Biswas M.; Sengupta S.; Gandhi K.A.; Gupta S.K.; Gera P.B.; Nayak B.S.; Jagadeb M.; Gota V.; Sonawane A.

Details: July, 2025

Abstract: Escherichia coli L-asparaginase (EcA), a key component of a multi-drug acute lymphatic leukemia (ALL) treatment regimen, has several limitations that reduce its therapeutic efficacy. The major disadvantages include immunogenicity, serum instability, shorter half-life, and accompanying glutaminase activity that causes neurotoxicity and pancreatitis. Pegylated asparaginase and Erwinase have better therapeutic potential, but they are expensive. Using site-directed mutagenesis, we created several EcA variants by substituting specific amino acid residues at the dimer-dimer interface and B-cell epitope regions. After several rounds of screening and selection, we identified two EcA variants viz. K288S/Y176F (KSY-17) and K288S/Y176F/W66Y (KSYW-17), which showed comparable asparaginase activity to wild-type (WT) and significantly less glutaminase activity (30.36 U/mg for WT vs 1.54 and 0.99 U/mg for KSY-17 and KSYW-17). KSYW-17 was less immunogenic than WT, eliciting 4.8–5.3-fold and 2.4–3.8-fold less IgG and IgM responses, respectively. Compared to WT EcA, we also observed significantly less (~1.5-2-fold) binding of these variants to pre-existing antibodies in ALL patients' serum. ALL xenograft mice studies showed a 90% and 70% reduction in leukemia burden in KSY-17 and KSYW-17 administered mice, respectively, as compared to 30% for WT after repeat dose administration, accompanied by significantly higher mice survival (100% vs. 70% vs. 10% for KSY-17 vs. KSYW-17 vs. WT). Overall, the engineered EcA variants' showed improved therapeutic efficacy, thus making them promising candidates for primary and relapsed ALL treatment. (Figure presented.)

URL: https://www.nature.com/articles/s41417-024-00865-6

SCHOLARLY PUBLICATIONS
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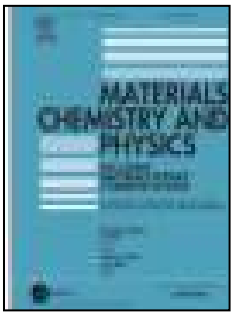
Journal Name: Materials Chemistry and Physics **IF: 4.7**

Title: Deciphering biosurfactant-salt interaction and its influence on biosurfactant activity in muga silk fibroin extraction

Author: Biswal B.; Das M.; Das D.; Prusty D.; Dan A.K.

Details: Volume 344, October 2025

Abstract: Degumming of silk cocoons is the initial technique employed to separate two silk proteins (fibroin and sericin), which further leads to the formulation of diverse silk-based biomaterials for biomedical applications. In this study, a novel approach has been implemented in a mixed system. Specifically, this paper emphasizes the impact of degumming on fibroin fiber, which was carried out using varying concentrations of sodium carbonate (Na_2CO_3) and crude biosurfactant extracted from Acacia concinna (Willd.) Dc. The study investigated the effectiveness of the degumming process under a specific concentration of Na_2CO_3 with crude biosurfactant extract, examining the influence of reaction time, temperature, and mixed reagent concentration. The results of the degumming process show that approximately 24.8 % degumming occurred when using 0.012 g/mL of biosurfactant extract with 3×10^{-4} g/mL of Na_2CO_3 as degumming reagents. Furthermore, SEM, XRD, TGA, and mechanical strength analyses suggest that the quality of fibers extracted using the crude biosurfactant (BSE) and Na_2CO_3 mixture in the degumming process yielded significant results. This innovative approach of degumming can extract the silk fibroin from the cocoons in the fastest and most effective way. Moreover, this strategy may significantly diminish the harmful contamination of sericin and degumming chemicals in the effluent.



URL: https://www.sciencedirect.com/science/article/pii/S0254058425008107?via%3Dihub

SCHOLARLY PUBLICATIONS
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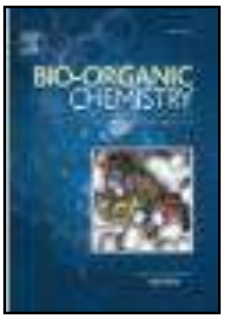
Journal Name: Bioorganic Chemistry **IF: 4.7**

Title: Design, synthesis and biological evaluation of 2-phenylquinoxaline carbonyl piperazine derivatives as novel FASN inhibitors with anticancer activity

Author: Singh S.; Paul S.; Martins F.G.; Sousa S.F.; Kundu C.N.; Karthikeyan C.; Moorthy N.S.H.N.

Details: Volume 163, August 2025

Abstract: Overexpression of fatty acid synthase (FASN) has been linked to the advancement of various cancers. FASN caters to the increased demand for lipids within tumor cells, facilitating tumor growth and progression, making it an attractive target for anticancer drug discovery. Herein we report a novel series of 2-phenylquinoxaline-6-carboxylic acid derivatives as novel potent FASN inhibitors with anticancer potential. Structure-activity relationship analysis demonstrated that all the synthesized compounds showed potent and selective cytotoxicity against the three cancer cell lines evaluated with IC_{50} values less than 10 µM. QNX-10 was identified as a promising lead molecule as it elicited potent FASN inhibition and selective cytotoxicity against the colorectal (HCT-116, Caco-2 cell lines) and breast cancer (MCF-7 cell line). Notably, QNX-10 induces apoptosis and cell cycle arrest at S-phase in HCT-116 cells in a dose-dependent manner. Western blot analysis indicated that QNX-10 inhibits FASN and promotes apoptosis in HCT-116 cells by upregulating pro-apoptotic protein Bax and downregulating anti-apoptotic protein Bcl-xL. Molecular docking and MD simulation studies with QNX-10 revealed the binding mode of the compound to the KR domain of FASN. Taken together, the study establishes compound QNX-10 to be a promising lead candidate for the development of anticancer therapeutics targeting the FASN enzyme.



URL: https://www.sciencedirect.com/science/article/abs/pii/S0045206825005772?via%3Dihub

SCHOLARLY PUBLICATIONS
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Journal Name: Materials Advances **IF: 4.7**

Title: Bactericidal activity of ZnO nanoparticles-anti-TB drug combination towards the H37Rv strain and multidrug-resistant isolates of Mycobacterium tuberculosis via SufB splicing inhibition

Author: Ojha D.K.; Mehra A.; Rout S.S.; Giri S.; Nayak S.

Details: Issue 15, 2025

Abstract: Tuberculosis (TB) remains a significant global health threat, claiming millions of lives annually. Despite advancements in treatment, the emergence of drug-resistant strains has hindered effective TB control. The current management of TB involves prolonged treatment duration with severe side effects, leading to poor patient compliance. However, the mycobactericidal potential of nanoparticles towards drug-resistant TB is not confirmed yet. This work explores the bactericidal potential of zinc oxide nanoparticles (ZnONPs, 40 nm) in managing both drug-sensitive and drug-resistant TB in combination with anti-TB drugs. It was found that ZnONPs inhibit the generation of active SufB protein via splicing inhibition, an essential event for Mycobacterium tuberculosis (Mtb) survival. While TEM and UV-visible spectroscopy identified NPs-protein interaction, SEM visualised extensive membrane damage in H37Rv and multidrug-resistant (MDR) Mtb cells. Alamar blue assay and the spread plate method detected minimum inhibitory concentration and minimum bactericidal concentration of ZnONPs towards the H37Rv strain and MDR Mtb isolates. In vitro studies identified a combination with ZnONPs that reduced effective doses for anti-TB drugs towards H37Rv and MDR Mtb isolates. A similar drug combination attenuated the mycobacterial load and inflammation in the spleen and lungs and protected against Mtb induced splenomegaly in infected mice. Thus, ZnONPs can be used as a potent additive in the anti-TB regimen to manage drug-susceptible and drug-resistant TB, addressing challenges such as prolonged therapy, drug toxicity and poor patient compliance.

URL: https://pubs.rsc.org/en/content/articlelanding/2025/ma/d4ma01224k

SCHOLARLY PUBLICATIONS
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Journal Name: Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy **IF:4.6**

Title: Spectroscopic investigation of hydrogen bond network stability and microplastic leaching in ethanol-based potentised medicines at extreme dilutions during prolonged plastic storage

Author: Chakraborty S.; Ghosh K.; Biswas S.; Roy Chaudhuri C.; Roy Chowdhury A.; Chakravarty R.; Nayak D.; Kaushik S.; Barui A.; Kundu S.

Details: Vol. 343, Dec 2025

Abstract: The quality and efficacy of pharmaceutical products stored under proper conditions are critical. This study examined the effects of long-term plastic storage on extremely diluted ethanol-based potentised (EP) medicines using advanced spectroscopic techniques. Four medicines, Arnica montana, Rhus toxicodendron, Conium maculatum, and Belladonna, at ultra-high (200C, 1 M) and moderate-high (30C, 200C) potencies, were stored in glass and plastic containers for one month. Glass-stored medicines showed increased antioxidant activity and zeta potential with higher potency, while plastic-stored samples showed a decreasing trend. Conductivity was inversely correlated with zeta potential, with glass-stored medicines showing a ~ 41.91 % reduction, while plastic-stored samples showed a ~ 36.29 % increase. Mid-IR spectra revealed a blue shift (~4–14 cm^{-1}) in O–H stretching and a red shift (~2–3 cm^{-1}) in H–O–H bending for glass-stored medicines, showing weaker inter-molecular H-bonds at higher potencies. In contrast, plastic-stored medicines showed opposite shifts (~2–17 cm^{-1}), implying more constrained H-bonding due to carbonyl-water interaction in presence of microplastics, disrupting the native ethanol-water H-Bond network. Far-IR spectra showed an enthalpic gain (~45.34 %) in glass-stored medicines, while plastic-stored samples showed an enthalpic loss (~56.60 %), confirming structural destabilisation of native water-network due to microplastic leaching. Our findings show that plastic containers compromised the efficacy of studied medicines by altering H-bond network stability and electrical properties. Further studies on different plastic grades and storage durations are needed to validate these findings and explore cost-effective alternatives for long-term storage of such medicines.

URL: https://www.sciencedirect.com/science/article/abs/pii/S1386142525009229?via%3Dihub

SCHOLARLY PUBLICATIONS
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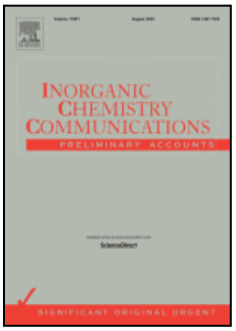
Journal Name: Inorganic Chemistry Communications **IF: 4.4**

Title: Bio-synthesized cerium oxide nano-particles for efficient adsorption of fluoride ion from aqueous solution

Author: Hansdah S.; Das J.; Mandal D.; Parhi P.K.

Details: Volume 178, Part 2, August 2025, 114583

Abstract: Cerium oxide (CeO_2) nanoparticles (NPs) were successfully synthesized via a facile biosynthesis route, utilizing a cost-effective and environmentally friendly bio-extract derived from fenugreek seeds, for the effective removal of fluoride ions from contaminated water. The synthesized CeO_2 NPs were characterized using UV, FTIR, XRD and SEM to determine the phase, purity, and size, revealing an average size of approximately 17.4 nm. The fluoride sorption behavior and mechanism on to the ceria NPs phase was confirmed through kinetics, isotherm, and thermodynamics investigations. The sorption affinity of fluoride ion with ceria NPs appears to be effective at solution pH 2.0. The fluoride sorption rate onto the nano-ceria phase was observed to follow a pseudo-second order kinetic model along with intra-particle diffusion. Among the three sorption adopted isotherm models; Langmuir, Freundlich and Temkin, the fluoride adsorption behavior revealed to follow Langmuir Isotherm with high regression coefficient value (R^2 = 0.993). The maximum fluoride adsorption loading capacity of CeO_2 NPs was determined to be 123.6 mg/g at the temp. 293 K. The fluoride ion adsorption with CeO_2 NPs is observed to be spontaneous and endothermic in nature which was strongly supported by the thermodynamics results; ΔH= 13.789 KJ/mol, and ΔS= +62.799. The phase transformation due to the sorption of fluoride onto the homogeneous ceria phase was ascertained isotherm results and EDX analysis resulted of fluoride ion loaded Ceria NPs.



URL: https://www.sciencedirect.com/science/article/pii/S1387700325006999?via%3Dihub

SCHOLARLY PUBLICATIONS
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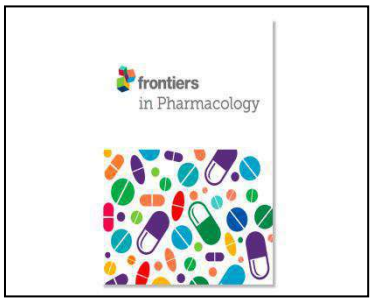
Journal Name: Frontiers in Pharmacology **IF: 4.4**

Title: Editorial: Emerging and reemerging neglected tropical diseases: epidemiology, transmission, mitigation, and vaccines and chemotherapy advancements

Author: Mohapatra R.K.; Mishra S.; Kandi V.; Sirka C.S.; Tuglo L.S.

Details: Volume 16, 2025, Article number 1545801

Abstract: Neglected tropical diseases (NTDs) are infectious diseases caused by bacteria, viruses, fungi and parasites, including ectoparasites like mites and fleas (Mohapatra et al., 2024; Kutikuppala et al., 2023; WHO, 2024). NTDs are an ongoing challenge to global public healthcare and community health. The main reason why such diseases remain collectively neglected is that they are considered “diseases of the poor”, primarily people in low- and middle-income countries (LMICs) with modest purchasing capacity. As a result of this, the commercial diagnostic, therapeutic and prophylactic efforts by the pharmaceutical companies are only skeletal as they do not envision a profitable market. Thus, although treatable, these diseases ultimately manifest as terminal diseases of the have-nots. The World Health Organisation (WHO) has compiled a list of the world’s most prevalent NTDs and updates it from time to time. Currently, there are 21 aetiologically, epidemiologically and clinically unique diseases (or groups of diseases) listed as NTDs by the WHO (Malecela and Ducker, 2021). The WHO has devised public health strategies and proposed a roadmap to eliminate NTDs by 2030 (WHO, 2021). However, as the majority of the NTD-affected subjects live in financially constrained third-world countries, this seems to be an uphill task and achieving it is by no means easy. Lack of NTD-related awareness and limited diagnostic resources in these regions severely affect their foolproof identification. This is evidenced by the constantly increasing number of diseases that fit into the WHO criteria for NTDs. Various NTDs re-emerged in the wake of the coronavirus disease 2019 (COVID-19) pandemic by the severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2), which hit the healthcare infrastructure hard worldwide and exposed its underbelly.



URL:https://www.frontiersin.org/journals/pharmacology/articles/10.3389/fphar.2025.1545801/full

SCHOLARLY PUBLICATIONS
School of Biotechnology
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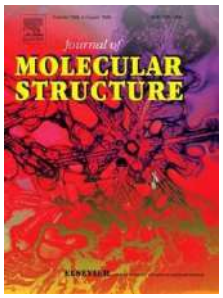
Journal Name: Journal of Molecular Structure **IF: 4.0**

Title: Antimicrobial activities of novel substituted spiropyrrolidine based heterocycles synthesized by multicomponent reaction against Bacillus subtilis and Pseudomonas aeruginosa

Author: Suresh Babu A.R.; Rani S.; Singh S.P.; Khera A.; Alajangi H.K.; Parandaman S.; Raj A.R.N.; Gavaskar D.; Gartia J.; Pandey A.; Yadav V.K.; Singh G.; Barnwal R.P.

Details: Volume 1339, 5 September 2025, Article number 142373

Abstract: The growing resistance of bacteria to antimicrobial agents has intensified the need for novel strategies to combat bacterial infections, particularly those associated with biofilm formation. Biofilms enhance bacterial resilience against hostile environments, immune responses, and antimicrobial treatments. The ability of biofilms to influence bacterial pathogenesis underscores the critical need for new antibacterial agents with anti-biofilm activity. This research aims to synthesize cost-effective, structurally diverse, chemical compounds with the biological significance of disrupting biofilm formation. Here, we report a facile sequential reaction for one-pot, four-component synthesis of spiropyrrolidine heterocycles with 1,3-dipolar cycloaddition of azomethine ylide. The multicomponent reaction (MCR) provides high yield and regioselectivity of the desired product, under mild reaction conditions. Preliminary screening for these novel compounds involves biofilm assays, which assess the developmental processes of biofilms, providing insights into the compounds' biological potential. Subsequent in vitro experiments assessed their antibacterial potential against B. subtilis and P. aeruginosa using the minimum inhibitory concentration (MIC) assay. A cell culture assay evaluated toxicity of these compounds in MDA-MB-231 cell lines. All these investigations cumulatively highlight the potential of these molecules as antibacterial agents for B. subtilis and P. aeruginosa.



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SCHOLARLY PUBLICATIONS
School of Biotechnology
KIIT Deemed to be University

Journal Name: Scientific Reports **IF: 3.9**

Title: Novel endophytic actinomycetes species Streptomyces panacea of Panax sokpayensis produce antimicrobial compounds against multidrug resistant Staphylococcus aureus

Author: Rai S.; Singh L.S.; Liriina K.; Jeyaram K.; Parija T.; Sahoo D.

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Abstract: Endophytic actinomycetes of medicinal plants have recently been in focus for developing novel antimicrobial compounds to combat multidrug-resistant pathogens. In this study, we isolated and characterised endophytic actinomycetes of Panax sokpayensis rhizome traditionally used as medicine in Sikkim-Himalayan region and assessed their antimicrobial activity against multidrug-resistant (MDR) clinical isolates of Staphylococcus aureus. Saccharopolyspora dominated as the endophytic actinomycetes of P. sokpayensis rhizome. However, a novel actinomycete strain PSRA5^T belongs to the genus Streptomyces, with the highest genome sequence similarity of 91.54% with its closest relative Streptomyces niveus NCIMB 11891 has shown an effective inhibition of six clinical isolates of MDR S. aureus during disc diffusion assay. Further comparative analysis of cellular fatty acids composition and phenotypic and biochemical characteristics of strain PSRA5^T with its phylogenetically closely related strain of S. niveus, classified as representing a novel species of the genus Streptomyces, for which the name Streptomyces panacea sp. nov. is proposed here with type strain PSRA5^T (= MCC5238^T). The minimum inhibition concentration of ethyl acetate crude extract of PSRA5^T culture supernatant against MDR S. aureus isolates was 5.5 to 13.5 µg/mL. Further correlation between biosynthetic gene clusters identified by genome search with LC-MS analysis-based chemical profiling of PSRA5^T culture extract and antibacterial activity of the representative compounds detected several compounds of aminoglycosides and polyketides with antimicrobial activity against MDR S. aureus isolates.

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SCHOLARLY PUBLICATIONS
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Title: Clinical and molecular epidemiology of chikungunya outbreaks during 2019-2022 in India

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Abstract: Chikungunya fever (CHIKF) is endemic in India, with multiple outbreaks occurring across the country since its reemergence in 2005. Suspected CHIKF patients were recruited from four clinical sites during 2019–2022, with data collected on sociodemographic, clinical, and epidemiological aspects. Sera samples were screened for IgM, IgG antibodies and viral RNA along with their neutralizing capacity. Envelope genes of Chikungunya virus (CHIKV) isolated were sequenced and further analysed. A total of 1312 suspected patients were screened during the study period; 258 patients were laboratory-confirmed with CHIKV infection. Severe clinical manifestation was observed in the patients during the viremic phase of infection. The neutralization potential was found to be increasing proportionally with the onset of illness, coinciding with the rise of IgG antibodies. Three of the four clinical sites had reported CHIKF outbreaks at different time points during the study period, and a distinct pattern of clinical presentation was observed across the sites. Phylogenetic and network analyses of E1, E2 and E3 genes from 62 CHIKV isolates demonstrated their evolution within the country. This study provides preliminary evidence of spatial and temporal variation in the clinical presentation and molecular evolution of virus in CHIKF outbreaks across India.

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Title: Small molecule based targeting of the CssA RNA thermometer: insights from computational and biophysical approaches

Author: Sharma A.; Gopi P.; Trivedi R.; Kumar D.; Gartia J.; Suresh Babu A.R.; Pandya P.; Singh G.; Barnwal R.P.

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Abstract: The exploration of RNA as a therapeutic target is relatively recent. The field of RNA targeting with small molecules remains elusive despite significant advances via approaches such as the development of bioinformatics tools and strategies facilitating improved modes of action. Non-coding RNAs like RNA thermometers reported in many bacterial pathogens are exciting targets due to the translational control exerted by these RNA elements. The current work involves virtual screening of an in house library of small molecules against CssA RNA thermometer from Neisseria meningitidis via docking and molecular dynamics (MD) simulations followed by in vitro experiments to affirm the binding of small molecules to the target RNA. Fluorescence binding assay and NMR provide evidence for RNA thermometer-small molecule binding. The present study would open new avenues in the domain of small molecule-based targeting of RNA. Interestingly, an RNA thermometer has never been exploited as a drug target. Targeting such RNA elements with small molecules would facilitate structure-based small molecule design with better affinity for the target RNA. From among spiro-pyrrolidine based heterocycles that showed the best binding affinity with the RNAs, a small molecule was identified as the top lead with the potential for targeting the CssA RNA thermometer.

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