SVKM'S NMIMS Deemed-to-be UNIVERSITY

SUNANDAN DIVATIA SCHOOL OF SCIENCE

ABSTRACT BOOK

National Conference on Computational Biology & AI in drug Discovery (CBAIDD-26)

February 6th & 7th 2026

Supported by

Anusandhan National Research Foundation

SDSOS Mentor Message

It gives me immense pleasure to extend my warm greetings to all participants of this national conference organized by SDSOS.

The **convergence of computational biology, artificial intelligence, and drug discovery** reflects the future of scientific innovation and translational research.

Such platforms are vital for **fostering interdisciplinary thinking, industry–academia collaboration**, and meaningful knowledge exchange.

Through focused mentorship, strategic vision and collective commitment, the school has steadily evolved and emerged to new heights of academic excellence and research impact.
I commend the organizing team for curating a conference that addresses emerging global challenges in healthcare and life sciences.

I encourage students and researchers to engage actively, question boldly and explore collaborative opportunities. I wish the conference every success and all participants a stimulating and enriching experience.

Dr Jayant P Gandhi

Honorary Secretary,

SVKM's NMIMS

Vice-Chancellor Message

It is a matter of great pride to welcome you to **the National Conference on Computational Biology & AI in Drug Discovery–26** being organized by **Sunandan Divatia School of Science, NMIMS.**

This conference represents our institutional vision of integrating advanced science and technology to address global healthcare needs. The convergence of computational biology and artificial intelligence is redefining the **future of drug discovery and precision medicine**.

Such scholarly platforms strengthen research culture and promote excellence across disciplines. I congratulate the Chair, Convener and organizing team for conceptualizing a conference of national relevance and impact. I am confident that the deliberations will lead to meaningful collaborations and knowledge advancement.

I wish the conference resounding success and enduring academic outcome.

Dr. Ramesh Bhat,
Vice-Chancellor,
NMIMS Deemed to be University, Mumbai.

Pro -Vice Chancellor Message

I am pleased to be associated with the **National Conference on Computational Biology & AI in Drug Discovery–26** being organized by **Sunandan Divatia School of Science, NMIMS.**

The conference offers an excellent opportunity for researchers and students to engage with emerging tools, methods and real-world applications.

Focused discussions on **AI-driven analytics, genomics and drug development** will enrich academic learning and research skills. Such interactions play a crucial role in bridging classroom knowledge with translational research and industry practices.

I commend the organizers for designing a program that encourages participation and interdisciplinary exchange. I urge young researchers to actively interact, question and explore new research directions.

I wish all participants a stimulating and rewarding academic experience.

Dr. Meena

Chintamaneni,

Pro-Vice

Chancellor,

NMIMS Deemed to be University, Mumbai.

Dean Message

It gives me great pleasure to welcome you to the **National Conference on Computational Biology & AI in Drug Discovery - 26**. This conference reflects the rapid convergence of computational biology, artificial intelligence and life sciences in addressing complex healthcare challenges. Recent advances in **AI-driven genomics, proteomics, molecular modelling and drug discovery** have transformed the way, we understand diseases and design targeted therapies. By integrating machine learning, data-driven modelling, and structural biology, the conference emphasizes innovation in personalized and precision medicine.

The platform brings together eminent academicians, industry experts, and young researchers to exchange ideas and showcase cutting-edge research. Such interdisciplinary dialogue is essential to translate computational insights into real-world clinical and industrial applications.

SVKMs NMIMS, Sunandan Divatia School of Science remains committed to nurturing scientific excellence, innovation and industry relevant research.

I congratulate the organizing committee for curating a timely and impactful scientific program. I wish all participants a stimulating, enriching and successful conference experience.

Dr. Jayakumar Bondili
Dean, SDSOS,
NMIMS Deemed to be University, Mumbai.

Convener Message

It is my great pleasure to welcome you to the **National Conference on Computational Biology & AI in Drug Discovery - 2026**. This conference has been organized to highlight the growing convergence of computational biology, artificial intelligence, and life sciences in addressing complex challenges in drug discovery and healthcare.Recent advances in machine learning, molecular modeling, systems biology, and AI-driven drug design have revolutionized our understanding of disease mechanisms and accelerated the development of targeted therapies. The conference aims to provide a multidisciplinary platform for academicians, researchers, industry professionals, and young scientists to share knowledge, exchange ideas, and discuss emerging trends in this rapidly evolving domain. By bringing together experts from diverse backgrounds, the conference emphasizes innovation, collaboration, and translational research with real-world impact. I am confident that the scientific deliberations, keynote lectures, and technical sessions will foster meaningful interactions, inspire new research directions, and strengthen academia–industry partnerships.

I sincerely thank all the speakers, participants, advisory members, and the organizing committee for their enthusiastic support and dedicated efforts in making this conference a success. I wish all participants a stimulating, enriching, and rewarding conference experience.

Dr. Bajarang Kumbhar
Convener-CBAIDD-26,
Assistant Professor, SDSOS
NMIMS Deemed to be University, Mumbai.

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Key-note Speaker - Dr. Dulal Panda, Director NIPER, Mohali **Title:** Opportunities and challenges of the development of microtubule-targeted anti- cancer drugs	10:30 am - 11:15 am
Tea Break (11.15 am to 11.30 am)	
Prof. Ravi Venkatramani, TIFR, Mumbai **Title**: How to Carry Out Statistically Sound Molecular Dynamics Simulations of Biomolecules	11:30 am – 12.00 pm
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Session Chair: Prof. Jagannath Sahoo, Dean SPPSPTM, NMIMS	
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Technical Program Session for the "National Conference on Computational Biology and AI in drug discovery-26"

Sessions and Speakers	Time Slot
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Mrs. Neha Sawant, MSc **SDSOS, NMIMS University,** **Mumbai** **Title:** Transcriptomic Insights of heterogenous regulator-mediated increase in fatty acid production	3.00 pm - 3.15 pm
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Invited Speaker - Abstracts

Opportunities and challenges of the development of microtubule-targeted anti-cancer drugs

Dulal Panda

National Institute of Pharmaceutical Education and Research, SAS Nagar (Mohali), Punjab

Abstract

Cancer is one of the leading causes of loss of lives in India. Cancer chemotherapy is a highly evolving research area. Anti-microtubule agents are in clinical use for the treatment of several types of cancer. Examples of successful microtubule-targeted anticancer drugs include estramustine, eribulin, taxol, vincristine, and vinblastine. Microtubule-targeting agents inhibit mitosis and generally trigger apoptotic cell death. In addition, microtubule targeting compounds also perturb several important cellular processes. However, microtubule-targeted drugs often cause severe toxicity in patients, limiting their effectiveness. Recent developments have established that targeted delivery can significantly reduce the toxicity of the drugs and thereby improve the efficacy of the anticancer drugs. I will discuss our strategy for discovering new anticancer agents. I will highlight the advantages of targeted drug delivery systems. I will also talk about the opportunities and challenges of current chemotherapeutic approaches.

How to Carry Out Statistically Sound Molecular Dynamics Simulations of Biomolecules

Ravi Venkatramani

Department of Chemical Sciences, Tata Institute of Fundamental Research, Mumbai, India,

Abstract

Molecular Dynamics (MD) simulations are an important tool which allow us to describe biomolecular dynamics and functions at very high atomic resolution and over picoseconds to millisecond timescales. However foundational issues like .1 Further, we propose a mode evolution metric (MEM) to deduce locally converged directions pointing towards undiscovered minima/meta-stable states in the underlying energy landscape2. I will discuss how these conceptual advances can be applied to extract insights on protein dynamics from MD simulations. I will also present a new software AutoSIM which integrates these concepts into an improved umbrella sampling scheme3 to generate reliable potentials of mean force for biomolecular conformational transitions.

Structural insights into the interaction of a Plasmodium falciparum translation enhancing factor with ribosomes

Ilamathy Pandiarajan, Swati Patankar, Sandip Kaledhonkar,

Department of Biosciences and Bioengineering, Indian Institute of Technology Bombay, Mumbai, India 400076

Abstract

Pregnancy-associated malaria (PAM), which affects 5.1% of pregnant women globally, is caused by Plasmodium falciparum. PAM occurs when the infected erythrocytes express a surface antigen VAR2CSA, that binds to chondroitin sulfate A (CSA) on the placental lining of the pregnant women. The expression of VAR2CSA is post-transcriptionally regulated by an upstream open reading frame (ORF). A protein named Plasmodium falciparum translation enhancing factor (PTEF) has been found to be involved in the expression of VAR2CSA, which was previously repressed by the upstream ORF. Our study investigates the structural role of PTEF in the expression of VAR2CSA. The C-terminal domain of PTEF houses a sterile alpha motif (SAM) that binds RNA and is suspected to play a role as a translation reinitiation factor. We demonstrated, using Bio-layer Interferometry and single-particle cryo-EM, that PTEF's C-terminal domain (PTEF-CTD), binds to the A-site of E. coli 70S ribosomes. This confirms its role as a potential translation reinitiation factor, offering structural insights may aid in developing new PAM treatments.

Keywords: Pregnancy-associated malaria, VAR2CSA, translation reinitiation

A systems-level perspective on host- Candida albicans interactions in vaginal infections

Susan Thomas

National Institute for Research in Reproductive and Child Health, Mumbai

Abstract

Candida spp. is a commensal fungus commonly present on the mucosal surfaces of its human host. Under conditions of host stress, it transforms into a pathogenic state, causing localised or systemic infections. Symptomatic infections caused by Candida spp in the reproductive tract of women are called vulvovaginal candidiasis (VVC). The treatment options for the management of VVC are limited to a few antifungal drugs, and several Candida spp. have been increasingly developing resistance to them. A better understanding of the host-pathogen interactions would pave the way to the identification of novel antifungal targets. We used an in vitro model of VVC wherein C. albicanswas co-cultured with the human vaginal epithelial cell line A-431 in conditions mimicking the host microenvironment. Untargeted multi-omics techniques were employed to gain a global overview of their interactions. Integrating the transcriptomics, proteomics and metabolomics profiles revealed significant perturbations in several metabolic pathways of both the host cell line as well as C. albicans. This multi-omics data was further integrated into genome-scale metabolic models of human and C. albicans to create an in-silico host-microbe model of VVC. Such a context-specific community model can help draw deeper insights into disease pathogenesis and facilitate the discovery of novel therapeutic targets.

Understanding molecular basis of antimicrobial resistance using Bioinformatics approaches

Kailas D. Sonawane[1], Sneha B.Paymal[2], Trupti K.Gade[2] , Deepak Jadhav[2], Vikram More[2] and Navnath M. Kumbhar[1]

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2. Department of Microbiology, Shivaji University, Kolhapur 416004, Maharashtra, India. Email: kds_biochem@unishivaji.ac.in

Abstract

Antibiotic resistance (AR) is the ability of a microorganism to tolerate the effects of an antibiotic. Antibiotic resistance is a serious challenge for the treatment against numorous infectious bacteria. Bacterial resistance to aminoglycoside antibiotics is primarily caused by the enzyme aminoglycoside phosphotransferases (APHs). Thus, efforts should be made to understand the cause of antibiotic resistance as well as to search an alternative strategy to address this issue. Various bioinformatics methods e.g. sequence analysis, homology modelling, molecular docking, and molecular dynamics (MD) simulation have been employed to understand the structural significance of APH from *B. cereus.* The mechanism of substrate and inhibitor binding to APH was studied using molecular docking, which identified GTP as more preferred substrate, whereas ZINC71575479 as most effective inhibitor. Similarly, a comprehensive structural analysis of dipeptide modifying D-Alanine: D-Serine ligase (Ddls) was performed to screen its inhibitors for combating vancomycin resistance. The structure- based virtual screening (SBVS) of oxadiazole derivatives performed by using modeled 3D structure of EgDdls from *E. gallinarum*. D-alanine-D-alanine ligases (Ddl) are interest ing because they use specific substrates e.g. D-amino acids which is vital to bacteria. The results of molecular docking showed that oxadiazole inhibitors could bind preferentially at ATP binding pocket with lowest binding energy. Further, docking and MD simulation results of EgDdls-inhibitor complex revealed interactions of ATP binding residues Phe172, Lys174, Gln210, Glu217, and Asn302 of EgDdls with virtually screened inhibitor. Thus, these studies could be useful to facilitate the design of new lead molecules.

Keywords: Antibiotic resistance, Homology modelling, Molecular docking

Temperature dependence of Intra-cellular Transport and Cytoplasmic Streaming

Ambarish Kunwar

Department of Biosciences and Bioengineering, Indian Institute of Technology Bombay, Mumbai, 400076, Maharashtra, India.

Abstract

Intra-cellular transport is essential for cell functioning and survival. Molecular motor proteins are an extremely important component of the intra-cellular transport system that harness chemical energy derived from ATP hydrolysis to carry out directed mechanical motion inside the cells. Transport properties of kinesin and dynein motors such as processivity, velocity, and their load dependence have been well established through single-molecule experiments. Temperature dependent biophysical properties of molecular motors are now being probed using single-molecule experiments. In the first part of the talk I will discuss our studies that implicate cytoplasmic dynein as a more thermally tunable motor and therefore a potential thermal regulator of microtubule-based intra-cellular transport. Our computational analysis further suggests that motor velocity changes can lead to qualitative changes in individual cargo motion and hence net intracellular cargo transport.

Cytoplasmic streaming is a phenomenon observed in plants where the circulation of cellular components occurs around the central vacuole. It is crucial for the spatio-temporal distribution of organelles in plant cells and thus has an important role in plant growth. It has been found that enhanced cytoplasmic streaming yielded higher growth and better foliage in plants. While cytoplasmic streaming in plants has been extensively studied, the in vivo quantification of the forces involved remains unexplored. In the second part of my talk, I will discuss how optical trapping combined with theoretical modelling enables us to measure collective transport properties such as the forces exerted by cargoes and their speeds during cytoplasmic streaming at different temperatures. A better understanding of how cytoplasmic streaming is regulated at different temperatures is essential to develop plants that can utilize nutrients more efficiently, thus increasing their yield and survival.

AI-Driven In silico Approaches for Next-Generation Antibacterial Discovery Against Multi-drug Resistant ESKAPE Pathogens

Sinosh Skariyachan

Department of Microbiology, St. Pius X College, Rajapuram- Kannur University, Kerala, India Email address: sinoshmicro@stpius.ac.in

Abstract

Antimicrobial resistance (AMR) has become one of the biggest threats to global public health in the twenty-first century. Infections caused by the ESKAPE pathogens are a critical and growing crisis due to their remarkable ability to escape nearly all available antibiotics. Addressing this issue requires a significant shift from traditional antimicrobial discovery methods to data-driven, next-generation strategies. In this setting, artificial intelligence (AI) has quickly emerged as a game-changer in antimicrobial research. The combination of AI with computational biology, systems bioinformatics, and medicinal chemistry allows detailed examination of complex biological and chemical environments on a large scale. By integrating multi-omics datasets—like genomic, proteomic, metabolomic, and chemical information—AI- powered platforms enable accurate predictions of drug-target interactions. They also uncover hidden resistance factors and help prioritize promising therapeutic candidates. Cutting-edge in silico techniques such as high-throughput virtual screening, molecular docking, molecular dynamics simulations, binding free-energy calculations, and AI-driven chemoinformatics speed up lead identification and optimization. These techniques significantly cut costs, time, and experimental failures. In addition, AI-driven bioinformatics tools have become essential for monitoring antimicrobial resistance in real-time, validating targets, and repurposing FDA- approved drugs. Using pathogen- and host-specific genomic signatures further improves precision antimicrobial therapy by allowing tailored treatment strategies that match changing resistance profiles. Together, these advancements are transforming the way we discover antimicrobials. This presentation highlights recent breakthroughs driven by AI at the intersection of computational biology and medicinal chemistry. It includes representative case studies from our lab. These combined technologies are redefining antibacterial drug discovery and preparing the field to effectively address the growing AMR threat posed by ESKAPE pathogens.

Keywords: Antimicrobial resistance (AMR), ESKAPE, Public health, Systems bioinformatics, Artificial intelligence, Molecular docking, Molecular dynamic simulations.

Hybrid Physics-Based and Machine Learning Frameworks for Predicting Fragment and Small-Molecule Binding Affinities

Andrew Lynn, Mrityunjay Singh, Shailendra Singh, and Smriti Mishra

School of Computational and Integrative Sciences, Jawaharlal Nehru University

Abstract

Accurately predicting binding affinities for small molecules and fragments remains a central challenge in computer-aided drug discovery. Physics-based approaches such as Molecular Mechanics Poisson–Boltzmann Surface Area (MM/PBSA) calculations provide a rigorous framework for estimating binding free energies, but their accuracy decreases for fragments due to weaker binding interactions, higher conformational variability, and sensitivity to solvation and entropic effects. Machine learning (ML) methods, on the other hand, can efficiently learn nonlinear relationships from data but often lack the physical interpretability and transferability necessary for general application.

In this study, we develop a hybrid framework that integrates MM/PBSA-derived energy components obtained from docked and simulated fragment and ligand complexes with data- driven molecular descriptors. Using a publicly available dataset containing quantum chemical and molecular dynamics features, we incorporate molecular fingerprint representations to extend chemical diversity and evaluate their complementarity with physics-based energy terms. The resulting model not only improves predictive accuracy across fragment and lead- like compounds but also allows systematic estimation of error contributions from individual components of the physical model.This work demonstrates that coupling MM/PBSA with ML-based corrections provides a robust and interpretable strategy for predicting fragment binding affinities, bridging the gap between physics-based and data-driven paradigms in computational drug discovery.

AI-Enabled Discovery of Choline Acetyltransferase Inhibitors for Theranostic Applications in AD

Rajnish Kumar

Indian Institute of Technology (BHU) Varanasi

Abstract:

Choline acetyltransferase (ChAT), is the key cholinergic enzyme that biosynthesizes the neurotransmitter acetylcholine, which plays a pivotal role in fundamental brain processes. There is a gradual decline in the cholinergic neurons at the early stages of Alzheimer's disease (AD) which results in the deficit of acetylcholine production. Thus, making it the definitive marker for the early-stage estimation of AD progression. The absence of specific, potent, blood-brain-barrier permeable small molecule ligands motivated us to discover novel ChAT ligands. Here we have screened an ultra-large library of small molecule database ZINC20 containing ~1.3 billion molecules by the help of deep learning integrated platform which is an Artificial Intelligence (AI) enabled structure-based virtual screening that enables 100-fold acceleration to the protocol by docking only a subset of a chemical library followed by a deep neural network that synchronously enables ligand-based predictions of the remaining compound library docking scores. The virtual screening was enriched with each iteration cycle until we have the top scoring five virtual hits. Molecular dynamic simulations were carried out to understand their dynamic interaction with ChAT. They also showed prominent interaction with the catalytic residue His324 which is necessary for inhibitory activity of ligands. The potential ChAT hits identified in this study can be utilized and further studied to be developed as novel ChAT ligands, which can also be used as ChAT tracer probes for the diagnosis of cholinergic dysfunction and to initiate timely therapeutic interventions to prevent or delay the progression of Alzheimer's disease.

Keywords: Choline-acetyltransferase, Alzheimer's disease, Deep Docking, Structure based virtual screening

Target AI – Drug sensitivity prediction for targeted cancer therapy

Pratik Chandrani
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Abstract

The aberrant alteration in genes, such as EGFR, resulting from somatic mutations, is associated with driver phenotype, making them a critical target in cancer therapy. This study aims to predict the response of Tyrosine Kinase Inhibitors (TKI) in cancer patients through an easy-to- use web server utilizing artificial intelligence (AI).

We developed an automated and scalable server, including modelling, molecular docking, and molecular dynamics (MD) simulations to elucidate the interactions of EGFR mutants (N ~ 700) with TKIs. These EGFR mutation models, molecular docking scores, and MD simulation reveal an interesting correlation between in-silico observations and clinical TKI sensitivity. We developed a machine-learning model utilizing features of protein sequence, structure, and dynamics.

The ML model achieves an accuracy of 93.7 % and an F1 Score of 97.9 % for the TKI- sensitivity prediction for mutations occurring in the kinase domain of EGFR. Using this model, we characterize the sensitivity of novel EGFR kinase domain mutations previously considered variants of unknown significance (VUS).

We present a new AI model capable of non-linear interpretation from complex data, allowing us to predict the sensitivity of novel EGFR VUS observed during clinical follow-up of cancer patients. The AI model is running over an easy-to-use web-server enabling biologists and clinicians to easily utilize in their practice. Further refinement and clinical validation of this model may provide valuable solutions to predetermine the drug sensitivity of patients in clinics.

Identifying regulatory DNA signatures from high-throughput experiments

Leelavati Naralikar

Indian Institute of Science Education and Research (IISER) Pune

Abstract

Machine learning algorithms are routinely used to answer problems in molecular biology. I will talk about a couple of examples from our lab, where we use mixture modeling to identify novel diverse regulatory mechanisms hidden in high-throughput data. I will focus on the regulatory architecture of promoters (especially in prokaryotes including M. tuberculosis) and if time permits, of regulatory regions in eukaryotes. I hope to make the case that not all machine learning methods are like a black-box.

InstaDock-v2: User-Friendly, Open-Source Tool for Multi-Target Docking and ADMET Analysis

Yash Mathur and Md. Imtaiyaz Hassan

Center for Interdisciplinary Research in Basic Sciences, Jamia Millia Islamia, New Delhi, India, 110025. E-mail: mihassan@jmi.ac.in

Abstract

Understanding drug-target interactions is central to drug discovery and development. Knowledge of these interactions facilitates the rational design of novel therapeutics. Here, we present InstaDock-v2, a Python-based, graphical user interface (GUI) tool designed to perform molecular docking experiments on both Windows and Linux platforms. InstaDock-v2 simplifies and automates the molecular docking pipeline, offering a user-friendly, feature-rich environment tailored especially for researchers with limited computational background. As a freely available, open-source, multi-platform tool, InstaDock-v2 supports both single- and multi-target docking, multiple scoring functions, and an integrated ADMET prediction model. Its modular framework includes utilities for ligand library generation, target preparation, docking, post-processing, and pharmacokinetic/toxicity filtering—all within a single cohesive platform. The tool also provides detailed analysis features such as a 2D interaction viewer and a 3D protein-ligand complex visualizer. By streamlining each stage of virtual screening into an intuitive interface, InstaDock-v2 significantly lowers the barrier to entry for non-specialists in cheminformatics and molecular modeling. We anticipate that its speed, simplicity, and comprehensive capabilities will accelerate structure-based drug design and enable new biological insights across a wide range of systems.

InstaDock-v2 is freely accessible at: **www.hassanlab.in/instadock-v2**

Keywords: Molecular Docking, Structure-Based Drug Design, High-Throughput Screening, Protein- Ligand Interaction, ADMET Prediction, Graphical User Interface, Multi-Target Docking

Computational and experimental approach to identify potential inhibitors against visceral leishmaniasis

Vijaykumar Prajapati

Delhi University South Campus, Delhi

Abstract

Visceral leishmaniasis (VL) is the deadliest form of leishmaniasis without a safer treatment option. This study implies drug repurposing to find a novel antileishmanial compound, namely febrifugine dihydrochloride (FFG) targeting Leishmania antioxidant system. Starting with virtual screening revealed the high binding affinity and lead likeness of FFG against the trypanothione reductase (TR) enzyme of Leishmania donovani, followed by experimental validation. The promastigotes inhibition assay gave the IC50 concentration of FFG and Miltefosine (positive control) as 7.16 ± 1.39 nM and 11.41 ± 0.29 μM, respectively. Their CC50 was found as 451 ± 12.73 nM and 135.9 ± 5.94 μM, respectively. FFG has been shown to increase the reactive oxygen species (ROS), leading to apoptosis-like cell death among L. donovani promastigotes. Spleen touch biopsy resulted in 62% and 55% decreased parasite load with FFG and miltefosine treatment, respectively. Cytokine profiling has shown an increased proinflammatory cytokine response post-FFG treatment. Moreover, FFG is safe on the liver toxicity parameter in mice post-treatment.

An HPC–AI Framework for Mapping Druggable Conformational Landscapes of Cancer Proteins Using Integrated Computing Environment (ICE)

Uddhavesh Sonavane

Centre for Development of Advanced Computing, Pune

Abstract

Protein conformational dynamics play a central role in cancer progression and drug response, yet capturing these transient states remains a major challenge in structure-based drug discovery. Recent advances in high-performance computing and AI-enabled automation provide new opportunities to efficiently explore biologically relevant conformational landscapes of cancer- associated proteins. We present an automated adaptive sampling molecular dynamics framework that accelerates the discovery of functionally important protein states relevant to drug binding. The workflow integrates large-scale molecular dynamics simulations with Markov state modeling–based analysis to iteratively identify metastable conformations and guide subsequent simulations toward underexplored regions of the conformational space. This closed-loop strategy enhances sampling efficiency while minimizing computational redundancy. The framework is deployed within an Integrated Computing Environment (ICE), enabling scalable execution, reproducibility, and seamless integration of simulation and analysis components. By combining AI-guided adaptive sampling with an automated HPC environment, this approach reduces time-to-insight and enables efficient mapping of druggable conformational states, supporting data-driven therapeutic discovery in computational oncology.

Unraveling Macromolecular Activation Mechanism and Protein-Protein Interactions in Health and Disease

Kakoli Bose

ACTREC, Tata Memorial Centre, Navi Mumbai, India Homi Bhabha

National Institute, India

Email: kbose@actrec.gov.in

Abstract

Uncontrolled cell proliferation due to the non-synchronous activity of pro- and anti-apoptotic proteins creates an imbalance in cellular homeostasis, often leading to 'apoptosis-evading' cancer. Therefore, understanding the intricate liaison between these antagonistic proteins becomes imperative to restore the balance and regulate the disease. HtrA2, a complex trimeric pyramidal serine protease, is involved in mitochondrial homeostasis and promotes apoptosis through multiple pathways, understanding of which is limited by obscurities of its intricate allosteric pathway, cellular targets, and substrate selectivity. This multitasking ability of HtrA2 and its omnipresence in the apoptotic pathway make it an important therapeutic target. Therefore, defining the signature(s) of HtrA2-substrate interactions, along with elucidating the mechanism of its activation, would help modulate the protease with desired characteristics. Despite the availability of structural details, the reports on HtrA2's mechanistic regulation remain non-concordant. Therefore, using a multidisciplinary approach in the presence of a wide array of substrates, we studied the mode of allosteric activation and the role of different domains in mediating catalytic activity and substrate selectivity of HtrA2. These helped proffer a hypothesis advocating activation through inter-subunit allosteric cross-talk, both via its N-terminus and C-terminal PDZ domain in a mutually exclusive yet synergistic manner. Furthermore, structural and computational snapshots confirmed the role of PDZs in maintaining structural stability and coordinating the reorganization of the N-terminal region. Revelation of a broad substrate specificity highlights its participation in multiple cellular pathways. Therefore, apart from providing cues for devising structure-guided, tailor-made therapeutic strategies, this study establishes a physiologically relevant working model of complex allosteric regulation through a trans-mediated cooperatively shared energy landscape.

Young Speaker - Abstracts

Design and optimization of CAR scFvs against the CD20 antigen using molecular modelling approach

Purva Khodke

Sunandan Divatia School of Science, SVKM's NMIMS Deemed-to-be University, Mumbai

Abstract:

CAR-T cell therapy faces significant efficacy hurdles when targeting the CD20 antigen due to its membrane-proximal location and short extracellular epitopes. To overcome these binding challenges, our study utilized a molecular modeling strategy to engineer and optimize scFvs derived from CD20 specific mAbs. By analysing binding modes and structural stability, our research identifies constructs that enhance affinity towards membrane-bound CD20. This computational approach provides a rational framework for developing next-generation CAR constructs with improved targeting and persistence in B-cell malignancies.

Transcriptomic Insights of heterogenous regulator-mediated increase in fatty acid production

Neha Sawant

Sunandan Divatia School of Science, SVKM's NMIMS Deemed-to-be University, Mumbai

Abstract:

Over a decade, microbial fatty acids (FA) have grabbed immense attention due to its diverse applications. These FA are conventionally harvested from algal and fungal sources. However, researchers are now transitioning towards microbial systems for FA production due to the inherent shortcomings and stresses generated during FA production in algal-fungal sources. Using recombinant DNA technology and transcriptome data analysis, we tried to mitigate the stresses generated during FA production and elucidate the molecular mechanism behind enhanced FA production in the recombinant strain.

Industry Sponsor- Abstracts

Bridging Physics-Based Modeling and AI: The Next Paradigm in Drug Design

Raghu.R CEO,

Molecular Solutions pvt ltd. Bangalore

Abstract

Pharmaceutical research and development is undergoing a profound digital transformation driven by advances in artificial intelligence (AI), machine learning (ML), and high- performance in silico methodologies. These technologies are fundamentally reshaping how drugs are discovered, optimized, and translated into clinical candidates, significantly reducing timelines, lowering costs, and improving overall success rates. Recent breakthroughs include chemical-space docking approaches capable of screening billions to trillions of compounds with hit rates approaching 40%, rapid prediction of binding and unbinding kinetics within minutes, and free energy perturbation (FEP) methods delivering highly accurate binding affinity predictions for small molecules, peptides, and complex targets within hours. In parallel, polymorphism prediction has reached accuracies of up to 98%, while AI/ML-driven formulation design is addressing solubility and stability challenges with predictive accuracies of approximately 85%. Further advances include the computation of more than 200 ADMET properties, high-throughput PBPK simulations, early pKa prediction to reduce late-stage attrition, and AI- and literature-driven retrosynthesis platforms that are transforming synthetic route design, process chemistry, and impurity prediction. The emergence of large language models (LLMs), generative AI, and AI-enabled atomistic simulations is further expanding the scope of digital drug design and development.

Collectively, these innovations are redefining hit identification, lead optimization, and translational decision-making. However, many academic institutions and research organizations continue to rely predominantly on traditional experimental approaches, underutilizing the power of modern digital drug discovery. This presentation will (i) explain the scientific principles and methodologies underlying these emerging technologies, (ii) present real-world case studies demonstrating measurable impact, and (iii) outline practical strategies for academia and research institutions to adopt AI-driven drug discovery and remain competitive in the evolving global R&D landscape.

Drug Design in the Digital Age: Harnessing Computational

Tools for Success

Anil Mhashal

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Abstract

The landscape of drug discovery is undergoing a rapid transformation driven by advances in artificial intelligence, high-performance computing, and data-centric modelling. In the digital age, traditional empirical approaches are increasingly complemented and often accelerated by computational platforms capable of predicting molecular properties, identifying therapeutic candidates, and optimizing formulations with unprecedented speed and accuracy. This work introduces PRinS3, an integrated digital suite designed to streamline end-to-end drug discovery workflows through three core pillars: predictive modelling, simulation, and smart screening. PRinS3 combines machine learning-based property prediction, molecular dynamics powered mechanistic insights, and automated virtual screening pipelines, enabling researchers to rapidly explore chemical space, evaluate candidate efficacy, accurate free energy estimations and enhance formulation performance. By unifying these capabilities within a single framework, PRinS3 significantly reduces development timelines, improves decision-making, and enhances the reliability of early-stage drug discovery. The suite represents a robust step toward fully digital, data-driven pharmaceutical innovation, accelerating the translation of molecular concepts into viable therapeutic solutions.

Artificial Intelligence and Machine Learning-Powered Cloud Platforms in Drug Discovery: Introducing SilicoXplore™ for Accelerated and Smarter Therapeutic Development

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Abstract
Artificial intelligence (AI) and machine learning (ML) are revolutionizing life science research by integrating computational intelligence with deep domain expertise in drug discovery and bioinformatics. In an era of increasingly complex biological data and fragmented research tools, AI/ML-powered platforms provide a unified in-silico ecosystem that accelerates the entire research continuum from intelligent hypothesis generation and target identification to predictive modeling, virtual screening, data interpretation, and translation toward clinical impact, dramatically reducing time, cost, and experimental burden while enabling discoveries that were previously unattainable. Cloud-based drug discovery platforms are very important in the pharmaceutical and biological sciences because they provide scientists with powerful computing resources without the need for expensive local machines. Researchers can easily share data and collaborate across the world in real time, run complex AI and simulations quickly, and access large libraries of compounds and biological information. This saves time, lowers costs, speeds up the search for new medicines, and helps bring life-saving drugs to patients faster. SilicoXplore™ is a powerful cloud-based platform, the flagship program of SilicoScientia, that accelerates, optimizes, and simplifies drug discovery. It brings together intelligent screening, predictive modeling, lead optimization, and data analysis tools in one simple place. By doing most of the early work on the computer rather than in the lab, SilicoXplore™ helps scientists quickly find promising drug candidates, make better predictions about how they will work in the body, reduce research costs, and speed up the journey from ideas to real medicines that can help patients.

Keywords: Artificial intelligence; Machine learning; Drug discovery; SilicoXplore

Poster - Abstracts

Deciphering the Binding Mechanisms of QLH11811 against Triple-Mutant EGFR for The Treatment of Non-Small Cell Lung Cancer through Integrated In-Silico Approaches

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Abstract

Non-small cell lung cancer (NSCLC) associated with triple-mutant epidermal growth factor receptor (EGFR) variants presents a major therapeutic challenge due to enhanced drug resistance. In this study, an extensive in-silico approach was employed to comparatively evaluate the inhibitory potential of QLH-11811, a clinical-stage EGFR inhibitor, and the FDA-approved drug Brigatinib against wild-type and triple-mutant EGFR proteins. Molecular docking analysis demonstrated that QLH-11811 exhibited a stronger binding affinity toward the triple-mutant EGFR, with a docking score of −7.737 kcal/mol, compared to Brigatinib (−6.783 kcal/mol). To further validate binding stability, MM-GBSA binding free energy calculations revealed a more favorable average binding energy for QLH-11811 (−189.375 kcal/mol) relative to Brigatinib (−170.465 kcal/mol), indicating enhanced thermodynamic stability of the QLH-11811–EGFR complex. These findings were further supported by molecular dynamics

simulations, including RMSD, RMSF, PCA, and DCCM analyses, which confirmed the superior stability and consistent interaction profile of QLH-11811 within the EGFR active site. Density functional theory (DFT) calculations provided insights into the electronic structure and reactivity of both ligands. In addition, pkCSM-based pharmacokinetic and toxicity predictions indicated favorable oral absorption, acceptable distribution characteristics, and non-mutagenic profiles for both compounds, supporting their drug-likeness and developability. Overall, the integrated computational results highlight QLH-11811 as a promising candidate with improved binding affinity, stability, and pharmacokinetic suitability against triple-mutant EGFR in resistant NSCLC.

Keywords: Triple-Mutant EGFR**,** Non-Small Cell Lung Cancer**,** Molecular Dynamics Simulation**,** QLH-11811

Harnessing 7-Hydroxy-4-Methylcoumarin–Phenyl Ether Hybrids for Antitubercular Drug Discovery: Integrating Synthesis, Molecular Modeling, and Biological Evaluation

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Abstract

Small-molecule discoveries continue to play a pivotal role in anti-tuberculosis drug development, particularly in combating drug-resistant *Mycobacterium tuberculosis* (MTb). Current research strategies emphasize both phenotypic and target-based screening approaches to identify compounds capable of disrupting essential mycobacterial pathways, including cell wall biosynthesis, energy metabolism, and protein homeostasis. Progress in medicinal chemistry, coupled with structure-guided molecular modeling, has facilitated the optimization of novel chemical scaffolds with enhanced potency and favorable pharmacokinetic profiles. In this study, a molecular hybridization approach was adopted to design

and develop new anti- tubercular and antibacterial agents by combining two privileged pharmacophores 7-hydroxy- 4-methylcoumarin and phenyl ether within a single molecular framework. This rational scaffold integration was intended to synergistically improve anti- mycobacterial activity. The synthesized hybrid compounds are anticipated to exhibit anti-TB activity against *M. tuberculosis* H37Rv with MIC values >25 µg/mL. Molecular modeling studies illustrate key interactions between the synthesized compounds and potential TB drug targets. Overall, the findings underscore coumarin-based molecular hybrids as promising candidates for tuberculosis treatment.

Key words: *Mycobacterium tuberculosis,* 7-hydroxy-4-methylcoumarin, molecular modeling.

Computational Framework for Identifying Potent Natural Therapeutic Leads in Parkinson's Disease Pathology

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Abstract

Parkinson's disease (PD) is a progressive neurodegenerative disorder characterized by interconnected pathological mechanisms such as oxidative stress, neuro-inflammation, and protein aggregation. The limited success of current disease-modifying therapies underscores the need for innovative multi-target therapeutic approaches. In this study, an integrative transcriptomic meta-analysis of twelve GEO datasets was performed to identify key regulatory genes implicated in PD pathology. Network-based and functional enrichment analyses were used to prioritize central molecular targets associated with major disease-relevant pathways.

A structure-based virtual screening strategy was employed to explore neuroprotective natural compounds targeting these prioritized proteins. Approximately three lakh purchasable compounds were obtained from the ZINC database and subjected to ADMET and blood–brain barrier permeability filtering to shortlist candidates for molecular docking. Docking studies identified compounds with strong binding affinities toward the selected targets. The top-ranked ligand– protein complexes were further assessed using molecular dynamics simulations, which demonstrated stable interactions as reflected by RMSD and RMSF analyses. Binding free energy calculations using the MM-PBSA approach confirmed favorable energetics primarily driven by van der Waals and electrostatic interactions.

Overall, this integrative computational framework highlights promising multi-target natural compounds as potential neuroprotective leads for Parkinson's disease and emphasizes the role of computational chemistry in accelerating sustainable drug discovery.

Keywords: Parkinson's disease, Oxidative stress, Natural Compounds, Drug Discovery.

Structure-Based Computer-Aided Discovery of Novel Antiviral Compounds

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Abstract

Computer-Aided Drug Design and Discovery (CADD) has emerged as a powerful approach to accelerate the identification and development of novel therapeutic agents by integrating computational chemistry, structural biology, and bioinformatics. In the context of emerging and re-emerging viral diseases, structure-based drug discovery offers a rational strategy for identifying antiviral compounds that specifically target essential viral proteins. This study presents a prospective analysis of structure-based computer-aided methodologies for identifying novel antiviral compounds using in silico techniques. The workflow involves the selection and preparation of viral target proteins, followed by virtual screening of small-molecule libraries using molecular docking to predict binding affinities and interaction profiles. Structural insights into protein–ligand interactions enable the identification of promising lead compounds with high specificity and stability. Computational analyses such as binding energy estimation, interaction mapping, and molecular property evaluation are employed to prioritize candidate molecules. The integration of advanced computational tools enhances screening efficiency while significantly reducing time and cost compared to conventional experimental approaches. The findings highlight the effectiveness of structure-based CADD in narrowing down potential antiviral leads and providing mechanistic insights into drug–target interactions. Furthermore, the incorporation of artificial intelligence and machine learning techniques holds promise for improving prediction accuracy and lead optimization. Overall, this study underscores the potential of computer-aided, structure-based strategies as a robust platform for accelerating antiviral drug discovery and supporting translational research in pharmaceutical development.

Keywords: Computer-Aided Drug Design, Structure-Based Drug Discovery, Antiviral Drug Discovery, Molecular Docking

Screening of Natural Ligands as Potential FKBP5 Inhibitors for Alcohol Use Disorder - A Bioinformatic Approach

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Abstract

Alcohol Use Disorder (AUD) is a complex neuropsychiatric condition marked by chronic stress, impaired neuroplasticity, and disrupted hippocampal function by compulsive alcohol use. Glucagon-like peptide-1 receptor (GLP-1R) agonists reduce alcohol intake and craving clinically, yet the hippocampal mechanisms underlying these effects remain unclear. This study uses an integrated bioinformatics workflow to define GLP-1R-associated signalling pathways in AUD.Differential expression analysis of the GSE44456 hippocampal transcriptome identified FKBP5 as significantly upregulated. Protein–protein interaction and network analyses revealed a functional GLP-1R-FKBP5-BDNF signalling axis. An inverse relationship between FKBP5 and BDNF expression across the CNS indicates opposing regulation of stress responsivity and neuroplasticity. Targeting FKBP5 mediated suppression of BDNF may therefore attenuate stress driven alcohol consumption. Six natural FKBP5 inhibitor candidates Ruscogenin, Rosavin, Ginsenosid, Quercetin, Curcumin, and Apigenin were evaluated using ADMET profiling, BBA permeability prediction, and molecular docking against FKBP51 with SAFIT1 as reference. Ruscogenin showed the strongest binding affinity (−7.7 kcal/mol) and favourable brain penetration, whereas Rosavin exhibited the most advantageous safety profile with minimal predicted hepatotoxicity. Overall, these findings position the GLP-1R-FKBP5-BDNF axis as a key regulator of hippocampal stress signalling and neuroplasticity in AUD and support FKBP5 as a mechanistically informed therapeutic target for intervention.

Keywords: Alcohol Use Disorder, FKBP5, Ruscogenin, DEG

SilicoXplore: A Next-Generation Cloud Platform for Scalable, Artificial Intelligence and Physics-Driven End-to-End Solution for Rapid Hit-to-Lead Optimization

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Abstract

SilicoXplore is a state-of-the-art, cloud-based, end-to-end in-silico drug discovery platform that integrates over 20 AI-powered modules to optimize early-stage therapeutic research. Combining advanced machine learning with physics-based simulations enables efficient exploration of chemical spaces, accurate target engagement prediction, and candidate prioritization, lowering experimental costs, timelines, and attrition in drug development. SilicoXplore empowers researchers to seamlessly explore vast-to-extra-large chemical spaces through an intuitive, no- code interface without requiring programming expertise. Core functionalities include AI- driven de novo molecules and peptides design, using generative models to create new scaffolds from user-defined queries, target structures, or physicochemical constraints. It excels at high-throughput virtual screening and precise large-scale docking across diverse chemical spaces, utilizing multiple scoring functions and advanced docking engines to identify potential hits. SilicoXplore also offers hassle-free MD simulations, seamless AI-powered ADMET profiling, rapid and precise quantum mechanical calculations, automated docking revalidation, effortless metallic compound docking, ML-accelerated QSAR modeling, and high-throughput virtual screening. Additional modules support sequence and structural bioinformatics for target prediction and validations. SilicoXplore's antimicrobial and anticancer projects showcase its power, delivering rapid identification of novel hits, optimized lead compounds, and mechanistic insights through integrated AI-driven screening and physics-based validation. Overall, SilicoXplore is an intuitive web interface, backed by a scalable cloud architecture, that facilitates automated workflows, collaborative data management, and reproducible analyses. SilicoXplore exemplifies the paradigm shift toward AI-accelerated, multi-parametric optimization in modern drug discovery. By bridging generative chemistry, predictive modeling, and simulation, it empowers researchers to narrow down candidates from millions to promising leads before experimental validation.

Keywords: SilicoXplore; Drug discovery; Cloud platform; Lead identification

Comparative structural and functional analysis of Parkinson's Disease associated SNCA mutants

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Abstract

Parkinson's disease (PD) is a neurodegenerative disorder affecting the neurons of the CNS. Alpha- synuclein (SNCA) misfolding and aggregation is associated with PD. The structural and functional impact of PD associated mutations on SNCA remain unexplored. This study presents a comparative in silico analysis of WT-SNCA and PD linked variants on the structure and function of SNCA.

Mutational impacts on protein stability (A30G, A30P, A53E, and A53T) were analysed using DynaMut2 and PremPS and A30G and A53E were found to be destabilising and showed intramolecular interaction changes The structural dynamics of WT and mutants were analysed using 100 ns molecular dynamics simulations using GROMACS. The A53T and A30P showed variation in RMSD in comparison with the WT. RMSF analysis showed higher residue fluctuations for all the mutants indicating loss of alpha helical structure. To study the functional relevance, equilibrated structures were docked against the P2RX7 receptor using HADDOCK and ClusPro with binding affinities analysed using Prodigy. Mutant SNCA variants demonstrated altered binding profiles relative to WT, with A53E and A53T showing enhanced predicted interaction strengths. Overall, these results suggest that PD associated SNCA mutations modulate α-synuclein stability, dynamics, and receptor interactions, potentially influencing P2RX7 mediated neuroinflammatory pathways associated with Parkinson's disease.

Keywords: Alpha-synuclein, Parkinson's Disease, Docking, P2RX7

Docking of Natural Products Targeting HIV- Leishmania Co-infection

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Abstract

HIV–Leishmania co-infection profoundly impairs immunity, accelerates disease progression, increases treatment failure, and poses a growing global public health crisis demanding novel targeted therapeutic interventions. Phytomolecules offer structurally diverse, multi-target bioactive scaffolds with lower toxicity, making them promising candidates for tackling the complex molecular interplay of HIV–Leishmania co-infection. This study explores the phytomolecular space to identify dual-acting natural products capable of simultaneously targeting key molecular pathways in HIV–Leishmania co-infection. The Natural Product Activity and Species Source database was explored for natural compounds, and possible hits were filtered using various drug- like filters. The binding affinities of screened compounds were assessed via molecular docking against HIV-1 reverse transcriptase and trypanothione reductase, key targets in HIV–Leishmania co-infection, with standard drugs docked as reference controls. The *in-silico* studies highlighted three phytomolecules: Eriocitrin, Silandrin and Narirutin that showed results comparable to the control molecules- Amphotericin B, Miltefosine and Nevirapine. The use of such natural compounds reduces the chemical load on the patient, chances of drug toxicity and associated adverse effects and can be used as lead compounds in drug development for HIV – Leishmania co-infection. Molecular Dynamics and in vitro experiments are further deemed necessary to validate the results.

Keywords: *Natural compounds, HIV-Leishmania co-infection, Molecular docking, Eriocitrin.*

CancerBiomeDB: A Knowledgebase on Gut Microbiome Signatures for Pan- Cancer Immunotherapy

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Abstract

Gut microflora composition constitutes a critical determinant in the regulation of response to anti- cancer therapies. Large scale metagenomic studies revealed compositional deviations in gut microflora serves as a contributing factor to heterogeneity in cancer therapeutic phenotypes. Despite investigating the impact of gut microflora in various cancer types limited efforts have been made to systemically integrate the gut microbial findings related to therapeutic response across cancer types. To offer a holistic and comprehensive landscape of gut microbial associations with clinical phenotypes we developed a manually curated CancerBiomeDB which compiles literature- based associations of gut microflora with therapeutic interventions. CancerBiomeDB consolidates 155 studies covering 22 countries. This knowledgebase incorporates human based 1744 curated gut microflora associations from 610 microbial taxa spanning 22 cancer histological subtypes.The CancerBiomeDB knowledgebase attributes an interactive web interface to facilitate browsing, retrieving and downloading curated entries. Furthermore, we mapped gut microflora deviations linked with anti-tumour medications and observed consistent microflora in various cancer types. Predominately documented gut microflora are *Faecalibacterium prausnitzii, Akkermansia muciniphila, Agathobacter rectalis,* and *Prevotella copri* with better prognosis whereas *Akkermansia muciniphila, Bacteroides thetaiotaomicron, Escherichia coli,* and *Hungatella hathewayi* in poor prognosis. This user-friendly knowledge base provides comprehensive insights into gut microbial influence on immunotherapy, aiding in the identification of potential predictive biomarkers for improved treatment strategies across pan-cancer patients.

Keywords: Cancer, Pan-cancer, Gut microbiota, Immunotherapy, Knowledgebase

Unravelling HER2/NRG1-Mediated Mechanisms of Osimertinib-Induced Cardiotoxicity: An Integrated

Computational Study

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Abstract

The emergence of osimertinib as a preferred therapy for EGFR-mutant non-small cell lung cancer (NSCLC) has been accompanied by increasing reports of cardiotoxicity, the mechanisms of which remain poorly understood. Given the cardioprotective role of the neuregulin-1 (NRG1)-HER2- HER4 signaling cascade, this study explored the hypothesis that off-target inhibition of HER2 may contribute to osimertinib-associated cardiac effects. Using an integrative computational approach, we compared the HER2-binding behavior of osimertinib with that of Trastuzumab and Lazertinib. Docking analyses revealed that osimertinib exhibited the strongest affinity toward HER2 (-9.526 kcal/mol), forming stable interactions within the ATP-binding site. Molecular dynamics simulations demonstrated minimal backbone deviation and enhanced complex stability, while principal component and dynamic correlation analyses indicated restricted conformational flexibility—features consistent with strong and persistent binding. MM-GBSA free-energy calculations further supported these results, showing a highly favorable ΔG_bind of –68.15 kcal/mol, dominated by van der Waals and lipophilic contributions. Together, these computational findings suggest that osimertinib's stable HER2 engagement may suppress HER2-mediated cardioprotective signaling, predisposing to cardiac dysfunction. The comparative weakness of lazertinib–HER2 interactions reinforces its lower cardiotoxic potential. This study provides molecular evidence linking HER2 inhibition to osimertinib-induced cardiotoxicity and highlights the importance of designing EGFR inhibitors with refined HER2 selectivity.

Keywords: Osimertinib, Non-Small Cell Lung Cancer, Cardiotoxicity, HER2

Machine Learning Techniques Applied to Identify Mycobacterial Cell Wall Inhibitors for Tuberculosis

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Abstract

Tuberculosis (TB), caused by Mycobacterium tuberculosis (Mtb), is a widespread chronic infection. The mycobacterial cell wall contains crucial arabinose polymers, primarily arabinogalactan, derived from decaprenylphosphoryl arabinofuranose (DPA). DprE1, an enzyme, plays a pivotal role in cell wall growth by converting decaprenylphosphoryl ribofuranose (DPR) to DPX. Here we present our efforts at designing a machine learning (ML) model for probable DprE1 inhibitors of Mtb.

A total of 255 molecules and their associated IC50 values, along with approximately 260 molecules and their corresponding MIC values, were extracted from the chemical classes of hydantoins, pyrrolothiadiazoles, and phenylpropanamides. The dataset was categorized into active and inactive compounds using a specific cutoff. Subsequently, 2D descriptors and four fingerprints were calculated. Eight machine learning algorithms, including Random Forest (RF), Decision Trees (DT), Support Vector Machine (SVM), and Extreme Gradient Boosting (XGBoost), were employed to develop a classification-based model. MACCS features outperform other feature sets in distinguishing structural and activity differences in molecules, yielding the highest average AUC values for both IC50 and MIC datasets. The results demonstrate that the XGBoost (XGB) algorithm exhibits the best performance (Accuracy: 0.81, AUC-ROC: 0.85, MCC: 0.47, F1: 0.88). The model was applied to different external datasets to assess its accuracy and reliability. The applicability domain and robustness of the model were also evaluated. Finally, a web app called "Quick Pred" has been developed and will be made freely available to detect potential DprE1 inhibitors of Mtb.

Keywords: Machine Learning, Mycobacterium tuberculosis, DprE1.

Comparative structural and functional analysis of Parkinson's Disease associated SNCA mutants

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Abstract

Parkinson's disease (PD) is a neurodegenerative disorder affecting the neurons of the CNS. Alpha-synuclein (SNCA) misfolding and aggregation is associated with PD. The structural and functional impact of PD associated mutations on SNCA remain unexplored. This study presents a comparative in silico analysis of WT-SNCA and PD linked variants on the structure and function of SNCA.

Mutational impacts on protein stability (A30G, A30P, A53E, and A53T) were analysed using DynaMut2 and PremPS and A30G and A53E were found to be destabilising and showed intramolecular interaction changes The structural dynamics of WT and mutants was analysed using 100 ns molecular dynamics simulations using GROMACS. The A53T and A30P showed variation in RMSD in comparison with the WT. RMSF analysis showed higher residue fluctuations for all the mutants indicating loss of alpha helical structure. To study the functional relevance, equilibrated structures were docked against the P2RX7 receptor using HADDOCK and ClusPro with binding affinities analysed using Prodigy. Mutant SNCA variants demonstrated altered binding profiles relative to WT, with A53E and A53T showing enhanced predicted interaction strengths. Overall, these results suggest that PD associated SNCA mutations modulate α-synuclein stability, dynamics, and receptor interactions, potentially influencing P2RX7 mediated neuroinflammatory pathways associated with Parkinson's disease.

Keywords: Alpha-synuclein, Parkinson's Disease, Docking, P2RX7

Structural Elucidation of lead compounds for Anti-fouling properties through computational strategies

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Abstract

Corrosion has long posed a significant challenge to human development and engineering systems, particularly in marine environments. Among the most critical threats to marine ecosystems and the maritime industry is the progressive colonization of submerged and wetted surfaces by microorganisms, plants, and invertebrates. This phenomenon, broadly referred to as marine biofouling, leads to increased fuel consumption, material degradation, and ecological imbalance. Traditionally, biofouling has been mitigated using synthetically derived antifouling agents; however, many of these compounds have demonstrated adverse environmental effects and face increasing regulatory restrictions due to concerns related to sustainability, toxicity, and long-term economic viability. The structural diversity of marine natural products (MNPs) and inherent bioactivity make them particularly suitable candidates for rational exploration using computer-aided drug design (CADD) methodologies. This presentation focuses on the application of integrated CADD strategies for the discovery and prioritization of novel antifouling compounds derived from marine sources.Ligand-based approaches, including quantitative structure–activity relationship (QSAR) modeling, were employed to design and generate potential leads targeting acetylcholinesterase, a key enzyme implicated in biofouling-related pathways. Structure-based techniques, such as molecular docking, were further utilized to investigate ligand–enzyme interactions and binding characteristics. Additionally, representative clusters of antifouling-relevant compound classes reported in the literature were considered to support rational lead selection. Overall, this poster highlights the role of CADD methodologies in accelerating the systematic exploration of marine natural products and supporting the development of ecologically safe and effective antifouling agents while reducing experimental complexity and resource expenditure.

Keywords- Computer-Aided Drug Design (CADD), Anti-Fouling Agents, Marine Natural Products (MNPs)

Computational Discovery of Dual-Target Inhibitors for Alzheimer's Disease Using Machine Learning and Pharmacokinetic Optimization

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Abstract

Alzheimer's disease (AD) is a progressive neurodegenerative condition with clinical manifestations of cognitive loss and memory degradation, which is primarily related to cholinergic dysfunction and amyloid-β aggregation. The enzymes acetylcholinesterase (AChE) and β-site amyloid precursor protein cleaving enzyme 1 (BACE1) are central to these pathological processes and are thus therapeutic targets of great importance in the treatment of AD. In the present work, a machine learning-supported model was designed to predict inhibitory activity (pIC_{50}) against both AChE and BACE1 simultaneously. Experimentally verified inhibitors were carefully selected from the ChEMBL database, and their molecular descriptors were calculated to build a dual-target prediction model by employing an optimized stacked ensemble regression strategy with Random Forest, XGBoost, SVR, and Ridge as base learners. Selection, removal of multicollinearity, and hyperparameter optimization using GridSearchCV improved model performance and generalizability. The completed dual-target model had excellent predictive performance in cross-validation and external validation sets and was then used to screen AI-generated novel ligands for the possibility of dual inhibitory activity. The highest-ranking candidates were docked against AChE and BACE1 active sites to investigate binding affinities as well as significant interactions. This combined AI/ML-based dual-target discovery workflow provides a rationale, cost-effective, and time-efficient methodology for the detection of novel multifunctional ligands with the potential to be therapeutically effective in Alzheimer's disease.

Keywords: Machine Learning, Alzheimer's disease, acetylcholinesterase (AChE), β-site amyloid precursor protein cleaving enzyme 1 (BACE1)

NatureCAN - Knowledgebase of evidence-based Ayurveda in Cancer Care

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Abstract

Cancer is a multifactorial disease managed with cytotoxic therapies. Therefore, there is an increasing demand to incorporate natural alternatives to cancer management. Studies report the use of medicinal plants to complement conventional cancer treatment, but a robust, evidence- driven, and computationally accessible resource connecting medicinal plants to their effects in cancer is lacking. Therefore, we developed NatureCAN to address this gap. We extracted 4010 medicinal plants used in Indian traditional medicine. Research articles and their metadata were automatically retrieved from PubMed. Natural Language Processing (NLP) and Large Language Model (LLM) based classification were employed to identify cancer types, study types, and brief experiment summaries for each retrieved article, followed by a rigorous statistical evaluation. Further, we deployed the knowledge base on a user-friendly web server. We used extracted medicinal plant names for automated evidence mining, yielding 131,533 PubMed articles. NLP models extracted specific cancer types from abstracts. While LLM classified studies into in vitro, in vivo, in silico, clinical, or review categories, resulting in 23,792 high-confidence classified entries. The extracted data yielded accuracy above 90% for cancer and study types, as verified manually. NatureCAN integrates programmatically mined evidence, AI-driven interpretation, and structured knowledge for Ayurveda-based cancer research. This resource provides a user-friendly interface and API, enabling researchers to explore medicinal plant evidence and support the development of integrative cancer care.

Keywords: NatureCan, Traditional Medicine, Natural Language Processing, Large Language Model

Computational Integration of Multi-omics and Pharmacological Data Using AI for Precision Therapeutics

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Abstract

Computational biology has moved from being a supportive analytical tool to becoming a central engine of biomedical innovation. When genomics and proteomics data are combined with artificial intelligence (AI), the healthcare sector can identify disease mechanisms faster, discover drug targets more precisely, and design candidate molecules with greater efficiency. This paper explains how genomics, proteomics, and multi-omics integration create a strong evidence base for drug discovery, and how AI methods such as machine learning, deep learning, and generative modelling convert complex biological signals into actionable therapeutic insights. It also highlights interdisciplinary innovation, where biology, clinical medicine, computer science, statistics, and regulatory governance work together to improve patient outcomes. At the same time, major challenges remain: data quality, bias, interpretability, reproducibility, privacy, and the translation gap between computational predictions and clinical success. By synthesizing recent literature and verifiable statistics, the paper proposes a practical view of how interdisciplinary teams can create a reliable pipeline from biological data to real- world healthcare innovation.

Keywords: computational biology, genomics, proteomics, multi-omics, AI, machine learning, drug discovery, precision medicine, biomarker, translational research

Network Pharmacology based Computational Investigation of Nelumbo nucifera derived alkaloids targeting GPCRs Associated with Schizophrenia

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Abstract

Schizophrenia is a complex neurological disorder characterized by hallucinations, cognitive impairment, and major health burdens. Current treatment emphasizes symptom control and relapse prevention primarily through dopamine-targeting antipsychotics despite notable physical and neurological side effects. Natural products have complementary therapeutic potential. Nelumbo nucifera (Sacred Lotus) contains bioactive alkaloids with considerable neuropharmacological potential, supporting exploration as adjunctive therapeutic candidates in schizophrenia. The present study provides a systematic and integrative evaluation of the antipsychotic potential of Nelumbo nucifera alkaloids using network pharmacology, molecular docking, and molecular dynamics simulations. Through multi database mining, 94 potential gene targets associated with nuciferine, nornuciferine, dehydronuciferine, and 7-hydroxydehydronuciferine (7-HDNF) were identified, of which 12 targets overlapped with schizophrenia associated and clinically relevant genes. This convergence highlights a meaningful pharmacological interface between Nelumbo nucifera alkaloids and schizophrenia-related molecular pathways.

Network analysis identified dopamine receptor D2 (DRD2) as the key hub gene, underscoring its central role in the schizophrenia pathophysiology and its relevance as a primary antipsychotic target. Molecular docking demonstrated favorable binding affinities of all four alkaloids toward DRD2, comparable to clinically used antipsychotic agents. Molecular dynamics simulations confirmed the structural stability of the DRD2–alkaloid complexes, supporting the plausibility of sustained receptor–ligand interactions under physiological conditions. Rather than replacing existing therapies, these findings support Nelumbo nucifera alkaloids as potential adjuvant agents in schizophrenia treatment. Their multi-target pharmacological profile and stable DRD2 interactions suggest complementary benefits, including enhanced therapeutic efficacy, reduced drug dosage, and mitigation of adverse effects providing a strong foundation for subsequent experimental and clinical validation.

Keywords: Schizophrenia, *Nelumbo nucifera*, Network pharmacology, Docking, MD simulations

Leveraging Genomic Technologies to Address Antimicrobial Resistance

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Abstract

Antimicrobial resistance (AMR) is a major global public health challenge driven by the increasing prevalence of drug-resistant bacterial pathogens. AMR occurs when microorganisms survive exposure to antimicrobial agents and continue to proliferate. Such resistance arises through genetic evolution, including spontaneous mutations and the acquisition of external genetic elements, which enhance microbial survival and fitness under selective pressures and adverse environmental conditions.Advances in high-throughput sequencing technologies have established genomics—the study of an organism's complete genetic material—as a powerful approach for investigating biological systems and disease mechanisms at the molecular level. Sequence-based strategies for AMR detection rely on advanced bioinformatics tools to analyse and visualize the genomic architecture of the microbial resistome, which comprises resistance genes and their precursors. Pathogen genomics has significantly improved understanding of the origin, molecular basis, and dissemination of antimicrobial resistance.This review focuses on pan-genome analysis as a key genomic approach for exploring the genetic diversity of pathogenic bacteria and elucidating mechanisms of AMR. Pan-genome analysis enables the characterization of core and accessory genomes, strain-specific genes, and mobile genetic elements, providing critical insights into bacterial evolution and the distribution of resistance determinants. In addition, commonly used bioinformatics tools and databases for genomic and pan-genomic analyses are summarized, along with a brief overview of major diseases associated with antimicrobial-resistant pathogens.

Keywords: Genomics, Antimicrobial resistance, Pan-genome analysis

AI-based Analysis of Gut Probiotic Microbiota And Its Role In Disease Presentation With Immune Modulation

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Abstract

The gut microbiome functions as an essential biological interface between microbial metabolism and host immunity, exerting long-term influence on immune equilibrium, inflammatory control, and systemic health of a human body. Increasing clinical and computational evidence indicates that alterations in microbial composition and function are closely linked with the initiation and progression of immune-related severe disorders such as autoimmune diseases, metabolic dysfunctions, neuroinflammatory conditions, and malignancies. To address the complexity of microbiome–immune interactions, the present study adopts a purely in-silico, artificial intelligence (ai) driven framework to decode immune relevant microbial patterns from small-scale to large-scale, publicly available microbiome datasets. Machine learning based classification models combined with multi-omic feature integration were used to identify microbial taxa and metabolic functions associated with immune stability. The analysis consistently highlighted probiotic-associated genera, particularly Lactobacillus and Bifidobacterium, along with enrichment of short-chain fatty acid linked metabolic pathways known to support intestinal barrier function and immune regulations. Predictive modelling further demonstrated that AI-assisted microbiome profiling can reliably differentiate inflammatory and non-inflammatory gut states, emphasizing its utility in immune risk predictions in the human healthcare sector. Additionally, computational simulations suggest that AI-guided precision nutrition and targeted probiotic formulations could serve as effective strategies for restoring microbial balance and mitigating chronic immune activation in human welfare society. Overall, this study demonstrates how ai can transform gut microbiome research by enabling scalable immune-centric analysis and supporting the rational design of microbiome-based preventive and therapeutic interventions.

Keywords: Gut microbiome, Artificial intelligence, Immune regulation, Probiotic modulation, Computational biology

Identification of natural alternatives for Targeted Therapy in Cancer

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Abstract

Cancer is a heterogeneous and multifactorial disease that requires a strategic approach for its treatment, including targeted therapy as a promising approach for targeting pathogenic genomic alterations. However, sometimes the patients harbour non-specific mutations to the designed drugs, leading to a less effective response or resistance. Therefore, we explore phytochemicals used in ayurvedic practice that can inhibit the activity of canonical EGFR mutants that are not targeted by known drugs. Therefore, we consider EGFR a model protein system for screening AYUSH phytochemicals, given the mutant EGFR observed in cancer patients. We define AYUSH phytochemicals as the well-studied plant-derived phytochemicals (N~1200) used in traditional medicine practice. Upon establishing the model system and pipelines for the virtual screening of the protein mutant library of M mutants and the ligand library of L phytochemicals, the screening was performed using Schrodinger 2025.1. Further, we sorted the phytochemicals based on ADMET analysis and MMGBSA rescoring. We also confirmed the binding affinities of potential phytochemicals using Molecular Dynamics Simulations. Our analysis identifies a phytochemical that shows selective affinity for EGFR mutants but not for wild-type EGFR. We propose that this phytochemical may be a potential compound complementary to conventional targeted therapy to address TKI resistance.

Keywords: Targeted Cancer Therapy, AYUSH Phytochemicals, Traditional Medicine, Virtual Screening

Design, Development and Characterisation of Rifabutin Loaded Nanostructure Lipid Carrier infused dissolving Microneedles

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Abstract

Methicillin-Resistant Staphylococcus aureus (MRSA) is a significant contributor to skin and soft tissue infections (SSTIs), often resistant to conventional antibiotics due to biofilm formation and poor tissue penetration. Rifabutin, known for its dual mechanism of RNA polymerase inhibition and biofilm disruption, holds therapeutic promise but is limited by poor solubility and systemic side effects. This study focused on formulating a transdermal drug delivery system using Rifabutin-loaded nanostructured lipid carriers (RFB-NLCs), further integrated into dissolving microneedles (DMNs) for localized delivery. RFB-NLCs were optimized using a Box-Behnken Design under a Quality by Design (QbD) framework. The final formulation exhibited a particle size of 122.5 ± 1.7 nm, polydispersity index (PDI) of 0.210, and entrapment efficiency of 78.4 ± 0.9%. Lyophilization with mannitol ensured redispersibility and stability. The NLCs were successfully incorporated into a 4×4 microneedle patch using a blend of PVA and PVP K30. The resulting DMNs demonstrated sharp morphology, uniformity, and sufficient mechanical strength for skin penetration, as validated by Parafilm® M insertion tests. In vitro release studies showed sustained Rifabutin release over 24 hours, following Korsmeyer- Peppas kinetics. Antibacterial activity confirmed superior inhibition zones for RFB-NLC-DMNs compared to plain drug and control, validating its efficacy against MRSA. The formulation remained stable over six months under specified storage conditions. This study presents a novel, non-invasive transdermal delivery platform that enhances Rifabutin's stability, localizes its action.

Keywords: Methicillin, Rifabutin, Microneedles, Antibacterial Activity.

Computational Design, Screening, and Validation of Novel Quinoline- Thiazole Hybrids Targeting M. tuberculosis

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Abstract

The rising incidence of Multi-Drug-Resistant Tuberculosis (MDR-TB) demands the prompt identification of novel therapeutic agents with unique mechanisms of action. This research focuses on the Mycobacterium tuberculosis enoyl-acyl carrier protein reductase (InhA), a crucial enzyme in the Type II fatty acid synthase (FAS-II) system necessary for mycolic acid biosynthesis and cell wall integrity. Using the crystal structure of InhA and Structure-Based Drug Design (SBDD) protocols, we created a library of 20 new heterocyclic molecules. The structural characteristics of these compounds were obtained from the co- crystallized ligand, 1-cyclohexyl-N-(3,5-dichlorophenyl)-5-oxopyrrolidine-3-carboxamide.

Comprehensive silico profiling validated that the library complies with Lipinski's Rule of Five and Veber's rules, forecasting advantageous oral bioavailability and pharmacokinetic characteristics. Molecular docking simulations also showed that the InhA active site has a high binding affinity and important hydrophobic interactions. Subsequently, these 20 derivatives were successfully synthesized and their chemical structures as well as purity was rigorously analysed using Thin Layer Chromatography (TLC), High- Performance Liquid Chromatography (HPLC), Mass Spectrometry, FT-IR, 1H NMR, and 13C NMR spectroscopy. This study effectively illustrates the rational design and synthesis of novel InhA inhibitors, thereby establishing a validated basis for subsequent biological evaluation and the advancement of potential antitubercular candidates.

Keywords: Molecular Docking; *in-silico* ADME Profiling, Tuberculosis; Structure-Based Drug Design

AI-Based In-Silico Screening of Small-Molecule Inhibitors Targeting DPP- IV and PTP1B

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Abstract

The type 2 diabetes mellitus (T2DM) is a complex metabolic disorder marked by impaired incretin activity and dysregulated insulin signaling. Dipeptidyl peptidase-IV (DPP-IV) and protein tyrosine phosphatase-1B (PTP1B) are key enzymes involved in glucose metabolism and insulin resistance, making them attractive therapeutic targets for diabetes management. In this study, a fully dry-lab, AI-assisted in-silico approach was employed to identify potential small- molecule inhibitors capable of targeting both DPP-IV and PTP1B. The three-dimensional crystal structures of the target proteins were retrieved and optimized using PyMOL and AutoDockTools for molecular docking studies. A compound library consisting of natural bioactive molecules and FDA-approved drugs was obtained from PubChem and prepared using Open Babel and AutoDockTools. Molecular docking was performed using AutoDock Vina with grid boxes centered on the active sites of both proteins. Protein–ligand interactions and binding modes were analyzed using PyMOL and Discovery Studio. The top-scoring compounds were further evaluated for drug-likeness, pharmacokinetic behavior, and toxicity profiles using SwissADME and pkCSM. The results identified several promising dual-target candidates, highlighting the potential of AI- integrated computational strategies to accelerate antidiabetic drug discovery and support the development of safer and more effective therapeutic agents.

Keywords: Type 2 diabetes mellitus; DPP-IV; PTP1B; In-silico drug discovery; Molecular docking; AI-assisted screening; Dual-target inhibitors

Fasting-Induced Metabolic Reprogramming: Exploiting Cancer Cell Vulnerabilities through Differential Cell Resistance

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Abstract

Cancer development is closely linked with the metabolic reprogramming of a cell that supports rapid and uncontrolled cell proliferation. A defining feature of cancer metabolism is the preference for aerobic glycolysis instead of oxidative phosphorylation, known as the Warburg effect, which basically prioritizes biosynthesis over maximal ATP production. Targeting these metabolic dependencies has gained increasing attention, as traditional therapies often lack selectivity for cancer cells. Understanding how nutrient availability influences cancer metabolism is significantly important. This study is based on a logical review of pre- existing literature, focusing on experimental and mechanistic research on cancer metabolism and fasting. Peer-reviewed articles focusing on the Warburg effect, mitochondrial function, and fasting-induced metabolic changes were examined to identify shared mechanisms and therapeutic implications. The analysis indicates that fasting induces metabolic changes in the body, including reduced glucose and insulin-like growth factor-1 (IGF-1) levels, suppression of mTOR signaling, activation of AMPK, and enhanced autophagy in normal cells. These adaptations promote cellular protection and stress resistance in normal cells. In contrast, cancer cells express limited metabolic flexibility due to their dependence on glucose and anabolic signaling, leading to increased metabolic stress under nutrient deprivation. This phenomenon, termed as differential stress resistance (DSR), explains the selective vulnerability of cancer cells when exposed to these conditions. Overall, the findings highlight how fasting-based interventions can exploit metabolic vulnerabilities in cancer cells. Combining metabolic profiling with computational modeling in future research could enable more precise personalized fasting strategies and increase their potential for use in cancer therapy.

Keywords: cancer metabolism, Warburg effect, fasting, differential stress resistance.

Exploring Potential Therapeutic Candidates for Monkeypox Virus

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Abstract

Monkeypox is an important virus as it was responsible for a worldwide epidemic recently between 2022-2023. Also, it was reported that this virus possesses high resistance and adaptability due to causing systemized mutations approximately forty-seven annually in current strains. Due to this, designing an effective treatment approach becomes necessary to solve this issue as best as possible. Here we are keeping focus on direct acting therapy of this virus via inhibiting its morphological changes in the structure. We are screening here a library of FDA approved, Investigational or orphan drugs which includes small molecules for determining the best possible candidate. Due to the virus's increasing endurance, we are also exploring a variety of short chain peptides for treatment as there is non-availability of FDA approved therapy based on peptides to expand resistance-management options for the infection caused by virus. After docking we are proposing synergistic therapy treatment by having potential candidates out of it and doing MD-simulation for both. Moreover, we are also trying to propose peptide-drug conjugate based on top hits to increase efficiency of the treatment and suggesting a newly advanced therapy option by docking the newly proposed candidates which can further synthesize in the lab to test its biological activity by doing experimental studies in future. If time permits, compare possible MD simulation of the top hit conjugate to see its comparison against top-ranked peptide and drug to study the possible effect.

Key words: Monkeypox, peptide, small molecules, treatment

High-Throughput Bioinformatics Pipeline for Automated Antimicrobial Resistance Profiling and Mutation Analysis

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Abstract:

Antimicrobial resistance (AMR) is an accelerating global health threat, with an estimated 10 million deaths per year projected by 2050. Although advances in genomic sequencing have improved accessibility, the downstream analysis of clinical isolates—particularly the identification of functional resistance arising from high-impact point mutations—remains a major bottleneck. Existing workflows are largely manual, fragmented, and time-consuming. This project presents a fully automated, coordinate-driven bioinformatics pipeline developed to streamline AMR profiling across clinical and environmental applications. The workflow is built on a proprietary technology stack hosted on GitHub and is based on a "Coordinate Hand-off" strategy to enhance both speed and analytical accuracy. The pipeline integrates four custom Python tools: Genome Extractor for rapid sequence retrieval, ABRicate Automator for high- throughput resistance gene screening, FastaAAExtractor for precise protein extraction, and WildTypeAligner & SubScan for protein alignment and polymorphism detection and finally PyMol Automator which visualises the mutated protein in PyMol. The utility of the pipeline is demonstrated through profiling of clinically significant resistance targets, delivering immediate and actionable insights to support antibiotic stewardship and infection-control decisions in hospital settings. By removing dependency on complex annotation files (GFF3) and fully automating the gene-to-protein analysis workflow, the system reduces processing time from hours to seconds per genome.

Keywords: antimicrobial resistance, bioinformatics pipeline, Python tools, antibiotic stewardship.

Identification and evaluation of PqsR-specific quorum-sensing inhibitors from natural products against Pseudomonas aeruginosa

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Abstract
Pseudomonas aeruginosa is an opportunistic pathogen responsible for chronic and drug-resistant infections, largely due to quorum sensing (QS)–mediated regulation of biofilm formation and virulence. Targeting QS represents an anti-virulence strategy that can attenuate pathogenicity without directly inhibiting bacterial growth. Among the QS networks in P. aeruginosa, the Pseudomonas quinolone signal (PQS) system plays a central role and is regulated by the transcriptional activator PqsR (MvfR), making it an attractive pathogen- specific target. In this study, we aimed to identify and evaluate natural-product-derived inhibitors of PqsR-mediated PQS signalling using an integrated in silico-to-in vitro discovery pipeline. Pharmacophore-based filtering and structure-guided virtual screening against the PqsR ligand-binding domain were employed to prioritise candidates from a curated natural- compound library, followed by hierarchical molecular docking. Top-ranking compounds were further assessed through in silico developability profiling, including drug-likeness, ADME, and toxicity prediction, as well as 100-ns all-atom molecular dynamics simulations to evaluate binding stability and interaction persistence. Shortlisted compounds were tested at sub- inhibitory concentrations in P. aeruginosa PAO1, where bacterial growth was monitored by OD_{600} growth-curve analysis. QS-regulated phenotypes were quantified using a crystal-violet microtitre biofilm reduction assay (OD_{595}) and an exopolysaccharide production assay based on Congo Red binding (A_{490}). Secreted virulence factors were evaluated through pyocyanin production, rhamnolipid production, and elastase activity assays, while relative expression of PQS-pathway genes (pqsR, pqsA, pqsH, phz,and phnB) was analysed by RT-qPCR using SYBR Green chemistry and normalised to a housekeeping gene. Treatment with the identified natural inhibitors resulted in an overall ~10–45% reduction in QS-linked virulence phenotypes, consistent with attenuation of PQS signalling under sub-inhibitory conditions.

Keywords: *Pseudomonas aeruginosa*, Quorum sensing, PqsR inhibitors, Molecular docking, Natural compound

Exploring therapeutic potential of Asparagus racemosus in polycystic ovarian syndrome: A computational study

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Abstract

Polycystic ovarian syndrome (PCOS) is a complex disorder with multiple contributing factors, marked by the disruption of several interconnected biological pathways. In modern medicine, treatment often involves therapies that focus on hormone balancing, while in Ayurvedic medicine, women's reproductive health is approached holistically, often using medicinal plants such as Asparagus racemosus, also known as Shatavari. Although most studies have focused on herb's ability to modulate female reproductive hormones, a thorough examination of its multiple target actions at the pathway level, influenced by its diverse bioactive components, remains limited. To address this knowledge gap, the present study employed an in-silico network pharmacology and molecular interaction approach to investigate the multi- target mechanisms of bioactive compounds derived from Asparagus racemosus in the context of PCOS. A comprehensive literature survey and database mining using IMPPAT database were conducted to identify 18 bioactive constituents of the plant. Putative gene targets of these compounds were retrieved using Chembl, Binding DB and GEO databases. A total of 2800 gene targets were identified, out of which 100 genes were enriched for their association with PCOS. Protein–protein interaction (PPI) analysis was performed using the STRING database and visualized in Cytoscape to identify key hub genes. A comprehensive compound–target– pathway interaction network was constructed to elucidate the multi-ligand, multi-target pharmacological profile of Asparagus racemosus. A docking-based screening was conducted to identify binding targets of the bioactive compounds. Notably, several new gene targets were discovered beyond the hormone modulation pathways. This research underscores the potential of Asparagus racemosus to influence molecular pathways related to PCOS that have not been extensively studied before.

Keywords: Polycystic ovarian syndrome, Asparagus racemosus, Network pharmacology, Molecular docking.

Machine learning and structure-based drug discovery approaches for identifying microtubule-depolymerizing agents

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Abstract

Schizophrenia is a chronic neuropsychiatric disorder with significant treatment limitations due to poor compliance, frequent dosing, systemic side effects, and low brain bioavailability of conventional antipsychotics; although Trifluoperazine hydrochloride (TFP) is effective in acute schizophrenia, its clinical utility is restricted by first-pass metabolism and dose-dependent adverse effects, prompting this study to develop and optimize TFP-loaded Nanostructured Lipid Carriers (TFP-NLCs) using a Quality-by-Design (QbD) approach, which demonstrated optimal particle size, stability, sustained drug release, improved pharmacokinetic bioavailability, and enhanced antipsychotic efficacy in in-vivo behavioral models, thereby highlighting TFP-NLCs as a promising lipid-based delivery system for improved schizophrenia management.

Keywords: Schizophrenia, Trifluoperazine hydrochloride,Nanostructured lipid carriers, Quality-by-Design, Sustained release, Bioavailability, Antipsychotic efficacy.

Designing Target-Specific Nematicides Through Synthetic Biology-Based Inhibition of β-1,4-Endoglucanase in Meloidogyne incognita

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Abstract

Plant-parasitic nematodes such as Meloidogyne incognita are responsible for substantial crop losses worldwide, creating an urgent need for control strategies that are both target-specific and environmentally sustainable. Synthetic biology offers a rational and integrative framework for identifying and evaluating molecular targets that are essential for nematode survival and host cell invasion. In the present study, we adopted a synthetic biology– guided, structure-based approach to investigate β-1,4-endoglucanase, a secreted cell wall– degrading enzyme of M. incognita, as a potential nematicide target. This enzyme plays a critical role in degrading plant cell walls and facilitating host tissue penetration, processes that are fundamental to successful nematode infection and establishment. The three-dimensional structure of β-1,4-endoglucanase was modelled computationally and subjected to molecular docking analyses with ten selected nematocidal compounds namely Quercetin, Kaempferol, Myricetin, Luteolin, Apigenin, Naringenin, Catechin, Rutin, Genistein and Baicalein. The results revealed strong and specific interactions between (-6.5 to -7.3 kcal/mol) the active site of the enzyme and several candidate molecules, suggesting a high potential for effective inhibition. From a synthetic biology perspective, this rational identification of a key pathogenic target and the structure-guided design of inhibitory molecules illustrate how biological systems can be analysed and strategically disrupted at the molecular level. Molecular docking and simulation analyses further support β-1,4-endoglucanase as a viable and selective target for the development of next-generation nematicides. Overall, this study highlights the value of synthetic biology–inspired computational strategies in plant–nematode management research and underscores their potential to contribute to the design of precise, sustainable approaches for nematode management.

Keywords: Synthetic biology; plant-parasitic nematodes; Meloidogyne incognita; β-1,4- endoglucanase; SBDD; molecular docking; MD; RMSD

Integrated computational approaches to investigate the potential herbal drugs for anti-osteoporosis

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Abstract

Osteoporosis is a multifactorial metabolic bone disorder marked by reduced bone mass and heightened fracture risk, necessitating a multitarget therapeutic approach, for which polyherbal formulations may offer synergistic benefits when selected and validated scientifically. This study aimed to design and validate such a formulation for osteoporosis management using network pharmacology and molecular docking. Osteoporosis-related targets were identified from databases and common disease–drug targets were analyzed using STRING, followed by network pharmacology to determine herbs acting on relevant signaling pathways. Molecular docking evaluated the binding affinities of major phytoconstituents with key targets including PPARG, HIF1A, and PTGS2. Based on in silico findings, selected herbal extracts underwent phytochemical screening and chromatographic analysis to confirm marker compounds, after which the finalized herbs were formulated into solid dosage forms and assessed for quality parameters. Results highlighted *Piper nigrum, Linum usitatissimum, Sesamum indicum, Boerhavia diffusa, Terminalia arjuna,* and *Zingiber officinale* as significantly associated with osteoporosis pathways, with their phytoconstituents exhibiting strong binding toward PPARG, HIF1A, and PTGS2. The phytochemical investigations verified the presence of key markers, and the developed formulation complied with quality standards. Overall, this study presents a rational, targetbased approach for selecting herbal drugs and developing scientifically validated polyherbal formulations for osteoporosis, demonstrating the utility of integrating network pharmacology with molecular docking.

Keywords Osteoporosis, Polyherbal formulation, Network pharmacology, Molecular docking, Phytochemical analysis

Molecular Docking of Phytochemicals against the Human PRC2–Histone 3 Complex

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Abstract

Polycomb repressive complex 2 (PRC2) proteins are recognized as epigenetic writers that imprint specific repressive chemical marks on histone proteins. The Histone-3-Lysine-27 (H3K27) residue is the primary target for methylation by the PRC2 complex, resulting in the compaction of the target DNA sequence. Dysregulation of PRC2 activity leads to aberrant gene expression and is implicated in cancer and neurodegenerative diseases. While dietary intake of bioactive phytochemicals, such as polyphenols, can reduce the risk of these diseases, the underlying epigenetic mechanisms of these effects remain incompletely understood. This study aimed to explore naturally occurring compounds capable of targeting the enzymatic function of the PRC2 complex using an in silico method. It investigated the interaction between 12 phytochemicals known for their anti-neurodegenerative properties and EZH2, the enzymatic subunit of PRC2, in complex with H3K27 and other subunits. To draw comparisons with small molecule drugs, an interaction study with four standard PRC2 inhibitors was also conducted. Docking results were evaluated in terms of free energy and dissociation constant values. The comparable outcomes between PRC2 inhibitors and phytochemical compounds underscore the potential application of naturally occurring compounds as small drug molecules.

Keywords: PRC2, Phytochemicals, Molecular Docking, Neurodegenerative disorders.

Machine Learning–Driven In Silico Discovery of Novel Breast Cancer Therapeutics through AI-Guided Molecular Design, Virtual Screening, and Pharmacokinetic Optimization

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Abstract

Triple-Negative Breast Cancer (TNBC) is an very aggressive and therapeutically challenging subtype that lacks estrogen (ER), progesterone (PR), and human epidermal growth factor receptor 2 (HER2) expressions, leaving fewer treatment options and a greater incidence of recurrence. Poly (ADP-ribose) polymerase (PARP) is the critical enzyme for DNA repair and a proven therapeutic target for TNBC treatment. Olaparib, Niraparib, Rucaparib and Talazoparib are FDA approved PARP inhibitors used for the treatment of TNBC, ovarian cancer. In the current work, a machine learning model was constructed with an aim to predict the activity of new PARP1 inhibitors. Experimentally confirmed PARP inhibitors (FDA-approved, clinical, and preclinical) were downloaded from the ChEMBL database along with their reported IC_{50} values. The HistGradientBoostingRegressor (HGBR) algorithm was used to build a pIC_{50} value predictive ML model. Feature correlation analysis, descriptor optimization, and hyperparameter optimization through GridSearchCV improved the predictivity of the model. Next, the developed model was used to predict the ic50 values of newly design or AI generated compounds for PARP inhibition. Lastly, molecular docking experiments were carried out to determine the binding affinities and salient interactions in the PARP1 active site. The optimized HGBR-based model demonstrated strong predictive performance and effectively identified potential novel PARP1 inhibitors. Docking analyses confirmed favorable binding modes and key interactions supporting the predicted activities. This integrated AI/ML–driven in silico platform is a fast and cost-effective approach for the discovery of novel PARP inhibitors.

Keywords: Poly (ADP-ribose) polymerase (PARP), Triple-Negative Breast Cancer (TNBC), molecular docking, Machine Learning

In Silico Identification and Network Analysis of Virulence-Associated Surface Proteins of Candida albicans

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Abstract

Candida albicans is an opportunistic fungal pathogen whose ability to adhere, invade, and damage host tissues is mediated by surface-exposed and secreted virulence factors. In the present study, a comprehensive computational biology approach was employed to identify and characterise potential virulence-associated surface cell wall proteins of C. albicans. The complete proteome was retrieved from UniProt and subjected to a multi-step in silico filtering pipeline involving signal peptide prediction, subcellular localisation, transmembrane domain exclusion, and effector prediction. This systematic screening resulted in the identification of 138 putative effector proteins.Protein–protein interaction (PPI) networks were constructed using the STRING database and analysed in Cytoscape to identify key hub proteins based on degree, betweenness centrality, and closeness centrality measures. In parallel, virulence-associated proteins were retrieved from the Database of Fungal Virulence Factors (DFVF) and integrated with the effector dataset to identify common high-confidence candidates. Furthermore, structural bioinformatics analysis was performed by docking selected virulence–effector proteins with host targets using the ClusPro server. Docking of secreted aspartyl proteinase SAP1 with human E-cadherin revealed a stable interaction involving the active site flap region, highlighting a possible molecular mechanism underlying host tissue invasion.Overall, this study demonstrates the utility of integrated computational proteomics, network biology, and structural modelling to prioritise candidate virulence factors of C. albicans, providing a strong foundation for downstream experimental validation.

Keywords: Virulence factors, Protein-Protein Interaction, Fungi – host Interaction.

Computational Screening and Molecular docking of Phytochemicals Targeting Arthritis

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Abstract

Arthritis, a chronic, inflammatory disorder affecting millions globally, demands safer and more effective therapeutic strategies beyond the use of conventional drugs like DMARDs, NSAIDs, Biologics, etc. Phytochemicals, with their structural diversity and bioactive potential, represent a promising resource for developing novel anti-arthritic agents. This study aims to screen and identify potent phytochemicals targeting key molecular regulators for arthritis – NLRP3 and CD28 (achieved through network pharmacology) using an integrated computational approach. A curated library of plant derived compounds from over 200 anti-arthritic plants was evaluated through virtual screening, including ADMET profiling and molecular docking. The interaction analysis was checked to assess binding affinity and molecule interactions. Based on these analyses, three top-ranking phytochemicals were shortlisted for each target exhibiting strong and specific interactions within the active binding domains of NLRP3 and CD28. The plant source of these top-ranking phytochemicals are: Chinese rhubarb, Bitter gourd, Ginger, and Amur barberry. These candidates are being further investigated through molecular dynamics simulations to validate structural stability and biological relevance. This study provides a translational framework linking natural compound discovery to therapeutic development.

Computational Design of Chimeric antigen receptor (CAR) against the CD20 antigen

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Abstract

CAR-T cell therapy has revolutionized immunotherapy, yet targeting the CD20 antigen remains challenging due to its limited extracellular epitope exposure at the membrane-proximal location. This study utilized a molecular modeling approach to engineer CAR-scFvs derived from Rituximab, focusing on the structural and functional impacts of two distinct linkers: Whitlow and G_4S_3. We employed MD simulations, free energy landscape analysis, and dynamic cross-correlation matrices to evaluate stability and binding affinity with CD20. Notably, binding energy calculations revealed that the scFv-Whitlow construct exhibited significantly higher energy compared to scFv-G_4S_3. The Whitlow linker promoted a flexible dynamic framework, allowing the V_H and V_L domains to maintain functional robustness. To validate these findings within a therapeutic context, the full CAR architecture, including hinge, transmembrane, and costimulatory domains was modelled using Alpha Fold. Analysis of the complete CAR in both unbound and CD20-docked states mirrored the scFv-only results, confirming that the Whitlow-based design shows better interaction dynamics compared to G_4S_3. These insights position the scFv-Whitlow CAR as a promising candidate for anti-CD20 therapies and provide a computational framework for the rational design of next-generation CAR constructs.

Keywords: CAR-T, CD20, MD simulation, scFv

Structure guided design of chimeric antigen receptor T-cells against the CD19 antigen for B-cell Malignancies

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Abstract

Chimeric Antigen Receptor (CAR) T-cell therapy has shown remarkable efficacy in relapsed or refractory B-cell malignancies, including B-cell acute lymphoblastic leukemia, chronic lymphocytic leukaemia, and non-Hodgkin's lymphoma. Currently approved CAR-T therapies predominantly target CD19; however, antigen escape remains a major cause of therapeutic failure. A clinically reported point mutation in CD19 (L174V), located within its extracellular domain, disrupts the binding of FMC63-based CARs and contributes to resistance and disease relapse. At present, no FDA- or CDSCO-approved CAR constructs specifically address this mutation. In this study, we employed a structure-guided computational strategy to design mutation-tolerant CAR single-chain fragment variables (CAR-scFvs) capable of recognizing both wild-type and L174V mutant CD19. Six humanized scFv models were generated, along with structural models of wild-type and mutant CD19, using AlphaFold followed by MD simulations to obtain global state conformations. Further, molecular docking was performed using HADDOCK to evaluate binding modes and relative affinities of scFv-CD19 complexes. This integrated in-silico workflow enables evaluation of CAR-scFv binding to wild-type and mutant CD19 variants and provides molecular insights into mutation-tolerant antigen recognition. The proposed framework supports the rational design of next-generation CAR constructs with the potential to enhance binding robustness and reduce antigen-escape- mediated failure in CD19-positive B-cell malignancies.

Keywords: CAR-T, CD19, Antibody, MD simulation.

Computational Analysis of ATP-Bound Fidgetin-Like 2 Hexamer Interactions with Neuronal β-Tubulin Isotypes

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Abstract

Microtubule dynamics are essential for neuronal development, maintenance, and intracellular transport, and are tightly regulated by microtubule-associated proteins, including microtubule- severing enzymes. Fidgetin-like 2 (FL2), a member of the AAA+ ATPase family, has emerged as an important regulator of microtubule remodeling in neuronal systems; however, its structural organization and interaction mechanisms with neuronal tubulin isotypes remain poorly characterized. In the present study, a structure-guided computational approach was employed to investigate the oligomeric organization and interaction behavior of FL2. A hexameric model of FL2 was constructed using AlphaFold-based multimer prediction. Subsequently, protein–protein docking studies were performed between the ATP-bound FL2 hexamer and the C-terminal tails of neuron-specific β-tubulin isotypes (β1, β2, β3, and β4), which are known to play critical roles in neuronal microtubule regulation. Docking analyses revealed distinct interaction patterns and binding propensities across tubulin isotypes, suggesting potential isotype-specific recognition or modulation by FL2. The predicted interaction interfaces were consistent with known functional regions involved in microtubule engagement by severing enzymes. Together, these findings provide structural insight into the ATP-dependent hexameric organization of FL2 and its differential interactions with neuronal tubulin isotypes. This study highlights the utility of integrative molecular modeling and docking approaches in elucidating the mechanistic basis of microtubule regulation and offers a foundation for future molecular dynamics simulations and functional investigations of FL2 in neuronal contexts.

Key words: Fidgetin-like 2, microtubule-severing enzymes, AAA+ ATPase.

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