

Program

Drug Discovery 2025: Emerging Trends and Future Prospects

February 24-26, 2025

Centre for Interdisciplinary Research in Basic Sciences,
Jamia Millia Islamia, New Delhi

DAY 1			24-Feb-2025 (Monday)		
9:00 -10:00		Registration			
10:00 - 11:15	Inaugural Session		Welcome Address Director's Speech Dean's Address Address by the Patron (Registrar) Address by Guest of Honor Address by the Chief Guest Address by the Chief Patron (Vice Chancellor) Vote of Thanks		
11:15 - 12:00		High Tea			
Session I 12:00 - 14:00		Chairs: Prof. Rajiv Bhat, JNU Prof. Savita Yadav, AIIMS		Structural Biology in Human Health	
12:00 - 12:25	Arockiasamy Arulandu International Centre for Genetic Engineering and Biotechnology, New Dlehi-110067. India,		Preclinical Drug Discovery for Novel Cardiovascular Disease Therapy		
12:25 - 12:50	Ruchi Anand Indian Institute of Technology Bombay, Mumbai		Combatting Ribosomal Methylation Based Antibiotic Resistance: A war at the microscopic level		
12:50 - 13:15	Sampa Biswas Saha Institute of Nuclear Physics, Kolkata		Mechanistic insight and inhibitor design of Falcipain 2; a potential drug target of malaria parasite		
13:15- 13:40	Prof. Timir Tripathi North-Eastern Hill University Shillong-793022, Meghalaya		Intrinsically Disordered FG-Nup98 and Tau Interact via Liquid-Liquid Phase Separation and form Droplets within Droplet		
13:40- 14:00	Mohd Mir General Manager – Medical Safety, Qinecsa Solutions		AMR & New Antimicrobial Development Challenges		
14:00 - 15:00		Lunch			
Session II 15:00 - 17:00		Chairs: Prof. Sonika Bhatnagar, NSUT Prof. Nagendra Singh, GBU		Precision Medicine	
15:00 - 15:25	Sathees C. Raghavan Indian Institute of Science, Bangalore		Discovery of a Novel BCL2 Inhibitor, Disarib as a Promising Cancer Therapeutic		
15:25 -15:50	Sri Rama Koti Ainavarapu Tata Institute of Fundamental Research, Mumbai		Liquid-liquid phase separation (LLPS) of ubiquitin-like proteins in crowded environments		
15:50 -16:15	Avinash Bajaj RCB, Faridabad		Engineering of Biomaterials for Targeting the Tumour Microenvironment		
16:15-16:40	Deepa Ghosh Institute of Nano Science and Technology, Mohali		Combating Progressive Cartilage Matrix Degeneration with Small Molecules		
16:40 -17:00	Sanjeev Kumar Singh Alagappa University, Tamil Nadu		Structural Bioinformatics and predictive modeling studies on Virus and Host Interaction to overcome HIV Latency		

17:00 - 17:30	Tea Break	
Session III 17:30 - 19:30	Chairs Dr. Naseem Gaur, ICGEB Dr. Hridayesh Prakash, Amity University, NOIDA	Next-Generation Therapeutics
17:30 - 17:55	R. Mahalakshmi Indian Institute of Science Education and Research, Bhopal	Lipid-Regulated Assembly and Stability of the Bacterial Barrel Assembly Machinery for Next-Generation Therapeutics
17:55 - 18:20	M.S. Madhusudhan Indian Institute of Science Education and Research, Pune	Peptide inhibitors that mimic antibody binding
18:20-18:45	Jeetender Chugh Indian Institute of Science Education and Research, Pune	Probing conformational heterogeneity in an RNA recognition motif: implications for fibril formation
18:45 - 19:10	Vikash Jain Indian Institute of Science Education and Research, Bhopal	Understanding phage infection in bacterium and its regulation: Development of phage-derived therapeutics against mycobacteria
19:10 - 19:30	Subhash Mohan Agarwal NICPR, NOIDA	Development of a systematic workflow design to compare virtual screening capabilities of identical protein structures
19:30 - 20:30	DINNER	

DAY 2:		25-Feb-2025 (Tuesday)
9:00 to 10:00	High Tea	
Session IV 10:00 - 12:00	Chairs: Prof. Sujata Sharma, AIIMS Dr. Bhupesh Taneja, IGIB	Biomolecular Assemblies
10:00 - 10:25	Bishwajit Kundu Indian Institute of Technology Delhi	<i>Salmonella typhi</i> Cell division Activator Protein (StCAP) is a DNA-binding protein orchestrating critical cellular events during pathogenesis.
10:25 - 10:50	M. Michael Gromiha Indian Institute of Technology Madras, Chennai	Computational approaches for understanding mutational effects on protein structure and function: implications to diseases
11:50 - 11:15	Shubhasis Haldar S. N. Bose National Centre for Basic Sciences, Kolkata	Characterizing the Mechanical Landscape of Protein-Drug Interactions: Correlating Mechanical Strength, Cell Migration, and Morphology with Novel Covalent Magnetic Tweezers
11:15 - 11:40	Shailja Singh Jawaharlal Nehru University New Delhi	CRISPR/Cas9-engineering of Kell null erythrocytes to unveil the repurposing of anti-diarrheal drug as irresistible antimalarial
11:40 - 12:05	Ranjan Sen CDFD Hyderabad	Sourcing novel proteins and peptides from bacteriophages with therapeutic potential
12:05 - 12:30	Hem Chandra Jha IIT Indore, Indore	Demethoxycurcumin and Rosmarinic acid as a potential anti-Epstein Barr Virus drug in neurological disorders
12:30 - 12:45	Safiya Habib Aligarh Muslim University	Oxidative synthetic hair dye pigment 4-chloro-orthophenylene diamine may induce inflammatory carcinogenesis
12:45 - 13:00	Shamila Fatima Aligarh Muslim University	Studies on Interaction Between Human Serum Albumin HSA and 3,4-Di Hydroxy Benzaldehyde DHB
13:00-14:00	Lunch	
14:00-15:00	Poster Presentation	
Session V 15:00 - 17:00	Chairs: Prof. Yasha Hasija, DTU Dr. Shalini Singh, NICPR	Integrative Approaches in Disease Mechanisms

15:00-15:25	Shashank Tripathi Indian Institute of Science, Bengaluru	Translating Virus-Host OMICs Data into Antiviral Interventions.
15:25-15:50	Shaiza Singh National Centre for Cell Science, Ganeshkhind, Pune	Leveraging Systems Biology to Target EGFR Autophagy in NSCLC Therapy
15:50-16:15	Punit Kaur All India Institute of Medical Sciences, New Delhi	Search for a Novel Drug Binding site in <i>Salmonella Typhi</i> DNA Gyrase for development of Drug candidates
16:15-16:40	Medicharla V. Jagannadham CSIR-CCMB, School of Life Sciences, University of Hyderabad	Membrane Vesicles: Evolutionary Conserved Mediators of Microbial Defence, Host Interaction, and Therapeutic Potential
16:40-17:00	Sinosh Skariyachan Kannur University, Kerala	Elucidation of the prospective molecular targets of drug-resistant <i>Acinetobacter baumannii</i> and <i>Pseudomonas aeruginosa</i> by computer aided screening and cheminformatics modelling
17:00-17:30	Tea	
Session VI 17:30 - 19:30	Chairs: Prof. Indrakant Singh, ACBR Dr. Harish Kumar, SERB	Computational Drug Discovery
17:30-17:50	Aditi Borkar University of Nottingham, UK	From Ice to Insight: Cryo-OrbiSIMS enables integrative modelling of RNA structures at atomic resolution to aid rational development of RNA therapeutics
17:50-18:10	Shubhra Ghosh Dastidar Bose Institute, Bidhannagar, Kolkata	Mechanistic insights into the Allosteric Changes in Drug Targets: MD Simulations and Machine Learning
18:10-18:30	Samudrala Gourinath Jawaharlal Nehru University, New Delhi	Targeting Cysteine Biosynthesis: Structural and Functional Insights into <i>E. histolytica</i> Enzymes
18:30-18:50	Krishnananda Chattopadhyay CSIR-Indian Institute of Chemical Biology, Kolkata	Conformational fluctuations of proteins: the physics, chemistry and biology of neuro-degenerations
18:50-19:10	Aditya Padhi IIT BHU, Varanasi	An integrated multiscale computational framework comprising protein design, machine learning, hybrid QM/MM, and clinical insights unveils resistance mutations in infectious diseases
19:10-20:00	Cultural Program	
20:00 onwards	Special Dinner	

DAY 3: 26-Feb-2025 (Wednesday)		
9:00 to 10:00	High Tea	
Session VII 10:00 - 12:30	Chairs: Prof. Laishram R. Singh, ACBR Dr. Parul Mehrotra, IIT Delhi	
10:00 - 10:25	Rajesh Pandey Institute of Genomic and Integrative Biology, New Delhi	Integrative Genomics-enabled understanding of Clinical Management: AMR and choice of Antibiotics
10:25 - 10:50	Amitava Das Department of Chemical Sciences, IISER Kolkata	Demonstration of a Proof of Concept for Using Small Molecule Aggregates as Therapeutic Options
10:50 - 11:15	Ramanathan Natesh IISER-Thiruvananthapuram	Targeting the DNA damage repair and transcription regulation in AMR
11:15 - 11:40	Sudhanshu Vrati Regional Centre for Biotechnology, Faridabad	Development of novel antivirals

11:40 –12:00	Saran Kumar Indian Institute of Technology Delhi, New Delhi	Tumor Vasculature: A Key Driver of Glioblastoma Heterogeneity
12:00 -12:15	Sana Akhtar Lehigh University, PA, USA	Mechanism of Ligand Binding to Theophylline RNA Aptamer
12:15- 12:30	Evanka Madan Sir Ganga Ram Hospital, New Delhi	Pre-Clinical evaluation of Sphingosine-1- phosphate kinase (SphK) in limiting Leishmania growth by inducing inflammation, autophagy and apoptosis in macrophages
12:30 - 12:45	Tara Kashav Central University of South Bihar	Mutational analysis of IRF6 Reveals Defects in Protein Stability, Oligomerization, and binding with p63
12:45 - 13:00	Rekha Barkatullah University	Codon usage, context and Synthetic biology approach to develop vaccine
13:00 - 14:00	Lunch	
14:00 - 15:00	Poster Presentation	
Session VIII 15:00 - 17:30	Dr. Jamal Akhtar, CCRUM Dr. Himanshu Ojha, INMAS	Oral Presentation
15:00 - 15:15	Rajendra V Joshi Surat Municipal Institute of Medical education & Research (SMIMER), Surat	Glaucoma due to Increased Intraocular Pressure is a Leading Cause of Blindness.
15:15-15:30	Puniti Mathur Amity University, NOIDA	Identification of peptidic Glucokinase activators through computational approaches
15:30-15:45	Tanya Arora Jamia Millia Islamia, New Delhi	An In-Silico study to categorise the Consensus Molecular Subtypes in Ovarian Carcinoma and Identify Potential Biomarkers
15:45-16:00	Fathima R. Karuvanthodikayil Indian Institute of Technology Madras, Chennai	Computational insights into binding affinity and mutation impact in membrane protein-protein complexes
16:00-16:15	Doha Omar Alghamdi King Abdulaziz University	Neuroprotective effect of a novel formulation of fisetin in an experimental model of Alzheimer's disease
16:15-16:30	Khushboo Bhagat School of Biochemical Engineering, IIT BHU	Resistance Profiling of Bebtelovimab-bound SARS-CoV-2 RBD mutants and validation with escape mutations, clinical results, and viral genome sequences
16:30-16:45	Harshil Samir Bhatt Centre for Bio Separation Technology, VIT-Vellore	2H-Chromene based Vibrio cholerae LpxC inhibitors: Docking, Molecular Dynamics Simulation and DFT Studies
16:45-17:00	Sneh Prabha Jamia Millia Islamia, New Delhi	Comprehensive Analysis of Hippocampal Gene Expression Datasets for the Identification of Alzheimer's Disease-Associated Molecular Biomarkers
17:00-17:15	Faisal Ashraf Bhat Aligarh Muslim University	Exploring the cardioprotective mechanism of SGLT2 inhibitors against Isoproterenol induced heart failure
17:15-17:30	Sudarshan Sarkar Raiganj University	Integrative Cross-Platform Transcriptomics and Machine Learning Approaches for Identifying Prognostic Biomarkers and Mechanisms of Disease Progression in Parkinson's Disease
18:30-19:00	Tea Break	
19:00 - 19:20	Concluding Session and Distribution of Prize	
19:30-20:30	Dinner	
Thanks.....		