

**Technical Program Session for the
“National Conference on Computational Biology and AI in drug discovery-26”**

Sessions and Speakers	Time slots
DAY 1 (6th February 2026)	
Registration & Breakfast	08:30 am - 09:30 am
Conference Inauguration program	10:00 am - 10:30 am
Session 1	
Session Chair: Prof. Hari Misra Distinguished Professor, SDSOS, NMIMS	10:30 am - 1:00 pm
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
Dr. Sandip Kaledhonkar, IIT Bombay Title: Structural insights into the interaction of a Plasmodium falciparum translation enhancing factor with ribosomes	12:00 pm - 12:30 pm
Dr. Susan Thomas, NIRRCH, Mumbai Title: A systems-level perspective on host- Candida albicans interactions in vaginal infections	12:30 am -1:00 pm
Poster Session Inauguration (1:00 pm - 1:30 pm)	
Lunch break (1.30 pm - 2:15 pm)	
Session 2	
Session Chair: Prof. Jagannath Sahoo, Dean SPPSPTM, NMIMS	2.30 pm - 5:00 pm
Prof. Kailas Sonawane, Shivaji University Kolhapur Title: Understanding molecular basis of antimicrobial resistance using bioinformatics approaches	2:30 pm – 3.00 pm
Prof. Ambarish Kunwar, IIT Bombay Title: Temperature dependence of Intra-cellular Transport and Cytoplasmic Streaming	3.00 pm – 3.30 pm
Dr. Sinosh Skariyachan, St. Pius X College Rajapuram, Kasargooda Title: Scope of computational data science and AI-powered drug discovery in curtailing antimicrobial resistance	3:30 pm – 4.00 pm
Tea Break	
Industry talks : Molecular Solutions Pvt ltd, Bangalore	4:20 pm – 5.00 pm
Poster Session, Networking	5.00 pm - 6.00 pm
Cultural Program	6.00 pm - 6.30 pm
Dinner	
6.30 pm onwards	

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Sessions and Speakers	Time Slot
DAY 2 (7th February 2026)	
Breakfast and Tea (8:00 am - 9:00 am)	
Session 3	
Session Chair: Prof. Ambarish Kunwar Department of Biosciences and Bioengineering, IIT Bombay	9.00 am to 12.30 pm
Key-note speaker: Prof. Andrew Lynn, JNU, New Delhi Title: Hybrid Physics-based and Machine Learning Framework for Predicting Fragment and Small-Molecule Binding Affinities	9:00 am - 9.45 am
Dr. Rajnish Kumar, IIT BHU Title: AI-Enabled Discovery of Choline Acetyltransferase Inhibitors for Theranostic Applications in AD	9:45 am - 10:15 am
Dr. Pratik Chandrani, ACTREC Mumbai Title: Target.AI – Drug sensitivity prediction for targeted cancer therapy	10:15 am - 10:45 am
Dr. Leelavati Narlikar, IISER Pune Title: Machine learning to understand transcriptional regulation	10:45 am - 11:15 am
Tea (11:15 am - 11.30 am)	
Session 4	
Session Chair: Prof. Andrew Lynn JNU, New Delhi	11.30 am to 1.15 pm
Key-note speaker: Prof. Imtiaz Hasan, JMI, Delhi Title: InstaDock-v2: User-Friendly, Open-Source Tool for Multi-Target Docking and ADMET Analysis	11:30 am - 12:15 am
Dr. Vijaykumar Prajapati, Delhi University Title: Computational and experimental approach to identify potential inhibitors against visceral leishmaniasis	12.15 am - 12.45 pm
Dr. Uddhvesh Sonavane, CDAC, Pune Title: An HPC–AI Framework for Mapping Druggable Conformational Landscapes of Cancer Proteins Using Integrated Computing Environment (ICE)	12.45 pm - 1:15 pm
Lunch break (1:15 am - 2:15 pm)	
Session 5	
Session Chair: Prof. Manu Lopus Associate Professor, University of Mumbai	2.15 pm to 4.00 pm
Prof. Kakoli Bose, ACTREC, Mumbai Title: Unraveling Macromolecular Activation Mechanism and Protein-Protein Interactions in Health and Disease	2:15 pm - 2:45 pm
Young Speakers	
Ms. Purva Khodke, MSc SDSOS, NMIMS University, Mumbai Title: Design and optimization of CAR scFvs against the CD20 antigen using molecular modelling approach	2.45 pm - 3.00 pm
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
Industry talk 1: Prescience Insilico pvt. ltd, Bangalore	3:15 pm - 3.45 pm
Industry talk 2: SilicoScientia pvt. ltd, Bangalore	3.45 pm - 4.15 pm
Valedictory: Poster Award ceremony, Vote of Thanks and Feedback (4.00 pm Onwards)	