

DAY 01

Tuesday, January 7, 2025

08:30-09:00 Registration

Session I: Inaugural Programme

09:00-10:40 Inaugural Session

10:40-11:00 Poster Inauguration followed by High Tea

Session II: Digital Twins in Biology and Medicine

Session Chair: Prof. Ravi Mahajan, Apollo Research Academy

11:00-11:45 "Digital You: The Virtual Future of Medicine" by Prof. Peter Coveney, University College London, UK

11:45-12:30 "Cancer, Data Science, and Prediction in Medicine: Perspectives for the Future" by Dr. Eric Stahlberg, MD Anderson Cancer Center, USA (ONLINE)

12:30-13:00 Bioinformatics@C-DAC: Transcending Three Decades

13:00-14:00 Lunch Break

Session III: Transcending Technologies and Enablers

Session Chair: Prof. Sunil Sherlekar, Sankhyasutra Labs, Bengaluru

14:00-14:30 "Advanced Methods and Applications for Extreme-Scale Biomolecular Simulations & EU-India collaboration efforts" by Dr. Rossen Apostolov, KTH, Sweden

14:30-15:00 "Solving 3D puzzles of biomolecular interactions by integrative modelling" by Prof. A.M.J.J Bonvin, Utrecht University, The Netherlands

15:00-15:30 "Transcending Technologies and Enablers" by Ms. Jaya Panvalkar, Kinetic Communications Ltd., Pune

15:30-16:00 "National Supercomputing Mission: Development of Supercomputing Ecosystem in the country" by Shri. Sanjay Wandhekar, C-DAC, Pune

16:00-16:15 Tea Break

16:15-17:30 Poster Session I

Session IV: Next Generation Drug Discovery, Repurposing and Toxicology

Session Chair: Prof. M.S. Madhusudan, IISER, Pune

17:30-18:00 "Hybrid Alchemical Free Energy/Machine Learning in the Design of Novel Lead Compounds from Fragment Seeds: Application to Cyclophilin Inhibitor Discovery" by Prof. Andrew Lynn, JNU, New Delhi

18:00-18:30 "Quadrivalent Lynch Syndrome Vaccine Product Development" by Dr. Shankar Gupta, NCI, USA

18:30-19:00 "Engineering RNA junctions for better stability and function" by Dr. Ashwani Sharma, IISER, Tirupati

Session V: Panel discussion on "Digital Twins in Biology: Challenges and Opportunities"

Session Chair: Prof. Shekhar Mande, SP Pune University

19:00-20:00 Session Members: Prof. Ravi Mahajan (Apollo Research Academy), Prof. Peter Coveney (University College London, UK), Dr. Sunil Sutar (Dassault Systèmes)

20:00 Dinner at Hotel Orchid

DAY 02

Wednesday, January 8, 2025

Session VI: Biomarker Discovery in Genomics

Session Chair: Dr. Pragya Yadav, National Institute of One Health, Nagpur

09:00-09:30 "Biomarkers And Their Effect On Personalized Cancer Treatment: The Connection Between Cancer Epigenetics And Metabolism" by Dr. Sanjay Gupta, ACTREC, Navi Mumbai

09:30-10:00 "Integrated omics approaches for divulging molecular signatures associated with agronomic traits" by Prof. Mukesh Jain, JNU, New Delhi

10:00-10:30 "AI-driven integrative and alternative Biomarkers: Cross-platform transcriptomics and the genomic language of DNA-shape" by Prof. Shandar Ahmad, JNU, New Delhi

10:30-11:00 "Accelerating disease biology research: Unravelling the mechanistic connection between biomarker mutations and genetic diseases through computational approaches" by Dr. Akash Ranjan, CDFD, Hyderabad

11:00-11:15 Tea Break

Session VII: Empowering Molecules: Multiscale simulations

Session Chair: Prof. Andrew Lynn, JNU, New Delhi

11:15-11:45 "A multiscale computational approach to identify novel viral epitopes by targeting MHC-TCR complexation" by Prof. Sanjib Senapati, IIT Madras

11:45-12:15 "Simulation-guided engineering of *Escherichia coli* for bioprocessing applications" by Prof. B. Gopal, IISc, Bengaluru

12:15-12:45 "Implications of Stoichiometric Compositions on Order and Disorder in Natural Proteins" by Prof. Aditya Mittal, IIT Delhi

12:45-13:15 "Understanding the building blocks of biological processes" by Dr. Chetan Gadgil, CSIR-NCL, Pune

13:15-14:15 Lunch Break

Session VIII: Computational applications in Traditional medicine

Session Chair: Dr. Sangeeta Sawant, SP Pune University

14:15-14:45 "Harnessing Indian Medicinal Plants as Sources of Potential Therapeutic Agents" by Prof. B. Jayaram, IIT Delhi

14:45-15:15 "Leveraging Computational Tools, Material Basis Approach for Advancing Ayurveda Therapeutics" by Dr. Kuldeep Choudhary, CARI, Mumbai

15:15-15:45 "Recent advances in AI/ML based methods for prediction of structure dynamics and ligand binding affinity of proteins" by Dr. Debasisa Mohanty, NII, New Delhi

15:45-16:45 Poster Session II

16:45-17:00 Tea Break

Session IX: Ideas to Impact

Session Chair: Dr. Arnab Mukherjee, IISER, Pune

17:00-17:30 "X-plat: a cross-platform transformation tool based on the nearest neighbor joining framework" by Prof. Binay Panda, JNU, New Delhi

17:30-18:00 "Environmental surveillance coupled with genomics for pathogen monitoring as an early warning system; a hope for pandemic preparedness?" by Dr. Mahesh Dharne, CSIR-NCL, Pune

18:00-18:30 "Towards a Digital wave in Drug Discovery and Development - Pharma 4.0" by Dr. Samiron Phukan, Aragen Life Sciences, Hyderabad

18:30-19:00 "Empowering Medical Insights with Genome Informatics" by Dr. Deeksha Bhartiya, GENOMIKI, Noida

19:00 onwards Festschrift for Dr. Rajendra Joshi
(followed by Gala Dinner at Hotel Orchid)

DAY 03

Thursday, January 9, 2025

Session X: Partners & Collaborators

Session Chair: Dr. Manali Joshi, SP Pune University

09:00-09:30 "Reading genomes" by Prof. M.S. Madhusudan, IISER, Pune

09:30-10:00 "Reinforcement Learning Helix Disrupting Mutation" by Dr. Arnab Mukherjee, IISER, Pune

10:00-10:30 "Marine Genomics and High-Performance Computing: The Indispensable Alliance" by Dr. Dharani Gopal, NIOT, Chennai

10:30-10:45 Tea Break

10:45-11:15 "Signatures of GPCR-lipid Interactions: Specificity, Synergy and Energetics" by Dr. Durba Sengupta, CSIR-NCL

11:15-11:45 "Salt Induced Transitions in the Conformational Ensembles of Intrinsically Disordered Proteins" by Dr. Govardhan Reddy, IISc, Bengaluru

11:45-13:00 Poster Session-III

13:00-14:00 Lunch Break

Session XI: Poster Oral Presentations

14:00-15:00 Chairs: Prof. Binay Panda, JNU; Dr. Durba Sengupta, CSIR-NCL; Dr. Akash Ranjan, CDFD

Session XII: Valedictory Programme

15:00-16:00 Session Chair: Dr. Rajendra Joshi, C-DAC

16:00-16:30 Valedictory Talk

16:30-17:00 Poster awards and feedback

17:00 Tea and Good Bye