



Schedule

Advances in Computer Simulations in Structural Biology and Biophysics

Venue: Committee Room, Convention Centre, JNU

Symposium 28th February 2025

DAY
01
FEB 28
2025

09:00 AM – 10:00 AM – Inauguration and Introduction to the School of Computational and Integrative Sciences

Session 1

10:00 AM – 11:30 AM - **Session Chair:** Dr. Shandar Ahmad (SCIS, JNU)

Speakers:

10:00 AM – 10:30 AM - Dr. Govardhan Reddy (IISc, Bangalore): Anionic Ligand Sensing by a Bacterial Riboswitch

10:30 AM – 11:00 AM - Dr. Nisanth N. Nair (IIT Kanpur): Exploring Rugged Energy Landscapes of Enzymatic Reactions

11:00 AM – 11:30 AM - Dr. Durba Sengupta (NCL, Pune): Benchmarking a Dual Scale Hybrid Simulation Framework for Small Globular Proteins Combining the CHARMM36 and Martini2/Martini3 models

11:30 AM – 12:00 PM - ☕ Tea Break

Session 2

12:00 PM – 01:30 PM - **Session Chair:** Dr. Devapriya Choudhury (SBT, JNU)

Speakers:

12:00 PM – 12:30 PM - Dr. Shubhra Ghosh Dastidar (Bose Institute, Kolkata): Allosteric Changes in Proteins Structure, Dynamics and Thermodynamics

12:30 PM – 01:00 PM - Dr. Rajesh Mishra (SBT, JNU): Osmolyte Assisted Refolding of Bacterial α -Amylase

01:00 PM – 01:30 PM - Dr. Hari O. S. Yadav (SCIS, JNU): Characterising the Hydrophobicity of Nanoscale surfaces

01:30 PM – 02:30 PM - 🍽️ Lunch Break

Session 3

02:30 PM – 03:30 PM - **Session Chair:** Dr. Andrew Lynn (SCIS, JNU)

Speakers:

02:30 PM – 03:00 PM - Dr. Sudhanshu Shanker (Mahindra University): Advancing Peptide Docking: Incorporating Non-Natural Amino Acids with AutoDock CrankPep v1.1

03:00 PM – 03:30 PM - Dr. Ananya Debnath (IIT Jodhpur): Plant Thylakoid Polymorphism and Dynamical Heterogeneity

03:30 PM – 05:00 PM - 📄 Poster + ☕ Tea Break

05:00 PM – 06:30 PM - **Session Honouring:** Dr. N. Subba Rao

Session Chair: Dr. Pradipta Bandyopadhyay (SCIS, JNU)

05:00 PM – 05:30 PM - Brief talks by the students and colleagues of Dr. N. Subba Rao:

Dr. N. Subba Rao (SCIS, JNU): My journey in chemistry and structural biology

07:30 PM onwards - 🍽️ Dinner

Session 4

10:00 AM – 11:30 AM - **Session Chair:** Dr. Debasisa Mohanty (NII)

Speakers:

10:00 AM – 10:30 AM - Dr. Ragothaman M Yennamalli (Sastra University): Deciphering Thermostability and Structural Dynamics in Carbohydrate-Active Enzymes

10:30 AM – 11:00 AM - Dr. Shailja Singh (SCMM, JNU): Target based Repurposing Anti-diarrheal Drugs as Irresistible Anti-malarial

11:00 AM – 11:30 AM - Dr. Sanjib Senapati (IIT Madras): Room Temperature DNA Storage to Enhanced Drug Bioavailability: Magic Molecules Ionic Liquids in action

11:30 AM – 12:00 PM - ☕ Tea Break

Session 5

12:00 PM – 01:00 PM - **Session Chair:** Dr. Sobhan Sen (SPS, JNU)

Speakers:

12:00 PM – 12:20 PM - Dr. Lipi Thukral (IGIB, Delhi): Simulation-driven Insights of the Autophagy Pathway

12:20 PM – 12:40 PM - Dr. Ajeet Kumar Yadav (Ashoka University): Exploring Hydration Thermodynamics through Analytical Model

12:40 PM – 01:00 PM - Dr. Sangeeta (SCIS, JNU): Unravelling the Role of Local DNA Deformation on the Target Search Dynamics of DNA Binding Proteins

01:00 PM – 01:30 PM - Conclusion

01:30 PM – 02:30 PM - 🍽️ Lunch Break

DAY
02
MAR 01
2025

Data Science and Molecular Dynamic Simulations for Drug Discovery

Venue: School of Computational and Integrative Sciences

Workshop 1st March 2025 | 03:00 PM – 05:30 PM

Speaker:

03:00 PM – 03:30 PM - Dr. Tarak Karmakar (IIT, Delhi): Thermodynamics and Kinetics of Biomolecular Recognition

03:30 PM – 05:30 PM - **Hands-on:**

Marvin Prakash and Anuj Kumar Sirohi