



Organises

Symposium cum Workshop

Symposium
**Advances in Computer Simulations
in Structural Biology and Biophysics**

Workshop
**Data Science and
Molecular Dynamics Simulation
for Drug Discovery**



 **Symposium**

**Advances in Computer Simulations
in Structural Biology and
Biophysics**

Since the first computer simulation of proteins in 1977 by McCammon, Gelin, and Karplus, the improvement of both theory/algorithm and hardware has been transformative and advanced this field to a great height. In this symposium, leading researchers will give talks on various aspects of computer simulation to solve various important biological problems. This will give an understanding of the current status of the field.

 **Workshop**

**Data Science and Molecular
Dynamics Simulation for Drug
Discovery**

The workshop aims to educate younger researchers to the cutting-edge techniques, both physics and AI-Based, used for simulation and computer aided drug discovery.



Invited Speakers

Dr. Sanjib Senapati IIT Madras

Dr. Nisanth Nair IIT Kanpur

Dr. Govardhan Reddy IISc Bangalore

Dr. Durba Sengupta NCL, Pune

Dr. Shubhra Ghosh Dastidar Bose Institute

Dr. Ragothaman M Yennamalli Sastra University

Dr. Ananya Debnath IIT Jodhpur

Dr. Tarak Karmakar IIT Delhi

Dr. Sudhanshu Shanker Mahindra University

Dr. Rajesh Mishra JNU New Delhi

Dr. Shailja Singh JNU New Delhi

Dr. Lipi Thukral IGIB Delhi

Dr. Hari O.S. Yadav JNU New Delhi

Dr. Ajeet Kumar Yadav Ashoka University

Dr. Sangeeta JNU New Delhi

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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