



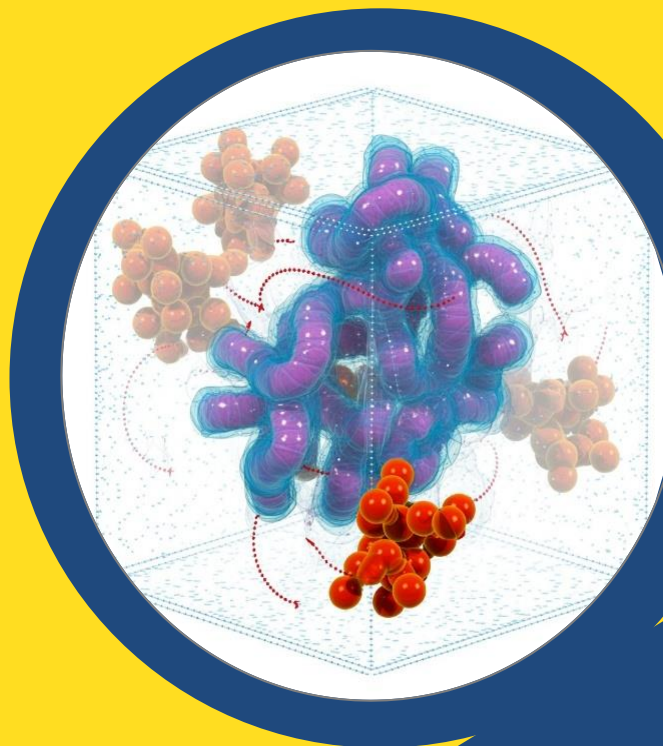
SHARDA
UNIVERSITY
Beyond Boundaries




Center for AI in Medicine, Imaging & Forensics
(CAIMIF)

is organizing

Certified FDP/Workshop on Protein-Ligand MD Using High - Performance Computing



 14th – 18th April

 10:00 AM - 04:30PM

 Center for AI in Medicine,
Imaging & Forensics Block 2,

1st Floor Room no- 103

Objectives of Event:

- Introduction to the Linux-based computational environment for molecular simulations.
- Hands-on training in biomolecular system preparation and MD simulations using GROMACS.
- Learning ligand parameterization and protein–ligand complex simulation workflows.
- Performing trajectory analysis, visualization, and GPU-accelerated HPC simulations.

**Registration
Fees**
(GST incl.)

Rs. 5000/-

Bank Name :	ICICI Bank Ltd.
Branch Address :	Krishna Apra Royal Plaza, D-2, E(acb), Alpha-1, Greater Noida, Gautam Budh Nagar, UP- 201306
Account Holder Name :	Sharda University-Seminar
Account No. :	025405005815 (CURRENT AC)
IFSC Code :	ICIC0000254
SWIFT Code :	ICICINBBCTS
MICR Code :	110229037

Scan QR Code



Registration Form Link: <https://surl.li/usytco>

WhatsApp Group Link: <https://surl.lu/nxkebf>

Training Schedule

DAY 1-ONLINE (14 th April, 2026)	Introduction to Linux and computational environment setup to prepare participants for running molecular dynamics workflows.
DAY 2 (15 th April, 2026)	Understanding MD theory and learning how to prepare and minimize biomolecular systems using GROMACS.
DAY 3 (16 th April, 2026)	Preparing ligands, building protein–ligand complexes, and running production molecular dynamics simulations.
DAY 4 (17 th April, 2026)	Performing trajectory analysis and visualizing structural and interaction dynamics from MD simulations.
DAY 5 (18 th April, 2026)	Learning GPU-accelerated MD simulations and HPC strategies for scaling simulations on DGX systems

Speakers

Dr. Ashok Kumar
Head, CAIMIF & Professor
Department of Physics, SSCS

Dr. Sunita Sharma
Assistant Professor
Department of Biotechnology,
SSBT

Ms. Shivani Singh
PhD Scholar
Department of Life Sciences,
SSBT

Resource Person

Shivani Singh
Department of Life Sciences,
SSBT

Manasvi
Department of Biotechnology,
SSBT

Yashaswini Pulastiya
Department of Biotechnology,
SSBT

Convenor

Dr. Ashok Kumar
Head, CAIMIF & Professor
Department of Physics, SSCS

Co-Convenor & Coordinator

Dr. Sunita Sharma
Assistant Professor
Department of Biotechnology, SSBT

Organizing Committee

Shivani Singh | Manasvi | Yashaswini Pulastiya

Sharda University- Plot No. 32, 34 - Knowledge Park 3, Greater Noida-201310, Delhi- NCR, India.

