



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



SHARDA
UNIVERSITY
Beyond Boundaries



is organizing

Certified FDP/Workshop

Protein-Ligand Molecular Simulations using High Performance Computing



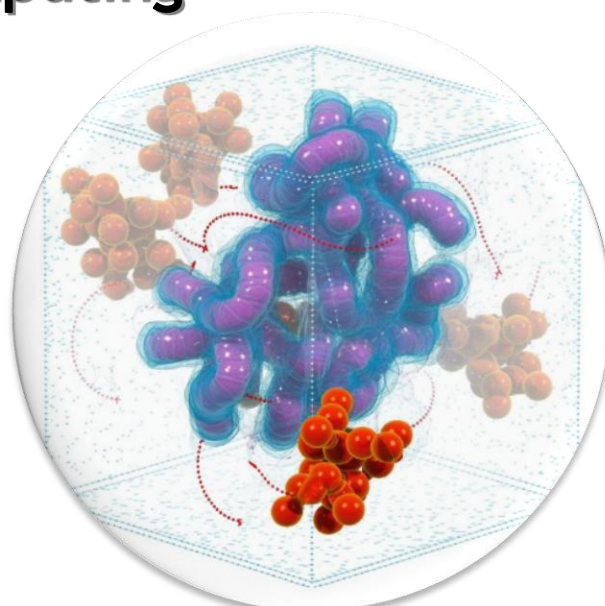
25th – 29th May, 2026



10:00 am – 4:30 pm



Center for AI in Medicine,
Imaging & Forensics, Block-2,
1st Floor, Lab 103 A/B



**Registration
Fees**

Rs. 5000/-*
(GST incl.)

*Special Group Offer for
Ph.D. Scholars

Register as a group of three and pay
only **₹3000 per person** (regular
fee: ₹5000).

SCAN to PAY



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

Objectives:

- ✓ 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 Form Link:

<https://surl.li/usytco>

WhatsApp Group Link:

<https://surl.li/nxkebf>

Training Schedule

DAY 1 (25 th May, 2026)	OFFLINE	Introduction to Linux and computational environment setup to prepare participants for running molecular dynamics workflows.
DAY 2 (26 th May, 2026)		Understanding MD theory and learning how to prepare and minimize biomolecular systems using GROMACS.
DAY 3 (27 th May, 2026)		Preparing ligands, building protein–ligand complexes, and running production molecular dynamics simulations.
DAY 4 (28 th May, 2026)		Performing trajectory analysis and visualizing structural and interaction dynamics from MD simulations.
DAY 5 (29 th May, 2026)		Learning GPU-accelerated MD simulations and HPC strategies for scaling simulations on DGX systems

Speakers

Dr. Sunita Sharma
Assistant Professor
Department of Biotechnology,
SSBT

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

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

Convenor

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

Resource Person

Shivani Singh
Department of Life Sciences,
SSBT

Manasvi
Department of Biotechnology,
SSBT

Yashaswini Pulastiya
Department of Biotechnology,
SSBT

Co-Convenor & Coordinator

Dr. Sunita Sharma
Assistant Professor
Department of Biotechnology, SSBT

Organizing Committee

Manasvi | Yashaswini | Aditya | Maihul | Khushboo |
Kushagra

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