



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



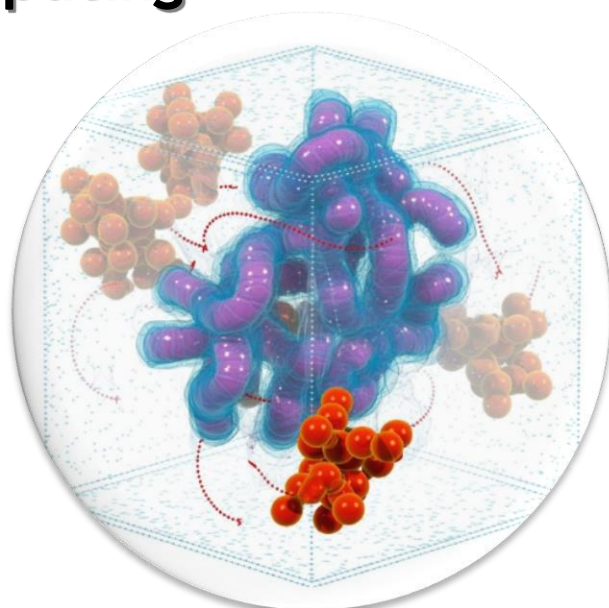
**14<sup>th</sup> – 18<sup>th</sup> April, 2026**



**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.)

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.lu/nxkebf>

# Training Schedule

<b>DAY 1</b> (14 <sup>th</sup> April, 2026)	<b>ONLINE</b>	Introduction to Linux and computational environment setup to prepare participants for running molecular dynamics workflows.
<b>DAY 2</b> (15 <sup>th</sup> April, 2026)	<b>OFFLINE</b>	Understanding MD theory and learning how to prepare and minimize biomolecular systems using GROMACS.
<b>DAY 3</b> (16 <sup>th</sup> April, 2026)		Preparing ligands, building protein–ligand complexes, and running production molecular dynamics simulations.
<b>DAY 4</b> (17 <sup>th</sup> April, 2026)		Performing trajectory analysis and visualizing structural and interaction dynamics from MD simulations.
<b>DAY 5</b> (18 <sup>th</sup> April, 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

Shivani Singh | Manasvi | Yashaswini Pulastiya

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

