

Centre for Advanced Training and Research  
Organizing Online Hands-on Workshop on

# Molecular Dynamics Simulation in Drug Discovery

25-29 June 2026, 6:30 PM IST (SUNDAY OFF)

This workshop provides participants with a comprehensive understanding of molecular dynamics (MD) simulation in drug discovery. Participants will gain theoretical knowledge and hands-on experience in configuring, executing, and interpreting MD simulations of protein-ligand complexes. By the end, participants will be equipped to independently conduct MD simulations, analyze results, and apply these techniques in drug discovery and other scientific fields, enhancing their contributions to computational biology and the pharmaceutical industry.

## Module

### Day 1: Introduction to Molecular Dynamics (MD) Simulation

- Basics of molecular dynamics and its relevance to drug discovery.
- Setting up MD simulations for protein-ligand complexes.
- Simulation parameters: force fields, solvation models, temperature, pressure, and time steps.
- **Hands-on:** Using **GROMACS** to set up a basic MD simulation.

### Day 2 & 3: Running MD Simulation

- Understanding solvation, ionization, energy minimization, equilibration, and production MD run.
- **Hands-on:** Executing a simulation for a specific protein-ligand complex using GROMACS.

### Day 4: Analyzing MD Simulation Results

- Extracting and interpreting MD trajectories: Root Mean Square Deviation (RMSD), Root Mean Square Fluctuation (RMSF) and binding free energy calculations.
- Stability assessment of protein-ligand interactions over time.
- Generating and visualizing dynamic trajectories.
- **Hands-on:** Using PyMOL to analyze MD results.

## Fee & Features

**Indian Participants: Rs 1400**

**Other Participants: \$ 75 US**

- E-Certificate to participants
- Hands-on Workshop
- Live and Interactive Sessions
- Session Recordings
- Software & Installation
- Soft Copy of Protocols
- Lecture PPTs to Participants

## Date & Time

 **25-29 June 2026**

 India 6:30 PM  
Dubai 5:00 PM  
Saudi Arabia 4:00 PM

**REGISTER HERE**

**Contact us:**

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