

Molecular Dynamics & Simulation Studies — Hands-on

Hands-on molecular dynamics from PDB to publication: parameterize systems, choose force fields wisely, equilibrate/produce safely, and turn trajectories into defensible insights.

Molecular Dynamics & Simulation Studies (GROMACS, AMBER, CHARMM)

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Session 1

Fee: Rs 6300 [Apply Now](#)

System Preparation & Force Fields

PDB cleanup, missing atoms, protonation, termini capping

[pdbfixer](#) [PDB2PQR](#) [propka](#)

Force fields, water models & ions; parameterization of ligands

[AMBER ff14SB/ff19SB](#) [CHARMM36m](#) [OPLS-AA/M](#)
[TIP3P/TIP4P-Ew](#) [antechamber/CGenFF](#)

Topology/coordinate generation and solvation boxes

[gmx](#) [pdb2gmx](#) [tleap](#) [CHARMM GUI basics](#)

Session 2

Fee: Rs 8400 Apply Now

Setup, Constraints & Equilibration

Energy minimization, NVT/NPT schedules, thermostats & barostats

grompp/mdrun **sander/pmemd** **CHARMM** **V-rescale/Langevin** **Parrinello–Rahman/Berendsen**

Constraints, cutoffs & long-range electrostatics

LINCS/SHAKE **PME** **PBC & neighbor lists**

Input file hygiene & GPU/CPU performance tips

mdp/in files **domain decomposition**
precision/constraints tradeoffs

Session 3

Fee: Rs 11200 Apply Now

Production Runs & Trajectory Analysis

Running stable production and monitoring simulation health

checkpointing **restraints** **log/EDR checks**

Core analyses: RMSD/RMSF, R_g , H-bonds, SASA, diffusion

gmx rms/gyrate/hbond/sasa **cpptraj** **VMD**

Advanced: PCA, clustering, free-energy projections

MDAnalysis **MDTraj** **PyEMMA/bioPCA**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: PDB → Insights

From prepared structure to short production and report bundle

Theory + Practical

Reproducibility: config templates, provenance & QC checklist

YAML/MDP versioning **Conda/Mamba** **Quarto**

Deliverables: figures, tables, README & manifest

PDF **CSV/TSV** **checksums**