Molecular Dynamics Simulations — Setup & Analysis — Hands-on

Learn how to set up, execute and analyze molecular dynamics (MD) simulations for proteins and protein–ligand complexes. From force field selection and system building through minimization, equilibration, production runs and trajectory analysis, you will construct MD workflows that are reproducible, physically sensible and ready to support docking, stability and mechanism studies.

Molecular Dynamics Simulations — Setup & Analysis

Help Desk · WhatsApp

Session Index

Session 1

Fee: Rs 12320 Apply Now

Force Fields, System Building & MD Basics

MD concepts and force fields

Newtonian dynamics idea | **AMBER / CHARMM / OPLS style fields** | **cutoffs and long range interactions**

Protein and complex preparation for MD

fixing missing atoms and residues | **protonation states and pH ideas** | **ligand parameter overview**

Solvation, ions and box definition

periodic boxes and shapes | water models (TIP3P like) | neutralizing and adding salt

Session 2

Fee: Rs 16520 Apply Now

Minimization, Equilibration & Production

Energy minimization strategies

steepest descent and conjugate gradient | restraints on heavy atoms | convergence criteria ideas

NVT / NPT equilibration design

thermostats and barostats | restraints and relaxation schedule | checking temperature and pressure stability

Production MD parameters and stability

time step and constraints | trajectory length planning | saving coordinates vs performance

Session 3

Fee: Rs 20720 Apply Now

Trajectory Analysis & Property Extraction

Basic stability and flexibility metrics

RMSD and RMSF time series | radius of gyration | secondary structure evolution ideas

Interactions and binding stability

H bond and contact analysis | salt bridges and hydrophobic contacts | distance and angle monitors

Advanced views and projections

PCA / essential dynamics concepts | clustering conformations | extracting representative snapshots

Session 4

Fee: Rs 26320 Apply Now

Best Practices, Reproducibility & Reporting

Good practice checklists for MD projects

documenting settings and versions | run logs and QC plots | common pitfalls and artefacts

Connecting MD to docking and free energy ideas

using MD for pose refinement | extracting frames for MM PBSA style work | identifying metastable states

Figures, tables and repositories for MD studies

time series and distribution plots | summaries for manuscripts | sharing inputs and trajectories overview