Molecular Dynamics for Binding Stability & Pathway Analysis — Hands-on

Learn how to plan, run and interpret molecular dynamics simulations for drug discovery questions. This module walks through system preparation, equilibration and production runs, quality checks, binding stability metrics and pathway level interpretation so that MD trajectories can be turned into clear, defensible design and mechanism insights.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

MD Foundations & System Preparation

Role of MD in modern drug discovery workflows

when MD adds value beyond docking **time scales and expectations** **force fields and simulation engines overview**

Protein–ligand system building basics

cleaning structures and fixing issues **protonation**

states and tautomers | ligand parameterization concepts

Solvation, ions and box setup choices

explicit solvent models and box types | neutralization and salt concentration | periodic boundary conditions basics

Session 2

Fee: Rs 11800 Apply Now

Equilibration, Production & QC

Minimization and equilibration protocols

energy minimization and restraint strategies | NVT / NPT phases | temperature and pressure coupling picks

Production MD setup for binding studies

time step and constraint choices | trajectory length and output frequency | replicate runs and seeds

Quick QC plots and stability indicators

energy drift and temperature stability | density and volume behavior | sanity checks before deeper analysis

Session 3

Fee: Rs 14800 Apply Now

Trajectory Analysis & Binding Stability

Core structural stability metrics

RMSD and RMSF trends | radius of gyration | secondary structure over time

Protein–ligand interaction persistence & stability

H bonds and salt bridge occupancy | contact maps and

distance traces | water networks and bridging interactions

Pathway and conformational change views

simple PCA / essential dynamics | projecting motion onto functional coordinates | relating motions to mechanism hypotheses

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: MD-Driven Pathway Insights

Designing a short MD study for a ligand–target system

Theory + Practical

Analyzing trajectories for binding stability & pathways

stability plots and interaction timelines | key conformational states | simple pathway or mechanism story

Deliverables: MD report and design suggestions

notebook or script for analysis | figures for binding stability & motion | concise recommendations for chemists