MD Analysis, Stability, Energetics & Binding Free Energy — Hands-on

Learn how to turn raw molecular dynamics trajectories into decision ready analyses. This module focuses on trajectory handling, stability and flexibility metrics, interaction and energetics analysis, and MM/PBSA style binding free energy workflows so that you can quantify complex stability and binding strength in a reproducible way.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Trajectory Handling & Quality Checks

MD trajectory formats and preprocessing steps

coordinate and topology files **removing PBC jumps and imaging** **fitting and alignment choices**

Basic run quality diagnostics vs time

temperature and pressure traces **density, energy and volume checks** **spotting instabilities and artefacts**

Region and selection management for analysis

whole protein vs domain selections | ligand and binding site groups | reference frames and subsets

Session 2

Fee: Rs 11800 Apply Now

Stability & Flexibility Metrics

Global stability measures

RMSD vs time for backbone and ligand | radius of gyration and compactness | equilibration window identification

Local flexibility and fluctuation analysis

RMSF per residue | mapping fluctuations onto structure | loop and binding site flexibility

Conformational descriptors and PCA ideas

principal component projections | essential dynamics interpretations | connecting motions to function

Session 3

Fee: Rs 14800 Apply Now

Interactions, Energetics & Clustering

Protein ligand interaction analysis over time

hydrogen bonds and salt bridges | hydrophobic contacts and pi stacking | contact maps and interaction fingerprints

Energetic decomposition concepts

Coulomb and Lennard Jones terms | per residue energy contributions idea | identifying key stabilizing residues

Clustering conformations and representative structures

distance metrics and clustering options **picking centroid structures** **link to docking and further calculations**

Session 4

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Mini Capstone: Binding Free Energy Report

MM PBSA style binding free energy workflow concepts

Theory + Practical

Prepare snapshots, run calculations and interpret results

snapshot selection from equilibrated window **per residue decomposition overview** **understanding uncertainty and limits**

Deliverables: MD stability and binding free energy dossier

plots for RMSD, RMSF and interactions **binding free energy tables** **written interpretation and next step guidance**