

Structural Bioinformatics & Molecular Mechanics — Hands-on

Bridge structure and physics: learn how molecular mechanics energy functions shape conformations, how to probe motions with normal modes/ENMs, and how electrostatics/solvation govern stability and function—then turn these into clear, reproducible analyses.

Structural Bioinformatics & Molecular Mechanics

[Help Desk](#) · [WhatsApp](#)

Session Index

[Session 1 — Energy Functions & Force Fields](#) [Session 2 — Conformational Analysis & Normal Modes](#) [Session 3 — Electrostatics, Solvation & Stability](#) [Session 4 — Mini Capstone: Mechanistic Story](#)

Session 1

Fee: Rs 6300 [Apply Now](#)

Energy Functions & Force Fields

Molecular mechanics terms: bonds, angles, dihedrals, vdW, Coulomb

Theory

Protein force fields & parameterization concepts

AMBER ff14SB/ff19SB **CHARMM36m** **OPLS-AA/M**
water/ions choices

Energy minimization & local landscape intuition

steepest/CG/L-BFGS **restraints & constraints**

Session 2

Fee: Rs 8400 Apply Now

Conformational Analysis & Normal Modes

Conformational space: rotamers, Ramachandran, dihedral scans

SCWRL **torsion profiles**

Normal mode analysis & elastic network models (ENMs)

GNM/ANM **ProDy** **low-frequency modes**

PCA of structures/trajectories & motion visualization

MDAAnalysis/MDTraj **morphs & arrows**

Session 3

Fee: Rs 11200 Apply Now

Electrostatics, Solvation & Stability

Continuum electrostatics & solvation models

PB/GB (APBS, GB models) **dielectric choices** **ionic strength**

pKa shifts, salt bridges & H-bond networks

PROPKA/PDB2PQR **network centrality**

Stability metrics & knowledge-based potentials

DOPE/DFIRE overview **packing & cavities**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Mechanistic Story

Link motions, energetics and electrostatics to a functional hypothesis

Theory + Practical

Assemble a concise analysis bundle with provenance

ProDy/ENM outputs **APBS maps** **config & scripts**

Deliverables: figures, tables, README & manifest

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