

Biophysics of Biomolecules: Thermodynamics & Kinetics — Hands-on

Bridge simulation and experiment to extract rigorous thermodynamics and kinetics for biomolecular processes. Learn to compute free energies and rate constants from simulations and interpret them alongside ITC/SPR/thermal data in transparent, reproducible workflows.

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Session 1

Fee: Rs 6300 [Apply Now](#)

Thermodynamics Foundations & Binding

State functions & ensembles; ΔG , ΔH , ΔS and partition functions

Theory

Binding thermodynamics & linking K_d to ΔG (ITC/van't Hoff)

[ITC/SPR interpretation](#) [van't Hoff/Eyring plots](#)

Simulation observables → thermodynamic quantities

[alchemical/endpoint overview](#) [convergence sanity](#)

Session 2

Fee: Rs 8400 Apply Now

Kinetics, MSMs & Rate Theory

Transition-state theory, Kramers, and reaction coordinates

barrier crossing committor concepts

Markov State Models (MSMs) for kinetics from MD

PyEMMA/MSMBuilder implied timescales

MFPT/residence time

$k_{\text{on}}/k_{\text{off}}$ estimation & uncertainty

bootstraps/CI model diagnostics

Session 3

Fee: Rs 11200 Apply Now

PMFs & Enhanced Sampling

Potential of mean force (PMF) along collective variables

umbrella sampling WHAM integration

Metadynamics & biasing strategies with PLUMED

well-tempered meta bias deposition & recovery

Toolchain & practice

GROMACS/AMBER PLUMED MDTraj/MDAnalysis

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: $\Delta G/\Delta H/\Delta S$ & k Extraction

From MD to PMF and MSM: compute ΔG and rate constants for a binding/folding step

Theory + Practical

Thermo–kinetic narrative with experiment links (ITC/SPR)

consistency checks **uncertainty reporting**

Deliverables: figures, tables, README & manifest

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