Free Energy Calculations — MM PBSA MM GBSA FEP — Hands-on

Learn how to estimate binding free energies for protein–ligand and protein–protein systems using MM-PBSA, MM-GBSA and introductory FEP style workflows. From MD trajectory preparation and definition of energy terms to convergence checks, uncertainty estimation and interpretation limits, you will construct free energy protocols that complement docking and MD and are suitable for decision support and publication.

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Session 1
Fee: Rs 12320 Apply Now

Concepts, Thermodynamic Cycles & Protocol Choice

Binding free energy fundamentals

ΔG, enthalpy, entropy ideas   absolute vs relative free energies   end point vs alchemical views

Thermodynamic cycles for binding

solution vs gas phase cycles   protein–ligand and

mutation scenarios link to experiment (Kd, IC50)

Choosing between MM PBSA, MM GBSA and FEP

data requirements and cost expected accuracy regimes screening vs refinement use cases

Session 2
Fee: Rs 16520 Apply Now

MM PBSA / MM GBSA Workflows

Preparing MD trajectories for analysis

equilibration checks and frame selection stripping waters and ions as required handling periodicity and imaging

Energy components in MM PBSA / GBSA

molecular mechanics (E_vdw, E_elec) polar & nonpolar solvation terms entropy estimation strategies overview

Running and interpreting MM PBSA / GBSA

single vs multiple trajectory approaches per residue decomposition ideas linking ∆G trends to SAR and mutations

Session 3
Fee: Rs 20720 Apply Now

FEP Concepts, Setup & Checks

Alchemical FEP foundations

alchemical vs physical pathways λ windows and soft core potentials relative binding free energy use cases

System and perturbation setup

mapping ligands and mutations topology and parameter consistency choosing number of windows

Convergence, overlap and error estimates

monitoring λ window overlaps BAR / MBAR style estimators (concepts) run length and hysteresis checks

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Session 4
Fee: Rs 26320 Apply Now

Best Practices, Uncertainty & Reporting

Uncertainty, replicates and robustness

technical vs physical replicates confidence intervals and error bars sensitivity to protocol choices

Integrating free energies into decision making

ranking ligands or variants combining with docking and SAR data flagging borderline and noisy cases

Documentation, plots and publication readiness

tabulating ΔG and components correlation plots vs experiment protocol descriptions for reviewers