

## Free Energy Calculations & Binding Affinity — Hands-on

From quick end-state estimates to rigorous alchemical workflows: set up, run, and analyze binding free energy calculations with best practices for convergence, uncertainty, and transparent reporting.

# Free Energy Calculations & Binding Affinity (MM-PBSA, FEP)

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### Session 1

**Fee: Rs 6300** [Apply Now](#)

## MM-PBSA/GBSA: Theory & Setup

End-state methods, dielectric models and entropy options

**Theory**

Running MM-PBSA/GBSA on MD snapshots

**gmx\_MMPBSA** **MMPBSA.py (AMBER)** **trajectory subsampling**

Interpreting components & sanity checks

**$\Delta E_{MM}$ ,  $\Delta G_{solv}$ ,  $T\Delta S$**  **per-residue decomposition**

### Session 2

Fee: Rs 8400 Apply Now

## Alchemical FEP/TI Workflows

$\lambda$ -schedules, soft-core potentials, restraints & standard states

Boresch restraints standard-state correction  
decoupling schemes

Tooling & engines (overview)

GROMACS+PLUMED OpenMM/pmx AMBER TI FEP+\*

Analysis: TI/BAR/MBAR and error propagation

BAR/MBAR overlap matrices CI/bootstraps

### Session 3

Fee: Rs 11200 Apply Now

## Convergence, Errors & Enhanced Sampling

Convergence diagnostics & window overlap checks

time-series decorrelation effective sample size  
replicates

Umbrella sampling & PMF with WHAM

reaction coordinates biasing & windows WHAM

Enhanced sampling (overview)

REST2/HREX metadynamics (PLUMED)

### Session 4

Fee: Rs 14000 Apply Now

## Mini Capstone: Affinity Report

Compute  $\Delta G$  with MM-PBSA and a small FEP/TI example;  
compare vs literature

**Theory + Practical**

Uncertainties, convergence plots & reproducibility checklist

**BAR/MBAR tables** **overlap matrices** **protocol**

**YAML/inputs**

Deliverables: figures, tables, README & manifest

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