Advanced Sampling, Metadynamics, Umbrella & Replica — Hands-on

Go beyond straightforward MD and learn how to map free-energy landscapes, cross barriers and sample rare events in biomolecular systems. This module covers reaction coordinates, metadynamics, umbrella sampling, replica-exchange concepts and practical workflows so that you can design and interpret advanced sampling simulations for real research problems.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Free Energy Landscapes & Reaction Coordinates

Why advanced sampling is needed beyond standard MD

rare events and high barriers | **metastable states and slow modes** | **connection to kinetics and thermodynamics**

Free-energy surfaces and collective variables (CVs)

1D vs 2D free-energy profiles | **distance, angle and**

RMSD based CVs | choosing CVs aligned with mechanism

Assessing CV quality and basic projection ideas

orthogonality and degeneracy issues | connection to PCA and slow coordinates | sanity checks using short MD runs

Session 2

Fee: Rs 11800 Apply Now

Metadynamics Concepts & Setup

Metadynamics basics and biasing along CVs

history dependent bias potentials | Gaussian height, width and stride | ordinary vs well tempered metadynamics idea

Practical metadynamics parameter choices

choosing bias factor and temperature | boundary handling and wall potentials | avoiding runaway bias and artefacts

Reconstructing free-energy surfaces from metadynamics

accumulated bias and FES reconstruction | monitoring convergence indicators | interpreting barriers and minima

Session 3

Fee: Rs 14800 Apply Now

Umbrella Sampling, Windows & PMF

Umbrella sampling concepts along a chosen coordinate

harmonic restraints and windows | initial structures and pulling runs | coverage and overlap requirements

Running umbrella windows and checking sampling quality

histogram overlap checks **equilibration vs production frames in each window** **troubleshooting poorly sampled regions**

PMF reconstruction and barrier interpretation

WHAM style reconstruction overview **error estimation and confidence bands** **relating PMF to binding or transition mechanisms**

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Replica & Advanced Campaign

Replica-exchange ideas and temperature/hamiltonian ladders

Theory + Practical

Design a small advanced sampling campaign for a case system

choosing CVs and method (meta or umbrella) **optional replica or multiple walkers concept** **running and monitoring a short pilot campaign**

Deliverables: FES/PMF plots and advanced sampling report

free-energy landscape or PMF profiles **parameter tables and convergence diagnostics** **written interpretation and limitations discussion**