Understand how proteins move across their conformational landscapes. This module connects normal mode analysis, molecular dynamics, essential dynamics and ensemble modelling so that you can characterize motions, identify functional states, and extract mechanistic insight for docking, design and allostery studies.

Conformational Landscapes — Normal Modes & Ensembles

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Session 1
Fee: Rs 19800 Apply Now

Conformational Landscapes & Normal Modes

Energy landscapes and conformational basins

minima, barriers and pathways native state ensembles rugged vs smooth landscapes

Normal mode analysis (NMA) foundations

Hessian matrices and eigenmodes low frequency collective motions elastic network models (ENM)

Visualizing mode motions and displacements

`arrow and morph animations` `overlap with experimental states` `link to functional domains`

Session 2
`Fee: Rs 23800` Apply Now

MD Trajectories, PCA & Essential Dynamics

Preparing and inspecting MD trajectories for analysis

`alignment and fitting choices` `removal of overall translation / rotation` `coordinate selection (backbone vs atoms)`

Principal component analysis (PCA) of motions

`covariance matrices` `eigenvectors and eigenvalues` `projection of trajectories onto PCs`

Essential dynamics and free energy projections

`2D landscapes along PC1/PC2` `population densities and basins` `linking PCs to experimental observables`

Session 3
`Fee: Rs 27800` Apply Now

Ensembles, Clustering & State Models

Generating and curating conformational ensembles

`downsampling long MD runs` `RMSD and PC based metrics` `removal of poorly equilibrated frames`

Clustering methods for conformations

`k-means and hierarchical clustering` `density based methods` `selection of representative structures`

From clusters to kinetic and state models

transition counts between states basic Markov state model (MSM) ideas estimating lifetimes and transition paths

Session 4
Fee: Rs 30800 Apply Now

Functional Motions, Allostery & Reporting

Relating modes and ensembles to function

open–closed transitions gating and loop motions mapping motions onto active sites

Allosteric pathways and communication routes

mode based allostery indicators network and graph views of motions coupling of distant sites

Deliverables: landscape figures, ensembles & narrative

free energy maps and projections representative structures per state mechanistic story for reports and slides