Membrane Proteins — Topology, Dynamics & MD Setup — Hands-on

Learn how to prepare, embed and simulate membrane proteins in realistic lipid bilayers. This module connects topology prediction, bilayer construction, MD setup and analysis so you can study orientation, dynamics and interactions of channels, transporters and receptors in silico.

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Session Index

Session 1

Fee: Rs 23800 Apply Now

Membrane Protein Classes & Topology

Classes and architectures of membrane proteins

single and multi pass helices **beta barrels** **channels, transporters and GPCRs**

Topology prediction and orientation in membranes

transmembrane segment prediction **inside outside topology mapping** **signal peptides and tail anchors**

Lipid environment and biophysical context

bilayer thickness and hydrophobic matching | lipid composition and asymmetry ideas | cholesterol and raft concepts

Session 2

Fee: Rs 27800 Apply Now

Bilayer Building & Embedding Workflows

Building lipid bilayers for simulations

choice of lipid types and mixtures | bilayer size and area per lipid | asymmetric leaflets and mixtures

Embedding membrane proteins in bilayers

alignment to membrane normal | packing lipids around the protein | removing overlaps and clashes

Solvation, ions and box setup for MD

water models and box geometry | ion placement and neutralization | checking overlaps and system sanity

Session 3

Fee: Rs 31800 Apply Now

MD Protocols for Membrane Systems

Force fields and parameters for membranes

protein and lipid force field choices | coarse grained vs all atom ideas | mixing and compatibility issues

Equilibration strategies for membrane systems

restrained minimization and short MD | releasing protein and lipid restraints | monitoring area per lipid and thickness

Production runs and trajectory management

time step and ensemble choices | long timescale planning | checkpointing and storage practices

Session 4

Fee: Rs 34800 Apply Now

Dynamics Analysis, Lipid Contacts & Reporting

Protein stability, orientation and dynamics readouts

RMSD and RMSF in membranes | helix tilt and rotation metrics | pore radius and channel opening ideas

Lipid interactions and local environment

annular lipid contacts | specific lipid binding sites | cholesterol and headgroup preferences

Deliverables: membrane MD report and figures

summary plots for bilayer properties | snapshots and movies of key events | structure to mechanism narrative