Membrane Proteins, Coarse-Grain & Lipid Systems — Hands-on

Learn how to prepare and simulate membrane protein systems using both atomistic and coarse-grained approaches. This module covers bilayer building, lipid composition choices, protein insertion/orientation, CG mapping and system setup so that you can generate robust membrane and lipid systems for MD, free-energy and design workflows.

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Membrane Protein Basics & Topology

Membrane protein classes and architecture overview

single pass and multi pass helices | **beta barrels and channels** | **peripheral vs integral proteins**

Topology prediction and orientation in the membrane

transmembrane segment detection ideas | **inside outside and tilt considerations** | **aligning structures to**

membrane normal

Preparing membrane protein structures for embedding

fixing loops and missing residues | removing unwanted partners and detergents | checking hydrophobic and polar exposure

Session 2

Fee: Rs 11800 Apply Now

Bilayer Building, Lipid Mixes & Insertion

Choosing bilayer composition and dimensions

simple vs mixed lipid systems | headgroup and tail saturation effects | asymmetric vs symmetric leaflets ideas

Bilayer building and quality checks before insertion

area per lipid and thickness checks | packing issues and voids | equilibration of pure lipid patches

Protein insertion and overlap removal concepts

punching lipids around the protein | preserving tilt and orientation | initial restrained equilibration of embedded system

Session 3

Fee: Rs 14800 Apply Now

Coarse-Grain Mapping & CG System Setup

Coarse-grain modeling principles for membranes

mapping atoms to beads concepts | trade off between speed and detail | when to choose CG vs atomistic

Protein and lipid mapping to CG force fields

standard mapping schemes overview | tuning elastic

networks for proteins | ensuring proper lipid phase behaviour

Setting up and equilibrating CG membrane systems

box size and timestep choices | CG specific thermostat and barostat settings | converting CG outputs into analysis ready trajectories

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Atomistic↔CG Membrane System

Select a membrane protein and define bilayer and CG strategy

Theory + Practical

Build atomistic and CG versions of the same system and equilibrate briefly

compare thickness, area per lipid and tilt | qualitative comparison of dynamics | prepare configurations for longer production runs

Deliverables: membrane system build files and comparison report

topology and coordinates for both resolutions | summary tables for bilayer properties | documented workflow for future membrane projects