Allostery Hotspots & Communication Pathways — Hands-on

Learn how to detect, visualize and interpret allosteric communication in proteins. This module connects networks, normal modes and MD-based pathway analysis to identify allosteric hotspots, characterize communication routes and propose allosteric design or modulation strategies for enzymes, receptors and complexes.

Allostery Hotspots & Communication Pathways

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Session Index

Session 1

Fee: Rs 26800 Apply Now

Allostery Concepts, Networks & Hotspots

Foundations of allostery and communication

concerted vs sequential models | **allosteric sites vs orthosteric sites** | **examples from enzymes and receptors**

Residue interaction networks from structures

building graphs from contacts | **edge definitions and cutoffs** | **centrality and community concepts**

Allosteric hotspot indicators

betweenness and degree centrality | interface and hinge-like regions | evidence from mutation and disease data

Session 2

Fee: Rs 30800 Apply Now

Normal Modes, ENMs & Communication Paths

Elastic network models and normal mode basics

coarse-grained ENM concepts | low-frequency collective modes | linking modes to functional motions

Pathways and communication metrics from ENMs

perturbation response ideas | coupling between distant sites | identifying residue chains along modes

Overlaying network and mode information

consensus allosteric hotspots | visualizing pathways on structures | prioritizing regions for deeper MD analysis

Session 3

Fee: Rs 34800 Apply Now

MD-Based Allosteric Pathways & Perturbations

Extracting communication from MD trajectories

dynamic interaction networks | correlations and mutual information | time-averaged vs state-specific networks

Pathway extraction and ranking from MD

shortest and highest-flow paths | comparison across

ligand/bound states | robust vs transient communication routes

Perturbation ideas and mutational impacts

virtual mutations at hotspots | effects on networks and pathways | connecting to experimentally observed variants

Session 4

Fee: Rs 37800 Apply Now

Allosteric Design Ideas, Reporting & Case Studies

Allosteric site prioritization and design ideas

ranking potential allosteric pockets | stabilizing or destabilizing pathways | linking to small-molecule or protein modulators

Case studies: enzymes, GPCRs and multi-domain proteins

known allosteric switches | mutational analysis of communication | translating insights to experiments

Deliverables: allosteric communication report & visuals

network and pathway figures | hotspot and site tables | design and mutation recommendations