Allostery, Hotspots & Protein Engineering — Hands-on

Learn how to think about proteins as dynamic, allosteric systems instead of static structures. This module focuses on detecting allosteric hotspots, reading conformational pathways and using this information to design mutations that modulate activity, stability and regulation, building a practical bridge between structural analysis and protein engineering decisions.

Allostery, Hotspots & Protein Engineering

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Allostery Concepts & Dynamic Networks

Allostery and long range communication in proteins

classical vs modern views of allostery **conformational selection and population shift** **active, inactive and intermediate states idea**

Networks on structures and paths of communication

residue contact and interaction graphs concept **centrality and path based measures sketch** **connecting network metrics to motions**

Inputs for allostery analysis from structures and MD style data

static snapshots vs trajectory information **contact frequency and correlated motions ideas** **caveats of limited sampling and resolution**

Session 2
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Hotspot Mapping & Conformational Pathways

Identifying allosteric hotspots on structures and ensembles

rigidity and flexibility patterns idea **network central residues and hubs** **experimental hints from mutagenesis or HDX**

Conformational pathways between functional states

interpolations and transition paths concept **mapping motions onto network edges** **visual summaries of domain shifts and loops**

Ranking hotspots for intervention and follow up work

combining structural, network and dynamics clues **filtering out positions with structural risk** **building shortlists for engineering or screening**

Session 3
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Allostery Aware Protein Engineering

Design strategies targeting allosteric sites and networks

stabilizing desired states idea **modulating communication rather than active site** **positive vs negative allosteric effects**

Mutation planning around hotspots and communication paths

side chain chemistry and packing concepts **balancing**

activity, stability and expression | avoiding clashes and aggregation motifs

Simple in silico readouts to triage designs before experiments

local stability and packing checks idea | quick dynamics or network metrics comparison | shortlists for experimental follow up

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Allosteric Design Notebook

Select a protein and define an allostery focused design question

Theory + Practical

Map hotspots, propose mutations and sketch expected effects

annotated structures and network diagrams | simple stability or communication checks | prioritized design set for experiments

Deliverables: allosteric design slides, tables and notes

figures of hotspots and pathways | mutation table with rationale | plan for follow up MD and wet lab tests