Protein Network Topology & Interfaces — Hands-on

Learn how to connect protein structure, interfaces and interaction data into coherent network based views. From building and annotating protein interaction graphs through mapping structural interfaces, hotspots and allosteric paths, you will use network topology and graph measures to prioritize residues, partners and regions that matter for function, mechanism and design.

Protein Network Topology & Interfaces

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Session Index

Session 1

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Interaction Data, Networks & Graph Basics

Protein interaction data sources and QC

experimental vs predicted interactions | **confidence scores and filtering ideas** | **binary vs complex level interactions**

Graph representation of protein networks

nodes, edges and edge weights concepts | **directed, undirected and bipartite views** | **network building from interaction tables**

Basic network descriptors and plots

degree distributions and hubs | connected components and subgraphs | simple layouts and visual cues

Session 2

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Structural Interfaces & Hotspot Annotation

Mapping interactions to structural interfaces

using complexes and docking models | buried surface area and contact residues | interface type and geometry views

Interface hotspot and energy contributions (concepts)

conserved and central interface residues | alanine scanning ideas | electrostatic and hydrophobic contributions

From residue level features to interface level labels

annotating edges with interface types | critical residues and mutation sensitivity | linking structural details to network edges

Session 3

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Network Topology, Paths & Communities

Centrality and importance measures

degree, betweenness and closeness ideas | eigenvector and pagerank style views | node and edge centrality for PPIs

Paths, communication routes and allostery (concepts)

shortest paths and path ensembles | connecting

binding sites via residue networks **simple models of information flow**

Communities, modules and sub networks

clustering and community detection ideas **functional modules and complexes** **mapping communities back to structures**

Session 4

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Workflows, Integration & Reporting

End to end network and interface workflows

from interaction tables to graphs and interfaces **combining centrality, communities and hotspots** **shortlisting residues, proteins and complexes**

Integration with omics and structural projects

overlaying expression and variant data **linking to docking, MD and free energy outputs** **pathway and disease module mapping**

Figures, tables and project ready summaries

network diagrams with highlighted hubs **interface and hotspot panels on structures** **ranked lists with clear interpretation notes**