Structural Epitope Mapping & Paratope Docking — Hands-on

Build an intuitive, structure informed view of how epitopes and paratopes interact in three dimensions. This module connects sequence based epitope ideas to 3D antigen structures, antibody binding sites, interfaces and docking concepts that support rational vaccine and antibody engineering decisions.

Structural Epitope Mapping & Paratope Docking

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Structural Immunology & 3D Data Basics

Antibody structure, paratopes and antigen binding sites (conceptual)

Fab, Fc and variable domains | **CDR loops and framework regions** | **paratope definition and features**

3D structure formats and basic viewing concepts (orientation)

PDB style coordinate files | **chains, residues and**

atoms | cartoon, surface and stick views

Antigen epitope types and structural context

linear versus conformational epitopes | surface exposure and topology | relationship to sequence based predictions

Session 2

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Epitope Mapping on Antigen Surfaces

Mapping sequence defined epitopes onto 3D structures (conceptual)

chain and residue indexing | highlighting epitope patches | handling missing loops and unresolved regions

Surface accessibility and flexibility as epitope features

solvent exposed versus buried | loops, turns and protruding regions | electrostatic and hydrophobic patches

Relating mapped epitopes to known antibody complexes (where available)

overlaying antigen alone and complex structures noting shifts and conformational changes | cross checking with experimental epitope data

Session 3

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Paratope Features & Docking Concepts

Describing paratopes and antigen binding interfaces (conceptual)

CDR contributions and contact residues | shape complementarity ideas | hydrogen bonds and salt

bridges overview

Docking outputs and scoring readouts (orientation only)

poses and interface geometries **energetic scores and rankings (conceptual)** **limits and uncertainty of docking predictions**

Interpreting structural changes upon binding (conceptual)

induced fit and conformational selection **rigid regions versus flexible loops** **implications for escape and mutation mapping**

Session 4

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Mini Case Study: From Sequence to Structural Story

Starting from antigen sequence and predicted epitopes (conceptual)

identify or approximate 3D structure **map epitope locations on the surface** **note accessibility and clustering**

Connecting to antibody binding hypotheses (conceptual)

sketch possible paratope engagement regions **highlight key contact residues to watch** **relate to known escape or mutation sites**

Summarising structural insights for design teams (conceptual)

simple images and annotated views **tables of epitopes and interface notes** **handoff to docking, engineering and wet lab modules**