Homology Modeling & Model Assessment — Hands-on

Learn how to construct and critically evaluate homology models of proteins suitable for docking, MD and mechanistic studies. You will perform template search, build alignments, generate and refine models, and interpret validation metrics so that final structures are robust, defensible and ready for downstream applications and publication.

Homology Modeling & Model Assessment

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Session Index

Session 1

Fee: Rs 12320 Apply Now

Templates, Alignments & Modeling Strategy

Homology modeling principles and limits

sequence identity regimes | **single vs multi template ideas** | **global vs domain wise modeling**

Template identification and curation

BLAST and HMM based searches | **coverage, gaps and insertions** | **template quality and ligand presence**

Alignments for modeling

pairwise and multiple alignments | manual curation of key motifs | handling low complexity and insertions

Session 2

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Model Building, Loops & Side Chains

Core model building workflows

MODELLER like pipelines | template superposition ensemble of starting models

Loop modeling and difficult regions

insertions and deletions handling | loop sampling concepts | terminal flexibility considerations

Side chain placement and packing

rotamers and packing quality | buried polar residues salt bridges and hydrogen bonds

Session 3

Fee: Rs 20720 Apply Now

Geometry Checks & Quantitative Validation

Local geometry and stereochemistry

Ramachandran analysis | bond and angle checks steric clashes and rotamers

Global model quality scores

DOPE like potentials | QMEAN and related indices | per residue error profiles

Template comparison and RMSD analysis

backbone RMSD vs templates | superposition of functional regions | aligning active and binding sites

Session 4

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Refinement, Comparison & Use in Workflows

Energy minimization and limited relaxation

force field based minimization ideas | restrained vs unrestrained schemes | avoiding over optimization

Selecting best models and documenting decisions

ranking by multi metric panels | keeping ensembles for uncertainty | figure and table summaries

Preparing models for docking and MD pipelines

protonation and missing atoms | defining binding site views | sharing models with full validation record