

Homology Modelling — Template Selection & Refinement — Hands-on

Gain end-to-end skills in comparative modelling, from template search and sequence–structure alignment through model building, loop refinement and assessment. This module focuses on producing docking- and simulation-ready homology models using reproducible structural bioinformatics workflows.

Homology Modelling — Template Selection & Refinement

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Session 1

Fee: Rs 12800 [Apply Now](#)

Template Search & Selection Strategy

Sequence analysis and domain architecture

[domain boundaries](#) [disordered regions](#) [signal peptides & transmembranes](#)

Template search strategies

[BLAST / PSI-BLAST](#) [HHblits / HHsearch](#) [PDB & AlphaFold DB as template sources](#)

Template evaluation and selection criteria

sequence identity & coverage **resolution / quality scores** **biological relevance & ligands**

Session 2

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Alignments & Core Model Building

Pairwise and multiple sequence alignments for modelling

MAFFT / Clustal Omega **profile-profile alignment**
alignment editing & masking

Building initial homology models

MODELLER **SWISS-MODEL / Phyre2** **multi-template vs single-template**

Handling insertions, deletions and gaps

loop regions vs conserved core **exposed vs buried changes** **alignment-structure consistency checks**

Session 3

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Loop Modelling & Sidechain Refinement

Loop modelling approaches

database-based loops **ab initio loop sampling**
flexible regions near active sites

Sidechain packing and local minimization

rotamer libraries **clash removal** **hydrogen-bond and salt-bridge optimization**

Energy refinement of homology models

restrained minimization **force fields & solvation**

models **avoiding over-refinement artifacts**

Session 4

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Model Assessment, Ranking & Polishing

Quality assessment of homology models

DOPE / GA341 / QMEAN **MolProbity / ProSA** **per-residue reliability scores**

Ranking and selecting final models

consensus scoring **functional site inspection**
comparison with AlphaFold predictions

Deliverables: modelling report & ready-to-use structure

final PDB with documentation **alignment and template set** **QC plots & decision log**