# Homology and Comparative Modeling Pipelines — Hands-on

Learn how to go from a protein sequence to a ready-to-use 3D model using modern homology and comparative modeling pipelines. This module walks through template search, alignment, model building, refinement, and validation so that your final models are fit for docking, dynamics, and design tasks.

## Homology and Comparative Modeling Pipelines

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**Session 1**

**Fee: Rs 8800** Apply Now

### Template Search & Target–Template Alignment

Sequence analysis and domain architecture of the target

- UniProt and domain annotation
- transmembrane and signal peptides
- disorder and low complexity regions

Template search strategies

- BLAST and PSI BLAST
- HMM based search (HHpred style)
- coverage, identity and e value thresholds

Target–template alignment and manual curation

multiple sequence alignment | gap handling in loops and termini | alignments for active site integrity

Session 2

Fee: Rs 11800 Apply Now

## Model Building, Loops & Side Chains

Core homology model building workflow

restraints based modeling concepts | single vs multi template models | model ensembles and variability

Loop modeling strategies

database based loop search | ab initio loop building | loops near active and binding sites

Side chain placement and optimization

rotamer libraries | clash reduction and packing | preserving catalytic residues geometry

Session 3

Fee: Rs 14800 Apply Now

## Multi-Template Models & Refinement

Combining multiple templates

local vs global template usage | handling insertions and deletions | chimeric models and domain swaps

Complex and oligomer modeling basics

modeling biologically relevant assemblies | interface conservation and contacts | ligand and cofactor transfer

Energy minimization and refinement

restrained minimization concepts relaxing clashes and bad geometry preparing for MD or docking

Session 4

Fee: Rs 18800 Apply Now

### Mini Capstone: End-to-End Homology Model

Select target, templates and build a full model

Theory + Practical

Refine, validate and compare model candidates

geometry and clash checks Ramachandran and rotamer statistics model ranking and selection

Deliverables: final model set and pipeline report

PDB files for selected models QC and comparison summary documented pipeline for reuse