



Computational Antibody Affinity Maturation — Hands-on

Systematically mature antibodies in silico. Learn to quantify paratope–epitope quality, run mutational scans, design focused libraries under developability constraints, and triage candidates with docking/MD/free-energy estimates—then bundle everything into clear, defensible reports.

Computational Antibody Affinity Maturation

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Session 1

Fee: Rs 6300 [Apply Now](#)

Interface Basics & Metrics

Paratope–epitope anatomy, contacts, hotspots & energetics

Theory

Quantifying interfaces and spotting liabilities

buried SASA **H-bonds/salt bridges** **hydrophobic patches**

Preparing structures for design

cleanup/repair **loop checks/glycans**

Session 2

Fee: Rs 8400 Apply Now

In Silico Mutational Scanning

$\Delta\Delta G$ prediction & hotspot discovery (overview & practice)

Rosetta ddG **FoldX** **DL predictors (overview)**

Saturation & combinatorial scanning in CDRs

single/double mutants **positional scoring** **synergy checks**

Quick sanity: clashes, geometry & interface recovery

minimization **contact maps**

Session 3

Fee: Rs 11200 Apply Now

Library Design & Multi-objective Triage

Focused library design under developability constraints

patchiness/aggregation **liabilities filters** **germline proximity**

Docking, MD & scoring for shortlist triage (overview)

RosettaDock/HADDOCK **short MD relax** **MM-GBSA snapshot**

Ranking & uncertainty: consensus and bootstraps

score ensembles **replicates**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Design → Rank → Report

Propose mutations, evaluate $\Delta\Delta G$, triage with docking/MD, and deliver a ranked shortlist

Theory + Practical

Provenance & reproducibility (configs, seeds, versions, logs)

YAML/JSON configs **workflow scripts** **Quarto**
summary

Deliverables: figures, tables, README & manifest

PDF **CSV/TSV** **checksums**