



Computational Enzymology & Protein Engineering — Hands-on

Design better enzymes with structure-guided, computation-first workflows. Identify catalytic residues, model substrate poses, predict mutation effects on stability/activity, and plan focused variant sets with transparent, reproducible reporting.

Computational Enzymology & Protein Engineering

[Help Desk](#) · [WhatsApp](#)

Session Index

[Session 1 — Catalytic Sites & Mechanistic Context](#) [Session 2 — Mutations: Stability/Activity Predictions](#) [Session 3 — Design Workflows & Variant Prioritization](#) [Session 4 — Mini Capstone: Engineer → Justify → Report](#)

Session 1

Fee: Rs 6300 [Apply Now](#)

Catalytic Sites & Mechanistic Context

Identify catalytic residues, cofactors and motifs; map conservation

[Catalytic Site Atlas](#) [BRENDA](#) [InterPro/PROSITE](#)
[ConSurf](#)

Substrate binding & pocket characterization

[fpocket](#) [PLIP/LigPlot+](#) [electrostatics \(APBS\)](#)

Kinetic/thermodynamic intuition for engineering

k_{cat}/K_m context **pK_a shifts** **stability vs activity**
tradeoffs

Session 2

Fee: Rs 8400 Apply Now

Mutations: Stability/Activity Predictions

In silico mutagenesis & $\Delta\Delta G$ predictions (stability)

FoldX **Rosetta ddG** **PoPMuSiC/DynaMut2**

Catalytic residue sensitivity & activity proxies

contact/packing metrics **electrostatic shifts**
substrate pose impact

Filter, rank, and sanity-check candidate variants

hotspot maps **stability windows** **tradeoff plots**

Session 3

Fee: Rs 11200 Apply Now

Design Workflows & Variant Prioritization

Rational & semi-rational design strategies; saturation hotspots

HotSpot Wizard **FireProt** **RosettaDesign***

Substrate docking/pose checks to guide mutations

Vina/Smina **PLIP contacts** **catalytic geometry**

Prioritization panels & experiment-ready variant sets

multi-objective ranking **risk flags** **variant tables**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Engineer → Justify → Report

Propose variants for improved stability/activity and justify with evidence

Theory + Practical

Build an experiment-ready candidate table with provenance

$\Delta\Delta G$ panels **contact/electrostatic maps** **config & scripts bundle**

Deliverables: figures, tables, README & manifest

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