Capstone End-to-End Structural Modeling Project — Hands-on

Apply everything learned in structural bioinformatics, docking and molecular dynamics to a single coherent project. This capstone walks through scoping a realistic problem, selecting targets and inputs, planning workflows, running modeling and simple dynamics style analyses and packaging the results into a reproducible report and presentation suitable for academic or industry review.

Capstone End-to-End Structural Modeling Project

Help Desk · WhatsApp

Session Index

Session 1

Fee: Rs 8800 Apply Now

Scoping, Targets & Inputs

Define a realistic structural modeling question

enzyme, receptor or complex of interest **ligands, partners or mutations in scope** **success criteria and outputs expectation**

Gather sequences, structures and experimental context

sequence variants and domain boundaries **PDB or**

AlphaFold like models as starting points **known ligands or assay conditions overview**

Decide modeling depth vs time and compute budget

structure only vs docking plus dynamics style **number of systems and replicates idea** **timeline and milestone sketch for project**

Session 2

Fee: Rs 11800 Apply Now

Workflow & Modeling Plan

Design an end to end modeling workflow outline

structure curation and preparation steps **docking and complex generation ideas** **MD style equilibration and production concepts**

Choose key analyses and readouts in advance

RMSD, contacts and simple energy views **binding site occupancy or pose stability** **variants or conditions comparison plan**

Plan directory layout, naming and tracking for reproducibility

clear folders for inputs, runs and results **simple metadata and log files concept** **script or notebook based automation ideas**

Session 3

Fee: Rs 14800 Apply Now

Execution, Analysis & Checks

Run modeling, docking and basic dynamics style steps

prepared structures and complexes **short MD like trajectories for stability views** **capture runs, parameters and seeds in notes**

Perform core analyses and sanity checks on outputs

time series for RMSD and key distances **interaction and contact pattern summaries** **simple convergence and quality checks**

Compare conditions, ligands or variants against objectives

tables of metrics across systems **short narrative on winners and losers** **flags for results needing caution**

Session 4

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Final Report, Slides & Repro Pack

Draft a structured report telling the project story

Theory + Practical

Prepare figures, tables and slides for presentation

key structure and trajectory snapshots **comparison charts across systems** **clear takeaway messages for each figure**

Assemble the reproducible project pack for handover

notebooks or scripts with instructions **input and config file checklist** **brief note on limits and future improvements**