Protein–Protein & Protein–Ligand Interaction Analysis — Hands-on

Dissect how biomolecules recognize each other: quantify interfaces, map small-molecule contacts, estimate per-residue contributions, and produce clear, reproducible figures and tables for manuscripts and reports.

Protein–Protein & Protein–Ligand Interaction Analysis

Help Desk · WhatsApp

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Session 1 — Protein–Protein Interfaces | Session 2 — Protein–Ligand Contacts | Session 3 — Energetics & Hotspots | Session 4 — Mini Capstone: Interaction Report

Session 1

Fee: Rs 6300 Apply Now

Protein–Protein Interfaces

Interface geometry, buried surface area and contact networks

PDBePISA **PDBsum** **FreeSASA** **Arpeggio**

Contact types and interaction patterns

H-bonds **salt bridges** **π–π** **cation–π** **hydrophobics**

Dimer vs crystal contacts and biological assembly checks

symmetry mates **biounits** **artifact screens**

Session 2
Fee: Rs 8400 Apply Now
Protein–Ligand Contacts & Pockets

Binding site detection and cavities

fpocket DoGSiteScorer ICM pocket finder

Contact mapping and interaction fingerprints

PLIP LigPlot+ Arpeggio

Pose sanity checks and ligand quality flags

clashes/strain chemistry validation 2D/3D concordance

Session 3
Fee: Rs 11200 Apply Now
Energetics & Hotspot Identification

Binding energy estimation and per-residue decomposition (overview)

MM/GBSA snapshot overview contact energetics interface scores

Alanine scanning and hotspot prediction

FoldX Rosetta ddG PRODIGY

Uncertainty, controls and reproducibility

ensemble checks parameter sensitivity reporting standards

Session 4
Fee: Rs 14000 Apply Now
Mini Capstone: Interaction Report

From structure to interaction maps and hotspot summary

Theory + Practical

Automated tables, plots and 2D diagrams for publication

PLIP/LigPlot+ exports | contact matrices | scene files

Deliverables: figures, tables, README & manifest

PDF | CSV/TSV | checksums