Structural Annotation & Visualization with AI Tools — Hands-on

Combine AI structure predictions with expert curation to produce clear, defensible annotations and visuals. Map domains, motifs, pockets and interfaces; overlay conservation/electrostatics; and generate publication-ready figures and interactive scenes with consistent styles and provenance.

Structural Annotation & Visualization with AI Tools

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Session Index

Session 1

Fee: Rs 6300 Apply Now

AI Structures & Core Annotation

From sequence to structure: using AlphaFold/ESMFold models responsibly (pLDDT/PAE)

Theory

Domain, motif & feature mapping

Pfam/InterPro **PROSITE/ELM** **Foldseek**

Conservation & function prediction (overview)

ConSurf DeepFRI-like cues

Session 2

Fee: Rs 8400 Apply Now

Pockets, Interfaces & Biophysics Overlays

Pockets/cavities & interface annotation

fpocket/DoGSite interface contacts ligand mapping

Electrostatics & surfaces for interpretation

APBS/PDB2PQR SASA/curvature hydrophobicity maps

Confidence-aware overlays (pLDDT/PAE masks) & caveats

disorder/linkers flexible regions

Session 3

Fee: Rs 11200 Apply Now

Publication-grade Visualization & Styles

Tooling & scene management

PyMOL ChimeraX VMD/Mol*

Figure aesthetics: lighting, palettes, labels & layout grids

ray tracing SVG/PNG exports alt-text/checklist

Scripting & templates for consistent styles

PyMOL/ChimeraX cmds scene presets

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Annotate → Visualize → Report

Pick a protein, aggregate AI predictions & annotations, then craft

a 2–3 figure story with panels

Theory + Practical

Deliver reproducible bundle: scenes, scripts, exports & README with provenance

Quarto/Markdown manifest/checksums

Final outputs: figures, tables, README & manifest

PDF CSV/TSV HTML