

Graph Neural Networks for Structural Biology — Hands-on

Learn geometric deep learning for proteins, ligands, and complexes. Represent structures as graphs and surfaces, train 2D/3D equivariant GNNs for pocket/interaction/affinity tasks, and ship reproducible evaluation reports with clear baselines and error bars.

Graph Neural Networks for Structural Biology

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Session 1

Fee: Rs 6300 [Apply Now](#)

Molecular/Protein Graphs & GNN Basics

Graphs for chemistry & proteins: atoms/residues, bonds/contacts, kNN & radius graphs

Theory

Message passing & attention; node/edge/global features

[PyTorch Geometric](#) [DGL](#) [GraphConv/GAT/GIN](#)

Featurization & loaders: PDB/mmCIF → graph datasets

[AA props/SS/ASA](#) [ligand/metal flags](#)

Session 2

Fee: Rs 8400 Apply Now

Protein Geometry: 3D, Surfaces & Equivariance

3D coordinates, frames & invariances; surface meshes & point clouds

triangulated surfaces **MaSIF-like features**

E(n)/SE(3)-equivariant GNNs for 3D proteins/complexes

EGNN/SE(3)-Transformer **SchNet/DimeNet** **TFN**
(overview)

Efficiency & stability: batching, cutoffs, neighbor lists

mixed precision **checkpointing**

Session 3

Fee: Rs 11200 Apply Now

Tasks: Pockets, Interfaces, Rescoring & Affinity

Pocket/surface site prediction & residue-level function

classification/segmentation **imbalanced data**

PPI & protein–ligand: interface prediction, docking rescoring, affinity regression

PDBbind **SAbDab/PP interfaces** **PR-AUC/RMSE/CI**

Generalization & controls: scaffold/time splits, leakage checks

bootstraps **calibration**

Session 4

Fee: Rs 14000 Apply Now

Mini Capstone: Train → Evaluate → Report

Build a small GNN (PyG/DGL) for a chosen task (e.g., docking)

pose rescoring or pocket detection)

Theory + Practical

Benchmarking & deployment: ONNX/TorchScript export,
inference profiling

baselines & CIs **error analysis**

Deliverables: figures, tables, README & manifest

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