CryoEM, X-ray & NMR Informed Modeling — Hands-on

Learn how to use experimental structural data from Cryo EM, X ray crystallography and NMR to guide modeling and refinement. This module focuses on map and density handling, restraints, hybrid and integrative modeling concepts and validation so that final structures are consistent with experimental evidence and suitable for docking, MD and design workflows.

CryoEM, X-ray & NMR Informed Modeling

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Session 1

Fee: Rs 8800 Apply Now

Experimental Data & Density Basics

Overview of CryoEM, X ray and NMR structural data

maps, structure factors and restraints | **resolution and information content** | **common file formats and metadata**

Density maps and grids concepts

voxels and grid spacing | **map sharpening and filtering ideas** | **masking, focus regions and noise**

Coordinate and map alignment considerations

fitting initial models into density | origin, symmetry and box size issues | visual inspection and sanity checks

Session 2

Fee: Rs 11800 Apply Now

CryoEM Maps, Fitting & Refinement Concepts

Rigid body and flexible fitting into CryoEM maps

global vs local fitting ideas | density fit scores and correlation | handling multi domain and multi body assemblies

Model refinement guided by density

restrained refinement concepts | maintaining geometry while improving fit | recognising overfitting to noisy maps

CryoEM specific validation ideas

local resolution and map variability | how fit varies across the structure | documenting limitations in low resolution areas

Session 3

Fee: Rs 14800 Apply Now

X-ray/NMR Restraints & Hybrid Modeling

X ray data, structure factors and refinement ideas

electron density maps overview | R factor and R free concepts | difference maps and model corrections

NMR restraints and ensemble guided modeling ideas

NOE like distance restraints concept | chemical shift and RDC information | link to flexible and disordered regions

Hybrid and integrative modeling concepts

combining EM, X ray and NMR cues **using sparse restraints with modeling** **representing uncertainty and alternative models**

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: Experiment Guided Model

Select a target and define which experimental data will guide modeling

Theory + Practical

Fit, refine and validate a model against maps or restraints

initial model placement and refinement steps **quantitative fit and quality metrics** **documenting uncertainty and unresolved regions**

Deliverables: experiment informed structure and report

refined coordinate file and summary tables **fit to density or restraints plots** **notes for use in docking and MD projects**