

## **Cryo-EM Map Fitting & Model Building — Hands-on**

Build confidence in working with cryo-EM density maps from database retrieval and visualization to rigid and flexible fitting, refinement and validation. This module focuses on creating chemically sensible, density supported atomic models that are ready for publication, docking and simulation.

# Cryo-EM Map Fitting & Model Building

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#### Session Index

Session 1 — Cryo-EM Maps, Resolution & Visualization | Session 2 — Rigid-Body Fitting & Domain

Placement Session 3 — Flexible Fitting, Refinement & Rebuilding Session 4 — Validation, Hybrid Modelling & Reporting

Session 1

Fee: Rs 15800 Apply Now

Cryo-EM Maps, Resolution & Visualization

Cryo-EM data types and map formats

EMDB and PDB entries map vs half maps MRC / CCP4 formats

Resolution, local resolution and map features

global vs local resolution FSC curves threshold selection and contouring

Visualization and map inspection toolkit

UCSF Chimerax PyMOL volume tools basic map

### filtering and sharpening

Session 2

Fee: Rs 19800 Apply Now

## Rigid-Body Fitting & Domain Placement

Rigid-body fitting strategies and search spaces

global vs local search cross-correlation scores symmetry and oligomeric state

Placing domains, subunits and known structures

docking of PDB models fitting homology and AlphaFold models assembly of multi-domain complexes

Practical tools for rigid fitting

ChimeraX fit commands Phenix real-space tools cryoSPARC and RELION interfaces

Session 3

Fee: Rs 23800 Apply Now

## Flexible Fitting, Refinement & Rebuilding

Flexible fitting concepts and methods

normal mode based fitting MDFF style approaches local vs global flexibility

Interactive rebuilding in density

Coot for real-space refinement ISOLDE in ChimeraX correcting register and loops

Real-space refinement and restraints

geometry and map restraints secondary structure
and Ramachandran restraints ligand and cofactor
handling

Session 4

Fee: Rs 26800 Apply Now

Validation, Hybrid Modelling & Reporting

Validation of models against cryo-EM density

map vs model correlation per residue fit metrics overfitting checks and cross validation

Hybrid and integrative structural modelling context

combining X-ray, NMR and XL-MS restraints fitting multiple conformational states ensembles and heterogeneity

Deliverables: deposition and reporting package

final model and map files validation and refinement summary figures for manuscripts and presentations