X Ray Crystallography Data Processing & Refinement — Hands-on

Gain a practical, workflow-level understanding of X-ray crystallography data processing. From raw diffraction images through indexing, integration, scaling, phasing, refinement and validation, you will learn how high-quality macromolecular structures are generated, assessed and prepared for deposition.

X Ray Crystallography Data Processing & Refinement

Help Desk · WhatsApp

Session Index

Session 1 — Data Collection Strategy & Image QC   Session 2 — Indexing, Integration & Scaling

Session 3 — Phasing, Model Building & Refinement   Session 4 — Validation, Deposition & Troubleshooting

Session 1
Fee: Rs 8800   Apply Now

Data Collection Strategy & Image QC

Crystal assessment and data collection strategy

unit cell screening   multiplicity & completeness   radiation damage considerations

Raw image inspection and quality indicators

spot shape & streaking   ice rings & overloads   resolution estimation

Overview of processing suites and file formats

XDS / DIALS concepts | HKL family overview | MTZ, HKL, CIF basics

Session 2
Fee: Rs 11800 Apply Now
Indexing, Integration & Scaling

Indexing and lattice determination

spot finding | unit cell refinement | space group ambiguity

Integration and profile fitting

peak profiles | partiality & overlaps | per-image statistics

Scaling, merging and data quality metrics

Rmerge / Rmeas / Rpim | I/σ(I) & CC1/2 | resolution cutoffs

Session 3
Fee: Rs 14800 Apply Now
Phasing, Model Building & Refinement

Phasing strategies and map calculation

MR / SAD / MAD overview | figure of merit | density modification ideas

Model building in electron density maps

backbone tracing | side chain fitting | water and ligand placement

Refinement cycles and parameter choices

Rwork / Rfree | B-factor models | restraints and weighting

Session 4
Fee: Rs 18800 Apply Now

Validation, Deposition & Troubleshooting

Geometry and model quality checks

Theory + Practical

Comprehensive validation and outlier analysis

Ramachandran plots **clash scores & rotamers** **map vs model inspection**

Deposition, documentation and common problems

PDB / mmCIF deposition **validation reports** **troubleshooting checklist**