X-ray & NMR Constraints in Structural Modelling — Hands-on

Learn how to bring experimental X-ray and NMR information directly into your structural models. This module focuses on using electron density and NMR-derived restraints to guide model building, refinement and validation, enabling robust, experimentally anchored structures for publications, docking and simulations.

X-ray & NMR Constraints in Structural Modelling

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Session Index

Session 1

Fee: Rs 16800 Apply Now

X-ray Data, Density Maps & Restraints

X-ray diffraction data and electron density maps

- structure factor amplitudes
- $2F_o-F_c$ and F_o-F_c maps
- map resolution and noise

Real-space interpretation of density

- contouring and map inspection
- density fit for sidechains and ligands
- disorder and alternate

conformations

X-ray restraints in refinement engines

geometry vs density weights B-factor refinement strategies Phenix and CCP4 toolchain overview

Session 2

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NMR Observables & Structural Restraints

NMR data types and what they report on

NOEs and distance information J couplings and dihedral angles RDCs and orientational restraints

Translating NMR observables into restraints

upper and lower distance bounds dihedral and torsion restraints RDC alignment tensors

NMR restraint formats and software ecosystem

CNS / XPLOR-NIH style restraints ARIA / CYANA workflows validation of NMR restraint sets

Session 3

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Hybrid Refinement Workflows

Combining experimental restraints with force fields

energy function plus restraint terms weight tuning and calibration avoiding overfitting to data

X-ray and NMR guided refinement in practice

real-space refinement with density restraint driven torsion optimization ensemble vs single model strategies

Software pipelines for hybrid refinement

Phenix with NMR constraints CNS / XPLOR-NIH hybrid runs automation via scripts and workflows

Session 4

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Integrative Modelling & Case Studies

Placing X-ray and NMR data in integrative context

combining with cryo-EM maps XL-MS and SAXS restraints heterogeneous data weighting

Case studies of hybrid X-ray/NMR structures

flexible regions and ensembles ligand and interface definition dynamic proteins and conformational exchange

Deliverables: experimentally anchored model package

final PDB and restraint files validation and refinement summary figures for reports and manuscripts