Integrative Structural Biology — Hybrid Data Fusion — Hands-on

Learn how to combine multiple structural and biophysical data sources into coherent hybrid models. This module focuses on restraint types, model fitting, scoring, uncertainty assessment and narrative building for integrative structural biology projects.

Integrative Structural Biology — Hybrid Data Fusion

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Session Index

Session 1

Fee: Rs 24800 Apply Now

Experimental Modalities & Restraint Types

Overview of structural and biophysical inputs

cryo-EM maps **X-ray crystallography** **NMR, SAXS, XL-MS, HDX-MS**

Restraint types and their interpretation

density restraints and map agreement **distance and contact restraints** **shape envelopes and radius of gyration**

Data quality, resolution and uncertainty basics

map resolution and local resolution | signal-to-noise and error bars | compatibility of different datasets

Session 2

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Model Fitting, Restraints & Scoring

Rigid-body and flexible fitting into density

placing domains and subunits | local vs global fitting concepts | avoiding over-interpretation

Encoding restraints in modelling protocols

distance and contact restraints | orientation, symmetry and connectivity | soft vs hard restraints and weights

Scoring functions and model ranking ideas

fit-to-data terms vs stereochemistry | consistency across datasets | ensembles vs single best model

Session 3

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Hybrid Modelling Workflows & Uncertainty

Designing hybrid modelling workflows

data inventory and hierarchy | iterative refine & reweight cycles | tracking model provenance

Ensembles, alternative solutions & flexibility

representing positional uncertainty | multi-state and multi-conformer models | clustering and representative models

Validation and cross-validation concepts

using held-out data where possible **agreement vs overfitting to restraints** **documenting assumptions and caveats**

Session 4

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Case-Based Hybrid Project & Reporting

Mini-project: build a hybrid model from mixed data

combine 2–3 data modalities **define restraints and workflow** **generate models and ensembles**

Figures, tables and narratives for hybrid studies

fit-to-data visualizations **restraint satisfaction summaries** **uncertainty and alternative models**

Deliverables: hybrid model package & FAIR readiness

coordinates, restraints and metadata **validation and provenance records** **deposition and sharing considerations**