Integrative Structural Modeling & Restraint Fusion — Hands-on

Build hybrid structural models by fusing restraints from multiple experimental techniques. This module walks through how to represent components, encode restraints from crystallography, cryo EM, NMR, SAXS and XL MS, generate and score ensembles of models, and validate integrative structures with transparent uncertainty and FAIR archiving.

Integrative Structural Modeling & Restraint Fusion

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Systems, Restraints & Representation

Integrative modeling concepts and use cases

large assemblies and complexes | **heterogeneous and flexible systems** | **motivation for hybrid approaches**

Sources and types of structural restraints

cryo EM maps and X ray contacts | **SAXS and NMR restraints** | **XL MS and distance bounds**

Representation of subunits, domains and coarse graining

rigid bodies and flexible linkers **bead based models** **coordinate and restraint bookkeeping**

Session 2

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Sampling, Scoring & Model Generation

Search strategies and sampling schemes

rigid body sampling **flexible linker sampling** **Monte Carlo and heuristic moves**

Scoring functions and restraint fusion

weighting different data types **penalising restraint violations** **avoiding double counting information**

Generating and storing model ensembles

independent sampling runs **clustering solutions** **tracking scores and metadata**

Session 3

Fee: Rs 14800 Apply Now

Ensemble Analysis, Validation & Uncertainty

Analysing ensembles of integrative models

RMSD and clustering of solutions **contact maps and distance distributions** **consensus versus alternative arrangements**

Validation against input data and cross validation

restraint satisfaction statistics **holdout and bootstrap strategies** **independent experimental checks**

Quantifying and communicating uncertainty

precision for different regions representative models and spreads visual encoding of confidence

Session 4

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Integrative Workflows, FAIR Archiving & Reporting

End to end integrative modeling workflow case study

Theory + Practical

Model formats, deposition and FAIR practices

PDB dev integrative formats overview restraint and protocol documentation reproducible scripts and configs

Figure ready panels and methods text for manuscripts

communicating ensembles and uncertainty reporting validation and limitations checklists for reviewers and depositions