Structural Ensembles, Conformers & Disorder — Hands-on

Learn how to work with structural ensembles, conformers and disordered regions rather than relying on a single static structure. This module covers conformer generation ideas, ensemble analysis and clustering, intrinsic disorder annotation and dynamics-aware interpretation so that your modeling and design decisions reflect the real conformational space of biomolecules.

Structural Ensembles, Conformers & Disorder

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Session Index

Session 1

Fee: Rs 8800 Apply Now

Ensemble & Conformer Concepts

Why structural ensembles matter beyond a single model

conformational heterogeneity **functional states and transitions** **link to dynamics and thermodynamics**

Conformer generation ideas and inputs

backbone and side chain sampling **local refinement vs global moves** **ensembles from docking or MD**

NMR like ensembles, models and restraints concepts

multiple models in PDB entries | experimental restraints as ensemble constraints | visualizing and comparing members

Session 2

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Ensemble Analysis & Clustering

Measuring diversity inside an ensemble

pairwise RMSD matrices | per residue RMSF ideas | global vs local variability

Clustering conformers and picking representatives

distance metrics and clustering options | centroid and medoid structures | link to docking and further modeling

Projecting ensembles to low dimensional spaces

PCA and essential dynamics sketches | free energy like views along components | identifying major motions and basins

Session 3

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Disorder, IDRs/IDPs & Flexibility Annotation

Intrinsic disorder and fuzzy complexes concepts

IDRs and IDPs role in biology | coupled folding and binding ideas | limits of static PDB views

Disorder prediction and annotation workflows

sequence based disorder predictors ideas | mapping scores onto structures | coils, linkers and low complexity regions

Combining ensemble and disorder information

flexible vs rigid segments **regions to treat as conformational ensembles** **implications for docking and design tasks**

Session 4

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Mini Capstone: Ensemble Interpretation

Select a target and define ensemble and disorder questions

Theory + Practical

Build or assemble an ensemble, cluster and annotate flexibility

identify representative conformers **map disorder and fluctuations** **relate conformers to function or binding**

Deliverables: ensemble figures, tables and interpretation note

plots for RMSD/RMSF and clustering **summary of key conformational states** **written guidance for downstream use**