Ab Initio & Fragment-Based Protein Modeling — Hands-on

Understand how ab initio and fragment based approaches generate protein structures when no close templates are available. This module focuses on fragment library design, coarse grained sampling, all atom refinement, scoring and decoy selection so that you can critically use de novo models for hypothesis generation and downstream structural analyses.

Ab Initio & Fragment-Based Protein Modeling

Help Desk · WhatsApp

Session Index

Session 1

Fee: Rs 8800 Apply Now

Ab Initio Modeling Concepts & Fold Space

When and why ab initio modeling is needed

no template scenarios **remote homology and dark proteome** **comparing to homology modeling**

Protein fold space and energy landscapes

energy funnels and frustration **compact vs extended states** **secondary structure propensities**

Overview of fragment based de novo approaches

fragment insertion philosophy | coarse grained representations | decoy generation at scale

Session 2

Fee: Rs 11800 Apply Now

Fragment Libraries, Assembly & Coarse Sampling

Building sequence based fragment libraries

secondary structure prediction use | fragment length choices | diversity and redundancy control

Fragment insertion and assembly strategies

move sets and Monte Carlo steps | growing and reshaping folds | constraints and filters overview

Generating and storing decoy ensembles

runtime and compute planning | trajectory and seed management | basic sanity checks on decoys

Session 3

Fee: Rs 14800 Apply Now

All Atom Refinement, Scoring & Model Selection

From coarse grained to all atom models

backbone reconstruction ideas | side chain placement local minimization for relaxation

Energy functions and decoy discrimination

knowledge based vs physics based terms | energy funnels and score vs RMSD plots | screening thousands of decoys

Clustering and selecting representative models

RMSD based clustering | centroid and medoid models

balancing score and diversity

Session 4

Fee: Rs 18800 Apply Now

De Novo Modeling Case Study & Downstream Use

End to end de novo modeling case study

Theory + Practical

Assessing reliability of ab initio models

confidence by region | sensitivity to constraints and inputs | comparison to AI based predictions

Using de novo models carefully in projects

mapping variants and motifs | early stage docking or design ideas | figure panels and limitations in manuscripts