RNA Structure Prediction, Docking & Dynamics — Hands-on

Learn how to predict, model and refine RNA structures and then use them in docking and dynamics style workflows. This module covers RNA specific structure basics, secondary and tertiary modeling ideas, RNA ligand or protein docking and simple dynamics interpretation so that you can build realistic RNA models for discovery and mechanism studies.

RNA Structure Prediction, Docking & Dynamics

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Session Index

Session 1

Fee: Rs 8800 Apply Now

RNA Structure Basics & Formats

RNA building blocks and structural motifs overview

nucleotides and sugar puckers **helices, loops and bulges** **pseudoknots and long range contacts**

PDB like coordinate formats for RNA and annotations

naming and residue conventions **modified nucleotides concepts** **chains, hetero atoms and ions**

Secondary structure representations and notations

dot bracket style views | secondary structure diagrams idea | connecting 2D views to 3D structures

Session 2

Fee: Rs 11800 Apply Now

RNA Secondary & Tertiary Modeling

Secondary structure prediction ideas and constraints

minimum free energy views concept | base pairing patterns and alternatives | using experimental or covariation hints

From secondary to tertiary structure modeling ideas

building helical segments and junctions | loop conformations and packing | global folding and compaction concepts

Refinement and basic quality checks for RNA models

geometry and clashes review | base pairing and stacking integrity | visual inspection for kinks and distortions

Session 3

Fee: Rs 14800 Apply Now

RNA Docking with Ligands & Proteins

Binding site and pocket concepts on RNA surfaces

grooves and cavities in RNA | metal and ion binding ideas | regions suitable for small molecules

Ligand and protein docking scenarios with RNA models

local vs global docking strategies | constraints from known contacts concept | handling flexibility and

alternative poses

Interaction fingerprints and scoring interpretations

hydrogen bonds and stacking interactions | electrostatic and ion mediated contacts | ranking poses with simple metrics

Session 4

Fee: Rs 18800 Apply Now

Mini Capstone: RNA Docking & Dynamics Story

Pick an RNA target and define a docking and dynamics question

Theory + Practical

Build or refine RNA model, dock partner and explore simple dynamics

short MD style stability checks concept | tracking key contacts over time | capturing representative bound conformers

Deliverables: RNA model, complex snapshots and interpretation note

coordinate files for RNA and complex | tables for key interactions and stability | written summary of mechanism or design ideas