Flexible Docking & Induced-Fit Paradigms — Hands-on

Go beyond rigid docking by explicitly modeling receptor and ligand flexibility. This module focuses on induced-fit strategies, sidechain and limited backbone motion, ensemble docking and short MD or minimization based refinement so that your interaction models better reflect realistic binding events.

Flexible Docking & Induced-Fit Paradigms

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Session Index

Session 1

Fee: Rs 18800 Apply Now

Flexibility Concepts & Receptor States

Why rigid docking can fail

sidechain rearrangements **backbone shifts & loop motion** **water and protonation effects**

Receptor conformational states for docking

open vs closed forms **apo vs holo structures** **MD derived snapshots**

Flexible degrees of freedom in docking engines

ligand torsions **sidechain rotamers** **limited backbone**

flexibility

Session 2

Fee: Rs 22800 Apply Now

Induced-Fit Protocols & Local Refinement

Induced-fit concepts and workflows

sequential docking and refinement | local sidechain remodeling | backrub and loop relaxation

Refining binding sites around docked ligands

minimization with positional restraints | hydrogen bond network optimization | rotamer exploration and pruning

Practical induced-fit workflows in pipelines

rigid pre-dock → local refinement | template based sidechain rebuilding | automation and job control scripts

Session 3

Fee: Rs 26800 Apply Now

Ensemble Docking & State Sampling

Generating receptor ensembles

MD snapshots and clustering | NMR models and experimental ensembles | rotamer and local sampling

Running and managing ensemble docking

multiple receptor grids | batch job orchestration | tracking pose provenance per state

Interpreting ensemble docking outcomes

state specific vs global ranking | population and occupancy ideas | selecting poses for refinement

Session 4

Fee: Rs 29800 Apply Now

Analysis, Validation & Reporting

Contact patterns and interaction fingerprints

H bonds, hydrophobics, salt bridges | water mediated contacts | flexible residue hotspot mapping

Short MD and energy based validation

local MD relaxation | stability of key contacts | basic MM GBSA checks

Deliverables: flexible docking report & design hints

ranked poses with receptor state info | figures of induced-fit changes | SAR and optimization suggestions