

Online Workshop On

Molecular Docking Series

Transform Your Docking Skills - From Basics to Biological Insights

24-28 April 2026, 6:30 PM IST

About The Course

Our docking training introducing key molecular docking techniques for protein-ligand, protein-protein, and protein-DNA/RNA interactions using tools like AutoDock, PyMOL, and HADDOCK — bridging computational skills with real-world drug discovery.

Course Benefits:

- Learn step-by-step molecular docking workflows used in drug discovery.
- Gain hands-on experience with real datasets and professional docking tools.
- Understand how to interpret and visualize docking results for publication.
- Get exposure to Protein–Ligand, Protein–Protein, and Protein–DNA/RNA Docking in a single course.

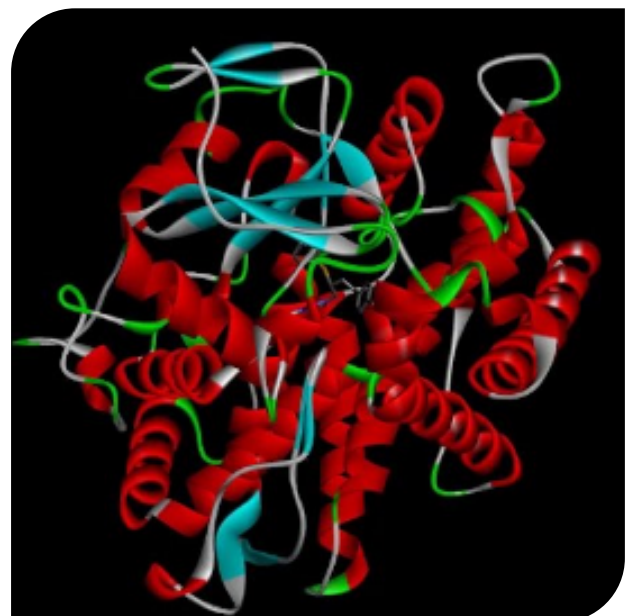
Fee & Features

₹999 (India) | \$55 US (International)

- E-Certificate to Participants
- Online by Google Meet Platform
- Live Sessions
- Interaction with Resource Person
- Lecture PPTs and Recordings to Participants

Who Can Join?

Graduate / Postgraduate / Research scholars/ Faculty/ Industrialist in the field of Life Sciences (ZBC, Biotech, BioChem, MicroBio etc.), MBBS/MD/MS, Pharmacy, Chemical Sciences, Medicine, Medical Professionals etc.



Course Module

Day 1–3: Protein–Ligand Docking

- **Module 1: Overview of the Drug Discovery Pipeline**
- **Module 2: Target Identification and Structure Retrieval**
Tools: PDB, UniProt
- **Module 3: Compound Generation and Databases**
Tools: MarvinSketch, PubChem, DrugBank
- **Module 4: Protein Preparation & Energy Minimization**
Tools: Schrodinger Maestro, Viewerlite
- **Module 5: Chemical File Format Conversion**
Tool: OpenBabel
- **Module 6: Introduction to Virtual Screening**
Tool: PyrX
- **Module 7: Molecular Docking Concepts**
Tools: MGLTools, AutoDock, Vina, PyrX
- **Module 8: Active Site Identification & Binding Pocket Detection**
Tools: CastP, PyMOL
- **Module 9: Protein–Ligand Interaction & Publication-Standard Image Generation**
Tools: PyMOL, Schrodinger Maestro
- **Module 10: ADMET Prediction**
Tools: SWISS-ADME, ProTox-II

Day 4: Protein–Protein Docking

- **Module 1: Introduction to Protein–Protein Docking**
- **Module 2: Docking Tools & Strategy**
Tools: ClusPro, HADDOCK
- **Module 3: Live Demo-ClusPro & HADDOCK Docking**
- **Module 4: Protein–Protein Interaction Analysis**
Tools: PDBePISA, PDBsum

Day 5: Protein–DNA/RNA Docking

- **Module 1: Concepts of Docking with Nucleic Acids**
- **Module 2: Tools & Preparation Tips**
Tools: HADDOCK, NPDock/HDOCK
- **Module 3: Live Demo — Protein–DNA Docking**
- **Module 4: Protein–DNA/RNA Interaction Analysis**
Tools: PDBePISA, PDBsum

