

Online Workshop On Molecular Docking Series

Transform Your Docking Skills - From Basics to Biological Insights

13-17 July 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.

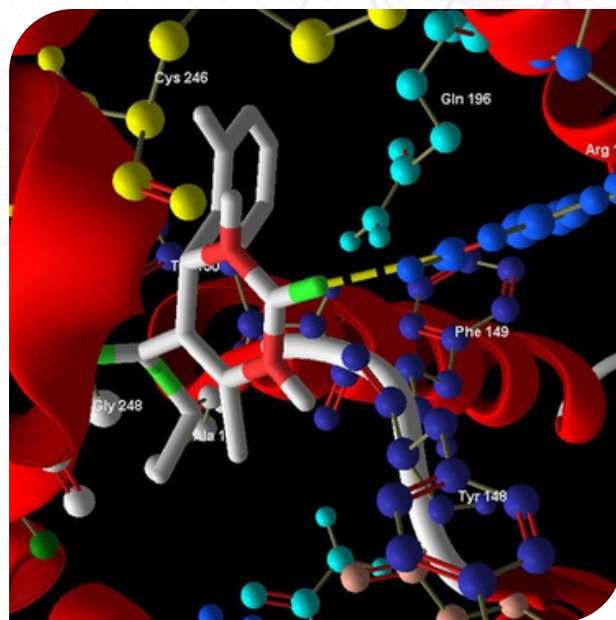
Fee & Features

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

- E-Certificate to Participants
- Online by Google Meet Platform
- Live Sessions
- Interaction with Resource Person
- LecturePPTs 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

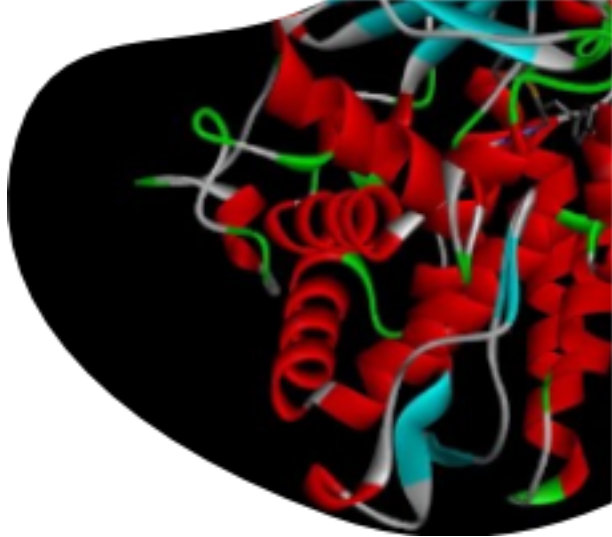
- Module 1: Overview of the Drug Discovery Pipeline
- Module 2: Target Identification and Structure Retrieval
Tools: PDB, UniProt
- Module 3: Compound Generation and Databases
Tools: MarvinSketch, PubChem, DrugBank
- Module 4: Protein Preparation & Energy Minimization
Tools: Schrodinger Maestro, Viewerlite
- 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



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