CATR
Centre for Advanced Training and Research

Online Workshop On

Molecular Docking Series

Transform Your Docking Skills – From Basics to Biological Insights

19-24 June 2026 (Sunday OFF), 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.

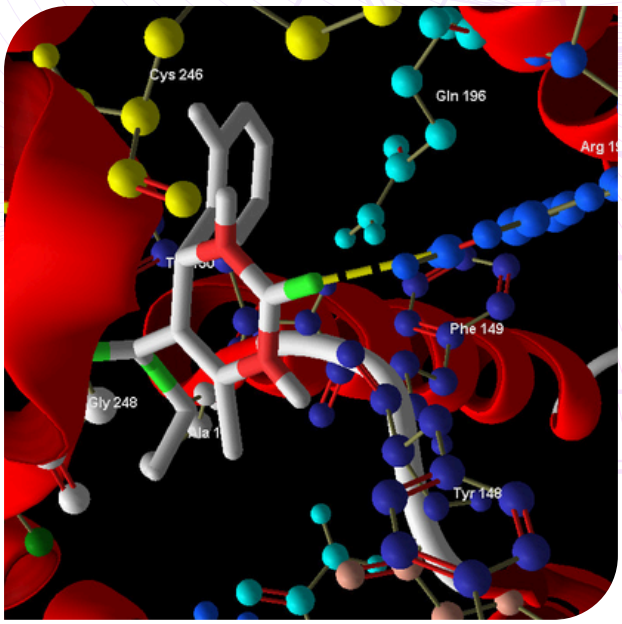
Course Benefits:

- 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.

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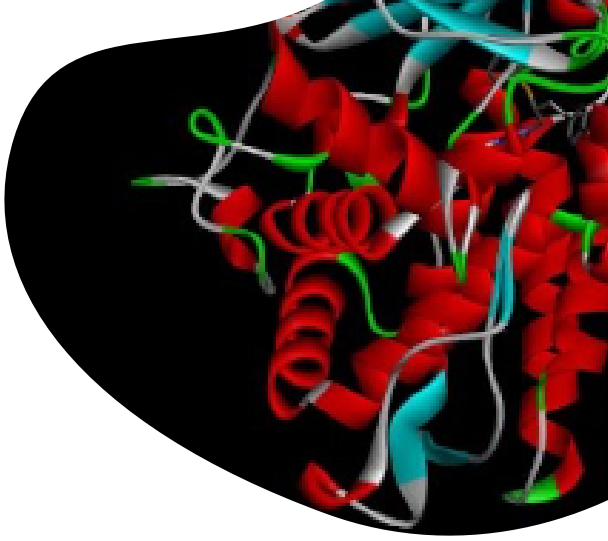
www.catredu.com

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

REGISTER NOW

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