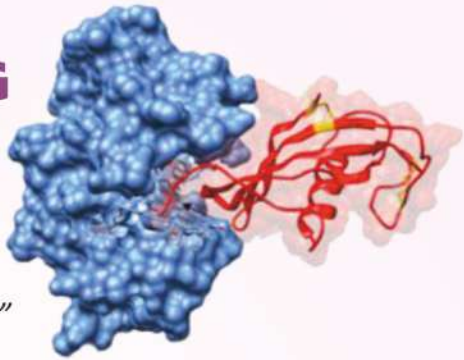
YENEPOYA
Homoeopathic Medical
College & Hospital

AYUSH Campus, Naringana, Mangaluru-575018
A CONSTITUENT COLLEGE OF YENEPOYA (DEEMED TO BE UNIVERSITY)

Research Consultancy on
MOLECULAR DOCKING FOR HOMEOPATHIC DRUGS



Tagline:

"Bridging Tradition and Molecular Science"

Molecular docking is a powerful computer tool that predicts how a drug binds to disease-related proteins. It adds a layer of biological proof beyond traditional symptom matching.

Why Use Molecular Docking?

- **Confirms** if a remedy can act on a disease target
- **Reveals** how and where the remedy binds inside the protein
- **Provides** modern scientific evidence for the drug's effect
- **Helps** discover stronger, more effective drugs with less trial-and-error.

Getting Started!

To begin, kindly review the literature to identify the lead and target molecules, and provide us with:

- **Lead Molecule** is the compound available in the drug. For example, the compound Atropine is found in the drug Belladona. You may search for the three dimensional structure of these lead molecules in databases like:

  PubChem: https://pubchem.ncbi.nlm.nih.gov/
  ChEMBL: https://www.ebi.ac.uk/chembl/
  DrugBank: https://go.drugbank.com/

  Provide the three dimensional structures of the lead molecules in **SMILES or SDF** file format. See overleaf for further instruction to search and download the lead molecule.

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Services Offered

- Computer-based docking with AutoDock Vina platform.
- Binding affinity predictions.
- Pose analysis and visualization.
- Interaction mapping between lead and target molecule

Your Comprehensive Report Includes:

- Docking results with optimal poses and binding energy.
- High-quality interaction maps & visualization images.
- A clear, step-by-step methodology

Fee and Timeline

- ₹600 + 18% GST per docking analysis
- Results within 4 working days (Mon–Fri) per docking.

Please contact us before payment

Payment link
https://rzp.io/rzp/shhU8bo

Ready to start your research?

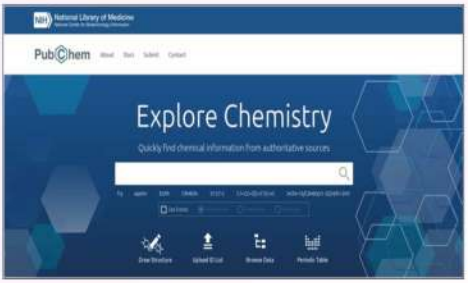
Contact us:
Coordinator,
Research & Development Cell, Yenepoya Homoeopathic Medical College,
AYUSH Campus, Naringana, Mangalore 575018
Email us: yhmcdocking@yenepoya.edu.in

Due to the computational nature of the work, fees are non-refundable once the process has begun

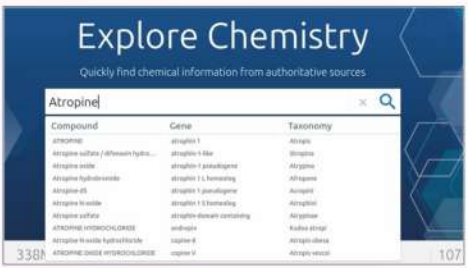
PROCEDURE TO DOWNLOAD LEAD MOLECULE AND TARGET PROTEIN

Lead Molecule

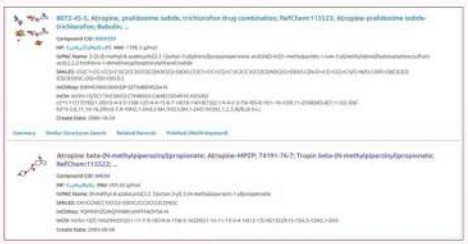
1. Identify the compound of interest through a thorough literature review.
2. Visit **PubChem** https://pubchem.ncbi.nlm.nih.gov/.



3. Use the search bar to find your compound (e.g., Atropine).



4. Select the correct molecule from the search results.



5. Scroll down to the **3D Conformer** section, click **Download,** and save the structure in **SDF format.**

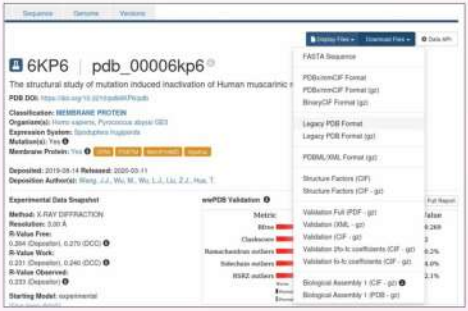
Target molecule

1. Identify the biological target (protein/receptor/enzyme) through a thorough literature review.
2. **Visit the Protein Data Bank (PDB) https://www.rcsb.org/.**

3. Use the search bar to find your protein target (e.g., Human muscarinic receptor M4).

4. Choose the correct protein entry and check key details (resolution, ligands, mutations, etc.).

5. Click **Download Files** (top right) → choose Legacy **PDB Format.**



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