

| Sr. No. | Database / Tools / Server | Description | Inputs | Results | URLs |
|---------|-----------------------------------|--|---|---|---|
| 1. | Therapeutic Target Database (TTD) | This database focuses on targeted therapeutics. One can get information for Patented Drugs, targets regulating microRNAs and transcription factors. Searches are provided for Targets, Drugs, Targets by Disease, Biomarkers and Drug Scaffolds. | For retrieval of targets: Enter the keyword in Search for Target box. Input: Text word | It will show tabular results for given drug name or a target. | http://db.idrblab.net/ttd/ |
| 2. | BindingDB | It is based on binding affinities of drug-targets and small drug-like molecules. There are different search and browse options for targets, compounds and special tools for docked congeneric series, Find My compounds Target, Find compounds for My Target, Do Virtual Screening and SCOP. | For retrieval of targets: Select Find My compounds Target Input: Draw a structure or Smiles or browse a file | It will show tabular results of targets based on similarity or substructure or exact match of compound that happens to bind the same protein. | https://www.bindingdb.org/bind/index.jsp |
| 3. | ChEMBL | Its database of bioactive drug-like small molecules. It is composed of properties like Molecular Weight, Lipinski Parameters, etc. and abstracted bioactivities like pharmacology and ADMET information. Data is curated from primary scientific literature. | Target data can be retrieved: Text word or Drawing a structure or by submitting sequence (blastp). | Compound Report Card will be shown. | https://www.ebi.ac.uk/chembl/ |
| 4. | canSAR | Integrated knowledge base which covers multi-disciplinary areas like chemistry, pharmacology, structural biology, cellular network and many more. It focuses on cancer research and drug discovery. | Target data can be retrieved: Text word keeping the compound filter ticked. | Result will be shown as per selected criteria. | https://cansarblack.icr.ac.uk/ |
| 5. | DrugBank | It's a database for approved drugs and drug targets. It contains information about pharmacological, pharmaceutical data of | Target data can be retrieved: keyword and selecting the Browse option, | List of associated targets are retrieved. | https://go.drugbank.com/ |

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| | | drugs. | drop down list will pop up select Drug Targets and search by keyword. | | |
| 6. | ECOdrug | This atabase has detailed information on the Evolutionary Conservation of human Drug targets in eukaryotes. Users can explore overview of species with an ortholog across taxonomic groups. | Drug target data can be retrieved : There is Drug target drop down and taxonomic range drop down, user defined selection can be done. | Predictions can be downloaded. | http://ecodrug.org/ |
| 7. | IUPHAR/BPS | It's a resource of ligand-activity-target relationships majorly focused on pharmacology and medical chemistry databases. | Target data can be retrieved: By selecting Target drop down. From that drop down either user can directly search via target search tool or else one can do BLAST. | Search result is shown | https://www.guidetopharmacology.org |
| 8. | PubChem | PubChem is a database of chemical molecules and their activities against biological assays. The system is maintained by the National Center for Biotechnology Information, a component of the National Library of Medicine, which is part of the United States National Institutes of Health. | Structure data can be retrieved by querying chemical names in the search box. | Search result is shown and structures can be downloaded | https://pubchem.ncbi.nlm.nih.gov |