eTOX Library

eTOX Library screens literature and the World Wide Web looking for relevant data related to drug toxicity
http://cadd.imim.es/etox-library/

Sung Kwang's ChemInfo

Chemical database, QSPR (Quantitative Structure Property Relationships), chemcial vitual library design, ADME/Tox prediction and QSRRs(Quantitative Structure Retention Relationships), ChemDB(web-based chemical database), PreADMET(web-based ADME prediction program). Ongoing work: chemical library design for High Throughtput Screening and Combi. Chem. and virtual screening using pharmacophore of active compounds or docking between ligand and target protein.
http://www.qspr.pe.kr

Click2Drug

Directory of computer-aided Drug Design tools. Click2Drug contains a comprehensive list of computer-aided drug design (CADD) software, databases and web services.These tools are classified according to their application field, trying to cover the whole drug design pipeline.
http://www.click2drug.org

Linux4Chemistry

Linux4Chemistry provides information about computational chemistry software for the Linux operating system (contributors).
http://www.linux4chemistry.info/

Bioinformatics Links Directory

The Bioinformatics Links Directory features curated links to molecular resources, tools and databases. The links listed in this directory are selected on the basis of recommendations from bioinformatics experts in the field.
http://bioinformatics.ca/links_directory/

Virtual Ligand Screening in 3D

Drug design tools, in silico drug design, structural bioinformatics, virtual screening tools, cheminformatics, drug-discover, ADMED-Tox prediction, a collection of tools by Bruno Villoutreix
http://www.vls3d.com/links.html

Worldwide Protein Data Bank

The Worldwide Protein Data Bank (wwPDB) consists of organizations that act as deposition, data processing and distribution centers for PDB data. Members are: RCSB PDB (USA), PDBe

(Europe) and PDBj (Japan), and BMRB (USA). The wwPDB's mission is to maintain a single PDB archive of macromolecular structural data that is freely and publicly available to the global community.
http://www.wwpdb.org/

Small Molecule Pathway Database

SMPDB (The Small Molecule Pathway Database) is an interactive, visual database containing more than 618 small molecule pathways found in humans. More than 70% of these pathways (>433) are not found in any other pathway database. SMPDB is designed specifically to support pathway elucidation and pathway discovery in metabolomics, transcriptomics, proteomics and systems biology. It is able to do so, in part, by providing exquisitely detailed, fully searchable, hyperlinked diagrams of human metabolic pathways, metabolic disease pathways, metabolite signaling pathways and drug-action pathways. All SMPDB pathways include information on the relevant organs, subcellular compartments, protein cofactors, protein locations, metabolite locations, chemical structures and protein quaternary structures. Each small molecule is hyperlinked to detailed descriptions contained in the HMDB or DrugBank and each protein or enzyme complex is hyperlinked to UniProt. All SMPDB pathways are accompanied with detailed descriptions and references, providing an overview of the pathway, condition or processes depicted in each diagram. The database is easily browsed and supports full text, sequence and chemical structure searching. Users may query SMPDB with lists of metabolite names, drug names, genes/protein names, SwissProt IDs, GenBank IDs, Affymetrix IDs or Agilent microarray IDs. These queries will produce lists of matching pathways and highlight the matching molecules on each of the pathway diagrams. Gene, metabolite and protein concentration data can also be visualized through SMPDB's mapping interface. All of SMPDB's images, image maps, descriptions and tables are downloadable.
http://www.smpdb.ca/

GDD, GPCR Decoy Database

The GDD, a GPCR Decoy Database, with its accompanying GPCR Ligand Library (GLL) have

been compiled to help in GPCR docking. The main characteristics of GLL and GDD are: 1)Sets of ligands and decoys for 147 GPCR targets. 2) For each ligand, 39 decoys were drawn from ZINC ensuring physical similarity of six properties (molecular weight, formal charge, hydrogen bond donors and acceptors, rotatable bonds and logP), but structural dissimilarity. GLL and GDD are developed by the Cavasotto Laboratory, and are freely available to the community
http://cavasotto-lab.net/Databases/GDD/

NuBBE database

NuBBE database (NuBBEDB) is a virtual database of natural products and derivatives from the Brazilian biodiversity containing the compounds obtained by the academic group NuBBE. NuBBEDB contains the main chemical and biological properties, and the 3D structure of the compounds. This database is the result of a collaborative research between the academic groups NuBBE and LQMC.
http://nubbe.iq.unesp.br/portal/nubbedb.html

KNApSAcK-3D

3D structure database of plant metabolites
http://knapsack3d.sakura.ne.jp/

FAF-Drugs2

Tools for accurate multiple conformation generator and rigid docking protocol for multi-step

virtual ligand screening, package to refine the 3D structures of compounds and of compounds docked into a protein target, in silico ADMET filtering, 3D conformation of small molecules using Distance Geometry and Automated Molecular Mechanics Optimization for in silico Screening
http://www.mti.univ-paris-diderot.fr/fr/downloads.html

Interactome3D

Web service for the structural annotation of protein-protein interaction networks
http://interactome3d.irbbarcelona.org/

2P2Idb

The chemical space of PPI (protein-protein interactions). it is not completely covered due to the limited amount of data currently available; however, the definition of what makes a PPI a potentially druggable target will become more and more reliable, as the number of 3D structures increases.
http://2p2idb.cnrs-mrs.fr/

TIMBAL database

Small molecules-inhibitors of protein-protein interaction database
http://mordred.bioc.cam.ac.uk/timbal

iPPI-DB

iPPI-DB contains 1650 non-peptidic inhibitors (iPPI) across 13 families of Protein-Protein Interactions. The chemical structures, the physicochemical and the pharmacological profiles of these iPPI are manually extracted from the literature and stored in iPPI-DB.
http://www.ippidb.cdithem.fr/