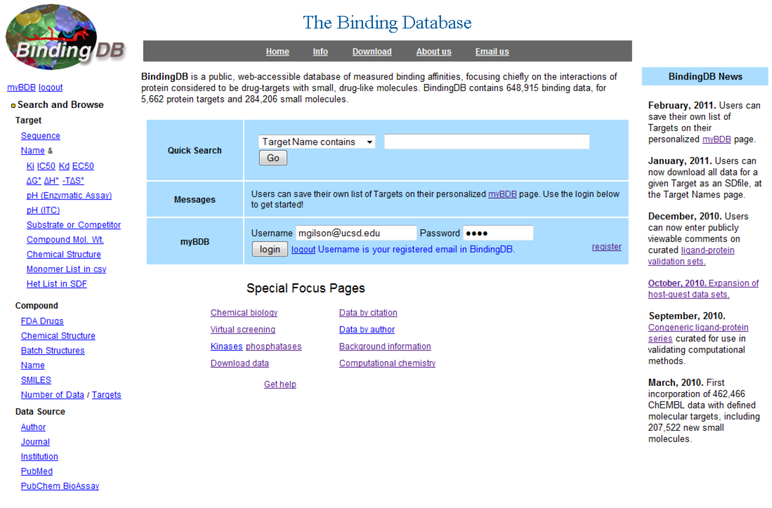
BindingDB: A Protein-Ligand Database for Drug Discovery

George Nicola, Tiqing Liu, Linda Hwang, and Michael Gilson
Skaggs School of Pharmacy and Pharmaceutical Sciences, University of California San Diego

www.BindingDB.org

Introduction:

The large and growing body of experimental data on biomolecular binding is of enormous value in developing a deeper understanding of molecular biology, in developing new therapeutics, and in various molecular design applications. However, most of these data are found only in the published literature and are therefore difficult to access and use. BindingDB is a public web-accessible database of measured binding affinities for various molecular types. The BindingDB allows queries based upon a range of criteria, including chemical similarity or substructure, sequence homology, numerical criteria and reactant names. The data specification includes significant experimental detail.



BindingDB contains 800,000 binding data, for 6,000 protein targets and 350,000 small molecules.

References

- Liu,T., Lin,Y., Wen,X., Jorrisen, R.N. and Gilson,M.K. *BindingDB: a web-accessible database of experimentally determined protein-ligand binding affinities* Nucleic Acids Research *35:D198-D201* (2007).
- Chen,X., Lin,Y. and Gilson,M.K. *The Binding Database: Overview and User's Guide* Biopolymers Nucleic Acid Sci. *61:127-141* (2002).
- Chen,X., Lin,Y., Liu,M. and Gilson,M.K. *The Binding Database: Data Management and Interface Design* Bioinformatics *18:130-139*(2002).
- Chen,X., Liu,M., and Gilson,M.K. *Binding DB: A web-accessible molecular recognition database* J. Combi. Chem. High-Throughput Screen *4:719-725* (2001).

Utilities and Features

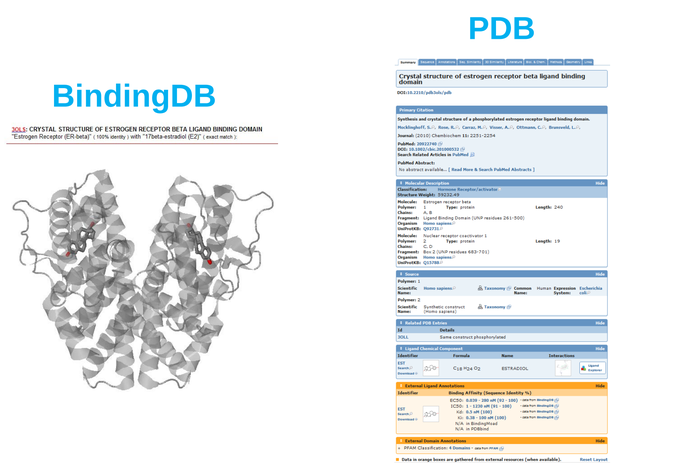
Chemical Similarity

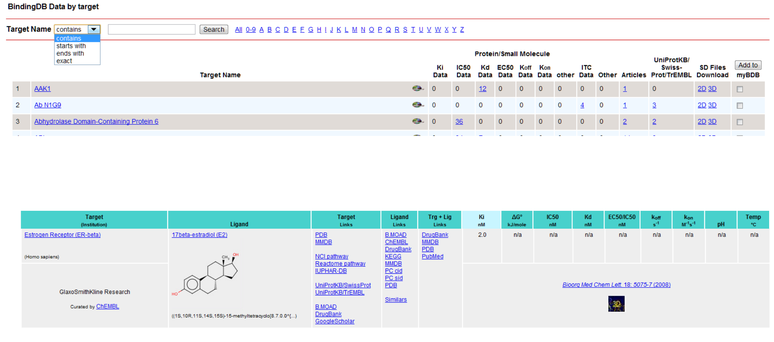
BindingDB provides users the ability to run a chemical similarity search with one of three methods:

1. Maximum similarity
2. Binary Kernel Discrimination (BKD)
3. Support Vector Machine (SVM)

Linking Affinity and Structure

Each affinity data is showcased in a separate page, and bidirectional links to the PDB are shown if available.

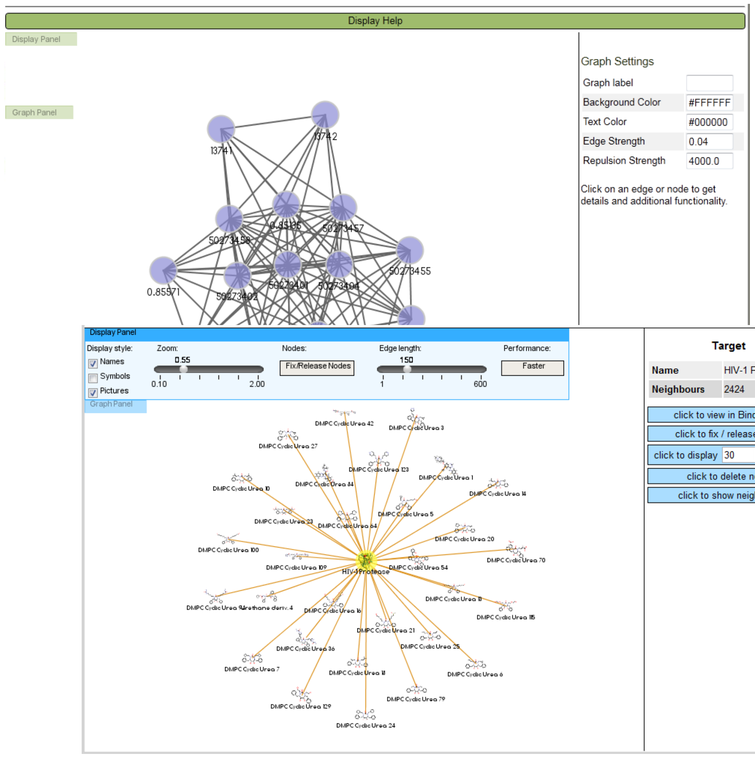




Under Development

Visual Representations

An interactive network representation was created using Cobweb to assist in viewing the target in the context of neighbors: http://bioinformatics.charite.de/bindingdb/index.php?id=eHIV-1+Protease



PSICQUIC

The BindingDB team is also working with the Proteomics Standards Initiative (PSI) consortium to make data available through the PSICQUIC service: http://www.ebi.ac.uk/Tools/webservices/psicquic/view/main.xhtml
This will allow visualization in applications such at Cytoscape and Reactome.