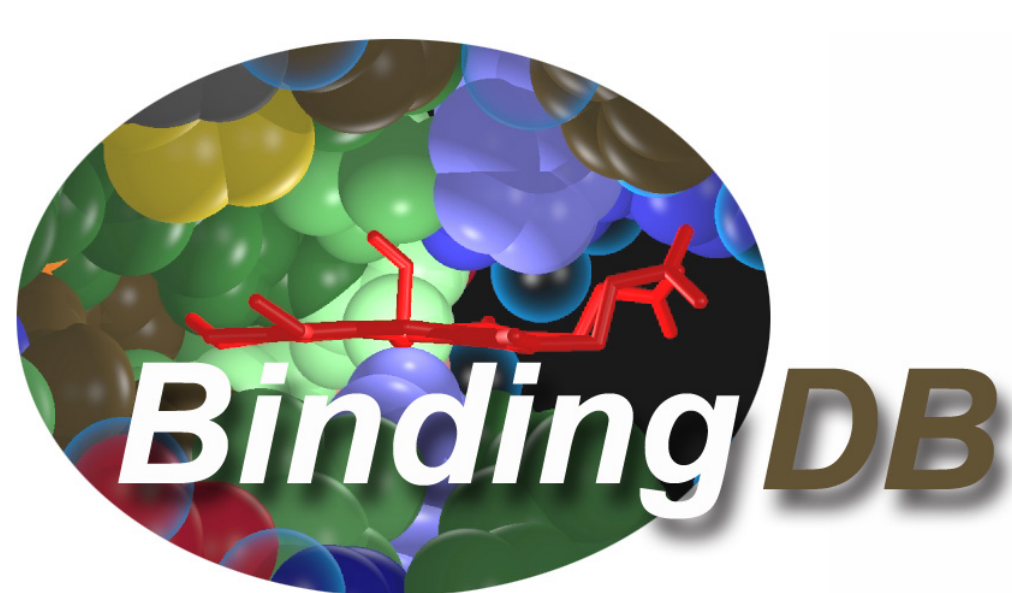




# BindingDB: A Protein-Ligand Database for Drug Discovery

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.

## 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

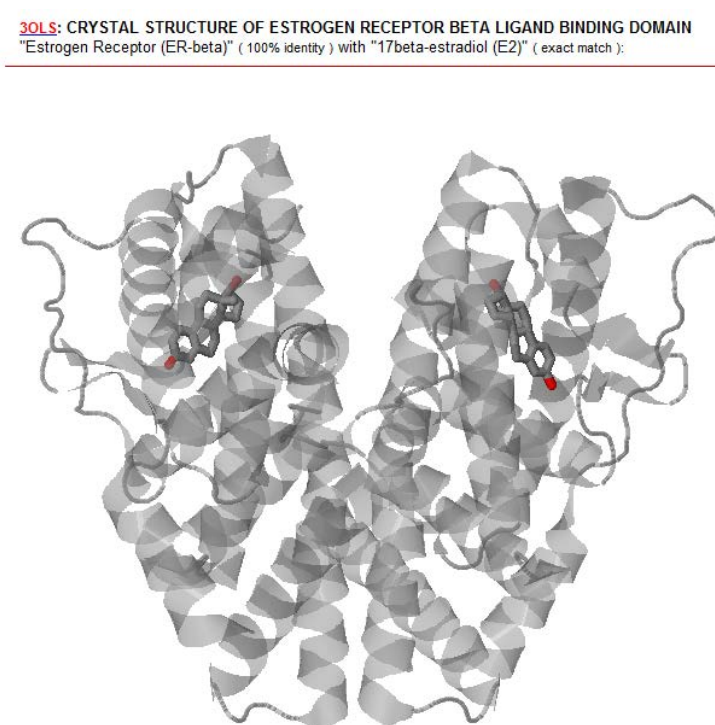
### Visual Representations

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>

### BindingDB News

- February, 2011. Users can save their own list of Targets on their personalized myBDB page.
- January, 2011. Users can now download all data for a given Target as an SDF file, at the Target Names page.
- December, 2010. Users can now enter publicly viewable comments on curated ligand-protein validation sets.
- October, 2010. Expansion of host-quest data sets.
- September, 2010. Conspecific ligand-protein series curated for use in validating computational methods.
- March, 2010. First incorporation of 462,466 ChEMBL data with defined molecular targets, including 207,522 new small molecules.

## BindingDB



## PDB

Same ligand and  
100 % sequence identity: 1437 structures in PDB  
>85 % sequence identity: 4146 structures in PDB

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

## References

- Liu, T., Lin, Y., Wen, X., Jorissen, 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).

Target	Ligand	Target Name	Ligand Name	Tri-Lig	Kd	IC50	Ki	EC50/IC50	Km	Kd	pH	Temp
Estrogen Receptor (ER-beta)	17beta-estradiol (E2)	PCB	1,2,3,4,6,7,8-Heptachlorocyclohexane	Yes	2.0	n/a	n/a	n/a	n/a	n/a	n/a	n/a
Glass/DmBkHase Research	(1S,10R,11S,14S,15S)-15-methylheptahydro-7,8-DI...)	BINDAD	1,2,3,4,6,7,8-Heptachlorocyclohexane	Similar								

## 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 as Cytoscape and Reactome.