MCULE - BindingDB subset

BindingDB, the first public molecular recognition database, enables research, education and practice in drug discovery, pharmacology and related fields. BindingDB contains 2.7M data for 1.2M Compounds and 9.0k Targets, as of May, 2023. BindingDB is based at the Skaggs School of Pharmacy and Pharmaceutical Sciences at the University of California, San Diego, La Jolla, CA.

In this subset we have collected the compounds of Mcule aggregated catalogs that have an equivalent BindingDB monomer pair. These pairs are presented in the following format:

SMILES	Mcule ID	BDBM ID	Affinity*	UniProt ID

*'Affinity' indicates the affinity data (Ki, IC50, or EC50) in nM on the target labeled with its UniProt ID in the following column. Compounds might have multiple Affinity-Target pairs in further columns .

To find BindingDB's data for a compound, use the following model URL: https://www.bindingdb.org/rwd/bind/chemsearch/marvin/MolStructure.jsp?monomerid=xxxxxxxx where xxxxxxxx is the BDBM ID in the Mcule BindingDB Subset listing.

For more information the BindingDB: bindingdb@gmail.com

References:

Gilson,M.K., Liu,T., Baitaluk,M., Nicola,G., Hwang, L. and Chong,J. BindingDB in 2015: A public database for medicinal chemistry, computational chemistry and systems pharmacology Nucleic Acids Research 44:D1045-D1053 (2015)

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)

If you would prefer other molecular format or further filtering - feel free to contact us at support@mcule.com.

Our professional laboratory services include

- Transferring samples to plates/vials as solid or DMSO solution
- Solubility characterization
- Temperature controlled shipping
- Quality control via LC-MS & NMR (on demand)

Please also reach out to our cheminformatics experts with projects related to

- Screening library building/expansion
- Generation of synthetically feasible chemical spaces based on your building blocks
- Filtering the Mcule database based on your criteria