Resource Summary Report

Generated by SPARC SAWG on Aug 9, 2026

Binding MOAD

RRID:SCR_002294
Type: Tool

Proper Citation

Binding MOAD (RRID:SCR_002294)

Resource Information

URL: http://www.bindingmoad.org/

Proper Citation: Binding MOAD (RRID:SCR_002294)

Description: Database of protein-ligand crystal structures that is a subset of the Protein Data Bank (PDB), containing every high-quality example of ligand-protein binding. The resolved protein crystal structures with clearly identified biologically relevant ligands are annotated with experimentally determined binding data extracted from literature. A viewer is provided to examine the protein-ligand structures. Ligands have additional chemical data, allowing for cheminformatics mining. The binding-affinity data ranges 13 orders of magnitude. The issue of redundancy in the data has also been addressed. To create a nonredundant dataset, one protein from each of the 1780 protein families was chosen as a representative. Representatives were chosen by tightest binding, best resolution, etc. For the 1780 best complexes that comprise the nonredundant version of Binding MOAD, 475 (27%) have binding data. This collection of protein-ligand complexes will be useful in elucidating the biophysical patterns of molecular recognition and enzymatic regulation. The complexes with binding-affinity data will help in the development of improved scoring functions and structure-based drug discovery techniques.

Abbreviations: Binding MOAD

Synonyms: BindingMOAD.org, Binding Mother of All Databases

Resource Type: database, data or information resource

Defining Citation: PMID:18055497, PMID:16168689, PMID:15971202

Keywords: drug, enzymatic, affinity, binding, binding-affinity, biological, chemical, cheminformatic, crystal, crystallography, intermolecular interaction, signaling pathway, ligand, protein, ligand-protein binding, protein crystal structure, protein-ligand, protein-ligand complex

Funding: MCB 546073

Availability: Free, Public, Acknowledgement requested

Resource Name: Binding MOAD

Resource ID: SCR_002294

Alternate IDs: OMICS_01900, nif-0000-21048

Record Creation Time: 20220129T080212+0000

Record Last Update: 20260808T190340+0000

Ratings and Alerts

No rating or validation information has been found for Binding MOAD.

No alerts have been found for Binding MOAD.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 18 mentions in open access literature.

Listed below are recent publications. The full list is available at SPARC SAWG .

Kadan A, et al. (2025) Guided multi-objective generative AI to enhance structure-based drug design. Chemical science, 16(29), 13196.

Schneuing A, et al. (2024) Structure-based drug design with equivariant diffusion models. Nature computational science, 4(12), 899.

Elkashlan M, et al. (2023) A review of SARS-CoV-2 drug repurposing: databases and machine learning models. Frontiers in pharmacology, 14, 1182465.

Wagle S, et al. (2023) Sunsetting Binding MOAD with its last data update and the addition of 3D-ligand polypharmacology tools. Scientific reports, 13(1), 3008.

Meli R, et al. (2022) Scoring Functions for Protein-Ligand Binding Affinity Prediction using Structure-Based Deep Learning: A Review. Frontiers in bioinformatics, 2.

Ma F, et al. (2021) Applications and analytical tools of cell communication based on ligand-receptor interactions at single cell level. Cell & bioscience, 11(1), 121.

Haddad Y, et al. (2021) Toward structure-based drug design against the epidermal growth factor receptor (EGFR). Drug discovery today, 26(2), 289.

K??lsch A, et al. (2020) Current limits of structural biology: The transient interaction between cytochrome c 6 and photosystem I. Current research in structural biology, 2, 171.

Smith RD, et al. (2019) Updates to Binding MOAD (Mother of All Databases): Polypharmacology Tools and Their Utility in Drug Repurposing. Journal of molecular biology, 431(13), 2423.

Rifaioglu AS, et al. (2019) Recent applications of deep learning and machine intelligence on in silico drug discovery: methods, tools and databases. Briefings in bioinformatics, 20(5), 1878.

Wu Z, et al. (2018) Network-Based Methods for Prediction of Drug-Target Interactions. Frontiers in pharmacology, 9, 1134.

Glaab E, et al. (2016) Building a virtual ligand screening pipeline using free software: a survey. Briefings in bioinformatics, 17(2), 352.

Basse MJ, et al. (2016) 2P2Idb v2: update of a structural database dedicated to orthosteric modulation of protein-protein interactions. Database : the journal of biological databases and curation, 2016.

Ahmed A, et al. (2015) Recent improvements to Binding MOAD: a resource for protein-ligand binding affinities and structures. Nucleic acids research, 43(Database issue), D465.

Mohamed R, et al. (2015) Composition of Overlapping Protein-Protein and Protein-Ligand Interfaces. PloS one, 10(10), e0140965.

Bauer-Mehren A, et al. (2012) Automatic filtering and substantiation of drug safety signals. PLoS computational biology, 8(4), e1002457.

Swapna LS, et al. (2012) Extent of structural asymmetry in homodimeric proteins: prevalence and relevance. PloS one, 7(5), e36688.

Benson ML, et al. (2008) Binding MOAD, a high-quality protein-ligand database. Nucleic acids research, 36(Database issue), D674.