# Resource Summary Report

Generated by dkNET on May 18, 2025

## 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:** 20250517T055526+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 17 mentions in open access literature.

**Listed below are recent publications.** The full list is available at dkNET.

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.

Kölsch 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.

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.

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.

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

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.

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

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

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.

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

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

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