

Resource Summary Report

Generated by [kravitz2](#) on Jul 31, 2026

Protein-Small Molecule Database

RRID:SCR_002112

Type: Tool

Proper Citation

Protein-Small Molecule Database (RRID:SCR_002112)

Resource Information

URL: <http://compbio.cs.toronto.edu/psmdb>

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Description: Database of non-redundant sets of protein - small-molecule complexes that are especially suitable for structure-based drug design and protein - small-molecule interaction research. PSMB supports: * Support frequent updates - The number of new structures in the PDB is growing rapidly. In order to utilize these structures, frequent updates are required. In contrast to manual procedures which require significant time and effort per update, generation of the PSMB database is fully automatic thereby facilitating frequent database updates. * Consider both protein and ligand structural redundancy - In the database, two complexes are considered redundant if they share a similar protein and ligand (the protein - small-molecule non-redundant set). This allows the database to contain structural information for the same protein bound to several different ligands (and vice-versa). Additionally, for completeness, the database contains a set of non-redundant complexes when only protein structural redundancy is considered (our protein non-redundant set). The following images demonstrate the structural redundancy of the protein complexes in the PDB compared to the PSMB. * Efficient handling of covalent bonds - Many protein complexes contain covalently bound ligands. Typically, protein-ligand databases discard these complexes; however, the PSMB simply removes the covalently bound ligand from the complex, retaining any non-covalently bound ligands. This increases the number of usable complexes in the database. * Separate complexes into protein and ligand files -The PSMB contains individual structure files for both the protein and all non-covalently bound ligands. The unbound proteins are in PDB format while the individual ligands are in SDF format (in their native coordinate frame).

Abbreviations: PSMB

Synonyms: Protein - Small-Molecule DataBase

Resource Type: data or information resource, database

Defining Citation: [PMID:19153135](#)

Keywords: drug, interaction, ligand, protein, small molecule, structure, protein-ligand binding

Availability: Free, Available for download, Freely available

Resource Name: Protein-Small Molecule Database

Resource ID: SCR_002112

Alternate IDs: nif-0000-20897

Record Creation Time: 20220129T080211+0000

Record Last Update: 20260729T044021+0000

Ratings and Alerts

No rating or validation information has been found for Protein-Small Molecule Database.

No alerts have been found for Protein-Small Molecule Database.

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We have not found any literature mentions for this resource.