ProtChemSI
RRID:SCR_006115
Type: Tool

Proper Citation

ProtChemSI (RRID:SCR_006115)

Resource Information

URL: http://pcidb.russelllab.org/

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Description: The database of protein-chemical structural interactions includes all existing 3D structures of complexes of proteins with low molecular weight ligands. When one considers the proteins and chemical vertices of a graph, all these interactions form a network. Biological networks are powerful tools for predicting undocumented relationships between molecules. The underlying principle is that existing interactions between molecules can be used to predict new interactions. For pairs of proteins sharing a common ligand, we use protein and chemical superimpositions combined with fast structural compatibility screens to predict whether additional compounds bound by one protein would bind the other. The current version includes data from the Protein Data Bank as of August 2011. The database is updated monthly.

Abbreviations: ProtChemSI

Synonyms: ProtChemSI - the database of protein-chemical structural interactions, Protein-Chemical Structural Interactions, ProtChemSI: protein-chemical interaction database

Resource Type: data or information resource, database

Defining Citation: PMID:21573205

Keywords: protein, chemical, 3d structure, biological network, interaction, ligand, prediction, fasta, fasta sequence, smiles string, complex, bio.tools

Availability: Acknowledgement requested
**Resource Name:** ProtChemSI

**Resource ID:** SCR_006115

**Alternate IDs:** nlx_151590, biotools:protchemsi

**Alternate URLs:** https://bio.tools/protchemsi

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### Ratings and Alerts

No rating or validation information has been found for ProtChemSI.

No alerts have been found for ProtChemSI.

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### Data and Source Information

**Source:** SciCrunch Registry

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### Usage and Citation Metrics

We found 2 mentions in open access literature.

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