Resource Summary Report

Generated by NIF on Apr 9, 2025

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

Resource Type: database, data or information resource

Defining Citation: PMID:21573205

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

Funding:

Availability: Acknowledgement requested

Resource Name: ProtChemSI

Resource ID: SCR_006115

Alternate IDs: nlx_151590, biotools:protchemsi

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

Record Creation Time: 20220129T080234+0000

Record Last Update: 20250409T060506+0000

Ratings and Alerts

No rating or validation information has been found for ProtChemSI.

No alerts have been found for ProtChemSI.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 3 mentions in open access literature.

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

Chen J, et al. (2024) RNA-binding protein biomarkers NR4A2 and NR4A3 in renal ischemia-reperfusion injury diagnosis. Medicine, 103(46), e40426.

Morelli X, et al. (2012) Searching for the Holy Grail; protein-protein interaction analysis and modulation. EMBO reports, 13(10), 877.

Kalinina OV, et al. (2011) Combinations of protein-chemical complex structures reveal new targets for established drugs. PLoS computational biology, 7(5), e1002043.