Resource Summary Report

Generated by NIF on May 19, 2025

Drug Design Data Resource

RRID:SCR_000497
Type: Tool

Proper Citation

Drug Design Data Resource (RRID:SCR_000497)

Resource Information

URL: http://drugdesigndata.org

Proper Citation: Drug Design Data Resource (RRID:SCR_000497)

Description: Project portal's database of protein-ligand data sets provided by pharmaceutical partners that provide atomic details of drug mechanisms that will be used to improve computer-aided drug-design methods and thus accelerate drug discovery. The project aims to help companies release the high-quality data they have generated, which has incredible value to researchers working to improve methods of computer-aided drug discovery. Everyone stands to benefit from the ability to develop new medications more quickly and inexpensively. What computational chemists globally are trying to do is to make faster, more accurate, more predictive programs to speed up the process. Part of their mission is to engage the community in these challenges to test newly developed predictive algorithms.

Abbreviations: D3R

Synonyms: Drug Design Data (D3R) Resource

Resource Type: database, data or information resource, portal

Keywords: computer-aided drug design, drug design, pharmaceutical, small molecule, ligand-protein interaction, protein, ligand, drug development, drug, binding, data set, affinity, computation, medicine, compound, structure

Funding: NIGMS 1U01GM111528

Resource Name: Drug Design Data Resource

Resource ID: SCR_000497

Alternate IDs: nlx_158375

Alternate URLs: https://api.datacite.org/dois?prefix=10.15782

Record Creation Time: 20220129T080201+0000

Record Last Update: 20250517T055432+0000

Ratings and Alerts

No rating or validation information has been found for Drug Design Data Resource.

No alerts have been found for Drug Design Data Resource.

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.

Mey ASJS, et al. (2018) Impact of domain knowledge on blinded predictions of binding energies by alchemical free energy calculations. Journal of computer-aided molecular design, 32(1), 199.

Réau M, et al. (2018) Decoys Selection in Benchmarking Datasets: Overview and Perspectives. Frontiers in pharmacology, 9, 11.

Amaro RE, et al. (2016) Drug Discovery Gets a Boost from Data Science. Structure (London, England : 1993), 24(8), 1225.