Resource Summary Report

Generated by dkNET on Apr 16, 2025

Community Structure-Activity Resource

RRID:SCR_002206
Type: Tool

Proper Citation

Community Structure-Activity Resource (RRID:SCR_002206)

Resource Information

URL: http://www.csardock.org

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Description: Experimental datasets of crystal structures and binding affinities for diverse protein-ligand complexes. Some datasets are generated in house while others are collected from the literature or deposited by academic labs, national centers, and the pharmaceutical industry. For the community to improve their approaches, they need exceptional datasets to train scoring functions and develop new docking algorithms. They aim to provide the highest quality data for a diverse collection of proteins and small molecule ligands. They need input from the community in developing target priorities. Ideal targets will have many high-quality crystal structures (apo and 10-20 bound to diverse ligands) and affinity data for 25 compounds that range in size, scaffold, and logP. It is best if the ligand set has several congeneric series that span a broad range of affinity, with low nanomolar to mid-micromolar being most desirable. They prefer Kd data over Ki data over IC50 data (no % activity data). They will determine solubility, pKa, logP/logD data for the ligands whenever possible. They have augmented some donated IC50 data by determining Kon/Koff and ITC data.

Abbreviations: CSAR

Resource Type: data set, data or information resource, service resource, data repository, storage service resource

Keywords: crystal structure, binding affinity, protein-ligand complex, protein, small molecule, ligand, compound

Funding: NIGMS

Availability: The community can contribute to this resource, Public domain, Account

required

Resource Name: Community Structure-Activity Resource

Resource ID: SCR_002206

Alternate IDs: nlx_154720

Record Creation Time: 20220129T080212+0000

Record Last Update: 20250416T063257+0000

Ratings and Alerts

No rating or validation information has been found for Community Structure-Activity Resource.

No alerts have been found for Community Structure-Activity Resource.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 15 mentions in open access literature.

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

Wang DD, et al. (2024) Structure-based, deep-learning models for protein-ligand binding affinity prediction. Journal of cheminformatics, 16(1), 2.

Mohamed Abdul Cader J, et al. (2024) Ensembling methods for protein-ligand binding affinity prediction. Scientific reports, 14(1), 24447.

Meli R, et al. (2022) Scoring Functions for Protein-Ligand Binding Affinity Prediction using Structure-Based Deep Learning: A Review. Frontiers in bioinformatics, 2.

Wang DD, et al. (2022) Protein-ligand binding affinity prediction based on profiles of intermolecular contacts. Computational and structural biotechnology journal, 20, 1088.

Kumar S, et al. (2021) SMPLIP-Score: predicting ligand binding affinity from simple and interpretable on-the-fly interaction fingerprint pattern descriptors. Journal of cheminformatics, 13(1), 28.

Araki M, et al. (2021) Exploring ligand binding pathways on proteins using hypersound-accelerated molecular dynamics. Nature communications, 12(1), 2793.

Son J, et al. (2021) Development of a graph convolutional neural network model for efficient prediction of protein-ligand binding affinities. PloS one, 16(4), e0249404.

Karlov DS, et al. (2020) graphDelta: MPNN Scoring Function for the Affinity Prediction of Protein-Ligand Complexes. ACS omega, 5(10), 5150.

Kalinowsky L, et al. (2018) A Diverse Benchmark Based on 3D Matched Molecular Pairs for Validating Scoring Functions. ACS omega, 3(5), 5704.

Gilson MK, et al. (2016) BindingDB in 2015: A public database for medicinal chemistry, computational chemistry and systems pharmacology. Nucleic acids research, 44(D1), D1045.

Gu J, et al. (2015) A Self-Adaptive Steered Molecular Dynamics Method Based on Minimization of Stretching Force Reveals the Binding Affinity of Protein-Ligand Complexes. Molecules (Basel, Switzerland), 20(10), 19236.

Atkovska K, et al. (2014) Multipose binding in molecular docking. International journal of molecular sciences, 15(2), 2622.

Anand P, et al. (2014) ABS-Scan: In silico alanine scanning mutagenesis for binding site residues in protein-ligand complex. F1000Research, 3, 214.

Lemmon G, et al. (2013) Towards ligand docking including explicit interface water molecules. PloS one, 8(6), e67536.

Huang SY, et al. (2010) Advances and challenges in protein-ligand docking. International journal of molecular sciences, 11(8), 3016.