

# Resource Summary Report

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## rDock

RRID:SCR\_002838

Type: Tool

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### Proper Citation

rDock (RRID:SCR\_002838)

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### Resource Information

**URL:** <http://rdock.sourceforge.net/>

**Proper Citation:** rDock (RRID:SCR\_002838)

**Description:** A fast and versatile Open Source docking software program that can be used to dock small molecules against proteins and nucleic acids.

**Resource Type:** software resource

**Defining Citation:** [PMID:24722481](https://pubmed.ncbi.nlm.nih.gov/24722481/)

**Keywords:** standalone software

**Funding:**

**Resource Name:** rDock

**Resource ID:** SCR\_002838

**Alternate IDs:** OMICS\_03835

**Record Creation Time:** 20220129T080215+0000

**Record Last Update:** 20250420T014125+0000

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### Ratings and Alerts

No rating or validation information has been found for rDock.

No alerts have been found for rDock.

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## Data and Source Information

**Source:** [SciCrunch Registry](#)

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## Usage and Citation Metrics

We found 96 mentions in open access literature.

**Listed below are recent publications.** The full list is available at [FDI Lab - SciCrunch.org](#).

Matsoukas MT, et al. (2025) Design of Small Non-Peptidic Ligands That Alter Heteromerization between Cannabinoid CB1 and Serotonin 5HT2A Receptors. *Journal of medicinal chemistry*, 68(1), 261.

Fan Y, et al. (2025) Isovitexin targets SIRT3 to prevent steroid-induced osteonecrosis of the femoral head by modulating mitophagy-mediated ferroptosis. *Bone research*, 13(1), 18.

Debnath A, et al. (2025) Identification of novel cyclin-dependent kinase 4/6 inhibitors from marine natural products. *PloS one*, 20(1), e0313830.

Ferla MP, et al. (2025) Fragmenstein: predicting protein-ligand structures of compounds derived from known crystallographic fragment hits using a strict conserved-binding-based methodology. *Journal of cheminformatics*, 17(1), 4.

Wang X, et al. (2025) A novel approach for target deconvolution from phenotype-based screening using knowledge graph. *Scientific reports*, 15(1), 2414.

Raubenolt B, et al. (2024) Generalized open-source workflows for atomistic molecular dynamics simulations of viral helicases. *GigaScience*, 13.

Loeffler HH, et al. (2024) Reinvent 4: Modern AI-driven generative molecule design. *Journal of cheminformatics*, 16(1), 20.

Lee CJ, et al. (2024) ELK3 destabilization by speckle-type POZ protein suppresses prostate cancer progression and docetaxel resistance. *Cell death & disease*, 15(4), 274.

Lee GE, et al. (2024) SPOP-mediated RIPK3 destabilization desensitizes LPS/sMAC/zVAD-induced necroptotic cell death. *Cellular and molecular life sciences : CMLS*, 81(1), 451.

Comajuncosa-Creus A, et al. (2024) Comprehensive detection and characterization of human druggable pockets through binding site descriptors. *Nature communications*, 15(1), 7917.

Tan LH, et al. (2024) RmsdXNA: RMSD prediction of nucleic acid-ligand docking poses using machine-learning method. *Briefings in bioinformatics*, 25(3).

Cubero E, et al. (2024) Discovery of allosteric regulators with clinical potential to stabilize alpha-L-iduronidase in mucopolysaccharidosis type I. *PloS one*, 19(5), e0303789.

Zhang LJ, et al. (2024) Identification of lipid senolytics targeting senescent cells through ferroptosis induction. *bioRxiv : the preprint server for biology*.

Borges KCM, et al. (2024) New antibacterial candidates against *Acinetobacter baumannii* discovered by in silico-driven chemogenomics repurposing. *PloS one*, 19(9), e0307913.

Khachatryan H, et al. (2024) Computational evaluation and benchmark study of 342 crystallographic holo-structures of SARS-CoV-2 Mpro enzyme. *Scientific reports*, 14(1), 14255.

Yao L, et al. (2024) mRNA-seq-based analysis predicts: AEG-1 is a therapeutic target and immunotherapy biomarker for pan-cancer, including OSCC. *Frontiers in immunology*, 15, 1484226.

Barroso M, et al. (2024) Use of the Novel Site-Directed Enzyme Enhancement Therapy (SEE-Tx) Drug Discovery Platform to Identify Pharmacological Chaperones for Glutaric Acidemia Type 1. *Journal of medicinal chemistry*, 67(19), 17087.

Cao Y, et al. (2023) Novel hKDR mouse model depicts the antiangiogenesis and apoptosis-promoting effects of neutralizing antibodies targeting vascular endothelial growth factor receptor 2. *Cancer science*, 114(1), 115.

Olenginski LT, et al. (2023) Virtual Screening of Hepatitis B Virus Pre-Genomic RNA as a Novel Therapeutic Target. *Molecules (Basel, Switzerland)*, 28(4).

Hagg A, et al. (2023) Open-Source Machine Learning in Computational Chemistry. *Journal of chemical information and modeling*, 63(15), 4505.