Resource Summary Report

Generated by kravitz2 on Jul 31, 2026

DOCK

RRID:SCR_000128
Type: Tool

Proper Citation

DOCK (RRID:SCR_000128)

Resource Information

URL: http://dock.compbio.ucsf.edu/

Proper Citation: DOCK (RRID:SCR_000128)

Description: An algorithm used to predict and analyse binding modes of docking molecules. Users can search ligand databases for compounds that inhibit enzymatic activity and bind to particular molecules and nucleic acid targets. Molecular docking is used to predict a predominant binding mode(s) of a ligand in three-dimensional structure. This method can be used for molecular biology and computer-assisted drug design.

Abbreviations: DOCK

Synonyms: UCSF DOCK

Resource Type: software resource

Keywords: molecule docking, ligand model, drug design, molecular biology

Availability: Available to the research community, Free for the academic community, License fee for industrial organizations, Available for download

Resource Name: DOCK

Resource ID: SCR_000128

Alternate IDs: OMICS_01598

License URLs: https://dock.compbio.ucsf.edu/Online_Licensing/index.htm

Record Creation Time: 20220129T080159+0000

Record Last Update: 20260725T190436+0000

Ratings and Alerts

No rating or validation information has been found for DOCK.

No alerts have been found for DOCK.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 16 mentions in open access literature.

Listed below are recent publications. The full list is available at kravitz2 .

Jayaprakash NG, et al. (2020) The barley lectin, horcolin, binds high-mannose glycans in a multivalent fashion, enabling high-affinity, specific inhibition of cellular HIV infection. The Journal of biological chemistry, 295(34), 12111.

Shen JJ, et al. (2018) Substrate Specificity of Acyltransferase Domains for Efficient Transfer of Acyl Groups. Frontiers in microbiology, 9, 1840.

Calhoun S, et al. (2018) Prediction of enzymatic pathways by integrative pathway mapping. eLife, 7.

Basith S, et al. (2018) Exploring G Protein-Coupled Receptors (GPCRs) Ligand Space via Cheminformatics Approaches: Impact on Rational Drug Design. Frontiers in pharmacology, 9, 128.

Wacker D, et al. (2017) Crystal Structure of an LSD-Bound Human Serotonin Receptor. Cell, 168(3), 377.

Patel BB, et al. (2017) Tumor stroma interaction is mediated by monocarboxylate metabolism. Experimental cell research, 352(1), 20.

Glaab E, et al. (2016) Building a virtual ligand screening pipeline using free software: a survey. Briefings in bioinformatics, 17(2), 352.

London N, et al. (2014) Covalent docking of large libraries for the discovery of chemical probes. Nature chemical biology, 10(12), 1066.

Novinec M, et al. (2014) Probing the activity modification space of the cysteine peptidase cathepsin K with novel allosteric modifiers. PloS one, 9(9), e106642.

Jamal MS, et al. (2014) Anticancer compound plumbagin and its molecular targets: a structural insight into the inhibitory mechanisms using computational approaches. PloS one, 9(2), e87309.

Fornander LH, et al. (2012) Ca2+ improves organization of single-stranded DNA bases in human Rad51 filament, explaining stimulatory effect on gene recombination. Nucleic acids research, 40(11), 4904.

Cheng T, et al. (2012) Structure-based virtual screening for drug discovery: a problem-centric review. The AAPS journal, 14(1), 133.

Yang XG, et al. (2012) 6-[(1-naphthylmethyl)sulfanyl]-9H-purine induces G2/M phase arrest and apoptosis in human hepatocellular carcinoma HepG2 cells. European journal of pharmacology, 695(1-3), 27.

Carlsson J, et al. (2011) Ligand discovery from a dopamine D3 receptor homology model and crystal structure. Nature chemical biology, 7(11), 769.

Biesiada J, et al. (2011) Survey of public domain software for docking simulations and virtual screening. Human genomics, 5(5), 497.

Lewis SN, et al. (2010) Virtual Screening as a Technique for PPAR Modulator Discovery. PPAR research, 2010, 861238.