Resource Summary Report

Generated by NIF on Apr 21, 2025

AutoDock

RRID:SCR_012746
Type: Tool

Proper Citation

AutoDock (RRID:SCR_012746)

Resource Information

URL: http://autodock.scripps.edu/

Proper Citation: AutoDock (RRID:SCR_012746)

Description: Software suite of automated docking tools. Designed to predict how small molecules, such as substrates or drug candidates, bind to receptor of known 3D structure. AutoDock consist of AutoDock 4 and AutoDock Vina. AutoDock 4 consists of autodock to perform docking of ligand to set of grids describing target protein, and autogrid to pre calculate these grids.

Abbreviations: autodock

Resource Type: software resource

Defining Citation: PMID:19399780

Keywords: Small molecules receptor binding, automated docking tools, 3D structure, AutoDock 4, AutoDock Vina, ligand, docking

Funding:

Availability: Free, Available for download, Freely available

Resource Name: AutoDock

Resource ID: SCR_012746

Alternate IDs: OMICS_01594, biotools:autodock

Alternate URLs: https://bio.tools/autodock, https://sources.debian.org/src/autodock/

Record Creation Time: 20220129T080312+0000

Record Last Update: 20250420T014618+0000

Ratings and Alerts

No rating or validation information has been found for AutoDock.

No alerts have been found for AutoDock.

Data and Source Information

Source: SciCrunch Registry

Usage and Citation Metrics

We found 9798 mentions in open access literature.

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

Bao Y, et al. (2025) Metformin blocks BIK1-mediated CPK28 phosphorylation and enhances plant immunity. Journal of advanced research, 68, 31.

Finke F, et al. (2025) Different receptor models show differences in ligand binding strength and location: a computational drug screening for the tick-borne encephalitis virus. Molecular diversity, 29(1), 281.

Eltabeeb MA, et al. (2025) Nanocomposite alginate hydrogel loaded with propranolol hydrochloride kolliphor® based cerosomes as a repurposed platform for Methicillin-Resistant Staphylococcus aureus-(MRSA)-induced skin infection; in-vitro, ex-vivo, in-silico, and in-vivo evaluation. Drug delivery and translational research, 15(2), 556.

Wang W, et al. (2025) Metal-free production of natural blue colorants through anthocyanin-protein interactions. Journal of advanced research, 68, 17.

Fan J, et al. (2025) 4?Methoxydalbergione inhibits the tumorigenesis and metastasis of lung cancer through promoting ferroptosis via the DNMT1/system Xc?/GPX4 pathway. Molecular medicine reports, 31(1).

Yu C, et al. (2025) A novel Alteromonas phage with tail fiber containing six potential iron-binding domains. Microbiology spectrum, 13(1), e0093424.

Zhang L, et al. (2025) The Therapeutic Mechanisms of Huayu Quban Capsule in Treating Acne Vulgaris Are Uncovered Through Network Pharmacology and Molecular Docking.

Journal of cosmetic dermatology, 24(1), e16632.

Yang L, et al. (2025) Mebendazole effectively overcomes imatinib resistance by dual-targeting BCR/ABL oncoprotein and ?-tubulin in chronic myeloid leukemia cells. The Korean journal of physiology & pharmacology : official journal of the Korean Physiological Society and the Korean Society of Pharmacology, 29(1), 67.

Espinheira RP, et al. (2025) Discovery and Characterization of Mannan-Specialized GH5 Endo-1,4-?-mannanases: a Strategy for Açaí (Euterpe oleracea Mart.) Seeds Upgrading. Journal of agricultural and food chemistry, 73(1), 625.

Sinko W, et al. (2025) ModBind, a Rapid Simulation-Based Predictor of Ligand Binding and Off-Rates. Journal of chemical information and modeling, 65(1), 265.

Oliveira Soté W, et al. (2025) Exploring Binding Sites in Chagas Disease Protein TcP21 Using Integrated Mixed Solvent Molecular Dynamics Approaches. Journal of chemical information and modeling, 65(1), 363.

Visitsatthawong S, et al. (2025) Mechanistic insights into allosteric regulation of the reductase component of p-hydroxyphenylacetate 3-hydroxylase by p-hydroxyphenylacetate: a model for effector-controlled activity of redox enzymes. RSC chemical biology, 6(1), 81.

Yan K, et al. (2025) Using network pharmacology and molecular docking technology, proteomics and experiments were used to verify the effect of Yigu decoction (YGD) on the expression of key genes in osteoporotic mice. Annals of medicine, 57(1), 2449225.

Shosha MI, et al. (2025) New thiazole derivative as a potential anticancer and topoisomerase II inhibitor. Scientific reports, 15(1), 710.

Wang HW, et al. (2025) Identification, characterization, and expression of Oryza sativa tryptophan decarboxylase genes associated with fluroxypyr-meptyl metabolism. The plant genome, 18(1), e20547.

Negru DC, et al. (2025) Evaluation of the Alkaloids as Inhibitors of Human Acetylcholinesterase by Molecular Docking and ADME Prediction. In vivo (Athens, Greece), 39(1), 236.

Nguyen MH, et al. (2025) In vitro and in silico hybrid approach to unveil triterpenoids from Helicteres hirsuta leaves as potential compounds for inhibiting Nrf2. RSC advances, 15(3), 1915.

Francis S, et al. (2025) Evaluating the potential of Kalanchoe pinnata, Piper amalago amalago, and other botanicals as economical insecticidal synergists against Anopheles gambiae. Malaria journal, 24(1), 25.

El-Azab AS, et al. (2025) Remarkable utilization of quinazoline-based homosulfonamide for in vitro cytotoxic effects with triple kinase inhibition activities: cell cycle analysis and molecular docking profile. RSC advances, 15(1), 541.

Wang LL, et al. (2025) Identification of Filovirus Entry Inhibitors from Marine Fungus-Derived

Indole Alkaloids. Marine drugs, 23(1).