

Resource Summary Report

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AutoDockTools

RRID:SCR_026401

Type: Tool

Proper Citation

AutoDockTools (RRID:SCR_026401)

Resource Information

URL: <https://autodocksuite.scripps.edu/adt/>

Proper Citation: AutoDockTools (RRID:SCR_026401)

Description: Software graphical user interface to help to set up which bonds will be treated as rotatable in the ligand and to analyze dockings. Used for automated docking with selective receptor flexibility. Designed to predict how small molecules, such as substrates or drug candidates, bind to receptor of known 3D structure.

Abbreviations: ADT

Synonyms: AutoDockTools: the Graphical User Interface for AutoDock

Resource Type: software resource, software application

Defining Citation: [PMID:19399780](#)

Keywords: automated docking, selective receptor flexibility, predict binding, bind to receptor of known 3D structure, ligand, analyze dockings

Funding: NIGMS RO1 GM069832

Availability: Free, Available for download, Freely available

Resource Name: AutoDockTools

Resource ID: SCR_026401

Alternate URLs: <https://autodock.scripps.edu/>

Record Creation Time: 20250208T060343+0000

Record Last Update: 20260731T043212+0000

Ratings and Alerts

No rating or validation information has been found for AutoDockTools .

No alerts have been found for AutoDockTools .

Data and Source Information

Source: [SciCrunch Registry](#)

Usage and Citation Metrics

We found 1612 mentions in open access literature.

Listed below are recent publications. The full list is available at [kravitz2](#) .

Wang Z, et al. (2026) Integrated Network Pharmacology, Single-Cell Transcriptomics Unveil the Mechanistic Role of Morusin in Aortic Dissection. *Journal of cellular and molecular medicine*, 30(1), e70971.

Lv X, et al. (2026) Blautia coccoides-derived metabolite trimethylamine-N-oxide exacerbates Alzheimer's disease progression via targeting HIF1 α signaling. *Gut microbes*, 18(1), 2605768.

Chiang YC, et al. (2026) Multi-Omics and Single-Cell Dissection of Exostosin Glycosyltransferases (EXT1/EXT2) Reveals Divergent Oncogenic Roles and Therapeutic Vulnerabilities in Gliomas. *Journal of Cancer*, 17(1), 177.

Pan L, et al. (2026) tRNA-Derived Fragment tRF-22 Promotes Immunosuppression by Inhibiting HnRNPAB Ubiquitination in Esophageal Squamous Cell Carcinoma. *Advanced science (Weinheim, Baden-Wurttemberg, Germany)*, 13(1), e05806.

Zhao Q, et al. (2026) Mafu Yishen Formula ameliorates membranous nephropathy by promotion of regulatory T cell differentiation: a multi-omics study. *Chinese medicine*, 21(1), 5.

Zhou Z, et al. (2026) Chromosome-level genome provides novel insights into the starch metabolism regulation and evolutionary history of *Tetraselmis helgolandica*. *Journal of advanced research*, 79, 251.

Capucho LR, et al. (2026) In Silico Design and Validation of a Novel HPPD-Inhibiting Herbicide Candidate Based on Benzofuran and Arylthioacetic Acid Scaffolds. *Chemistry & biodiversity*, 23(1), e03221.

Al-Shami AS, et al. (2025) Early-life bisphenol A exposure causes neuronal pyroptosis in juvenile and adult male rats through the NF- κ B/IL-1 β /NLRP3/caspase-1 signaling pathway: exploration of age and dose as effective covariates using an in vivo and in silico modeling approach. *Molecular and cellular biochemistry*, 480(4), 2301.

Lv C, et al. (2025) Psoralen and Isopsoralen Activate Nuclear Factor Erythroid 2-Related Factor 2 Through Interaction With Kelch-Like ECH-Associated Protein 1. *Food science & nutrition*, 13(1), e4768.

Lyu C, et al. (2025) Ameliorative effects of Asiasarum root and rhizome extract on high fat diet-induced obesity in mice through regulation of the SIRT1/PGC1 α /AMPK pathways in muscle and liver tissues. *Molecular medicine reports*, 31(3).

Chen X, et al. (2025) Network pharmacology and molecular docking to explore mechanisms of clozapine-induced cardiac arrest. *Journal of psychiatry & neuroscience : JPN*, 50(1), E1.

Zhang L, et al. (2025) Ganoderic Acid A Alleviates Severe Acute Pancreatitis by Modulating Gut Homeostasis and Inhibiting TLR4-NLRP3 Signaling. *Journal of agricultural and food chemistry*, 73(2), 1563.

Chen F, et al. (2025) Tanshinone IIA affects the proliferation of A549/Tax by affecting the expression of MMP7 through the PI3K-AKT-mTOR signaling pathway. *Discover oncology*, 16(1), 369.

Yuan Y, et al. (2025) A new paradigm for drug discovery in the treatment of complex diseases: drug discovery and optimization. *Chinese medicine*, 20(1), 40.

Ahamad Khan MM, et al. (2025) Unveiling ferroptosis genes and inhibitors in diabetic retinopathy through single-cell analysis and docking simulations. *Biochemistry and biophysics reports*, 41, 101932.

Jia J, et al. (2025) Network Pharmacology and Molecular Docking to Explore the Mechanism of Compound Qilian Tablets in Treating Diabetic Retinopathy. *Current computer-aided drug design*, 21(3), 333.

Jin G, et al. (2025) Integrated metabolomics and network pharmacology analysis to reveal the mechanisms of Wenshenyang decoction in the treatment of chronic kidney disease. *Frontiers in pharmacology*, 16, 1500463.

Zhang J, et al. (2025) Targeting MAN1B1 potently enhances bladder cancer antitumor immunity via deglycosylation of CD47. *Cancer communications (London, England)*, 45(9), 1090.

Guo Y, et al. (2025) Caffeic acid phenethyl ester protects *Clostridioides difficile* infection by toxin inhibition and microbiota modulation. *eLife*, 13.

Liu Q, et al. (2025) Green development of whey protein-based complex system for the intestinal delivery of curcumin: Focus on formation mechanism, stability, and in vitro digestive characteristics. *Food chemistry: X*, 28, 102563.