

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 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 application, software resource

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: 20260912T200503+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 2063 mentions in open access literature.

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

Ruankham W, et al. (2026) Unraveling Network Pharmacology-Based Therapeutics of Anthranilate Sulfonamides via Sirtuins/FOXO3a Cascade in Alzheimer's Disease. Journal of neurochemistry, 170(2), e70377.

Jiang YY, et al. (2026) Ze-qi Decoction Inhibits Neutrophil Extracellular Trap Formation to Suppress the Progression and Metastasis of Non-Small Cell Lung Cancer. Integrative cancer therapies, 25, 15347354261420750.

Liu A, et al. (2026) Soluble Uric Acid Drives CD8+ T-cell Exhaustion by Inducing KSR1-Mediated MAPK Hyperactivation. Cancer research, 86(14), 3459.

Dong X, et al. (2026) Gut-microbiota-derived 3-indoleacrylic acid alleviates neonatal necrotizing enterocolitis by inhibiting epithelial necroptosis. Cell reports. Medicine, 7(4), 102721.

Sinyavskiy S, et al. (2026) Benzo[e][1,2,4]triazolo[1,5-c][1,2,3]triazines: Design, Synthesis, and Cytotoxic Effects. Chemistry & biodiversity, 23(6), e71416.

Roy S, et al. (2026) Design, Synthesis, Molecular Docking, Pharmacokinetic Properties, and Molecular Dynamics Simulation of Sulfonyl Derivatives of Benzimidazole against Parkinson's Disease. Current medicinal chemistry, 33(5), 1096.

Beigh S, et al. (2026) Ginkgolide as a Promising Multi-Target Therapeutic for Alzheimer's Disease: Targeting ApoE4 and Beyond. Current pharmaceutical design, 32(15), 1200.

Zhang S, et al. (2026) Microcystin-LR Triggers Renal Tubular Ferroptosis Through Epigenetic Repression of GPX4: Implications for Environmental Nephrotoxicity. Advanced science (Weinheim, Baden-Wurttemberg, Germany), 13(9), e14349.

Zhang S, et al. (2026) Deciphering the therapeutic mechanism of kaempferol in diabetic retinopathy via the P21/Thioredoxin axis. Molecular and cellular biochemistry, 481(1), 457.

Liu Y, et al. (2026) A Comparative Study of Deep Learning and Classical Modeling Approaches for Protein-Ligand Binding Pose and Affinity Prediction in Coronavirus Main Proteases. Journal of chemical information and modeling, 66(1), 731.

Wang J, et al. (2026) Network toxicology and Mendelian randomization reveal pathogenic factors of monoethyl phthalate-induced thyroid cancer. *European thyroid journal*, 15(1).

Guo F, et al. (2026) A Comprehensive Multiomics Approach Illuminates the Biosynthetic Mechanism of Scoparone in *Artemisia capillaris*. *Plant biotechnology journal*, 24(1), 346.

Jiang YQ, et al. (2026) GR/HDAC2/synaptic complexes in hippocampal CA1 mediate the antidepressant effects of magnolol. *Biomedical journal*, 49(3), 100961.

Chen H, et al. (2026) SELE is associated with reduced breast cancer susceptibility: Evidence from Mendelian randomization and single-cell transcriptome. *Translational oncology*, 66, 102713.

Fan Q, et al. (2026) Sinensetin attenuates post-stroke depression via dual modulation of TLR4/NF- κ B-NRF2/GPX4 pathways. *Scientific reports*, 16(1).

Bao X, et al. (2026) Jichuan decoction alleviates constipation by inhibiting the PI3K/Akt/mTOR signaling pathway: an integrated network pharmacology and experimental study. *Scientific reports*, 16(1).

Pellegrino M, et al. (2026) Molecular insights into Silodosin's anti-cancer effects: a promising repurposing strategy for breast cancer. *Cell death discovery*, 12(1).

Zhang W, et al. (2026) Decoding resistance in *Diutina catenulata* by validating clinically relevant Erg11/Fks1 mutations. *Frontiers in cellular and infection microbiology*, 16, 1776442.

Li Y, et al. (2026) Neuroimmunological Mechanisms of Xiao-Yao-San Against Chronic Stress-Induced Colorectal Cancer: A Bioinformatics and Single-Cell Sequencing Study. *Cancer management and research*, 18, 567746.

Li S, et al. (2026) Identification of a Diagnostic Gene Signature Associated with Centrosome Amplification in Pressure Injuries: A Cross-Sectional Transcriptome and Machine Learning Study. *Journal of inflammation research*, 19, 580289.