

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 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: 20260905T133521+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.

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

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.

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.

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.

Schedlbauer A, et al. (2026) Aminolevulinate inhibition of human coproporphyrinogen oxidase clarifies coproporphyrin III accumulation in porphyrias. Bioscience reports, 46(3).

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

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

Yang X, et al. (2026) An integrated study combining network toxicology machine learning and molecular simulation reveals the molecular mechanisms of permanent hair dyes in breast cancer. *Discover oncology*, 17(1).

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.

Kobzar OL, et al. (2026) Heterocycle-Tethered Aurones: Synthesis and Evaluation of ??-Glucosidase Inhibition. *BioMed research international*, 2026(1), e5193886.

Badarala L, et al. (2026) Q-CaDD: accelerating in silico methodologies with quantum computation and machine learning for Epidermal growth factor receptor. *Scientific reports*, 16(1).

Andrade MC, et al. (2026) Tagitinin C-Rich Extract From *Tithonia diversifolia* (hemsl.) A. Gray Exerts Activity Against Pathogenic Bacteria and Biofilms. *APMIS : acta pathologica, microbiologica, et immunologica Scandinavica*, 134(3), e70185.

Elshemy HM, et al. (2026) Photodynamic larvicidal activity of magnesium chlorophyllin and magnesium chlorophyllin zinc oxide nanocomposite against *Spodoptera frugiperda* with non-target safety assessment. *Scientific reports*, 16(1).

Zhang C, et al. (2026) Combining bioinformatics prediction with experimental validation to explore the ameliorative effect of *Psoralea corylifolia* on vitiligo. *Molecular medicine reports*, 33(6).

Kardoudi A, et al. (2026) Computational Identification of Natural Inhibitors Targeting Fiber Proteins of FAdV-1 and FAdV-4 Through Integrated Virtual Screening and Molecular Dynamics Simulations. *Veterinary sciences*, 13(3).

Fu Y, et al. (2026) Wine-Processed *Cornus officinalis* Ameliorates Osteoarthritis via Modulating M1/M2 Macrophage Polarization. *Journal of cellular and molecular medicine*, 30(7), e71113.