Resource Summary Report

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Autogrid

RRID:SCR_015982 Type: Tool

Proper Citation

Autogrid (RRID:SCR_015982)

Resource Information

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

Proper Citation: Autogrid (RRID:SCR_015982)

Description: THIS RESOURCE IS NO LONGER IN SERVICE. Documented on February 23,2023.Software for automated docking analysis to precalculate the set of grids describing the target protein. It is a part of automated molecular modeling simulation software AutoDock.

Synonyms: Autogrid toolkit, Autogrid: automated grid

Resource Type: data analysis software, software application, software resource, simulation software, data processing software

Defining Citation: PMID:16862531

Keywords: software, automated, docking, analysis, tool, precalculate, set, grid, ligand, protein, target, molecular, simulation, modeling, protein-ligand interaction, data

Funding: The Scripps Research Institute ; San Diego ; California

Availability: THIS RESOURCE IS NO LONGER IN SERVICE

Resource Name: Autogrid

Resource ID: SCR_015982

Alternate URLs: http://mgl.scripps.edu/forum

License: GNU General Public License

Record Creation Time: 20220129T080328+0000

Record Last Update: 20250403T061157+0000

Ratings and Alerts

No rating or validation information has been found for Autogrid.

No alerts have been found for Autogrid.

Data and Source Information

Source: <u>SciCrunch Registry</u>

Usage and Citation Metrics

We found 1082 mentions in open access literature.

Listed below are recent publications. The full list is available at FDI Lab - SciCrunch.org.

R V, et al. (2025) In vitro and In silico investigation deciphering novel antifungal activity of endophyte Bacillus velezensis CBMB205 against Fusarium oxysporum. Scientific reports, 15(1), 684.

Chatterjee P, et al. (2025) A computational and structural approach to identify malignant nonsynonymous FOXM1 single nucleotide polymorphisms in triple-negative breast cancer. Scientific reports, 15(1), 964.

Lu S, et al. (2025) Cortisol regulates neonatal lung development via Smoothened. Respiratory research, 26(1), 27.

Liu T, et al. (2025) Deciphering the therapeutic effects of Xiyanping injection: insights into pulmonary and gut microbiome modulation, SerpinB2/PAI-2 targeting, and alleviation of influenza a virus-induced lung injury. Virology journal, 22(1), 19.

Wu Q, et al. (2025) Identification of Oligopeptides in the Distillates from Various Rounds of Soy Sauce-Flavored Baijiu and Their Effect on the Ester-Acid-Alcohol Profile in Baijiu. Foods (Basel, Switzerland), 14(2).

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).

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.

Fuochi V, et al. (2025) Antiviral efficacy of heparan sulfate and enoxaparin sodium against SARS-CoV-2. Archiv der Pharmazie, 358(1), e2400545.

Silva E, et al. (2025) Aqueous extracts of Moringa oleifera and Cinnamomum cassia as promising sources of antibiofilm compounds against mucoid and small colony variants of Pseudomonas aeruginosa and Staphylococcus aureus. Biofilm, 9, 100250.

Ao Y, et al. (2025) Cellular senescence-associated genes in rheumatoid arthritis: Identification and functional analysis. PloS one, 20(1), e0317364.

Shuvo AUH, et al. (2025) Evaluation of Xanthine Oxidase Inhibitors Febuxostat and Allopurinol on Kidney Dysfunction and Histological Damage in Two-Kidney, One-Clip (2K1C) Rats. Scientifica, 2025, 7932075.

Vitale RM, et al. (2025) Identification of Cannabidiolic and Cannabigerolic Acids as MTDL AChE, BuChE, and BACE-1 Inhibitors Against Alzheimer's Disease by In Silico, In Vitro, and In Vivo Studies. Phytotherapy research : PTR, 39(1), 233.

Summat R, et al. (2025) Phytomedicine Potential of Oroxylum indicum Root and Its Constituents: Targeting Alzheimer's Disease. Plants (Basel, Switzerland), 14(2).

Joshi R, et al. (2025) Exploring pyrazolines as potential inhibitors of NSP3-macrodomain of SARS-CoV-2: synthesis and in silico analysis. Scientific reports, 15(1), 767.

Haufe Y, et al. (2024) Symmetrical Bispyridinium Compounds Act as Open Channel Blockers of Cation-Selective Ion Channels. ACS pharmacology & translational science, 7(3), 771.

Lv MT, et al. (2024) In silico and in vitro analyses of a novel FoxO1 agonist reducing A? levels via downregulation of BACE1. CNS neuroscience & therapeutics, 30(3), e14140.

Zens B, et al. (2024) Lift-out cryo-FIBSEM and cryo-ET reveal the ultrastructural landscape of extracellular matrix. The Journal of cell biology, 223(6).

Shi F, et al. (2024) Integrated analysis of single cell-RNA sequencing and Mendelian randomization identifies lactate dehydrogenase B as a target of melatonin in ischemic stroke. CNS neuroscience & therapeutics, 30(5), e14741.

Schottlender G, et al. (2024) Bacterial cytochrome P450s: a bioinformatics odyssey of substrate discovery. Frontiers in microbiology, 15, 1343029.

Lin K, et al. (2024) Analgesic and anti-inflammatory effects of galangin: a potential pathway

to inhibit transient receptor potential vanilloid 1 receptor activation. The Korean journal of pain, 37(2), 151.