

# AutoDock Vina 1.2.0: New Docking Methods, Expanded

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Citation Report

#	ARTICLE	IF	CITATIONS
1	Interaction of (+)-Strebloside and Its Derivatives with Na <sup>+</sup> /K <sup>+</sup> -ATPase and Other Targets. <i>Molecules</i> , 2021, 26, 5675.	1.7	6
4	Identification of antiviral phytochemicals as a potential SARS-CoV-2 main protease (Mpro) inhibitor using docking and molecular dynamics simulations. <i>Scientific Reports</i> , 2021, 11, 20295.	1.6	24
5	Novel Anti-Hepatitis B Virus Activity of <i>Euphorbia schimperii</i> and Its Quercetin and Kaempferol Derivatives. <i>ACS Omega</i> , 2021, 6, 29100-29110.	1.6	22
6	Antidepressant-like effect of rosmarinic acid during LPS-induced neuroinflammatory model: The potential role of cannabinoid receptors/PPAR $\gamma$ signaling pathway. <i>Phytotherapy Research</i> , 2021, 35, 6974-6989.	2.8	15
7	Improving ligand ranking of AutoDock Vina by changing the empirical parameters. <i>Journal of Computational Chemistry</i> , 2022, 43, 160-169.	1.5	19
8	Kinetic Studies of Newly Patented Aminoalkanol Derivatives with Potential Anticancer Activity as Competitive Inhibitors of Prostate Acid Phosphatase. <i>International Journal of Molecular Sciences</i> , 2021, 22, 11761.	1.8	4
9	Antilymphoma Effect of Incomptine A: In Vivo, In Silico, and Toxicological Studies. <i>Molecules</i> , 2021, 26, 6646.	1.7	4
11	DockStream: a docking wrapper to enhance de novo molecular design. <i>Journal of Cheminformatics</i> , 2021, 13, 89.	2.8	24
12	Redesigning of the cap conformation and symmetry of the diphenylethyne core to yield highly potent pan-genotypic NS5A inhibitors with high potency and high resistance barrier. <i>European Journal of Medicinal Chemistry</i> , 2022, 229, 114034.	2.6	1
13	Multi-stage structure-based virtual screening approach towards identification of potential SARS-CoV-2 NSP13 helicase inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2022, 37, 563-572.	2.5	15
14	In-silico investigation of antibacterial herbal compounds in order to find new antibiotic against <i>Staphylococcus aureus</i> and its resistant subtypes. <i>Informatics in Medicine Unlocked</i> , 2022, 28, 100843.	1.9	9
16	NMR Detection and Structural Modeling of the Ethylene Receptor LeETR2 from Tomato. <i>Membranes</i> , 2022, 12, 107.	1.4	0
17	Inhibition of Collagenase Q1 of <i>Bacillus cereus</i> as a Novel Antivirulence Strategy for the Treatment of Skin Wound Infections. <i>Advanced Therapeutics</i> , 2022, 5, 2100222.	1.6	4
18	Docking and Molecular Dynamic of Microalgae Compounds as Potential Inhibitors of Beta-Lactamase. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1630.	1.8	7
19	Computational Analysis of Molnupiravir. <i>International Journal of Molecular Sciences</i> , 2022, 23, 1508.	1.8	28
20	Understanding the Anti-Diarrhoeal Properties of Incomptines A and B: Antibacterial Activity against <i>Vibrio cholerae</i> and Its Enterotoxin Inhibition. <i>Pharmaceuticals</i> , 2022, 15, 196.	1.7	4
21	Modeling glycosaminoglycan-protein complexes. <i>Current Opinion in Structural Biology</i> , 2022, 73, 102332.	2.6	16
22	New dimer and trimer of chalcone derivatives from anti-inflammatory and antinociceptive extracts of <i>Schinopsis brasiliensis</i> roots. <i>Journal of Ethnopharmacology</i> , 2022, 289, 115089.	2.0	3

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23	Network Pharmacology and Molecular Docking Elucidate the Pharmacological Mechanism of the OSTEOWONDER Capsule for Treating Osteoporosis. <i>Frontiers in Genetics</i> , 2022, 13, 833027.	1.1	2
24	In Silico Screening of Bioactive Compounds of Representative Seaweeds to Inhibit SARS-CoV-2 ACE2-Bound Omicron B.1.1.529 Spike Protein Trimer. <i>Marine Drugs</i> , 2022, 20, 148.	2.2	19
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26	Defining Diffuse Large B-Cell Lymphoma Immunotypes by CD8+ T Cells and Natural Killer Cells. <i>Journal of Oncology</i> , 2022, 2022, 1-13.	0.6	4
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29	Lotus Seed Green Embryo Extract and a Purified Glycosyloxyflavone Constituent, Narcissoside, Activate TRPV1 Channels in Dorsal Root Ganglion Sensory Neurons. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 3969-3978.	2.4	4
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37	In Silico Structure-Based Approach for Group Efficiency Estimation in Fragment-Based Drug Design Using Evaluation of Fragment Contributions. <i>Molecules</i> , 2022, 27, 1985.	1.7	2
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40	In silico vaccine design: A tutorial in immunoinformatics. <i>Healthcare Analytics</i> , 2022, 2, 100044.	2.6	18
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43	Phenolic Compound Ethyl 3,4-Dihydroxybenzoate Retards Drug Efflux and Potentiates Antibiotic Activity. <i>Antibiotics</i> , 2022, 11, 497.	1.5	5
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48	Assessment of antimicrobial and enzymes inhibition effects of <i>Allium kastambulense</i> with in silico studies: Analysis of its phenolic compounds and flavonoid contents. <i>Arabian Journal of Chemistry</i> , 2022, 15, 103810.	2.3	12
49	Ethylenediamine- $\beta$ -cyclodextrin modified graphene oxide nanocomposite membranes for highly efficient chiral separation of tryptophan and propranolol enantiomers. <i>Separation and Purification Technology</i> , 2022, 290, 120833.	3.9	15
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58	Genotoxic and cytotoxic effects of pethoxamid herbicide on <i>Allium cepa</i> cells and its molecular docking studies to unravel genotoxicity mechanism. <i>Environmental Science and Pollution Research</i> , 2022, 29, 63127-63140.	2.7	13
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61	CB-Dock2: improved protein-ligand blind docking by integrating cavity detection, docking and homologous template fitting. <i>Nucleic Acids Research</i> , 2022, 50, W159-W164.	6.5	219
62	fastDRH: a webserver to predict and analyze protein-ligand complexes based on molecular docking and MM/PB(GB)SA computation. <i>Briefings in Bioinformatics</i> , 2022, 23, .	3.2	34
63	Interaction of <i>Pelargonium sidoides</i> Compounds with Lactoferrin and SARS-CoV-2: Insights from Molecular Simulations. <i>International Journal of Environmental Research and Public Health</i> , 2022, 19, 5254.	1.2	5
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66	Semi-Synthesis of N-Aryl Amide Analogs of Piperine from <i>Piper nigrum</i> and Evaluation of Their Antitrypanosomal, Antimalarial, and Anti-SARS-CoV-2 Main Protease Activities. <i>Molecules</i> , 2022, 27, 2841.	1.7	10
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69	Accelerating AutoDock Vina with GPUs. <i>Molecules</i> , 2022, 27, 3041.	1.7	28
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74	Antimalarial potential of naphthalene-sulfonic acid derivatives: Molecular electronic properties, vibrational assignments, and in-silico molecular docking studies. <i>Journal of Molecular Structure</i> , 2022, 1264, 133298.	1.8	76
75	Regulation of $\beta$ -Disaccharide Accumulation by $\beta$ -Glucosidase Inhibitors to Enhance Cellulase Production in <i>Trichoderma reesei</i> . <i>Fermentation</i> , 2022, 8, 232.	1.4	6
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84	Optimization of pyrazolo[1,5-a]pyrimidine based compounds with pyridine scaffold: Synthesis, biological evaluation and molecular modeling study. <i>Arabian Journal of Chemistry</i> , 2022, 15, 104015.	2.3	12
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87	Synthesis, In Vitro Antiproliferative Activity, and In Silico Evaluation of Novel Oxiranyl-Quinoxaline Derivatives. <i>Pharmaceuticals</i> , 2022, 15, 781.	1.7	3
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94	AI-Based Protein Structure Prediction in Drug Discovery: Impacts and Challenges. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3142-3156.	2.5	36
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107	Molecular Modeling of ABHD5 Structure and Ligand Recognition. <i>Frontiers in Molecular Biosciences</i> , 0, 9, .	1.6	4
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117	Influence of Association on Binding of Disaccharides to YKL-39 and hHyal-1 Enzymes. <i>International Journal of Molecular Sciences</i> , 2022, 23, 7705.	1.8	0

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