AutoDock4 and AutoDockTools4: Automated docking with selective receptor flexibility

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543	Coumarin-based derivatives targeting Trypanosoma cruzi cruzain and Trypanosoma brucei cathepsin L-like proteases.	0
542	Structural and functional characterization of 1-deoxy-D-xylulose-5-phosphate synthase (DXS) from Acinetobacter baumannii: identification of promising lead molecules from virtual screening, molecular docking and molecular dynamics simulations. 1-14	0
541	GC/MS Analysis, Cytotoxicity, and Antiviral Activities of Annona glabra Hexane Extract Supported by In Silico Study. **2023**, 28, 1628	0
540	Inhibitory effect and underlying mechanism of cinnamon and clove essential oils on Botryosphaeria dothidea and Colletotrichum gloeosporioides causing rots in postharvest bagging-free apple fruits. 14,	0
539	Scalable Inhibitors of the Nsp3–Nsp4 Coupling in SARS-CoV-2. **2023**, 8, 5349-5360	0
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530	Synthesis and Spectroscopic Characterization of Novel Pyridine-based N-acyl Hydrazone Derivatives and Molecular Docking Studies on Glucosamine-6-Phosphate. **2023**, 13, 135-152	0
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527	Biophysical insights on the interaction of anticoagulant drug dicoumarol with calf thymus-DNA: deciphering the binding mode and binding force with thermodynamics. 1-12	0
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460	Synthesis, in silico studies and investigations on antimicrobial, antimalarial activities of p-toluenesulphonamoyl Leu-Gly dipeptide carboxamide derivatives. **2023**, 1285, 135529	0
459	Design, synthesis and molecular docking studies of 5,6-difluoro-1H-benzo[d]imidazole derivatives as effective binders to GABAA receptor with potent anticonvulsant activity. **2023**, 1285, 135502	0
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443	Design, synthesis and biological evaluation of purine-based derivatives as novel JAK2/BRD4(BD2) dual target inhibitors. **2023**, 132, 106386	0
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417	Comparative Genomics of Histoplasma capsulatum and Prediction of New Vaccines and Drug Targets. **2023**, 9, 193	1
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411	Structural Basis for Agonistic Activity and Selectivity toward Melatonin Receptors hMT1 and hMT2. **2023**, 24, 2863	1
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399	Universal Approach to De Novo Drug Design for Target Proteins Using Deep Reinforcement Learning. **2023**, 8, 5464-5474	1
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387	Exploring anticancer potential of nintedanib conjugated magnetic nanoparticles: In-vitro and in-silico studies. **2023**, 81, 104213	0
386	Dinuclear Phenoxo-Bridged Nickel(II) and Copper(II) Complexes of Phenolate-Based Tripodal Ligand: Theoretical and Experimental Insights. 1-20	0
385	Targeting Acanthamoeba proteins interaction with flavonoids of Propolis extract by in vitro and in silico studies for promising therapeutic effects. 11, 1274	0
384	Phlorizin isolated from seagrass Syringodium isoetifolium inhibits diethylnitrosamine and carbon tetrachloride-induced hepatocellular carcinoma in BALB/c mice. **2023**, 155, 1-15	0
383	N-Amidation of Nitrogen-Containing Heterocyclic Compounds: Can We Apply Enzymatic Tools?. **2023**, 10, 222	0
382	Identification of pyrrolizidine alkaloids and flavonoid glycosides through HR-LCMS/MS analysis, biological screening, DFT and molecular docking studies on Heliotropium dasycarpum Ledeb.. **2023**, 16, 104655	0
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367	Resveratrol analog, triacetylresveratrol, a potential immunomodulator of lung adenocarcinoma immunotherapy combination therapies. 12,	0
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169	Synthesis, Characterization and Structural Studies of Novel Pyrazoline Derivatives as Potential Inhibitors of NAD+ Synthetase in Bacteria and Cytochrome P450 51 in Fungi. **2023**, 8,	0
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167	Rigid Scaffolds are Promising for Designing Macrocyclic Kinase Inhibitors.	0
166	Synthesis, characterization, docking and antimicrobial studies of binol based amide linked symmetrical bistriazoles. **2023**, 100, 100973	0
165	Combination of furosemide, gold, and dopamine as a potential therapy for breast cancer. **2023**, 23,	0
164	Efficient screening of protein-ligand complexes in lipid bilayers using LoCoMock score. **2023**, 37, 217-225	0
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162	Computer-Aided Drug Design and Synthesis of Rhenium Clotrimazole Antimicrobial Agents. **2023**, 12, 619	0
161	Purification and activity evaluation of novel anti-inflammatory peptides from pearl oyster (Pinctada martensii) hydrolysates.	0
160	Drug repurposing for Mpox: Discovery of small molecules as potential inhibitors against DNA-dependent RNA polymerase using molecular modeling approach.	0
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155	Unraveling the Aquaporin-3 Inhibitory Effect of Rottlerin by Experimental and Computational Approaches. **2023**, 24, 6004	0
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134	Investigation of the Entry Pathway and Molecular Nature of 1 Receptor Ligands. **2023**, 24, 6367	0
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118	Synthesis of Novel 2,9-Disubstituted-6-morpholino Purine Derivatives Assisted by Virtual Screening and Modelling of Class I PI3K Isoforms. **2023**, 15, 1703	0
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113	Green biosynthesis of rare DHA-phospholipids by lipase-catalyzed transesterification with edible algal oil in solvent-free system and catalytic mechanism study. 11,	0
112	Development of New Targeted Nanotherapy Combined with Magneto-Fluorescent Nanoparticles against Colorectal Cancer. **2023**, 24, 6612	0
111	Quantitative structure activity relationship studies of androgen receptor binding affinity of endocrine disruptor chemicals with index of ideality of correlation, their molecular docking, molecular dynamics and ADME studies. 1-16	0
110	Therapeutic Role of DGJ (1-deoxygalactonojirimycin) in Fabry Disease: Theoretical Insights. **2023**, 8,	0
109	Synthesis, X-ray Crystal Structure, Anticancer, Hirshfeld Surface Analysis, DFT, TD-DFT, ADMET, and Molecular Docking of 3-Phenyl-1,2,4-triazolo[3,4-h]-13,4-thiaza-11-crown-4. **2023**, 28, 3166	0
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101	Biologically potent organotin(iv) complexes of N-acetylated □-amino acids with spectroscopic, X-ray powder diffraction and molecular docking studies. **2023**, 13, 10768-10789	0
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83	Exploring polyamine interactions and binding pockets in SARS-CoV-2 ORF3a. **2023**, 122, 108487	0
82	Green Synthesis, Antimycobacterial Evaluation and Molecular Docking Studies of Novel 2,3-Dihydro-1H-pyrazol-4-ylnaphthalene-1,4-diones. **2023**, 135556	0
81	Comparative modeling and enzymatic affinity of novel haloacid dehalogenase from Bacillus megaterium strain BHS1 isolated from alkaline Blue Lake in Turkey. 1-14	0
80	Tool and Techniques on Computer-Aided Drug Design for Targeted Cancer Therapy. **2023**, 781-829	0
79	Molecular interactions, binding stability, and synergistic inhibition on Acetylcholinesterase activity of Safranin O in combination with Quercetin and Gallic acid: In vitro and in silico study. **2023**, 1286, 135562	0
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61	Identification of Potential p38□Inhibitors via In Silico Screening, In Vitro Bioassay and Molecular Dynamics Simulation Studies. **2023**, 24, 7360	0
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56	Drug-target interaction prediction based on spatial consistency constraint and graph convolutional autoencoder. **2023**, 24,	0
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51	Discovery of Highly Potent HDAC8 PROTACs with Anti-tumor Activity. **2023**, 106546	0
50	In Silico Analysis of Anti-Inflammatory and Antioxidant Properties of Bioactive Compounds from Crescentia cujete L.. **2023**, 28, 3547	0
49	Study on molecular mechanisms of destabilizing A□(1₴42) protofibrils by licochalcone A and licochalcone B using molecular dynamics simulations. **2023**, 108500	0
48	Zeolite@-Ag-S-CH2-COOH catalyzed synthesis of bis-cyclohexenones and their antibacterial evaluation and molecular docking study. **2023**, 122710	0

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46	Small Molecule Attenuates Bacterial Virulence by Targeting Conserved Response Regulator.	0
45	The Cytotoxicity Profile, Apoptosis Mechanism, and Molecular Docking Studies of a Series of Benzimidazolium Derivative Morpholine-Substituted Ag(I) Heterocyclic Carbene Complexes.	0
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43	Identification of Novel Compounds Inhibiting the Kinase Activity of the CDK5/p25 Complex via Direct Binding to p25.	0
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41	Solvent effect on molecular, electronic parameters, topological analysis and Fukui function evaluation with biological studies of Imidazo [1, 2-a] pyridine-8-carboxylic acid. **2023**, 121863	0
40	Potential profound fluctuation in tacrolimus concentration on consumption of pomegranate rind extract: A Pharmacokinetic Experiment. 14,	0
39	Catalytic resilience of multicomponent aromatic ring-hydroxylating dioxygenases in Pseudomonas for degradation of polycyclic aromatic hydrocarbons. **2023**, 39,	0
38	Structure based virtual screening, molecular dynamic simulation to identify the oxadiazole derivatives as inhibitors of Enterococcus D-Ala-D-Ser ligase for combating vancomycin resistance. **2023**, 106965	0
37	Study of the binding interaction of salmon sperm DNA with nintedanib, a tyrosine kinase inhibitor using multi-spectroscopic, thermodynamic, and in silico approaches. 1-11	0
36	Allosteric modulation of GluN1/GluN3 NMDA receptors by GluN1-selective competitive antagonists. **2023**, 155,	0
35	Concussion Diagnostics: A New Diagnostic Approach Using PET Technology. **2023**, 4,	0
34	Molecular Structure, Hydrogen Bonding Interactions and Docking Simulations of Nicotinamide (Monomeric and Trimeric Models) by Using Spectroscopy and Theoretical Approach. 1-19	0
33	Insight into the phytochemical profile and antimicrobial activities of Amomum subulatum and Amomum xanthioides: an in vitro and in silico study. 14,	0
32	Biocatalytic Access to Chiral Benzazepines Using Imine Reductases. 6185-6194	0
31	Repurposing of phytocompounds-derived novel bioactive compounds possessing promising anticancer and cancer therapeutic efficacy through molecular docking, MD simulation, and drug-likeness/ADMET studies. **2023**, 201-222	0
30	Synthesis, Spectroscopic, Crystallographic, Quantum and Molecular Docking Investigations of cis-4,5-diphenylimidazolidine-2-thione. **2023**, 135633	0

29	Characterizing Soft Matter Self-Assembly and Material Properties with Advanced Molecular Dynamics and Data-Driven Methods. **2023**, 1197-1220	0
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22	Investigation of the inhibitory behavior of XFE and mitoxantrone molecules in interaction with AKT1 protein: a molecular dynamics simulation study. **2023**, 29,	0
21	Homology Modeling, Screening, and Identification of Potential FOXO6 Inhibitors Curtail Gastric Cancer Progression: an In Silico Drug Repurposing Approach.	0
20	Molecular dynamics simulation of the interaction of a raspberry polygalacturonase (RiPG) with a PG inhibiting protein (RiPGIP) isolated from ripening raspberry (Rubus idaeus cv. Heritage) fruit as a model to understand proteins interaction during fruit softening. **2023**, 108502	0
19	In Silico Interactions of Natural and Synthetic Compounds with Key Proteins Involved in Alzheimer's Disease: Prospects for Designing New Therapeutics Compound.	0
18	The signal conversion strategy using the lytic transglycosylase Cag4-double nanoporous gold co-catalysis for the rapid screening of drugs against Helicobacter pylori infection. **2023**, 115345	0
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15	Development of quinazolinone and vanillin acrylamide hybrids as multi-target directed ligands against Alzheimer's disease and mechanistic insights into their binding with acetylcholinesterase. 1-18	0
14	VirtualFlow 2.0 - The Next Generation Drug Discovery Platform Enabling Adaptive Screens of 69 Billion Molecules.	0
13	Uni-Dock: GPU-Accelerated Docking Enables Ultralarge Virtual Screening.	0
12	In-silico method in predicting potential targets from marine natural products in the waters of South Sulawesi, Indonesia. **2023**,	0

11	Proximity-Induced Nucleic Acid Degrader (PINAD) Approach to Targeted RNA Degradation Using Small Molecules.	0
10	Experimental and Theoretical Investigation of Inclusion Complexes of β-Cyclodextrin with Fingolimod. **2023**, 97, 469-476	0
9	Targeting the vital non-structural proteins (NSP12, NSP7, NSP8 and NSP3) from SARS-CoV-2 and inhibition of RNA polymerase by natural bioactive compound naringenin as a promising drug candidate against COVID-19. **2023**, 1287, 135642	0
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7	The difference in the cellular uptake of tocopherol and tocotrienol is influenced by their affinities to albumin. **2023**, 13,	0
6	Discovery of pyrimidine-5-carboxamide derivatives as novel salt-inducible kinases (SIKs) inhibitors for inflammatory bowel disease (IBD) treatment. **2023**, 256, 115469	0
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4	Genomic analyses provide insights into the polyploidization-driven herbicide adaptation in Leptochloa weeds.	0
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2	Exploring the Antioxidant and Anti-Inflammatory Potential of Wilckia maritima: In Vitro and In Silico Investigations. **2023**, 11, 1497	0
1	Spectroscopic analysis of 2-amino-1-naphthalenesulfonic acid, molecular docking, and evaluation of the electronic properties of several solvents. 1-20	0