Automated docking using a Lamarckian genetic algorithm and an empirical binding free energy function

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630	In-silico interactions of eugenol and temephos with metabolic detoxifying enzymes of Aedes aegypti (Diptera: Culicidae). **2022**, 42, 1987	
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482	The Progress of Business Analytics and Knowledge Management for Enterprise Performance Using Artificial Intelligence and Man-machine Coordination. **2022**, 30, 0-0	1
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269	A New Naphthopyran Derivative Combines c-Myb Inhibition, Microtubule-Targeting Effects, and Antiangiogenic Properties.	1
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253	A Comprehensive Study to Unleash the Putative Inhibitors of Serotype2 of Dengue Virus: Insights from an In Silico Structure-Based Drug Discovery.	0
252	Identification of Potential Antiviral Disaccharide Leading Compounds against SARS-CoV-2 through A Computer Aided Study.	0
251	Biophysical insights into the binding capability of Cu(II) schiff base complex with BSA protein and cytotoxicity studies against SiHa. **2022**, e11345	0
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246	Phytochemical Variability, In Vitro and In Vivo Biological Investigations, and In Silico Antibacterial Mechanisms of Mentha piperita Essential Oils Collected from Two Different Regions in Morocco. **2022**, 11, 3466	0
245	Characterization of the interaction of metal-protoporphyrins photosensitizers with lactoglobulin. **2022**, 106918	0
244	Microwave assisted synthesis of 2-amino-4-chloro-pyrimidine derivatives: Anticancer and computational study on potential inhibitory action against COVID-19. **2022**, 15, 104366	1
243	Dual modulators of aggregation and dissociation of amyloid beta and tau: In vitro, in vivo, and in silico studies of Uncaria rhynchophylla and its bioactive components. **2022**, 156, 113865	0
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235	Photophysical evaluation on the electronic properties of synthesized biologically significant pyrido fused imidazo[4,5-c]quinolines. **2023**, 287, 122081	0
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229	Guava Leaf Essential Oil as a Potent Antioxidant and Anticancer Agent: Validated through Experimental and Computational Study. **2022**, 11, 2204	1
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227	Biochemical Targets and Molecular Mechanism of Ginsenoside Compound K in Treating Osteoporosis Based on Network Pharmacology. **2022**, 23, 13921	0
226	7,8-Dihydroxycoumarin derivatives: In silico molecular docking and in vitro anticholinesterase activity. **2022**, 134535	0
225	The essential oil from Drimys winteri possess activity: Antioxidant, theoretical chemistry reactivity, antimicrobial, antiproliferative and chemical composition. 1,	0
224	Binding Properties of Photosynthetic Herbicides: Photosynthetic Activity and Molecular Docking Approach towards 1,4-Dihydropyridines Derivatives.	0

223	Synthesis, Spectroscopic, Computational, Biological and Molecular docking studies on 3-allyl 2,6-diaryl piperidin-4-ones. **2022**, 7,	0
222	An immunoinformatic approach employing molecular docking and molecular dynamics simulation for evaluation of l-asparaginase produced by Bacillus velezensis. 1-15	0
221	Amine-Reactive BODIPY Dye: Spectral Properties and Application for Protein Labeling. **2022**, 27, 7911	0
220	Antiviral activity of Turbinaria ornata against white spot syndrome virus in freshwater crab (Paratelphusa hydrodromous).	0
219	Novel Uracil-Based Inhibitors of Acetylcholinesterase with Potency for Treating Memory Impairment in an Animal Model of Alzheimer Disease. **2022**, 27, 7855	0
218	Virtual screening and zebrafish models in tandem, for drug discovery and development.	0
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216	Structural and spectroscopic analysis, solvent effect on the molecular properties and molecular docking of trans-2-(4-(dimethylamino) styryl)-benzothiazole. **2022**, 140192	0
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214	Characterization of binding properties of ephedrine derivatives to human alpha-1-acid glycoprotein. **2022**, 106333	0
213	Identification of Active Compounds against Melanoma Growth by Virtual Screening for Non-Classical Human DHFR Inhibitors. **2022**, 23, 13946	0
212	Novel 1,2,4-triazoles derived from Ibuprofen: synthesis and in vitro evaluation of their mPGES-1 inhibitory and antiproliferative activity.	0
211	Icotinib derivatives as tyrosine kinase inhibitors with anti-esophageal squamous carcinoma activity. 13,	0
210	Computational drug discovery under RNA times. 1-21	0
209	Exploring the dual effect of novel 1,4-diarylpyranopyrazoles as antiviral and anti-inflammatory for the management of SARS-CoV-2 and associated inflammatory symptoms. **2022**, 106255	3
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205	In silico and docking studies on the binding activities of Keap1 of antioxidant compounds in non-oilseed legumes. **2022**, 104414	0
204	The Charge Transfer Complex between 2, 3-diamino-5-bromopyridine and Chloranilic acid: Preparation, Spectroscopic Characterization, DNA binding, and DFT/PCM analysis. **2022**, 99, 100799	0
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201	Interaction between C-Reactive Protein and Phytochemical(s) from <i>Calotropis procera</i>: An Approach on Molecular Docking. 61, 43-55	1
200	In vitro and in silico investigation of inhibitory activities of 3-arylcoumarins and 3-phenylazo-4-hydroxycoumarin on MAO isoenzymes.	0
199	S-allylCysteine Ester/Caffeic Acid Amide Hybrids as Promising Antiprotozoal Candidates: Synthesis, Biological Evaluation and Molecular Modeling Studies. 58,	0
198	Improving the kinetic resolution of rac-2-(diphenylthiophosphinoferrocene) methanol catalyzed by Thermomyces lanuginosus lipase immobilized on immobead-150. **2023**, 535, 112867	0
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196	Computational insights for predicting the binding and selectivity of peptidomimetic plasmepsin IV inhibitors against cathepsin D. **2022**, 13, 602-614	0
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193	One-pot reproducible Sonosynthesis of trans-[Br(N?N)Cu(μBr)2Cu(N?N)Br] dimer:[HBr S(9)] synthons, spectral, DFT/XRD/HSA, thermal, docking and novel LOX/COX enzyme inhibition. **2023**, 1275, 134626	0
192	Synthesis, crystal structure, theoretical chemical activitiy, electrophilicity-based charge transfer (ECT) with DNA bases and molecular docking studies of 2-amino-4-(2,4-dimethoxyphenyl)-5,6-dihydrobenzo[H]quinoline-3-carbonitrile. **2023**, 1275, 134641	0
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190	Understanding the in silico aspects of bacterial catabolic cascade for styrene degradation.	0
189	Understanding hypocholesterolemic activity of soy isoflavones: Completing the puzzle through computational simulations. 1-7	0
188	Entropy-based Lamarckian Quantum-behaved Particle Swarm Optimization for Flexible Ligand Docking.	0

187	Synthesis and study of the biological activity of thiourea-containing amiridine derivatives as potential multi-target drugs for the treatment of Alzheimer disease. **2022**, 71, 2404-2415	0
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184	Spectroscopic, computational DFT, in vitro, and molecular docking investigations of newly isolated 2, 3, 9, and 10-tetrahydroacridin-3-one from the methanolic extract of nilavembu kudineer chooranam.	0
183	New Ni(II) and Pd(II) complexes bearing derived sulfa drug ligands: synthesis, characterization, DFT calculations, and in silico and in vitro biological activity studies.	0
182	Zinc sulfide nano aqua formulation as antifungal nanopriming agent against phytopathogens of paddy seeds: in silico, in vitro and seed treatment studies.	1
181	An in-silico investigation of fluoride ions impact on pancreatic lipase.	0
180	Isolation, purification and biochemical characterization of Conopomorpha cramerella farnesol dehydrogenase.	0
179	Design, synthesis, characterization and analysis of anti-inflammatory properties of novel N-(benzo[d]thiazol-2-yl)-2-[phenyl(2-(piperidin-1-yl) ethylamino] benzamides and N-(benzo[d]thiazol-2-yl)-2-[phenyl (2-morpholino) ethylamino] benzamides derivatives through in vitro and in silico approach.	0
178	amino carbonyl derivatives: Synthesis, Molecular Docking, ADMET, Molecular Dynamic and Herbicidal studies.. **2022**, 7,	3
177	Alpha-Lipoic Acid and Its Enantiomers Prevent Methemoglobin Formation and DNA Damage Induced by Dapsone Hydroxylamine: Molecular Mechanism and Antioxidant Action. **2023**, 24, 57	0
176	(-)-Epigallocatechin-3-gallate Directly Binds Cyclophilin D: A Potential Mechanism for Mitochondrial Protection. **2022**, 27, 8661	0
175	Molecular docking, ADMET profiling of gallic acid and its derivatives (N-alkyl gallamide) as an anti-breast cancer agent. 11, 1453	0
174	Design of ionic liquids containing glucose and choline as drug carriers, finding the link between QM and MD studies. **2022**, 12,	0
173	Discovery of anti-colon cancer agents targeting wild-type and mutant p53 using computer-aided drug design. 1-19	0
172	SARS-CoV-2 main protease inhibitors: Structure-based enhancement to anti-viral pre-clinical GC376 encourages further development.	0
171	Chemical Survey of Three Species of the Genus Rauhia Traub (Amaryllidaceae). **2022**, 11, 3549	2
170	Molecular spectroscopic and docking analysis of the interaction of fluorescent thiadicarbocyanine dye with biomolecule bovine serum albumin. 1-11	0

169	Ligand-guided investigation of a series of formamidine-based thiuram disulfides as potential dual-inhibitors of COX-1 and COX-2.	0
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165	Comprehensive Survey of Consensus Docking for High-Throughput Virtual Screening. **2023**, 28, 175	0
164	Decoding the binding interaction of steroidal pyridines with bovine serum albumin using spectroscopic and molecular docking techniques. **2022**, 109156	0
163	3D-QSAR, drug-likeness, ADMET prediction, and molecular docking studies in silico of novel 5-oxo-1-thioxo-4,5-dihydro-1H-thiazolo[3,4-a]quinazoline derivatives as MALT1 protease inhibitors for the treatment of B cell lymphoma.	1
162	Absolute binding free energies of the antiviral peptide ATN-161 with protein targets of SARS-CoV-2. 1-12	0
161	A new serotonin 2A receptor antagonist with potential benefits in non-alcoholic fatty liver disease. **2022**, 121315	0
160	Evaluating Khaya senegalensis for dipeptidyl peptidase-IV inhibition using in vitro analysis and molecular dynamic simulation of identified bioactive compounds.	0
159	A Biologically Active Chromone from Bomarea setacea (alstroemeriaceae): Leishmanicidal, Antioxidant and Multilevel Computational Studies. **2022**, 7,	0
158	In Vitro Study of Cytotoxic Mechanisms of Alkylphospholipids and Alkyltriazoles in Acute Lymphoblastic Leukemia Models. **2022**, 27, 8633	0
157	Destabilizers of the thymidylate synthase homodimer accelerate its proteasomal degradation and inhibit cancer growth. 11,	0
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155	Investigation of the Interaction between Aloe´vera Anthraquinone Metabolites and c-Myc and C-Kit G-Quadruplex DNA Structures. **2022**, 23, 16018	0
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153	The Impact of Software Used and the Type of Target Protein on Molecular Docking Accuracy. **2022**, 27, 9041	0
152	Scanning aldoxime dehydratase sequence space and characterization of a new aldoxime dehydratase from Fusarium vanettenii. **2022**, 110187	1

151	Determining the stoichiometry and binding constant of Lamotrigine with human serum albumin using voltammetry analysis and molecular modeling. 1-8	0
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149	Experimental and Theoretical Investigations of Argania spinosa Extracts on the Antioxidant Activity and Mild Steel Corrosion Inhibition in 1 M HCl. **2022**, 12, 12641	0
148	Efficient Antibacterial/Antifungal Activities: Synthesis, Molecular Docking, Molecular Dynamics, Pharmacokinetic, and Binding Free Energy of Galactopyranoside Derivatives. **2023**, 28, 219	4
147	Intestinal epithelium penetration of liraglutide via cholic acid pre-complexation and zein/rhamnolipids nanocomposite delivery. **2023**, 21,	0
146	Electrochemical, Ultrasensitive, and Selective Detection of Nitrite and H2O2: Novel Macrostructured Phthalocyanine with Composite MWCNTs on a Modified GCE.	0
145	Synthesis, crystal structure, DFT, Hirshfeld surface analysis, energy framework, docking and molecular dynamic simulations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one as anticancer agent. 1-20	0
144	Pyridine derivatives complexes of Co (II) and Ni (II) 3-Bromobenzoates: Crystal Structure, in silico Anti-SARS-CoV-2 potential, Serum Albumin Binding Properties and Cytotoxicity.	0
143	Molecular Insights into Substrate Binding of the Outer Membrane Enzyme OmpT. **2023**, 13, 214	0
142	Chetomin, a SARS-CoV-2 3C-like Protease (3CLpro) Inhibitor: In Silico Screening, Enzyme Docking, Molecular Dynamics and Pharmacokinetics Analysis. **2023**, 15, 250	0
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140	Butein Inhibits the Glycation of Crystallin: An Approach in Prevention of Retinopathy.	0
139	Structural Investigation of Beta-Cyclodextrin Complexes with Cannabidiol and Delta-9-Tetrahydrocannabinol in 1:1 and 2:1 Host-Guest Stoichiometry: Molecular Docking and Density Functional Calculations. **2023**, 24, 1525	0
138	Design, synthesis, anti-acetylcholinesterase evaluation and molecular modelling studies of novel coumarin-chalcone hybrids. 1-13	0
137	Modes of action of lysophospholipids as endogenous activators of the TRPV4 ion channel.	0
136	Carbohydrate-Small Molecule Hybrids as Lead Compounds Targeting IL-6 Signaling. **2023**, 28, 677	0
135	Assessment of Neurotoxic Effects of Oxycodone and Naloxone in SH-SY5Y Cell Line. **2023**, 24, 1424	0
134	Neural Networks in the Design of Molecules with Affinity to Selected Protein Domains. **2023**, 24, 1762	0

133	In silico insights into procathepsin S maturation mediated by glycosaminoglycans. **2023**, 108406	0
132	Exploration of phytochemicals and probing potential effects of Priva cordifolia active extract on PACAP 38 and its nociceptor in the human trigeminovascular system. **2023**, 13,	0
131	Syntheses, Structural Characterization, and Cytotoxicity Assessment of Novel Mn(II) and Zn(II) Complexes of Aroyl-Hydrazone Schiff Base Ligand.	0
130	In Silico Analysis of a Drosophila Parasitoid Venom Peptide Reveals Prevalence of the Cation–Polar–Cation Clip Motif in Knottin Proteins. **2023**, 12, 143	0
129	A Schiff Base with Polymorphic Structure (Z? = 2): Investigations with Computational Techniques and in Silico Predictions. 1-26	0
128	Antileishmanial Activity of Clinanthus milagroanthus S. Leiva & Meerow (Amaryllidaceae) Collected in Peru. **2023**, 12, 322	0
127	Investigation of the interactions of HSA and SARS-CoV-2 papain-like protease against eugenol for novel COVID-19 drug discovery: spectroscopic and insilico study. 1-10	0
126	Exploiting HOPNO-dicopper center interaction to development of inhibitors for human tyrosinase. **2023**, 248, 115090	0
125	Design, synthesis and antifungal activity of novel pyrazole amides derivates. **2023**, 1277, 134881	0
124	Spectral studies, crystal structures, DNA binding, and anticancer potentials of Pd(II) complexes with iminophosphine ligands: Experimental and computational methods. **2023**, 547, 121368	0
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121	An Approach to Antifungal Efficacy through Well Diffusion Analysis and Molecular Interaction Profile of Polyherbal Formulation. **2022**, 15, 2069-2084	0
120	Design, Synthesis, Characterization, and Analysis of Antimicrobial Property of Novel Benzophenone Fused Azetidinone Derivatives through In Vitro and In Silico Approach. **2023**, 45, 92-109	0
119	Modelación estructural de la proteína de la cápside del virus a de la papa (PVA, <i>Potyvirus</i>). **2017**, 33, 75-84	0
118	Small Molecules Targeting the RNA-Binding Protein HuR Inhibit Tumor Growth in Xenografts. **2023**, 66, 2032-2053	0
117	Exploration of the Product Specificity of chitosanase CsnMY002 and Mutants Using Molecular Dynamics Simulations. **2023**, 28, 1048	0
116	Conjugates of Tacrine and Salicylic Acid Derivatives as New Promising Multitarget Agents for Alzheimer's Disease. **2023**, 24, 2285	0

115	Novel 3,9-Disubstituted Acridines with Strong Inhibition Activity against Topoisomerase I: Synthesis, Biological Evaluation and Molecular Docking Study. **2023**, 28, 1308	0
114	Identification of thrombin inhibiting antithrombin-III like protein from Punica granatum using in silico approach and in´vitro validation of thrombin inhibition activity in crude protein. 1-13	0
113	In silico Identification of Triclosan Derivatives as Potential Inhibitors of Mutant Mycobacterium tuberculosis InhA.	0
112	Novel Benzo[4,5]imidazo[1,2-a]pyrimidine derivatives as selective Cyclooxygenase-2 Inhibitors: Design, synthesis, docking studies, and biological evaluation.	0
111	Interaction of copper potential metallodrugs with TMPRSS2: A comparative study of docking tools and its implications on COVID-19. 11,	0
110	Divulging the Intricacies of Crosstalk Between NF-kB and Nrf-2/Keap1 Pathway in the Treatment of Arthritis by Dimethyl Fumarate.	1
109	Repulsive Scaling Replica Exchange Molecular Dynamics in Modeling Protein-Glycosaminoglycan Complexes. **2023**, 153-167	0
108	The Effect of Alkali Iodide Salts in the Inclusion Process of Phenolphthalein in Cyclodextrin: A Spectroscopic and Theoretical Study. **2023**, 28, 1147	0
107	Molecular Docking in the Study of Ligand-Protein Recognition: An Overview.	0
106	Design, Synthesis and Biological Evaluation of Conjugates of 3-O-Descladinose-azithromycin and Nucleobases against rRNA A2058G- or A2059G-Mutated Strains. **2023**, 28, 1327	0
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103	Druggable sites identification in Streptococcus mutans VicRK system evaluated by catechols. 1-16	0
102	MetaDOCK: A Combinatorial Molecular Docking Approach.	0
101	Interaction mechanisms of the binding of polychlorinated biphenyls to thyroid hormone transporters revealed based on quantum chemistry and spectroscopy. **2023**, 1281, 135104	0
100	Combined theoretical and experimental insights on DNA and BSA binding interactions of Cu(ii) and Ni(ii) complexes along with the DPPH method of antioxidant assay and cytotoxicity studies. **2023**, 13, 7632-7644	0
99	Catalytic Mechanism of Pyridoxal 5?-Phosphate-Dependent Aminodeoxychorismate Lyase: A Computational QM/MM Study. **2023**, 63, 1313-1322	0
98	Hoop layouts optimization for vibration reduction of L-shaped pipeline based on substructure-analytical model and genetic algorithm. **2023**, 45,	0

97	Machine learning-enabled globally guaranteed evolutionary computation.	0
96	New ferrocene integrated amphiphilic guanidines: Synthesis, spectroscopic elucidation, DFT calculation and in vitro □amylase and □glucosidase inhibition combined with molecular docking approach. **2023**, 9, e14919	0
95	Antiviral effect of melatonin on Japanese encephalitis virus infection involves inhibition of neuronal apoptosis and neuroinflammation in SH-SY5Y cells. **2023**, 13,	0
94	SCEOMOO: A novel Subspace Clustering approach using Evolutionary algorithm, Off-spring generation and Multi-Objective Optimization. **2023**, 139, 110185	0
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92	DNA-binding affinity and molecular docking studies of the PEGylated binuclear palladacycle, BTC2, an efficient metallodrug against triple-negative breast cancer. **2023**, 243, 112191	0
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89	Quantum chemical, spectroscopic and molecular docking studies on methyl 2-chloro-6-methyl pyridine-4-carboxylate: A potential inhibitor for irritable bowel syndrome. **2023**, 294, 122544	0
88	Molecular structure, spectral, computational, IEFPCM investigation, and topological study on the biologically potent; cardiotonic drug 2-chloroquinolin-3-amine with structural optimization. **2023**, 6, 100193	0
87	Rational engineering of glycosaminoglycan-based Dickkopf-1 scavengers to improve bone regeneration. **2023**, 297, 122105	0
86	Synthesis, characterization and antimicrobial properties of silver complexes derived from 5,6-Dimethylbenzimidazol-2-ylidene. **2023**, 237, 116383	0
85	New palladium (II) complexes from halogen substituted Schiff base ligands: Synthesis, spectroscopic, biological activity, density functional theory, and molecular docking investigations. **2023**, 552, 121505	0
84	Design, synthesis and evaluation of benzo[cd]indol-2(1H)-one-donepezil hybrids as cholinesterase inhibitors and living cell imaging agents. **2023**, 1285, 135511	0
83	Design and development of novel spiro-oxindoles as potent antiproliferative agents using quantitative structure activity based Monte Carlo method, docking molecular, molecular dynamics, free energy calculations, and pharmacokinetics /toxicity studies. **2023**, 1284, 135404	0
82	Effective bioactive compounds and their antiviral properties from some selected aquatic plants through in silico and in vitro approaches. **2023**, 573, 739574	0
81	Covalent interaction, solvent effects, electrochemical, and spectroscopic characterization of novel (4Z)-4-{2-[amino(hydroxy)methyl]hydrazinylidene}-2,6-di(furan-2-yl)-3-methylpiperidin-1-ol derivative- anti-microbial activity study. **2023**, 374, 121272	0
80	Polymerized stimuli-responsive microgels for the removal of organic dye from water. **2023**, 375, 121267	0

79	Computational analyses of the interactome between TNF and TNFR superfamilies. **2023**, 103, 107823	0
78	Antioxidant activity and enzymatic of lichen substances: A study based on cyclic voltammetry and theoretical. **2023**, 372, 110357	1
77	A computational strategy for therapeutic development against superoxide dismutase (SOD1) amyloid formation: effect of polyphenols on the various events in the aggregation pathway. **2023**, 25, 6232-6246	0
76	Construction of Biocatalysts Using the P450 Scaffold for the Synthesis of Indigo from Indole. **2023**, 24, 2395	0
75	Biocontrol efficacy of apigenin isolated from Anisomeles indica (L.) Kuntze against immature stages of Culex quinquefasciatus (Say, 1823) and its in silico studies. **2023**, 48, 102637	0
74	4-Hydroxy Enigmol, a 1-Deoxyphytosphingolipid that Exhibit Good Activity against Prostate and Colon Cancer. **2023**, 8,	0
73	Anticancer cytotoxicity of indole-thiazolidinone hybrids, in silico study of mechanisms of their action. **2022**, 38, 257-277	0
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71	Synthesis, spectroscopic profiling, biological evaluation, DFT, molecular docking and mathematical studies of 3,5-diethyl-2r,6c-diphenylpiperidin-4-one picrate. **2023**, 121,	0
70	Computational modeling of cyanobacterial phytoconstituents against toll-like receptors of skin cancer. 1-13	0
69	Synthesis and anti-HIV activity of non-nucleoside reverse-transcriptase inhibitor DB02 phosphate derivatives based on water-soluble optimization.	0
68	Design, Synthesis, and Molecular Docking Study of 6-Aryl-3-(quinolin-3-yl)-7H-[1,2,4]triazolo[3,4-b][1,3,4]thia□diazines as Novel Antimicrobial Agents. **2022**, 58, 1851-1860	0
67	Synthesis, molecular docking study and anticancer activity of novel 1,3,4-oxadiazole derivatives as potential tubulin inhibitors. **2023**, 9, e13460	0
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65	Potency of Hexaconazole to Disrupt Endocrine Function with Sex Hormone-Binding Globulin. **2023**, 24, 3882	0
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