Open Babel: An open chemical toolbox

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Citation Report

#	Article	IF	Citations
1	Molecular Modeling of Nucleic Acid Structure. Current Protocols in Nucleic Acid Chemistry, 2001, 6, Unit 7.5.	0.5	9
2	3D-QSPR Method of Computational Technique Applied on Red Reactive Dyes by Using CoMFA Strategy. International Journal of Molecular Sciences, 2011, 12, 8862-8877.	1.8	6
3	Modeling the Mechanism of GR/c-Jun/Erg Crosstalk in Apoptosis of Acute Lymphoblastic Leukemia. Frontiers in Physiology, 2012, 3, 410.	1.3	3
4	ChemBioServer: a web-based pipeline for filtering, clustering and visualization of chemical compounds used in drug discovery. Bioinformatics, 2012, 28, 3002-3003.	1.8	57
5	Toward the Prediction of FBPase Inhibitory Activity Using Chemoinformatic Methods. International Journal of Molecular Sciences, 2012, 13, 7015-7037.	1.8	4
6	SwissSidechain: a molecular and structural database of non-natural sidechains. Nucleic Acids Research, 2012, 41, D327-D332.	6.5	100
7	ChemProt-2.0: visual navigation in a disease chemical biology database. Nucleic Acids Research, 2012, 41, D464-D469.	6.5	50
8	Comment on â€œFast and Accurate Modeling of Molecular Atomization Energies with Machine Learningâ€. Physical Review Letters, 2012, 109, 059801; author reply 059802.	2.9	38
9	ZINCPharmer: pharmacophore search of the ZINC database. Nucleic Acids Research, 2012, 40, W409-W414.	6.5	311
10	First identification of small-molecule inhibitors of Pontin by combining virtual screening and enzymatic assay. Biochemical Journal, 2012, 443, 549-559.	1.7	36
11	CDRUG: a web server for predicting anticancer activity of chemical compounds. Bioinformatics, 2012, 28, 3334-3335.	1.8	43
12	H++ 3.0: automating pK prediction and the preparation of biomolecular structures for atomistic molecular modeling and simulations. Nucleic Acids Research, 2012, 40, W537-W541.	6.5	1,314
13	Cheminformatics. Communications of the ACM, 2012, 55, 65-75.	3.3	21
14	Peripheral Ligand-binding Site in Cytochrome P450 3A4 Located with Fluorescence Resonance Energy Transfer (FRET). Journal of Biological Chemistry, 2012, 287, 6797-6809.	1.6	65
15	Synthesis of 6â€³-triazole-substituted Î±-GalCer analogues as potent iNKT cell stimulating ligands. Bioorganic and Medicinal Chemistry, 2012, 20, 7149-7154.	1.4	14
16	A geometrical correction for the inter- and intra-molecular basis set superposition error in Hartree-Fock and density functional theory calculations for large systems. Journal of Chemical Physics, 2012, 136, 154101.	1.2	556
17	Freely Available Conformer Generation Methods: How Good Are They?. Journal of Chemical Information and Modeling, 2012, 52, 1146-1158.	2.5	178
18	New Insights into the Molecular Structures, Compositions, and Cation Distributions in Synthetic and Natural Montmorillonite Clays. Chemistry of Materials, 2012, 24, 4376-4389.	3.2	79

#	Article	IF	Citations
19	Classification of Ligand Molecules in PDB with Fast Heuristic Graph Match Algorithm COMPLIG. Journal of Molecular Biology, 2012, 424, 379-390.	2.0	15
20	Coarse-Grained Simulations of Protein Backbone Dynamics. 1. Local Sterics Define the Dihedral Angles. Journal of Chemical Theory and Computation, 2012, 8, 4732-4745.	2.3	2
21	Automation of the CHARMM General Force Field (CGenFF) I: Bond Perception and Atom Typing. Journal of Chemical Information and Modeling, 2012, 52, 3144-3154.	2.5	1,409
22	A Single Sign-On Infrastructure for Science Gateways on a Use Case for Structural Bioinformatics. Journal of Grid Computing, 2012, 10, 769-790.	2.5	39
23	A Study on Cheminformatics and its Applications on Modern Drug Discovery. Procedia Engineering, 2012, 38, 1264-1275.	1.2	46
24	Ligand and Decoy Sets for Docking to G Protein-Coupled Receptors. Journal of Chemical Information and Modeling, 2012, 52, 1-6.	2.5	103
25	Iterative Fragment Selection: A Group Contribution Approach to Predicting Fish Biotransformation Half-Lives. Environmental Science & Technology, 2012, 46, 8253-8260.	4.6	67
26	idTarget: a web server for identifying protein targets of small chemical molecules with robust scoring functions and a divide-and-conquer docking approach. Nucleic Acids Research, 2012, 40, W393-W399.	6.5	150
27	Avogadro: an advanced semantic chemical editor, visualization, and analysis platform. Journal of Cheminformatics, 2012, 4, 17.	2.8	6,063
28	Molecular Fingerprint-Based Artificial Neural Networks QSAR for Ligand Biological Activity Predictions. Molecular Pharmaceutics, 2012, 9, 2912-2923.	2.3	102
29	In silico evaluation of TERT inhibition by anticancer drugs. Journal of Molecular Modeling, 2012, 18, 4739-4744.	0.8	3
30	In Silico Mutagenesis and Docking Study of Ralstonia solanacearum RSL Lectin: Performance of Docking Software To Predict Saccharide Binding. Journal of Chemical Information and Modeling, 2012, 52, 1250-1261.	2.5	34
31	Inhibition of forebrain Î¼-opioid receptor signaling by low concentrations of rimonabant does not require cannabinoid receptors and directly involves Î¼-opioid receptors. Neurochemistry International, 2012, 61, 378-388.	1.9	18
32	A canonical form of the complex reaction mechanism. Energy, 2012, 43, 64-72.	4.5	5
33	Modeling, Synthesis and Biological Evaluation of Potential Retinoidâ€...X Receptorâ€Selective Agonists: Novel Halogenated Analogues of 4â€[1â€(3,5,5,8,8â€Pentamethylâ€5,6,7,8â€tetrahydroâ€2â€naphthyl)ethynyl]benzoic Acid (Bexarotene). ChemMedChem, 2012, 7, 1551-1566.	2.6	13
34	The semantics of Chemical Markup Language (CML) for computational chemistry : CompChem. Journal of Cheminformatics, 2012, 4, 15.	2.8	24
35	Towards a Universal SMILES representation - A standard method to generate canonical SMILES based on the InChI. Journal of Cheminformatics, 2012, 4, 22.	2.8	179
36	mol2chemfig, a tool for rendering chemical structures from molfile or SMILES format to LATE X code. Journal of Cheminformatics, 2012, 4, 24.	2.8	5

#	Article	IF	Citations
37	CheS-Mapper - Chemical Space Mapping and Visualization in 3D. Journal of Cheminformatics, 2012, 4, 7.	2.8	41
38	Structure-based design of eugenol analogs as potential estrogen receptor antagonists. Bioinformation, 2012, 8, 901-906.	0.2	14
39	COSMOsim3D: 3D-Similarity and Alignment Based on COSMO Polarization Charge Densities. Journal of Chemical Information and Modeling, 2012, 52, 2149-2156.	2.5	21
40	admetSAR: A Comprehensive Source and Free Tool for Assessment of Chemical ADMET Properties. Journal of Chemical Information and Modeling, 2012, 52, 3099-3105.	2.5	1,439
41	Modeling flexibility in metalâ€“organic frameworks: Comparison between Density-Functional Tight-Binding and Universal Force Field approaches for bonded interactions. Microporous and Mesoporous Materials, 2012, 163, 215-220.	2.2	31
42	Computational Design of New Refrigerant Fluids Based on Environmental, Safety, and Thermodynamic Characteristics. Industrial & Engineering Chemistry Research, 0, , 120917100332001.	1.8	25
43	Computational Prediction of Blood-Brain Barrier Permeability Using Decision Tree Induction. Molecules, 2012, 17, 10429-10445.	1.7	77
44	Large-scale reverse docking profiles and their applications. BMC Bioinformatics, 2012, 13, S6.	1.2	34
45	chemf: A purely functional chemistry toolkit. Journal of Cheminformatics, 2012, 4, 38.	2.8	6
46	The Effective Fragment Molecular Orbital Method for Fragments Connected by Covalent Bonds. PLoS ONE, 2012, 7, e41117.	1.1	28
47	FragIt: A Tool to Prepare Input Files for Fragment Based Quantum Chemical Calculations. PLoS ONE, 2012, 7, e44480.	1.1	39
48	Simulation of Intramolecular Hydrogen Bond Dynamics in Manzamine A as a Sensitive Test for Charge Distribution Quality. Natural Product Communications, 2012, 7, 1934578X1200700.	0.2	0
49	Sequence analysis and homology modeling of peroxidase from Medicago sativa. Bioinformation, 2012, 8, 974-979.	0.2	18
50	OBGMX: A webâ€based generator of GROMACS topologies for molecular and periodic systems using the universal force field. Journal of Computational Chemistry, 2012, 33, 2204-2208.	1.5	70
51	Redefining Cheminformatics with Intuitive Collaborative Mobile Apps. Molecular Informatics, 2012, 31, 569-584.	1.4	25
52	Copper Complexes of â€œSuperpodalâ€•Amine Ligands and Reactivity Studies towards Dioxygen. European Journal of Inorganic Chemistry, 2012, 2012, 3000-3013.	1.0	10
53	Web tools for predictive toxicology model building. Expert Opinion on Drug Metabolism and Toxicology, 2012, 8, 791-801.	1.5	10
54	DecoyFinder: an easy-to-use python GUI application for building target-specific decoy sets. Bioinformatics, 2012, 28, 1661-1662.	1.8	155

#	Article	IF	Citations
55	LigMerge: A Fast Algorithm to Generate Models of Novel Potential Ligands from Sets of Known Binders. Chemical Biology and Drug Design, 2012, 80, 358-365.	1.5	17
56	Structural Basis for Substrate Targeting and Catalysis by Fungal Polysaccharide Monooxygenases. Structure, 2012, 20, 1051-1061.	1.6	257
57	Packaging free software chemistry programs in Debian GNU/Linux: past, present and future. Journal of Cheminformatics, 2012, 4, .	2.8	0
58	A tandem regression-outlier analysis of a ligand cellular system for key structural modifications around ligand binding. Journal of Cheminformatics, 2013, 5, 21.	2.8	0
59	Random forests for feature selection in QSPR Models - an application for predicting standard enthalpy of formation of hydrocarbons. Journal of Cheminformatics, 2013, 5, 9.	2.8	60
60	Python Materials Genomics (pymatgen): A robust, open-source python library for materials analysis. Computational Materials Science, 2013, 68, 314-319.	1.4	2,392
61	Quinazoline-based multi-tyrosine kinase inhibitors: Synthesis, modeling, antitumor and antiangiogenic properties. European Journal of Medicinal Chemistry, 2013, 67, 373-383.	2.6	59
62	The Molecule Calculator: A Web Application for Fast Quantum Mechanics-Based Estimation of Molecular Properties. Journal of Chemical Education, 2013, 90, 1093-1095.	1.1	36
63	Protein structure prediction using distributed parallel particle swarm optimization. Natural Computing, 2013, 12, 29-41.	1.8	6
64	GPUâ€accelerated molecular mechanics computations. Journal of Computational Chemistry, 2013, 34, 2249-2260.	1.5	16
65	DockoMatic 2.0: High Throughput Inverse Virtual Screening and Homology Modeling. Journal of Chemical Information and Modeling, 2013, 53, 2161-2170.	2.5	26
66	Integrative relational machine-learning for understanding drug side-effect profiles. BMC Bioinformatics, 2013, 14, 207.	1.2	48
67	QVibeplot: A Program To Visualize Molecular Vibrations in Two Dimensions. Journal of Chemical Education, 2013, 90, 944-946.	1.1	31
68	Competitive Binding of Natural Amphiphiles with Graphene Derivatives. Scientific Reports, 2013, 3, 2273.	1.6	61
69	Three-dimensional quantitative structureâ€“activity relationship CoMFA/CoMSIA on pyrrolidine-based tartrate diamides as TACE inhibitors. Medicinal Chemistry Research, 2013, 22, 4192-4201.	1.1	12
70	TargetHunter: An In Silico Target Identification Tool for Predicting Therapeutic Potential of Small Organic Molecules Based on Chemogenomic Database. AAPS Journal, 2013, 15, 395-406.	2.2	171
71	Design, synthesis, biological evaluation and docking study of 5-oxo-4,5-dihydropyrano[3,2-c]chromene derivatives as acetylcholinesterase and butyrylcholinesterase inhibitors. European Journal of Medicinal Chemistry, 2013, 68, 260-269.	2.6	91
72	Design, synthesis, docking study and biological evaluation of some novel tetrahydrochromeno [3â€²,4â€²:5,6]pyrano[2,3-b]quinolin-6(7H)-one derivatives against acetyl- and butyrylcholinesterase. European Journal of Medicinal Chemistry, 2013, 68, 291-300.	2.6	50

#	Article	IF	Citations
73	Synthesis of Some New 3â€‹scp›C‹/scp›oumaranone and Coumarin Derivatives as Dual Inhibitors of Acetylâ€•and Butyrylcholinesterase. Archiv Der Pharmazie, 2013, 346, 577-587.	2.1	27
74	An analysis of a â€˜community-drivenâ€™ reconstruction of the human metabolic network. Metabolomics, 2013, 9, 757-764.	1.4	30
75	5,6-Dimethoxybenzofuran-3-one derivatives: a novel series of dual Acetylcholinesterase/Butyrylcholinesterase inhibitors bearing benzyl pyridinium moiety. DARU, Journal of Pharmaceutical Sciences, 2013, 21, 15.	0.9	30
76	Homology Modeling, Molecular Docking and DNA Binding Studies of Nucleotide Excision Repair UvrC Protein from M. tuberculosis. Protein Journal, 2013, 32, 467-476.	0.7	25
77	AutoGrow 3.0: An improved algorithm for chemically tractable, semi-automated protein inhibitor design. Journal of Molecular Graphics and Modelling, 2013, 44, 104-112.	1.3	48
78	StreptomeDB: a resource for natural compounds isolated from Streptomyces species. Nucleic Acids Research, 2013, 41, D1130-D1136.	6.5	107
79	Lessons Learned in Empirical Scoring with smina from the CSAR 2011 Benchmarking Exercise. Journal of Chemical Information and Modeling, 2013, 53, 1893-1904.	2.5	675
80	Machine learning based search space optimisation for drug discovery. , 2013, , .		5
81	Inhibition of dipeptidyl peptidase IV and xanthine oxidase by amino acids and dipeptides. Food Chemistry, 2013, 141, 644-653.	4.2	124
82	Exploring the Biologically Relevant Chemical Space for Drug Discovery. Journal of Chemical Information and Modeling, 2013, 53, 2820-2828.	2.5	39
83	Beyond Terrestrial Biology: Charting the Chemical Universe of Î±-Amino Acid Structures. Journal of Chemical Information and Modeling, 2013, 53, 2851-2862.	2.5	40
84	In silico QSAR analysis of quercetin reveals its potential as therapeutic drug for Alzheimer's disease. Journal of Young Pharmacists, 2013, 5, 173-179.	0.1	57
85	Deriving Static Atomic Multipoles from the Electrostatic Potential. Journal of Chemical Information and Modeling, 2013, 53, 3410-3417.	2.5	25
86	Small-Molecule 3D Structure Prediction Using Open Crystallography Data. Journal of Chemical Information and Modeling, 2013, 53, 3127-3130.	2.5	17
87	Binary Classification of a Large Collection of Environmental Chemicals from Estrogen Receptor Assays by Quantitative Structureâ€“Activity Relationship and Machine Learning Methods. Journal of Chemical Information and Modeling, 2013, 53, 3244-3261.	2.5	66
88	Nonlinear Scoring Functions for Similarity-Based Ligand Docking and Binding Affinity Prediction. Journal of Chemical Information and Modeling, 2013, 53, 3097-3112.	2.5	45
89	Visually Interpretable Models of Kinase Selectivity Related Features Derived from Field-Based Proteochemometrics. Journal of Chemical Information and Modeling, 2013, 53, 3021-3030.	2.5	30
90	Discovery of novel cannabinoid receptor ligands by a virtual screening approach: Further development of 2,4,6-trisubstituted 1,3,5-triazines as CB2 agonists. European Journal of Pharmaceutical Sciences, 2013, 48, 9-20.	1.9	15

#	Article	IF	Citations
91	A knowledge-based halogen bonding scoring function for predicting protein-ligand interactions. Journal of Molecular Modeling, 2013, 19, 5015-5030.	0.8	35
92	K-Map: connecting kinases with therapeutics for drug repurposing and development. Human Genomics, 2013, 7, 20.	1.4	25
93	KNIME-CDK: Workflow-driven cheminformatics. BMC Bioinformatics, 2013, 14, 257.	1.2	119
94	Rubabel: wrapping open Babel with Ruby. Journal of Cheminformatics, 2013, 5, 35.	2.8	8
95	WhichCyp: prediction of cytochromes P450 inhibition. Bioinformatics, 2013, 29, 2051-2052.	1.8	57
96	CVDHD: a cardiovascular disease herbal database for drug discovery and network pharmacology. Journal of Cheminformatics, 2013, 5, 51.	2.8	45
97	Conformational Analysis of the Antiâ€obesity Drug Lorcaserin in Water: How To Take Advantage of Longâ€Range Residual Dipolar Couplings. Chemistry - A European Journal, 2013, 19, 14989-14997.	1.7	27
98	Inhibitors of the aminoglycoside 6â€²-N-acetyltransferase type Ib [AAC(6â€²)-Ib] identified by in silico molecular docking. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 5694-5698.	1.0	24
99	Fast and Accurate Electrostatics in Metal Organic Frameworks with a Robust Charge Equilibration Parameterization for High-Throughput Virtual Screening of Gas Adsorption. Journal of Physical Chemistry Letters, 2013, 4, 3056-3061.	2.1	90
100	Batch tautomer generation with MolTPC. Journal of Computational Chemistry, 2013, 34, 2485-2492.	1.5	5
101	Molecular modeling of butyrylcholinesterase inhibition by cresyl saligenin phosphate. Russian Chemical Bulletin, 2013, 62, 2527-2537.	0.4	17
102	The dissociation of glycolateâ€"astrochemical and prebiotic relevance. Physical Chemistry Chemical Physics, 2013, 15, 16615-16625.	1.3	10
103	CNA web server: rigidity theory-based thermal unfolding simulations of proteins for linking structure, (thermo-)stability, and function. Nucleic Acids Research, 2013, 41, W340-W348.	6.5	118
104	Extensions to In Silico Bioactivity Predictions Using Pathway Annotations and Differential Pharmacology Analysis: Application to Xenopus laevis Phenotypic Readouts. Molecular Informatics, 2013, 32, 1009-1024.	1.4	13
105	Experimental validation of in silico target predictions on synergistic protein targets. MedChemComm, 2013, 4, 278-288.	3.5	7
106	Sequence Matters: Modulating Electronic and Optical Properties of Conjugated Oligomers via Tailored Sequence. Macromolecules, 2013, 46, 1384-1392.	2.2	67
107	The chemical interactome space between the human host and the genetically defined gut metabotypes. ISME Journal, 2013, 7, 730-742.	4.4	21
108	Step-by-step thermal transformations of a new porous coordination polymer [(H2O)5CuBa(Me2mal)2]n (Me2mal2â^'=dimethylmalonate): Thermal degradation to barium cuprate. Journal of Solid State Chemistry, 2013, 197, 379-391.	1.4	33

#	Article	IF	Citations
109	G4LDB: a database for discovering and studying G-quadruplex ligands. Nucleic Acids Research, 2013, 41, D1115-D1123.	6.5	137
110	Comprehensive Classification and Diversity Assessment of Atomic Contacts in Proteinâ€“Small Ligand Interactions. Journal of Chemical Information and Modeling, 2013, 53, 241-248.	2.5	13
111	In Silico and in Vitro Physicochemical Screening of Rigidoporus sp. Crude Laccase-assisted Decolorization of Synthetic Dyesâ€”Approaches for a Cost-effective Enzyme-based Remediation Methodology. Applied Biochemistry and Biotechnology, 2013, 169, 911-922.	1.4	17
112	Characterization of Small Molecule Binding. I. Accurate Identification of Strong Inhibitors in Virtual Screening. Journal of Chemical Information and Modeling, 2013, 53, 114-122.	2.5	41
113	Aldoâ€“keto reductases in retinoid metabolism: Search for substrate specificity and inhibitor selectivity. Chemico-Biological Interactions, 2013, 202, 186-194.	1.7	31
114	Molecular dynamics simulations and statistical coupling analysis reveal functional coevolution network of oncogenic mutations in the CDKN2Aâ€“CDK6 complex. FEBS Letters, 2013, 587, 136-141.	1.3	9
115	Consensus Docking: Improving the Reliability of Docking in a Virtual Screening Context. Journal of Chemical Information and Modeling, 2013, 53, 384-390.	2.5	194
116	CovalentDock: Automated covalent docking with parameterized covalent linkage energy estimation and molecular geometry constraints. Journal of Computational Chemistry, 2013, 34, 326-336.	1.5	117
117	Novel coumarin-3-carboxamides bearing N-benzylpiperidine moiety as potent acetylcholinesterase inhibitors. European Journal of Medicinal Chemistry, 2013, 70, 623-630.	2.6	106
118	Synthesis of PDE IV inhibitors. First asymmetric synthesis of two of GlaxoSmithKline's highly potent Rolipram analogues. Organic and Biomolecular Chemistry, 2013, 11, 8082.	1.5	17
119	Modeling, Synthesis, and Biological Evaluation of Potential Retinoid X Receptor (RXR) Selective Agonists: Novel Analogues of 4-[1-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydro-2-naphthyl)ethynyl]benzoic Acid (Bexarotene) and (E)-3-(3-(1,2,3,4-tetrahydro-1,1,4,4,6-pentamethylnaphthalen-7-yl)-4-hydroxyphenyl)acrylic Acid (CD3254). Journal of Medicinal Chemistry, 2013, 56, 8432-8454.	2.9	23
120	iCDI-PseFpt: Identify the channelâ€“drug interaction in cellular networking with PseAAC and molecular fingerprints. Journal of Theoretical Biology, 2013, 337, 71-79.	0.8	113
121	Subpocket Analysis Method for Fragment-Based Drug Discovery. Journal of Chemical Information and Modeling, 2013, 53, 131-141.	2.5	23
122	Farnesyl Diphosphate Synthase Inhibitors from In Silico Screening. Chemical Biology and Drug Design, 2013, 81, 742-748.	1.5	42
123	Psoralen Derivatives as Inhibitors of NF-ÎºB/DNA Interaction: Synthesis, Molecular Modeling, 3D-QSAR, and Biological Evaluation. Journal of Medicinal Chemistry, 2013, 56, 1830-1842.	2.9	34
124	Crystal structure determination by combined synchrotronpowder X-ray diffraction and crystal structure prediction: 1â€‰:â€‰1 l-ephedrine<scp>d</scp>-tartrate. CrystEngComm, 2013, 15, 1853-1859.	1.3	17
125	Analysis of Chemical and Biological Features Yields Mechanistic Insights into Drug Side Effects. Chemistry and Biology, 2013, 20, 594-603.	6.2	50
126	An Augmented Volume-Based Model of the Glass Transition Temperature of 209 Molecular Liquids. Journal of Pharmaceutical Sciences, 2013, 102, 1970-1980.	1.6	5

#	Article	IF	Citations
127	STAAR: Statistical analysis of aromatic rings. Journal of Computational Chemistry, 2013, 34, 518-522.	1.5	31
128	Profiling 976 ToxCast Chemicals across 331 Enzymatic and Receptor Signaling Assays. Chemical Research in Toxicology, 2013, 26, 878-895.	1.7	162
129	MolShaCS: A free and open source tool for ligand similarity identification based on Gaussian descriptors. European Journal of Medicinal Chemistry, 2013, 59, 296-303.	2.6	22
130	Efficient Computational Screening of Organic Polymer Photovoltaics. Journal of Physical Chemistry Letters, 2013, 4, 1613-1623.	2.1	161
131	Structural Insights into the Theoretical Model ofPlasmodium falciparumNADH Dehydrogenase and its Interaction with Artemisinin and Derivatives: Towards Global Health Therapeutics. OMICS A Journal of Integrative Biology, 2013, 17, 231-241.	1.0	10
132	Oxidation-Induced Photoluminescence of Conjugated Polymers. Journal of Physical Chemistry B, 2013, 117, 4528-4535.	1.2	14
133	Evaluation and Optimization of Virtual Screening Workflows with DEKOIS 2.0 â€“ A Public Library of Challenging Docking Benchmark Sets. Journal of Chemical Information and Modeling, 2013, 53, 1447-1462.	2.5	134
134	Hybrid Metaheuristic Approach for Nonlocal Optimization of Molecular Systems. Journal of Chemical Theory and Computation, 2013, 9, 2137-2149.	2.3	16
135	Prediction of Cytochrome P450 Xenobiotic Metabolism: Tethered Docking and Reactivity Derived from Ligand Molecular Orbital Analysis. Journal of Chemical Information and Modeling, 2013, 53, 1294-1305.	2.5	38
136	Identification of Key Nodes of Type 2 Diabetes Mellitus Protein Interactome and Study of their Interactions with Phloridzin. OMICS A Journal of Integrative Biology, 2013, 17, 302-317.	1.0	14
137	Tocopheramines and tocotrienamines as antioxidants: ESR spectroscopy, rapid kinetics and DFT calculations. Bioorganic and Medicinal Chemistry, 2013, 21, 5039-5046.	1.4	16
138	Virtual screening of low molecular weight mushrooms compounds as potential Mdm2 inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2013, 28, 569-575.	2.5	11
139	Synthesis and evaluation of 4-substituted coumarins as novel acetylcholinesterase inhibitors. European Journal of Medicinal Chemistry, 2013, 64, 252-259.	2.6	100
140	MOFomics: Computational pore characterization of metalâ€“organic frameworks. Microporous and Mesoporous Materials, 2013, 165, 32-39.	2.2	113
141	Noncontiguous Atom Matching Structural Similarity Function. Journal of Chemical Information and Modeling, 2013, 53, 2511-2524.	2.5	9
142	CH5M3D: an HTML5 program for creating 3D molecular structures. Journal of Cheminformatics, 2013, 5, 46.	2.8	6
143	Nemesis - a molecular modeling package. Journal of Cheminformatics, 2013, 5, .	2.8	1
144	FAst MEtabolizer (FAME): A Rapid and Accurate Predictor of Sites of Metabolism in Multiple Species by Endogenous Enzymes. Journal of Chemical Information and Modeling, 2013, 53, 2896-2907.	2.5	47

#	Article	IF	Citations
145	Design of Linear Ligands for Selective Separation Using a Genetic Algorithm Applied to Molecular Architecture. Journal of Chemical Information and Modeling, 2013, 53, 1638-1660.	2.5	4
146	Quantum-Chemical Electron Densities of Proteins and of Selected Protein Sites from Subsystem Density Functional Theory. Journal of Chemical Theory and Computation, 2013, 9, 2425-2440.	2.3	43
147	Mail-Order Metalâ€“Organic Frameworks (MOFs): Designing Isoreticular MOF-5 Analogues Comprising Commercially Available Organic Molecules. Journal of Physical Chemistry C, 2013, 117, 12159-12167.	1.5	64
148	Comparison of ultraâ€fast 2<scp>D</scp> and 3<scp>D</scp> ligand and target descriptors for side effect prediction and network analysis in polypharmacology. British Journal of Pharmacology, 2013, 170, 557-567.	2.7	15
149	Molecular Modeling of Nucleic Acid Structure. Current Protocols in Nucleic Acid Chemistry, 2013, 54, 7.5.1-7.5.13.	0.5	10
150	A Î²-cyclodextrinâ€“resveratrol inclusion complex and the role of geometrical and electronic effects on its electronic induced circular dichroism. RSC Advances, 2013, 3, 10242.	1.7	19
151	Dissociation of Multisubunit Proteinâ€“Ligand Complexes in the Gas Phase. Evidence for Ligand Migration. Journal of the American Society for Mass Spectrometry, 2013, 24, 1573-1583.	1.2	15
152	5-Methylation of Cytosine in CG:CG Base-Pair Steps: A Physicochemical Mechanism for the Epigenetic Control of DNA Nanomechanics. Journal of Physical Chemistry B, 2013, 117, 16436-16442.	1.2	22
153	CSBB-ConeExclusion, Adapting Structure Based Solution Virtual Screening to Libraries on Solid Support. Journal of Chemical Information and Modeling, 2013, 53, 3156-3162.	2.5	1
154	Volarea â€“ A Bioinformatics Tool to Calculate the Surface Area and the Volume of Molecular Systems. Chemical Biology and Drug Design, 2013, 82, 743-755.	1.5	26
155	Exploring the energy landscapes of flexible molecular loops using higherâ€dimensional continuation. Journal of Computational Chemistry, 2013, 34, 234-244.	1.5	7
156	Glycogen Synthase Kinase 3 as an Anticancer Drug Target: Novel Experimental Findings and Trends in the Design of Inhibitors. Current Pharmaceutical Design, 2013, 19, 665-679.	0.9	25
157	PTID: an integrated web resource and computational tool for agrochemical discovery. Bioinformatics, 2013, 29, 292-294.	1.8	20
158	Discovery of Anthelmintic Drug Targets and Drugs Using Chokepoints in Nematode Metabolic Pathways. PLoS Pathogens, 2013, 9, e1003505.	2.1	69
159	A Comprehensive Survey of Small-Molecule Binding Pockets in Proteins. PLoS Computational Biology, 2013, 9, e1003302.	1.5	103
160	Predicting Drugs Side Effects Based on Chemical-Chemical Interactions and Protein-Chemical Interactions. BioMed Research International, 2013, 2013, 1-8.	0.9	23
161	iEzy-Drug: A Web Server for Identifying the Interaction between Enzymes and Drugs in Cellular Networking. BioMed Research International, 2013, 2013, 1-13.	0.9	73
162	Navigating the Chemical Space of HCN Polymerization and Hydrolysis: Guiding Graph Grammars by Mass Spectrometry Data. Entropy, 2013, 15, 4066-4083.	1.1	38

#	Article	IF	Citations
163	Consistent Estimation of Gibbs Energy Using Component Contributions. PLoS Computational Biology, 2013, 9, e1003098.	1.5	231
164	Using Existing Drugs as Leads for Broad Spectrum Anthelmintics Targeting Protein Kinases. PLoS Pathogens, 2013, 9, e1003149.	2.1	36
165	Prediction of the P. falciparum Target Space Relevant to Malaria Drug Discovery. PLoS Computational Biology, 2013, 9, e1003257.	1.5	47
166	Structure-Based Discovery of the Novel Antiviral Properties of Naproxen against the Nucleoprotein of Influenza A Virus. Antimicrobial Agents and Chemotherapy, 2013, 57, 2231-2242.	1.4	115
167	Chemical annotation of small and peptide-like molecules at the Protein Data Bank. Database: the Journal of Biological Databases and Curation, 2013, 2013, bat079.	1.4	14
168	Dimeric Sfh3 has structural changes in its binding pocket that are associated with a dimerâ€“monomer state transformation induced by substrate binding. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 313-323.	2.5	12
169	LigSearch: a knowledge-based web server to identify likely ligands for a protein target. Acta Crystallographica Section D: Biological Crystallography, 2013, 69, 2395-2402.	2.5	2
170	Metabolite Identification through Machine Learningâ€" Tackling CASMI Challenge Using FingerID. Metabolites, 2013, 3, 484-505.	1.3	24
171	In silicomodelling for predicting the cationic hydrophobicity and cytotoxicity of ionic liquids towards theLeukemiarat cell line,Vibrio fischeriandScenedesmus vacuolatusbased on molecular interaction potentials of ions. SAR and QSAR in Environmental Research, 2013, 24, 863-882.	1.0	51
172	Yeast-based automated high-throughput screens to identify anti-parasitic lead compounds. Open Biology, 2013, 3, 120158.	1.5	32
173	Novel phytochemical–antibiotic conjugates as multitarget inhibitors of Pseudomononas aeruginosa GyrB/ParE and DHFR. Drug Design, Development and Therapy, 2013, 7, 449.	2.0	10
174	PyPLIF: Python-based Protein-Ligand Interaction Fingerprinting. Bioinformation, 2013, 9, 325-328.	0.2	49
175	Prospecting for Novel Plant-Derived Molecules of Rauvolfia serpentina as Inhibitors of Aldose Reductase, a Potent Drug Target for Diabetes and Its Complications. PLoS ONE, 2013, 8, e61327.	1.1	45
176	Use of Natural Products as Chemical Library for Drug Discovery and Network Pharmacology. PLoS ONE, 2013, 8, e62839.	1.1	299
177	Interface of the Polarizable Continuum Model of Solvation with Semi-Empirical Methods in the GAMESS Program. PLoS ONE, 2013, 8, e67725.	1.1	13
178	An In Silico Analysis of the Binding Modes and Binding Affinities of Small Molecule Modulators of PDZ-Peptide Interactions. PLoS ONE, 2013, 8, e71340.	1.1	18
179	iGPCR-Drug: A Web Server for Predicting Interaction between GPCRs and Drugs in Cellular Networking. PLoS ONE, 2013, 8, e72234.	1.1	106
180	Ligand Pose and Orientational Sampling in Molecular Docking. PLoS ONE, 2013, 8, e75992.	1.1	139

#	Article	IF	Citations
181	Combining Machine Learning Systems and Multiple Docking Simulation Packages to Improve Docking Prediction Reliability for Network Pharmacology. PLoS ONE, 2013, 8, e83922.	1.1	268
182	lazar: a modular predictive toxicology framework. Frontiers in Pharmacology, 2013, 4, 38.	1.6	124
183	Small Molecule Identification with MOLGEN and Mass Spectrometry. Metabolites, 2013, 3, 440-462.	1.3	32
184	The Critical Assessment of Small Molecule Identification (CASMI): Challenges and Solutions. Metabolites, 2013, 3, 517-538.	1.3	35
185	Open Source Software and Web Services for Designing Therapeutic Molecules. Current Topics in Medicinal Chemistry, 2013, 13, 1172-1191.	1.0	25
186	CASMI: And the Winner is . . .. Metabolites, 2013, 3, 412-439.	1.3	30
187	The Curious Case of Benzbromarone: Insight into Super-Inhibition of Cytochrome P450. PLoS ONE, 2014, 9, e89967.	1.1	26
188	Rational Modification of Estrogen Receptor by Combination of Computational and Experimental Analysis. PLoS ONE, 2014, 9, e102658.	1.1	8
189	Cheminformatics Models for Inhibitors ofSchistosoma mansoniThioredoxin Glutathione Reductase. Scientific World Journal, The, 2014, 2014, 1-9.	0.8	18
190	Evaluation of 11 Scoring Functions Performance on Matrix Metalloproteinases. International Journal of Medicinal Chemistry, 2014, 2014, 1-9.	2.2	10
191	Multipose Binding in Molecular Docking. International Journal of Molecular Sciences, 2014, 15, 2622-2645.	1.8	51
192	Computational Redesign of Bacterial Biotin Carboxylase Inhibitors Using Structure-Based Virtual Screening of Combinatorial Libraries. Molecules, 2014, 19, 4021-4045.	1.7	10
193	Solving CASMI 2013 with MetFrag, MetFusion and MOLGEN-MS/MS. Mass Spectrometry, 2014, 3, S0036-S0036.	0.2	16
194	Molecular Docking and Reaction Kinetic Studies of Chrysin Binding to Serum Albumin. Natural Product Communications, 2014, 9, 1934578X1400900.	0.2	1
195	XTMS: pathway design in an eXTended metabolic space. Nucleic Acids Research, 2014, 42, W389-W394.	6.5	96
196	Recent Advances in the Open Access Cheminformatics Toolkits, Software Tools, Workflow Environments, and Databases. Methods in Pharmacology and Toxicology, 2014, , 257-296.	0.1	5
197	Molecular cloning and in-silico characterization of high temperature stress responsive pAPX gene isolated from heat tolerant Indian wheat cv. Raj 3765. BMC Research Notes, 2014, 7, 713.	0.6	18
198	FADB: a food additive molecular database forin silicoscreening in food toxicology. Food Additives and Contaminants - Part A Chemistry, Analysis, Control, Exposure and Risk Assessment, 2014, 31, 792-798.	1.1	14

#	Article	IF	Citations
199	The IUPHAR/BPS Guide to PHARMACOLOGY: an expert-driven knowledgebase of drug targets and their ligands. Nucleic Acids Research, 2014, 42, D1098-D1106.	6.5	826
200	Extending in silico mechanism-of-action analysis by annotating targets with pathways: application to cellular cytotoxicity readouts. Future Medicinal Chemistry, 2014, 6, 2029-2056.	1.1	19
201	Metabolite identification through multiple kernel learning on fragmentation trees. Bioinformatics, 2014, 30, i157-i164.	1.8	87
202	PLIC: proteinâ€“ligand interaction clusters. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau029.	1.4	37
203	rDock: A Fast, Versatile and Open Source Program for Docking Ligands to Proteins and Nucleic Acids. PLoS Computational Biology, 2014, 10, e1003571.	1.5	404
204	Pathway Thermodynamics Highlights Kinetic Obstacles in Central Metabolism. PLoS Computational Biology, 2014, 10, e1003483.	1.5	249
205	Pairwise input neural network for target-ligand interaction prediction. , 2014, , .		20
206	Sequence Matters: Determining the Sequence Effect of Electronic Structure Properties in Ï€-Conjugated Polymers. ACS Symposium Series, 2014, , 379-393.	0.5	4
207	MolBridge: a program for identifying nonbonded interactions in small molecules and biomolecular structures. Journal of Applied Crystallography, 2014, 47, 1772-1776.	1.9	16
208	Analysis of Subpocket Selectivity and Identification of Potent Selective Inhibitors for Matriptase and Matriptase-2. Journal of Medicinal Chemistry, 2014, 57, 10198-10204.	2.9	31
209	Anadenanthera colubrina (Vell.) Brenan produces steroidal substances that are active against Alternaria alternata (Fr.) Keissler and that may bind to oxysterolâ€binding proteins. Pest Management Science, 2014, 70, 1815-1822.	1.7	11
210	Code interoperability and standard data formats in quantum chemistry and quantum dynamics: The Q5/D5Cost data model. Journal of Computational Chemistry, 2014, 35, 611-621.	1.5	22
211	iLOGP: A Simple, Robust, and Efficient Description of n-Octanol/Water Partition Coefficient for Drug Design Using the GB/SA Approach. Journal of Chemical Information and Modeling, 2014, 54, 3284-3301.	2.5	560
212	Gradientâ€driven molecule construction: An inverse approach applied to the design of smallâ€molecule fixating catalysts. International Journal of Quantum Chemistry, 2014, 114, 838-850.	1.0	27
213	Structure-based discovery of the first allosteric inhibitors of cyclin-dependent kinase 2. Cell Cycle, 2014, 13, 2296-2305.	1.3	48
214	Crystal Structure of a Bacterial Unsaturated Glucuronyl Hydrolase with Specificity for Heparin. Journal of Biological Chemistry, 2014, 289, 4787-4797.	1.6	8
215	Using chiral molecules as an approach to address lowâ€druggability recognition sites. Journal of Computational Chemistry, 2014, 35, 2114-2121.	1.5	4
216	<scp>R</scp>ingâ€<scp>H</scp>ydroxylating <scp>O</scp>xygenase database: a database of bacterial aromatic ringâ€hydroxylating oxygenases in the management of bioremediation and biocatalysis of aromatic compounds. Environmental Microbiology Reports, 2014, 6, 519-523.	1.0	27

#	Article	IF	Citations
217	Shapeâ€based virtual screening with volumetric aligned molecular shapes. Journal of Computational Chemistry, 2014, 35, 1824-1834.	1.5	24
218	Moxidectin causes adult worm mortality of human lymphatic filarial parasite Brugia malayi in rodent models. Folia Parasitologica, 2014, 61, 561-570.	0.7	12
219	CheS-Mapper 2.0 for visual validation of (Q)SAR models. Journal of Cheminformatics, 2014, 6, .	2.8	14
220	Direct computation of parameters for accurate polarizable force fields. Journal of Chemical Physics, 2014, 141, 194114.	1.2	28
221	ParaPep: a web resource for experimentally validated antiparasitic peptide sequences and their structures. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau051-bau051.	1.4	60
222	HAMMER: automated operation of mass frontier to construct in silico mass spectral fragmentation libraries. Bioinformatics, 2014, 30, 581-583.	1.8	36
223	A Systematic Computational Analysis of Biosynthetic Gene Cluster Evolution: Lessons for Engineering Biosynthesis. PLoS Computational Biology, 2014, 10, e1004016.	1.5	164
224	TIPdb-3D: the three-dimensional structure database of phytochemicals from Taiwan indigenous plants. Database: the Journal of Biological Databases and Curation, 2014, 2014, bau055-bau055.	1.4	29
225	Exploring Large Scale Receptor-Ligand Pairs in Molecular Docking Workflows in HPC Clouds. , 2014, , .		11
226	The Potential Utility of Predicted One Bond Carbon-Proton Coupling Constants in the Structure Elucidation of Small Organic Molecules by NMR Spectroscopy. PLoS ONE, 2014, 9, e111576.	1.1	12
227	Computerized Models of Carbohydrates. , 2014, , 1-38.		2
228	A Coarse-Grained Molecular Dynamics Simulation Using NAMD Package to Reveal Aggregation Profile of Phospholipids Self-Assembly in Water. Journal of Chemistry, 2014, 2014, 1-6.	0.9	10
229	Efficient ring perception for the Chemistry Development Kit. Journal of Cheminformatics, 2014, 6, 3.	2.8	25
230	Modeling T cell receptor recognition of CD1-lipid and MR1-metabolite complexes. BMC Bioinformatics, 2014, 15, 319.	1.2	5
231	Design, synthesis, docking study and cytotoxic activity evaluation of some novel letrozole analogs. DARU, Journal of Pharmaceutical Sciences, 2014, 22, 83.	0.9	12
232	SMMRNA: a database of small molecule modulators of RNA. Nucleic Acids Research, 2014, 42, D132-D141.	6.5	29
233	MotiveValidator: interactive web-based validation of ligand and residue structure in biomolecular complexes. Nucleic Acids Research, 2014, 42, W227-W233.	6.5	11
234	Crystal structure of atomoxetine hydrochloride (Strattera), C₁₇H₂₂NOCl. Powder Diffraction, 2014, 29, 269-273.	0.4	79

#	Article	IF	Citations
235	The challenges of understanding glycolipid functions: An open outlook based on molecular simulations. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2014, 1841, 1130-1145.	1.2	35
236	Use of Freely Available and Open Source Tools for In Silico Screening in Chemical Biology. Journal of Chemical Education, 2014, 91, 602-604.	1.1	13
237	Mapping the Cellular Response to Small Molecules Using Chemogenomic Fitness Signatures. Science, 2014, 344, 208-211.	6.0	217
238	Sharing Chemical Relationships Does Not Reveal Structures. Journal of Chemical Information and Modeling, 2014, 54, 37-48.	2.5	7
239	Computing Clinically Relevant Binding Free Energies of HIV-1 Protease Inhibitors. Journal of Chemical Theory and Computation, 2014, 10, 1228-1241.	2.3	123
240	Prediction of hydration free energies for the SAMPL4 data set with the AMOEBA polarizable force field. Journal of Computer-Aided Molecular Design, 2014, 28, 235-244.	1.3	16
241	Decreasing acidity in a series of aldose reductase inhibitors: 2-Fluoro-4-(1H-pyrrol-1-yl)phenol as a scaffold for improved membrane permeation. Bioorganic and Medicinal Chemistry, 2014, 22, 2194-2207.	1.4	20
242	Novel Mycosin Protease MycP₁ Inhibitors Identified by Virtual Screening and 4D Fingerprints. Journal of Chemical Information and Modeling, 2014, 54, 1166-1173.	2.5	14
243	Progress in computational toxicology. Journal of Pharmacological and Toxicological Methods, 2014, 69, 115-140.	0.3	91
244	In silico approaches to predict the potential of milk protein-derived peptides as dipeptidyl peptidase IV (DPP-IV) inhibitors. Peptides, 2014, 57, 43-51.	1.2	113
245	Structure modeling and hybrid virtual screening study of Alzheimerâ€™s associated protease kallikrein 8 for the identification of novel inhibitors. Medicinal Chemistry Research, 2014, 23, 3516-3527.	1.1	3
246	Machine learning-based prediction of drugâ€“drug interactions by integrating drug phenotypic, therapeutic, chemical, and genomic properties. Journal of the American Medical Informatics Association: JAMIA, 2014, 21, e278-e286.	2.2	264
247	De Novo Design of Drug-Like Molecules by a Fragment-Based Molecular Evolutionary Approach. Journal of Chemical Information and Modeling, 2014, 54, 49-56.	2.5	51
248	AlzPlatform: An Alzheimerâ€™s Disease Domain-Specific Chemogenomics Knowledgebase for Polypharmacology and Target Identification Research. Journal of Chemical Information and Modeling, 2014, 54, 1050-1060.	2.5	177
249	g_mmpbsaâ€”A GROMACS Tool for High-Throughput MM-PBSA Calculations. Journal of Chemical Information and Modeling, 2014, 54, 1951-1962.	2.5	3,304
250	Applicability Domain Analysis (ADAN): A Robust Method for Assessing the Reliability of Drug Property Predictions. Journal of Chemical Information and Modeling, 2014, 54, 1500-1511.	2.5	51
251	Improvement of Virtual Screening Results by Docking Data Feature Analysis. Journal of Chemical Information and Modeling, 2014, 54, 1401-1411.	2.5	25
252	Open-Source Tools, Techniques, and Data in Chemoinformatics. , 2014, , 1-92.		1

#	Article	IF	Citations
253	Conformation-independent QSAR on c-Src tyrosine kinase inhibitors. Chemometrics and Intelligent Laboratory Systems, 2014, 134, 47-52.	1.8	10
254	Identification and analysis of synthesis routes in complex catalytic reaction networks for biomass upgrading. Applied Catalysis B: Environmental, 2014, 145, 149-160.	10.8	16
255	Conformational Polymorphism. Chemical Reviews, 2014, 114, 2170-2191.	23.0	590
256	Multivariate SAR and QSAR of cucurbitacin derivatives as cytotoxic compounds in a human lung adenocarcinoma cell line. Journal of Molecular Graphics and Modelling, 2014, 48, 70-79.	1.3	15
257	Docking Studies in Target Proteins Involved in Antibacterial Action Mechanisms: Extending the Knowledge on Standard Antibiotics to Antimicrobial Mushroom Compounds. Molecules, 2014, 19, 1672-1684.	1.7	44
258	LIBSA â€“ A Method for the Determination of Ligand-Binding Preference to Allosteric Sites on Receptor Ensembles. Journal of Chemical Information and Modeling, 2014, 54, 530-538.	2.5	14
259	Predicting hexadecaneâ€“air equilibrium partition coefficients (L) using a group contribution approach constructed from high quality data. SAR and QSAR in Environmental Research, 2014, 25, 51-71.	1.0	22
260	DiSCuS: An Open Platform for (Not Only) Virtual Screening Results Management. Journal of Chemical Information and Modeling, 2014, 54, 347-354.	2.5	5
261	EC-BLAST: a tool to automatically search and compare enzyme reactions. Nature Methods, 2014, 11, 171-174.	9.0	112
262	molBLOCKS: decomposing small molecule sets and uncovering enriched fragments. Bioinformatics, 2014, 30, 2081-2083.	1.8	32
263	iSyn: WebGL-Based Interactive De Novo Drug Design. , 2014, , .		5
264	Inhibition of NarL of Mycobacterium Tuberculosis: an in silico approach. Interdisciplinary Sciences, Computational Life Sciences, 2014, 6, 292-299.	2.2	10
265	A drug similarity network for understanding drug mechanism of action. Journal of Bioinformatics and Computational Biology, 2014, 12, 1441007.	0.3	1
266	In silico site of metabolism prediction for human UGT-catalyzed reactions. Bioinformatics, 2014, 30, 398-405.	1.8	29
267	Stochastic atomistic simulation of polycyclic aromatic hydrocarbon growth in combustion. Physical Chemistry Chemical Physics, 2014, 16, 7969-7979.	1.3	52
268	Application of the 4D Fingerprint Method with a Robust Scoring Function for Scaffold-Hopping and Drug Repurposing Strategies. Journal of Chemical Information and Modeling, 2014, 54, 2834-2845.	2.5	12
269	Insights into the structure and function of fungal Î²â€mannosidases from glycoside hydrolase familyÂ2 based on multiple crystal structures of the TrichodermaÂharzianum enzyme. FEBS Journal, 2014, 281, 4165-4178.	2.2	22
270	Imidazo[2,1-b]thiazole derivatives as new inhibitors of 15-lipoxygenase. European Journal of Medicinal Chemistry, 2014, 87, 759-764.	2.6	30

#	Article	IF	Citations
271	Simultaneous Virtual Prediction of Anti-Escherichia coli Activities and ADMET Profiles: A Chemoinformatic Complementary Approach for High-Throughput Screening. ACS Combinatorial Science, 2014, 16, 78-84.	3.8	51
272	Relativistic Force Field: Parametric Computations of Protonâ€“Proton Coupling Constants in ¹H NMR Spectra. Journal of Organic Chemistry, 2014, 79, 8397-8406.	1.7	74
273	Discovery of New Uncompetitive Inhibitors of Glucose-6-Phosphate Dehydrogenase. Journal of Biomolecular Screening, 2014, 19, 1362-1371.	2.6	25
274	Discovery, Biological Evaluation, and Crystal Structure of a Novel Nanomolar Selective Butyrylcholinesterase Inhibitor. Journal of Medicinal Chemistry, 2014, 57, 8167-8179.	2.9	220
275	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. Advances in Protein Chemistry and Structural Biology, 2014, 96, 235-265.	1.0	214
276	Complex Chemical Reaction Networks from Heuristics-Aided Quantum Chemistry. Journal of Chemical Theory and Computation, 2014, 10, 897-907.	2.3	100
277	Reaction analysis and visualization of ReaxFF molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2014, 53, 13-22.	1.3	79
278	Generalized Workflow for Generating Highly Predictive in Silico Off-Target Activity Models. Journal of Chemical Information and Modeling, 2014, 54, 2411-2422.	2.5	8
279	Fragment-Based Docking: Development of the CHARMMing Web User Interface as a Platform for Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2014, 54, 2612-2620.	2.5	21
280	Automated and reproducible read-across like models for predicting carcinogenic potency. Regulatory Toxicology and Pharmacology, 2014, 70, 370-378.	1.3	12
281	6-(Hetero)Arylpurine nucleotides as inhibitors of the oncogenic target DNPH1: Synthesis, structural studies and cytotoxic activities. European Journal of Medicinal Chemistry, 2014, 85, 418-437.	2.6	22
282	Markov Logic Networks for Optical Chemical Structure Recognition. Journal of Chemical Information and Modeling, 2014, 54, 2380-2390.	2.5	19
283	Enrichment of Chemical Libraries Docked to Protein Conformational Ensembles and Application to Aldehyde Dehydrogenase 2. Journal of Chemical Information and Modeling, 2014, 54, 2105-2116.	2.5	17
284	Endocrine Disruptomeâ€”An Open Source Prediction Tool for Assessing Endocrine Disruption Potential through Nuclear Receptor Binding. Journal of Chemical Information and Modeling, 2014, 54, 1254-1267.	2.5	113
285	A set of descriptors for identifying the proteinâ€“drug interaction in cellular networking. Journal of Theoretical Biology, 2014, 359, 120-128.	0.8	22
286	In Silico Design of Three-Dimensional Porous Covalent Organic Frameworks via Known Synthesis Routes and Commercially Available Species. Journal of Physical Chemistry C, 2014, 118, 23790-23802.	1.5	40
287	Molecular Docking of Bacosides with Tryptophan Hydroxylase: A Model to Understand the Bacosides Mechanism. Natural Products and Bioprospecting, 2014, 4, 251-255.	2.0	8
288	Bringing the MMFF force field to the RDKit: implementation and validation. Journal of Cheminformatics, 2014, 6, .	2.8	121

#	Article	IF	Citations
289	Disodium cromoglycate: exploiting its properties as a NMR weak-aligning medium for small organic molecules. Organic and Biomolecular Chemistry, 2014, 12, 1957-1965.	1.5	32
290	Prediction of Cosolvent Effect on Solvation Free Energies and Solubilities of Organic Compounds in Supercritical Carbon Dioxide Based on Fully Atomistic Molecular Simulations. Journal of Physical Chemistry B, 2014, 118, 11769-11780.	1.2	32
291	Synthesis of novel bridged dinitrogen heterocycles and their evaluation as potential fragments for the design of biologically active compounds. Tetrahedron, 2014, 70, 7854-7864.	1.0	18
292	QM Computations on Complete Nucleic Acids Building Blocks: Analysis of the Sarcinâ€“Ricin RNA Motif Using DFT-D3, HF-3c, PM6-D3H, and MM Approaches. Journal of Chemical Theory and Computation, 2014, 10, 2615-2629.	2.3	32
293	Chemo- and bioinformatics resources for inÂsilico drug discovery from medicinal plants beyond their traditional use: a critical review. Natural Product Reports, 2014, 31, 1585-1611.	5.2	104
294	A Theoretical Structural Study of Isoniazid Complexes with Thiotriazoline. Chemistry of Heterocyclic Compounds, 2014, 50, 438-443.	0.6	3
295	Autogrid-based clustering of kinases: selection of representative conformations for docking purposes. Molecular Diversity, 2014, 18, 611-619.	2.1	3
296	TCMSP: a database of systems pharmacology for drug discovery from herbal medicines. Journal of Cheminformatics, 2014, 6, 13.	2.8	2,919
297	A rotation-translation invariant molecular descriptor of partial charges and its use in ligand-based virtual screening. Journal of Cheminformatics, 2014, 6, 23.	2.8	21
298	iDrug: a web-accessible and interactive drug discovery and design platform. Journal of Cheminformatics, 2014, 6, 28.	2.8	30
299	Cytochrome P450 site of metabolism prediction from 2D topological fingerprints using GPU accelerated probabilistic classifiers. Journal of Cheminformatics, 2014, 6, 29.	2.8	26
300	Molpher: a software framework for systematic chemical space exploration. Journal of Cheminformatics, 2014, 6, 7.	2.8	32
301	Consistency of sugar structures and their annotation in the PDB. Journal of Cheminformatics, 2014, 6, .	2.8	0
302	QSAR modeling of aromatase inhibition by flavonoids using machine learning approaches. Chemical Papers, 2014, 68, .	1.0	9
303	Small molecule interaction with lipid bilayers: A molecular dynamics study of chlorhexidine. Journal of Molecular Graphics and Modelling, 2014, 48, 96-104.	1.3	19
304	inSARa: Intuitive and Interactive SAR Interpretation by Reduced Graphs and Hierarchical MCS-Based Network Navigation. Journal of Chemical Information and Modeling, 2014, 54, 1578-1595.	2.5	10
305	ProTox: a web server for the in silico prediction of rodent oral toxicity. Nucleic Acids Research, 2014, 42, W53-W58.	6.5	400
306	DDI-CPI, a server that predicts drugâ€“drug interactions through implementing the chemicalâ€“protein interactome. Nucleic Acids Research, 2014, 42, W46-W52.	6.5	63

#	Article	IF	Citations
307	Bromide Ion Exchange with a Keggin Polyoxometalate on Functionalized Polymeric Membranes: A Theoretical and Experimental Study. Journal of Physical Chemistry B, 2014, 118, 2396-2404.	1.2	9
308	Sterol Carrier Protein-2: Binding Protein for Endocannabinoids. Molecular Neurobiology, 2014, 50, 149-158.	1.9	35
309	The Flavonoid Derivative 2-(4â€² Benzyloxyphenyl)-3-hydroxy-chromen-4-one Protects Against Aî²42-Induced Neurodegeneration in Transgenic Drosophila: Insights from In Silico and In Vivo Studies. Neurotoxicity Research, 2014, 26, 331-350.	1.3	34
310	WebChem Viewer: a tool for the easy dissemination of chemical and structural data sets. BMC Bioinformatics, 2014, 15, 159.	1.2	0
311	Insight into the Binding Mechanism of Imipenem to Human Serum Albumin by Spectroscopic and Computational Approaches. Molecular Pharmaceutics, 2014, 11, 1785-1797.	2.3	191
312	OOMMPPAA: A Tool To Aid Directed Synthesis by the Combined Analysis of Activity and Structural Data. Journal of Chemical Information and Modeling, 2014, 54, 2636-2646.	2.5	9
313	Automated Building of Organometallic Complexes from 3D Fragments. Journal of Chemical Information and Modeling, 2014, 54, 1919-1931.	2.5	31
314	MDWiZ: A platform for the automated translation of molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2014, 48, 80-86.	1.3	10
315	NRLiSt BDB, the Manually Curated Nuclear Receptors Ligands and Structures Benchmarking Database. Journal of Medicinal Chemistry, 2014, 57, 3117-3125.	2.9	42
316	Indolinone-based acetylcholinesterase inhibitors: Synthesis, biological activity and molecular modeling. European Journal of Medicinal Chemistry, 2014, 84, 375-381.	2.6	73
317	BCRP Inhibition: from Data Collection to Ligandâ€Based Modeling. Molecular Informatics, 2014, 33, 322-331.	1.4	27
318	Structure determination from powder data without prior indexing, using a similarity measure based on cross-correlation functions. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2014, 70, 347-359.	0.5	32
319	Identification of a novel polyfluorinated compound as a lead to inhibit the human enzymes aldose reductase and AKR1B10: structure determination of both ternary complexes and implications for drug design. Acta Crystallographica Section D: Biological Crystallography, 2014, 70, 889-903.	2.5	28
320	Incorporating post-translational modifications and unnatural amino acids into high-throughput modeling of protein structures. Bioinformatics, 2014, 30, 1681-1689.	1.8	8
321	Synthesis and anti-cholinesterase activity of new 7-hydroxycoumarin derivatives. European Journal of Medicinal Chemistry, 2014, 82, 536-544.	2.6	69
322	Antigen specific immune enhancement of innate and acquired immunity by pearl in ashed form. International Immunopharmacology, 2014, 21, 82-93.	1.7	4
323	3D Flexible Alignment Using 2D Maximum Common Substructure: Dependence of Prediction Accuracy on Target-Reference Chemical Similarity. Journal of Chemical Information and Modeling, 2014, 54, 1850-1863.	2.5	33
324	Reverse docking: a powerful tool for drug repositioning and drug rescue. Future Medicinal Chemistry, 2014, 6, 333-342.	1.1	106

#	Article	IF	Citations
325	Synthesis, biological evaluation and docking study of 3-aroyl-1-(4-sulfamoylphenyl)thiourea derivatives as 15-lipoxygenase inhibitors. European Journal of Medicinal Chemistry, 2014, 82, 308-313.	2.6	51
326	QSAR models for thiophene and imidazopyridine derivatives inhibitors of the Polo-Like Kinase 1. European Journal of Pharmaceutical Sciences, 2014, 62, 171-179.	1.9	6
327	Pharmacological evaluation and docking studies of Î±,Î²-unsaturated carbonyl based synthetic compounds as inhibitors of secretory phospholipase A2, cyclooxygenases, lipoxygenase and proinflammatory cytokines. Bioorganic and Medicinal Chemistry, 2014, 22, 4151-4161.	1.4	50
328	Exploration of the dihydropyrimidine scaffold for the development of new potential anti-inflammatory agents blocking prostaglandin E2 synthase-1 enzyme (mPGES-1). European Journal of Medicinal Chemistry, 2014, 80, 407-415.	2.6	61
329	Graphlet signature-based scoring method to estimate proteinâ€“ligand binding affinity. Royal Society Open Science, 2014, 1, 140306.	1.1	6
330	Drug-Induced Conformational Population Shifts in Topoisomerase-DNA Ternary Complexes. Molecules, 2014, 19, 7415-7428.	1.7	7
331	Quantum chemistry structures and properties of 134 kilo molecules. Scientific Data, 2014, 1, 140022.	2.4	887
332	Molecular Dynamics Simulation-Based Evaluation of the Binding Free Energies of Computationally Designed Drug Candidates: Importance of the Dynamical Effects. Chemical and Pharmaceutical Bulletin, 2014, 62, 661-667.	0.6	11
333	TINAGL1 and B3GALNT1 are potential therapy target genes to suppress metastasis in non-small cell lung cancer. BMC Genomics, 2014, 15, S2.	1.2	66
334	Genes associated with genotype-specific DNA methylation in squamous cell carcinoma as candidate drug targets. BMC Systems Biology, 2014, 8, S4.	3.0	36
335	Generic strategies for chemical space exploration. International Journal of Computational Biology and Drug Design, 2014, 7, 225.	0.3	26
336	WikiHyperGlossary (WHG): an information literacy technology for chemistry documents. Journal of Cheminformatics, 2015, 7, 22.	2.8	3
337	Drug discovery for breast cancer based on big data analytics techniques. , 2015, , .		2
338	Targeting kinases with anilinopyrimidines: discovery of N-phenyl-Nâ€™-[4-(pyrimidin-4-ylamino)phenyl]urea derivatives as selective inhibitors of class III receptor tyrosine kinase subfamily. Scientific Reports, 2015, 5, 16750.	1.6	53
339	Sulfonoquinovosyl diacylglyceride selectively targets acute lymphoblastic leukemia cells and exerts potent anti-leukemic effects in vivo. Scientific Reports, 2015, 5, 12082.	1.6	7
340	Mechanistic analysis of a synthetic inhibitor of the Pseudomonas aeruginosa LasI quorum-sensing signal synthase. Scientific Reports, 2015, 5, 16569.	1.6	57
341	In silico Spleen Tyrosine Kinase Inhibitor Screening by ChooseLD. IPSJ Transactions on Bioinformatics, 2015, 8, 14-20.	0.2	0
342	A large-scale crop protection bioassay data set. Scientific Data, 2015, 2, 150032.	2.4	18

#	Article	IF	Citations
343	The PubChemQC project: A large chemical database from the first principle calculations. AIP Conference Proceedings, 2015, , .	0.3	10
344	9Hâ€Carbazole Derivatives Containing the Nâ€Benzylâ€1,2,3â€triazole Moiety as New Acetylcholinesterase Inhibitors. Archiv Der Pharmazie, 2015, 348, 366-374.	2.1	29
345	Synthesis and Anticholinergic Activity of 4â€hydroxycoumarin Derivatives Containing Substituted Benzylâ€1,2,3â€triazole Moiety. Chemical Biology and Drug Design, 2015, 86, 1215-1220.	1.5	42
346	The Chemical Validation and Standardization Platform (CVSP): large-scale automated validation of chemical structure datasets. Journal of Cheminformatics, 2015, 7, 30.	2.8	20
347	ChemDIS: a chemicalâ€“disease inference system based on chemicalâ€“protein interactions. Journal of Cheminformatics, 2015, 7, 25.	2.8	13
348	Smiles2Monomers: a link between chemical and biological structures for polymers. Journal of Cheminformatics, 2015, 7, 62.	2.8	10
349	Combined use of computational chemistry and chemoinformatics methods for chemical discovery. AIP Conference Proceedings, 2015, , .	0.3	3
350	In Silico Predictions of Drug â€“ Drug Interactions Caused by CYP1A2, 2C9 and 3A4 Inhibition â€“ a Comparative Study of Virtual Screening Performance. Molecular Informatics, 2015, 34, 431-457.	1.4	15
351	Inhibition of Osteoclast Differentiation by Ginsenoside Rg3 in RAW264.7 Cells via RANKL, JNK and p38 MAPK Pathways Through a Modulation of Cathepsin K: An In Silico and In Vitro Study. Phytotherapy Research, 2015, 29, 1286-1294.	2.8	30
352	Universal Structure Conversion Method for Organic Molecules: From Atomic Connectivity to Threeâ€Dimensional Geometry. Bulletin of the Korean Chemical Society, 2015, 36, 1769-1777.	1.0	36
353	Perspectives of Halogen Bonding Description in Scoring Functions and QSAR/QSPR: Substituent Effects in Aromatic Core. Molecular Informatics, 2015, 34, 404-416.	1.4	12
354	Phytochemica: a platform to explore phytochemicals of medicinal plants. Database: the Journal of Biological Databases and Curation, 2015, 2015, bav075.	1.4	53
355	ONRLDBâ€”manually curated database of experimentally validated ligands for orphan nuclear receptors: insights into new drug discovery. Database: the Journal of Biological Databases and Curation, 2015, 2015, bav112.	1.4	16
356	Optimizing the affinity and specificity of ligand binding with the inclusion of solvation effect. Proteins: Structure, Function and Bioinformatics, 2015, 83, 1632-1642.	1.5	12
357	Prediction of Protein-Ligand Binding Sites for Cisplatin and Transplatin based on Hydrogen Bonds. Journal of Proteomics and Bioinformatics, 2015, 8, .	0.4	0
358	The eNanoMapper database for nanomaterial safety information. Beilstein Journal of Nanotechnology, 2015, 6, 1609-1634.	1.5	92
359	The relevance of piroxicam for the prevention and treatment of nonmelanoma skin cancer and its precursors. Drug Design, Development and Therapy, 2015, 9, 5843.	2.0	35
360	Molecular docking analysis of known flavonoids as duel COX-2 inhibitors in the context of cancer. Bioinformation, 2015, 11, 543-549.	0.2	14

#	Article	IF	Citations
361	Potential Broad Spectrum Inhibitors of the Coronavirus 3CLpro: A Virtual Screening and Structure-Based Drug Design Study. Viruses, 2015, 7, 6642-6660.	1.5	57
362	Common Amino Acid Subsequences in a Universal Proteomeâ€"Relevance for Food Science. International Journal of Molecular Sciences, 2015, 16, 20748-20773.	1.8	23
363	A Structural Hierarchy Matching Approach for Molecular Similarity/Substructure Searching. Molecules, 2015, 20, 8791-8799.	1.7	0
364	Charting a Path to Success in Virtual Screening. Molecules, 2015, 20, 18732-18758.	1.7	62
365	Physicochemical characteristics of structurally determined metabolite-protein and drug-protein binding events with respect to binding specificity. Frontiers in Molecular Biosciences, 2015, 2, 51.	1.6	9
366	DockBench: An Integrated Informatic Platform Bridging the Gap between the Robust Validation of Docking Protocols and Virtual Screening Simulations. Molecules, 2015, 20, 9977-9993.	1.7	40
367	Structure- and Ligand-Based Virtual Screening Identifies New Scaffolds for Inhibitors of the Oncoprotein MDM2. PLoS ONE, 2015, 10, e0121424.	1.1	14
368	A Modularity-Based Method Reveals Mixed Modules from Chemical-Gene Heterogeneous Network. PLoS ONE, 2015, 10, e0125585.	1.1	2
369	Linear Interaction Energy Based Prediction of Cytochrome P450 1A2 Binding Affinities with Reliability Estimation. PLoS ONE, 2015, 10, e0142232.	1.1	23
370	The LUX Score: A Metric for Lipidome Homology. PLoS Computational Biology, 2015, 11, e1004511.	1.5	16
371	Novel Broad Spectrum Inhibitors Targeting the Flavivirus Methyltransferase. PLoS ONE, 2015, 10, e0130062.	1.1	58
372	Computational Structure-Based De Novo Design of Hypothetical Inhibitors against the Anti-Inflammatory Target COX-2. PLoS ONE, 2015, 10, e0134691.	1.1	24
373	A Database of Force-Field Parameters, Dynamics, and Properties of Antimicrobial Compounds. Molecules, 2015, 20, 13997-14021.	1.7	48
374	Modeling, molecular dynamics, and docking assessment of transcription factor rho: a potential drug target in Brucella melitensis 16M. Drug Design, Development and Therapy, 2015, 9, 1897.	2.0	41
375	Prediction of Drug Indications Based on Chemical Interactions and Chemical Similarities. BioMed Research International, 2015, 2015, 1-14.	0.9	3
376	Amino Acids in Nine Ligand-Prefer Ramachandran Regions. BioMed Research International, 2015, 2015, 1-10.	0.9	2
377	Molecular Docking Study Characterization of Rare Flavonoids at the Nac-Binding Site of the First Bromodomain of BRD4 (BRD4 BD1). Journal of Cancer Research, 2015, 2015, 1-15.	0.7	18
378	Chemoinformatics Approach to Antibacterial Studies of Essential Oils. Natural Product Communications, 2015, 10, 1934578X1501000.	0.2	9

#	Article	IF	Citations
379	Identification of Ellagic acid analogues as potent inhibitor of protein Kinase CK2:A chemopreventive role in oral cancer. Bioinformation, 2015, 11, 21-26.	0.2	8
380	AHTPDB: a comprehensive platform for analysis and presentation of antihypertensive peptides. Nucleic Acids Research, 2015, 43, D956-D962.	6.5	143
381	MemGen: a general web server for the setup of lipid membrane simulation systems. Bioinformatics, 2015, 31, 2897-2899.	1.8	71
382	Calculating an optimal box size for ligand docking and virtual screening against experimental and predicted binding pockets. Journal of Cheminformatics, 2015, 7, 18.	2.8	160
383	Digital NMR Profiles as Building Blocks: Assembling ¹H Fingerprints of Steviol Glycosides. Journal of Natural Products, 2015, 78, 658-665.	1.5	18
384	GLASS: a comprehensive database for experimentally validated GPCR-ligand associations. Bioinformatics, 2015, 31, 3035-3042.	1.8	92
385	Luscus: molecular viewer and editor for MOLCAS. Journal of Cheminformatics, 2015, 7, 16.	2.8	25
386	Chemometrics and cheminformatics in the analysis of biologically active peptides from food sources. Journal of Functional Foods, 2015, 16, 334-351.	1.6	74
387	Synthesis and antiproliferative activity of Î±-branched Î±,Î²-unsaturated ketones in human hematological and solid cancer cell lines. European Journal of Medicinal Chemistry, 2015, 98, 30-48.	2.6	6
388	Structure-Based Small Molecule Modulation of a Pre-Amyloid State: Pharmacological Enhancement of IAPP Membrane-Binding and Toxicity. Biochemistry, 2015, 54, 3555-3564.	1.2	11
389	How Does the Methodology of 3D Structure Preparation Influence the Quality of pK_a Prediction?. Journal of Chemical Information and Modeling, 2015, 55, 1088-1097.	2.5	10
390	Tyrosinase inhibitory potential of purpurin in Rubia cordifoliaâ€"A bioactivity guided approach. Industrial Crops and Products, 2015, 74, 319-326.	2.5	24
391	Computational Simulation Techniques to Understand Rifampicin Resistance Mutation (S425L) of rpoB in M. leprae. Journal of Cellular Biochemistry, 2015, 116, 1278-1285.	1.2	11
392	QuickFF: A program for a quick and easy derivation of force fields for metalâ€organic frameworks from ab initio input. Journal of Computational Chemistry, 2015, 36, 1015-1027.	1.5	132
393	An Ab Initio Method for Designing Multiâ€Target Specific Pharmacophores using Complementary Interaction Field of Aspartic Proteases. Molecular Informatics, 2015, 34, 380-393.	1.4	8
394	Properties of Organic Liquids when Simulated with Long-Range Lennard-Jones Interactions. Journal of Chemical Theory and Computation, 2015, 11, 2938-2944.	2.3	116
395	ChemCom: A Software Program for Searching and Comparing Chemical Libraries. Journal of Chemical Information and Modeling, 2015, 55, 1292-1296.	2.5	1
396	Computational identification and binding analysis of orphan human cytochrome P450 4X1 enzyme with substrates. BMC Research Notes, 2015, 8, 9.	0.6	15

#	Article	IF	Citations
397	Drug discovery for breast cancer based on big data analytics techniques. , 2015, , .		3
398	A novel approach to identify shared fragments in drugs and natural products. , 2015, , .		0
399	Challenges and Modifications for Creating a MoSGrid Science Gateway for US and European Infrastructures. , 2015, , .		3
400	LigDig: a web server for querying ligandâ€“protein interactions. Bioinformatics, 2015, 31, 1147-1149.	1.8	13
401	Chemozart: a web-based 3D molecular structure editor and visualizer platform. Journal of Cheminformatics, 2015, 7, 56.	2.8	8
402	Synthesis and biological evaluation of new C-10 substituted dithranol pleiotropic hybrids. Bioorganic and Medicinal Chemistry, 2015, 23, 7251-7263.	1.4	4
403	AtomicChargeCalculator: interactive web-based calculation of atomic charges in large biomolecular complexes and drug-like molecules. Journal of Cheminformatics, 2015, 7, 50.	2.8	50
404	Toxicity Predictions using Compound Descriptions. , 2015, , .		0
405	Molecular docking studies on InhA, MabA and PanK enzymes from Mycobacterium tuberculosis of ellagic acid derivatives from Ludwigia adscendens and Trewia nudiflora. In Silico Pharmacology, 2015, 3, 10.	1.8	14
406	ChemDes: an integrated web-based platform for molecular descriptor and fingerprint computation. Journal of Cheminformatics, 2015, 7, 60.	2.8	235
407	PEPstrMOD: structure prediction of peptides containing natural, non-natural and modified residues. Biology Direct, 2015, 10, 73.	1.9	164
408	Standards-based curation of a decade-old digital repository dataset of molecular information. Journal of Cheminformatics, 2015, 7, 43.	2.8	8
409	Metrabase: a cheminformatics and bioinformatics database for small molecule transporter data analysis and (Q)SAR modeling. Journal of Cheminformatics, 2015, 7, 31.	2.8	47
410	CancerPPD: a database of anticancer peptides and proteins. Nucleic Acids Research, 2015, 43, D837-D843.	6.5	253
411	An affinity improved single-chain antibody from phage display of a library derived from monoclonal antibodies detects fumonisins by immunoassay. Analytica Chimica Acta, 2015, 867, 74-82.	2.6	35
412	RIFM fragrance ingredient safety assessment, 2,6-Dimethyl-5-heptenal, CAS Registry Number 106-72-9. Food and Chemical Toxicology, 2015, 82, S89-S96.	1.8	1
413	Mechismo: predicting the mechanistic impact of mutations and modifications on molecular interactions. Nucleic Acids Research, 2015, 43, e10-e10.	6.5	95
414	Insights from the molecular docking of hydrolytic products of methyl iso cyanate (MIC) to inhibition of human immune proteins. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 287.	2.2	1

#	Article	IF	Citations
415	A Binding Mode Hypothesis of Tiagabine Confirms Liothyronine Effect on Î³-Aminobutyric Acid Transporter 1 (GAT1). Journal of Medicinal Chemistry, 2015, 58, 2149-2158.	2.9	44
416	Super Natural IIâ€"a database of natural products. Nucleic Acids Research, 2015, 43, D935-D939.	6.5	279
417	Biasing Potential Replica Exchange Multisite Î»-Dynamics for Efficient Free Energy Calculations. Journal of Chemical Theory and Computation, 2015, 11, 1267-1277.	2.3	32
418	Discriminating precursors of common fragments for large-scale metabolite profiling by triple quadrupole mass spectrometry. Bioinformatics, 2015, 31, 2017-2023.	1.8	18
419	Contributions of Ionic Interactions and Protein Dynamics to Cytochrome P450 2D6 (CYP2D6) Substrate and Inhibitor Binding. Journal of Biological Chemistry, 2015, 290, 5092-5104.	1.6	86
420	Computational prediction of microRNA networks incorporating environmental toxicity and disease etiology. Scientific Reports, 2014, 4, 5576.	1.6	51
421	Mechanism-Based Discovery of Novel Substrates of Haloalkane Dehalogenases Using in Silico Screening. Journal of Chemical Information and Modeling, 2015, 55, 54-62.	2.5	23
422	Similarity-based prediction for Anatomical Therapeutic Chemical classification of drugs by integrating multiple data sources. Bioinformatics, 2015, 31, 1788-1795.	1.8	59
423	Virtual screening of molecular properties of chitosan and derivatives in search for druggable molecules. International Journal of Biological Macromolecules, 2015, 74, 392-396.	3.6	9
424	MACE: mutation-oriented profiling of chemical response and gene expression in cancers. Bioinformatics, 2015, 31, 1508-1514.	1.8	5
425	Synthesis, biological evaluation and docking analysis of a new series of methylsulfonyl and sulfamoyl acetamides and ethyl acetates as potent COX-2 inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 810-820.	1.4	21
426	Todralazine Protects Zebrafish from Lethal Effects of Ionizing Radiation: Role of Hematopoietic Cell Expansion. Zebrafish, 2015, 12, 33-47.	0.5	12
427	Computational methods in metabolic engineering for strain design. Current Opinion in Biotechnology, 2015, 34, 135-141.	3.3	121
428	In silico analysis of conformational changes induced by normal and mutation of macrophage infectivity potentiator catalytic residues and its interactions with Rapamycin. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 326.	2.2	0
429	CFam: a chemical families database based on iterative selection of functional seeds and seed-directed compound clustering. Nucleic Acids Research, 2015, 43, D558-D565.	6.5	6
430	Scoring Functions for AutoDock. Methods in Molecular Biology, 2015, 1273, 467-474.	0.4	23
431	Predicting Hepatotoxicity Using ToxCast in Vitro Bioactivity and Chemical Structure. Chemical Research in Toxicology, 2015, 28, 738-751.	1.7	124
432	Bridging from syntactic to statistical methods: Classification with automatically segmented features from sequences. Pattern Recognition, 2015, 48, 3749-3756.	5.1	4

#	Article	IF	Citations
433	JP-10 combustion studied with shock tube experiments and modeled with automatic reaction mechanism generation. Combustion and Flame, 2015, 162, 3115-3129.	2.8	80
434	Atomsk: A tool for manipulating and converting atomic data files. Computer Physics Communications, 2015, 197, 212-219.	3.0	1,021
435	RIFM fragrance ingredient safety assessment, Î±-Irone, CAS registry number 79-69-6. Food and Chemical Toxicology, 2015, 82, S105-S113.	1.8	2
436	Open Drug Discovery Toolkit (ODDT): a new open-source player in the drug discovery field. Journal of Cheminformatics, 2015, 7, 26.	2.8	140
437	In Silico Analysis of Conformational Changes Induced by Normal and Mutation of Macrophage Infectivity Potentiator Catalytic Residues and its Interactions with Rapamycin. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 326-333.	2.2	6
438	Potent inhibition of miR-27a by neomycinâ€“bisbenzimidazole conjugates. Chemical Science, 2015, 6, 5837-5846.	3.7	33
439	Self-Assembly of Catecholic Moiety-Containing Cationic Random Acrylic Copolymers. Journal of Physical Chemistry B, 2015, 119, 8369-8379.	1.2	17
440	Nonlinear Optical Properties of Fluorescent Dyes Allow for Accurate Determination of Their Molecular Orientations in Phospholipid Membranes. Journal of Physical Chemistry B, 2015, 119, 9706-9716.	1.2	10
441	Modeling Epoxidation of Drug-like Molecules with a Deep Machine Learning Network. ACS Central Science, 2015, 1, 168-180.	5.3	130
442	Identification and Characterization of Novel Broad-Spectrum Inhibitors of the Flavivirus Methyltransferase. ACS Infectious Diseases, 2015, 1, 340-349.	1.8	51
443	Essential Domains of Anaplasma phagocytophilum Invasins Utilized to Infect Mammalian Host Cells. PLoS Pathogens, 2015, 11, e1004669.	2.1	33
444	Investigation of protonated and sodiated leucine-enkephalin by hydrogenâ€“deuterium exchange and theoretical calculations. Analytical Methods, 2015, 7, 5551-5556.	1.3	8
445	SANCDB: a South African natural compound database. Journal of Cheminformatics, 2015, 7, 29.	2.8	77
446	Synthesis and biological evaluation of 5-benzylidenerhodanine-3-acetic acid derivatives as AChE and 15-LOX inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2015, 30, 389-395.	2.5	22
447	Molecular Orientation and Structural Transformations in Phthalic Anhydride Thin Films on MgO(100)/Ag(100). Langmuir, 2015, 31, 7806-7814.	1.6	16
448	FlexAID: Revisiting Docking on Non-Native-Complex Structures. Journal of Chemical Information and Modeling, 2015, 55, 1323-1336.	2.5	54
449	How useful is molecular modelling in combination with ion mobility mass spectrometry for â€˜small moleculeâ€™ ion mobility collision cross-sections?. Analyst, The, 2015, 140, 6814-6823.	1.7	50
450	Discovery of TRAF-2 and NCK-interacting kinase (TNIK) inhibitors by ligand-based virtual screening methods. MedChemComm, 2015, 6, 1564-1572.	3.5	5

#	Article	IF	Citations
451	PockDrug-Server: a new web server for predicting pocket druggability on holo and apo proteins. Nucleic Acids Research, 2015, 43, W436-W442.	6.5	142
452	Identification of small-molecule inhibitors of calcineurin-NFATc signaling that mimic the PxIxIT motif of calcineurin binding partners. Science Signaling, 2015, 8, ra63.	1.6	22
453	Automated computational screening of the thiol reactivity of substituted alkenes. Journal of Computer-Aided Molecular Design, 2015, 29, 725-735.	1.3	19
454	LiSiCA: A Software for Ligand-Based Virtual Screening and Its Application for the Discovery of Butyrylcholinesterase Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1521-1528.	2.5	70
455	Vascular endothelial growth factor receptor-2 (VEGFR-2) inhibitors: development and validation of predictive 3-D QSAR models through extensive ligand- and structure-based approaches. Journal of Computer-Aided Molecular Design, 2015, 29, 757-776.	1.3	9
456	Ligand- and receptor-based docking with LiBELa. Journal of Computer-Aided Molecular Design, 2015, 29, 713-723.	1.3	13
457	Benzo[e]pyrimido[5,4-b][1,4]diazepin-6(11H)-one derivatives as Aurora A kinase inhibitors: LQTA-QSAR analysis and detailed systematic validation of the developed model. Molecular Diversity, 2015, 19, 965-974.	2.1	10
458	Detection of Binding Site Molecular Interaction Field Similarities. Journal of Chemical Information and Modeling, 2015, 55, 1600-1615.	2.5	45
459	Many InChIs and quite some feat. Journal of Computer-Aided Molecular Design, 2015, 29, 681-694.	1.3	19
460	Insights into the Interactions of Fasciola hepatica Cathepsin L3 with a Substrate and Potential Novel Inhibitors through In Silico Approaches. PLoS Neglected Tropical Diseases, 2015, 9, e0003759.	1.3	17
461	Computing stoichiometric molecular composition from crystal structures. Journal of Applied Crystallography, 2015, 48, 85-91.	1.9	133
462	Large-Scale Chemical Similarity Networks for Target Profiling of Compounds Identified in Cell-Based Chemical Screens. PLoS Computational Biology, 2015, 11, e1004153.	1.5	70
463	EpiDBase: a manually curated database for small molecule modulators of epigenetic landscape. Database: the Journal of Biological Databases and Curation, 2015, 2015, .	1.4	17
464	The chemical component dictionary: complete descriptions of constituent molecules in experimentally determined 3D macromolecules in the Protein Data Bank. Bioinformatics, 2015, 31, 1274-1278.	1.8	110
465	PDBest: a userâ€“friendly platform for manipulating and enhancing protein structures: Fig. 1.. Bioinformatics, 2015, 31, 2894-2896.	1.8	5
466	Novel type of virtual ligand screening on the basis of quantum-chemical calculations for proteinâ€“ligand complexes and extended clustering techniques. Computational and Theoretical Chemistry, 2015, 1061, 12-22.	1.1	19
467	Isolation and characterization of a 17-kDa FKBP-type peptidyl-prolyl cis/trans isomerase from Vibrio anguillarum. Protein Expression and Purification, 2015, 110, 130-137.	0.6	6
468	Diarylsulfonamides and their bioisosteres as dual inhibitors of alkaline phosphatase and carbonic anhydrase: Structure activity relationship and molecular modelling studies. Bioorganic and Medicinal Chemistry, 2015, 23, 2435-2444.	1.4	39

#	Article	IF	Citations
469	The Purchasable Chemical Space: A Detailed Picture. Journal of Chemical Information and Modeling, 2015, 55, 915-924.	2.5	38
470	Highly Selective Phosphatidylinositol 4-Kinase IIIÎ² Inhibitors and Structural Insight into Their Mode of Action. Journal of Medicinal Chemistry, 2015, 58, 3767-3793.	2.9	54
471	Comparative interactions of withanolides and sterols with two members of sterol glycosyltransferases from Withania somnifera. BMC Bioinformatics, 2015, 16, 120.	1.2	13
472	Identification ofPlasmodium falciparumapicoplast-targeted tRNA-guanine transglycosylase and its potential inhibitors using comparative genomics, molecular modelling, docking and simulation studies. Journal of Biomolecular Structure and Dynamics, 2015, 33, 2404-2420.	2.0	8
473	Large-scale virtual high-throughput screening for the identification of new battery electrolyte solvents: computing infrastructure and collective properties. Physical Chemistry Chemical Physics, 2015, 17, 3394-3401.	1.3	56
474	Psoralen derivatives as inhibitors of NF- $$upkappa hbox {B/DNA}$$ Îº B/DNA interaction: the critical role of the furan ring. Molecular Diversity, 2015, 19, 551-561.	2.1	6
475	Molecular dynamics to enhance structure-based virtual screening on cathepsin B. Journal of Computer-Aided Molecular Design, 2015, 29, 707-712.	1.3	19
476	Non-target screening with high-resolution mass spectrometry: critical review using a collaborative trial on water analysis. Analytical and Bioanalytical Chemistry, 2015, 407, 6237-6255.	1.9	489
477	<italic>In-silico</italic> Studies Show Potent Inhibition of HIV-1 Reverse Transcriptase Activity by a Herbal Drug. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2015, 12, 1355-1364.	1.9	5
479	Automated Discovery of Reaction Pathways, Rate Constants, and Transition States Using Reactive Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2517-2524.	2.3	155
480	Molecular mechanism of statin-mediated LOX-1 inhibition. Cell Cycle, 2015, 14, 1583-1595.	1.3	36
481	Design, synthesis and anticholinesterase activity of novel benzylidenechroman-4-ones bearing cyclic amine side chain. European Journal of Medicinal Chemistry, 2015, 97, 181-189.	2.6	29
482	Cheaper faster drug development validated by the repositioning of drugs against neglected tropical diseases. Journal of the Royal Society Interface, 2015, 12, 20141289.	1.5	97
483	SEABED: Small molEcule activity scanner weB servicE baseD. Bioinformatics, 2015, 31, 773-775.	1.8	8
484	PDB4DNA: Implementation of DNA geometry from the Protein Data Bank (PDB) description for Geant4-DNA Monte-Carlo simulations. Computer Physics Communications, 2015, 192, 282-288.	3.0	33
485	The Electrolyte Genome project: A big data approach in battery materials discovery. Computational Materials Science, 2015, 103, 56-67.	1.4	150
486	Site of Reactivity Models Predict Molecular Reactivity of Diverse Chemicals with Glutathione. Chemical Research in Toxicology, 2015, 28, 797-809.	1.7	70
487	Multi-Step Protocol for Automatic Evaluation of Docking Results Based on Machine Learning Methodsâ€"A Case Study of Serotonin Receptors 5-HT₆ and 5-HT₇. Journal of Chemical Information and Modeling, 2015, 55, 823-832.	2.5	12

#	Article	IF	Citations
488	Big Data Meets Quantum Chemistry Approximations: The Î”-Machine Learning Approach. Journal of Chemical Theory and Computation, 2015, 11, 2087-2096.	2.3	579
489	NutriChem: a systems chemical biology resource to explore the medicinal value of plant-based foods. Nucleic Acids Research, 2015, 43, D940-D945.	6.5	40
490	Quantitative Structureâ€“Property Relationship Predictions of Critical Properties and Acentric Factors for Pure Compounds. Journal of Chemical & Engineering Data, 2015, 60, 1377-1387.	1.0	18
491	Searching molecular structure databases with tandem mass spectra using CSI:FingerID. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 12580-12585.	3.3	695
492	Facts and fictions about polymorphism. Chemical Society Reviews, 2015, 44, 8619-8635.	18.7	499
493	Recognizing drug targets using evolutionary information: implications for repurposing FDA-approved drugs against Mycobacterium tuberculosis H37Rv. Molecular BioSystems, 2015, 11, 3316-3331.	2.9	20
494	Natural product (â^')â€gossypol inhibits colon cancer cell growth by targeting RNAâ€binding protein Musashiâ€1. Molecular Oncology, 2015, 9, 1406-1420.	2.1	116
495	Pharmacophore Modeling: Methods and Applications. Methods in Pharmacology and Toxicology, 2015, , 167-188.	0.1	4
496	NPDock: a web server for proteinâ€“nucleic acid docking. Nucleic Acids Research, 2015, 43, W425-W430.	6.5	180
497	Insights from the Molecular Docking of Hydrolytic Products of Methyl Isocyanate (MIC) to Inhibition of Human Immune Proteins. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 287-294.	2.2	11
498	Chemically Aware Model Builder (camb): an R package for property and bioactivity modelling of small molecules. Journal of Cheminformatics, 2015, 7, 45.	2.8	32
499	Molecular Rift: Virtual Reality for Drug Designers. Journal of Chemical Information and Modeling, 2015, 55, 2475-2484.	2.5	88
500	Principal component analysis-based unsupervised feature extraction applied to in silico drug discovery for posttraumatic stress disorder-mediated heart disease. BMC Bioinformatics, 2015, 16, 139.	1.2	46
501	FESetup: Automating Setup for Alchemical Free Energy Simulations. Journal of Chemical Information and Modeling, 2015, 55, 2485-2490.	2.5	92
502	Deciding when to stop: efficient experimentation to learn to predict drug-target interactions. BMC Bioinformatics, 2015, 16, 213.	1.2	6
503	A Cell-Based High-Throughput Screening for Inducers of Myeloid Differentiation. Journal of Biomolecular Screening, 2015, 20, 1150-1159.	2.6	14
504	Predicting Adsorption Affinities of Small Molecules on Carbon Nanotubes Using Molecular Dynamics Simulation. ACS Nano, 2015, 9, 11761-11774.	7.3	89
505	PoLi: A Virtual Screening Pipeline Based on Template Pocket and Ligand Similarity. Journal of Chemical Information and Modeling, 2015, 55, 1757-1770.	2.5	36

#	Article	IF	Citations
506	CancerHSP: anticancer herbs database of systems pharmacology. Scientific Reports, 2015, 5, 11481.	1.6	43
507	Communication: Accurate hydration free energies at a wide range of temperatures from 3D-RISM. Journal of Chemical Physics, 2015, 142, 091105.	1.2	60
508	Three Dimensional (3D) Printing: A Straightforward, User-Friendly Protocol To Convert Virtual Chemical Models to Real-Life Objects. Journal of Chemical Education, 2015, 92, 1398-1401.	1.1	57
509	Identification of disulfide isomerase ERp57 as a target for small molecule cardioprotective agents. RSC Advances, 2015, 5, 74605-74610.	1.7	12
510	SerpentinaDB: a database of plant-derived molecules of Rauvolfia serpentina. BMC Complementary and Alternative Medicine, 2015, 15, 262.	3.7	20
511	First-Principles Prediction of Enthalpies of Formation for Polycyclic Aromatic Hydrocarbons and Derivatives. Journal of Physical Chemistry A, 2015, 119, 11329-11365.	1.1	38
512	Some new indoleâ€“coumarin hybrids; Synthesis, anticancer and Bcl-2 docking studies. Bioorganic Chemistry, 2015, 63, 101-109.	2.0	62
513	Ligand similarity guided receptor selection enhances docking accuracy and recall for non-nucleoside HIV reverse transcriptase inhibitors. Journal of Molecular Modeling, 2015, 21, 282.	0.8	5
514	A novel benzimidazole derivative binds to the DNA minor groove and induces apoptosis in leukemic cells. RSC Advances, 2015, 5, 93194-93208.	1.7	40
515	CAVITY: Mapping the Druggable Binding Site. Methods in Pharmacology and Toxicology, 2015, , 111-132.	0.1	3
516	Transition state geometry prediction using molecular group contributions. Physical Chemistry Chemical Physics, 2015, 17, 32173-32182.	1.3	42
517	How to estimate solid-electrolyte-interphase features when screening electrolyte materials. Physical Chemistry Chemical Physics, 2015, 17, 22799-22808.	1.3	36
518	Accounting for Intraligand Interactions in Flexible Ligand Docking with a PMF-Based Scoring Function. Journal of Chemical Information and Modeling, 2015, 55, 2121-2137.	2.5	5
519	A fast topological analysis algorithm for large-scale similarity evaluations of ligands and binding pockets. Journal of Cheminformatics, 2015, 7, 42.	2.8	4
520	Cardiolipin Interactions with Proteins. Biophysical Journal, 2015, 109, 1282-1294.	0.2	116
521	Relationship between Enzyme/Substrate Properties and Enzyme Efficiency in Hydrolases. ACS Catalysis, 2015, 5, 5877-5887.	5.5	31
522	Towards quantifying the role of exact exchange in predictions of transition metal complex properties. Journal of Chemical Physics, 2015, 143, 034104.	1.2	93
523	End-to-end solution for accessible chemical diagrams. , 2015, , .		21

#	Article	IF	Citations
524	A Comparative Study of 2D UMI and 3D Zernike Shape Descriptor for ATS Drugs Identification. Advances in Intelligent Systems and Computing, 2015, , 237-249.	0.5	3
525	On the use of molecular dynamics simulation to calculate X-ray thermal diffuse scattering from molecular crystals. Journal of Applied Crystallography, 2015, 48, 1420-1428.	1.9	7
526	Systems pharmacology and molecular docking strategies prioritize natural molecules as cardioprotective agents. RSC Advances, 2015, 5, 77042-77055.	1.7	12
527	Ligand binding studies, preliminary structureâ€“activity relationship and detailed mechanistic characterization of 1-phenyl-6,6-dimethyl-1,3,5-triazine-2,4-diamine derivatives as inhibitors of Escherichia coli dihydrofolate reductase. European Journal of Medicinal Chemistry, 2015, 103, 600-614.	2.6	22
528	Expanding the chemical space of human serine racemase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2015, 25, 4297-4303.	1.0	22
529	Photobiological properties of 3-psoralenacetic acids. Photochemical and Photobiological Sciences, 2015, 14, 2074-2086.	1.6	3
530	A General Guidebook for the Theoretical Prediction of Physicochemical Properties of Chemicals for Regulatory Purposes. Chemical Reviews, 2015, 115, 13093-13164.	23.0	116
531	First-Principles Molecular Structure Search with a Genetic Algorithm. Journal of Chemical Information and Modeling, 2015, 55, 2338-2348.	2.5	83
532	RIFM fragrance ingredient safety assessment, allyl (cyclohexyloxy)acetate, CAS registry number 68901-15-5. Food and Chemical Toxicology, 2015, 82, S59-S65.	1.8	2
533	RIFM fragrance ingredient safety assessment, allyl phenylacetate, CAS registry number 1797-74-6. Food and Chemical Toxicology, 2015, 82, S66-S73.	1.8	0
534	RIFM fragrance ingredient safety assessment, borneol, CAS registry number 507-70-0. Food and Chemical Toxicology, 2015, 82, S81-S88.	1.8	8
535	Novel and selective acetylcholinesterase inhibitors for Tetranychus cinnabarinus (Acari:) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50	1.2	14
536	Optimal graphâ€based and Simplified Molecular Input Line Entry Systemâ€based descriptors for quantitative structureâ€“activity relationship analysis of arylalkylaminoalcohols, arylalkenylamines, and arylalkylamines as Ïƒ₁ receptor ligands. Journal of Chemometrics, 2015, 29, 13-20.	0.7	5
537	Some insight into the mode of cytotoxic action of organotin compounds with protective 2,6-di-tert-butylphenol fragments. Journal of Organometallic Chemistry, 2015, 782, 96-102.	0.8	23
538	Characterizing the pocketome of Mycobacterium tuberculosis and application in rationalizing polypharmacological target selection. Scientific Reports, 2014, 4, 6356.	1.6	25
539	EDCs DataBank: 3D-Structure database of endocrine disrupting chemicals. Toxicology, 2015, 327, 87-94.	2.0	36
540	Catalytic activity of copper(II) benzenetricarboxylate (HKUST-1) in reactions of aromatic aldehydes condensation with nitromethane: Kinetic and diffusion study. Inorganica Chimica Acta, 2015, 426, 119-125.	1.2	18
541	Molecular insights into cold active polygalacturonase enzyme for its potential application in food processing. Journal of Food Science and Technology, 2015, 52, 5484-5496.	1.4	23

#	Article	IF	Citations
542	Designing of promiscuous inhibitors against pancreatic cancer cell lines. Scientific Reports, 2014, 4, 4668.	1.6	19
543	Indexing volumetric shapes with matching and packing. Knowledge and Information Systems, 2015, 43, 157-180.	2.1	5
544	Automatic GROMACS Topology Generation and Comparisons of Force Fields for Solvation Free Energy Calculations. Journal of Physical Chemistry B, 2015, 119, 810-823.	1.2	88
545	Cyanobacteria as photosynthetic biocatalysts: a systems biology perspective. Molecular BioSystems, 2015, 11, 60-70.	2.9	51
546	Virtual screening-based identification of lead molecules as selective TACE inhibitors. Medicinal Chemistry Research, 2015, 24, 226-244.	1.1	19
547	Efficient searching and annotation of metabolic networks using chemical similarity. Bioinformatics, 2015, 31, 1016-1024.	1.8	47
548	XenoSite server: a web-available site of metabolism prediction tool. Bioinformatics, 2015, 31, 1136-1137.	1.8	64
549	Redox-active porous coordination polymer based on trinuclear pivalate: Temperature-dependent crystal rearrangement and redox-behavior. Journal of Solid State Chemistry, 2015, 223, 122-130.	1.4	6
550	Molecular fingerprint similarity search in virtual screening. Methods, 2015, 71, 58-63.	1.9	506
551	New tetracyclic tacrine analogs containing pyrano[2,3-c]pyrazole: Efficient synthesis, biological assessment and docking simulation study. European Journal of Medicinal Chemistry, 2015, 89, 296-303.	2.6	70
552	Polypharmacology modelling using proteochemometrics (PCM): recent methodological developments, applications to target families, and future prospects. MedChemComm, 2015, 6, 24-50.	3.5	109
553	Advances in molecular quantum chemistry contained in the Q-Chem 4 program package. Molecular Physics, 2015, 113, 184-215.	0.8	2,561
554	Internal threshold of toxicological concern values: enabling route-to-route extrapolation. Archives of Toxicology, 2015, 89, 941-948.	1.9	33
555	In silico interaction of methyl isocyanate with immune protein responsible for Mycobacterium tuberculosis infection using molecular docking. Toxicology and Industrial Health, 2016, 32, 162-167.	0.6	10
556	3D-QSAR and SVM Prediction of BRAF-V600E and HIV Integrase Inhibitors: A Comparative Study and Characterization of Performance with a New Expected Prediction Performance Metric. American Journal of Biochemistry and Biotechnology, 2016, 12, 253-262.	0.1	6
557	Internet Databases of the Properties, Enzymatic Reactions, and Metabolism of Small Moleculesâ€"Search Options and Applications in Food Science. International Journal of Molecular Sciences, 2016, 17, 2039.	1.8	20
558	Glutamine Synthetase Drugability beyond Its Active Site: Exploring Oligomerization Interfaces and Pockets. Molecules, 2016, 21, 1028.	1.7	12
559	Glycyrrhizic Acid Reduces Heart Rate and Blood Pressure by a Dual Mechanism. Molecules, 2016, 21, 1291.	1.7	14

#	Article	IF	Citations
560	Molecular docking and molecular dynamics simulation study of inositol phosphorylceramide synthase â€“ inhibitor complex in leishmaniasis: Insight into the structure based drug design. F1000Research, 2016, 5, 1610.	0.8	10
561	An explicit-solvent conformation search method using open software. PeerJ, 2016, 4, e2088.	0.9	6
562	Mechanical Properties of Boehmite Evaluated by Atomic Force Microscopy Experiments and Molecular Dynamic Finite Element Simulations. Journal of Nanomaterials, 2016, 2016, 1-13.	1.5	31
563	Treating Diabetes Mellitus: Pharmacophore Based Designing of Potential Drugs fromGymnema sylvestreagainst Insulin Receptor Protein. BioMed Research International, 2016, 2016, 1-14.	0.9	32
564	Prediction of selective estrogen receptor beta agonist using open data and machine learning approach. Drug Design, Development and Therapy, 2016, Volume 10, 2323-2331.	2.0	28
565	An antagonist of the platelet-activating factor receptor inhibits adherence of both nontypeable Haemophilus influenzae and Streptococcus pneumoniae to cultured human bronchial epithelial cells exposed to cigarette smoke. International Journal of COPD, 2016, Volume 11, 1647-1655.	0.9	36
566	Metabolic Complementation in Bacterial Communities: Necessary Conditions and Optimality. Frontiers in Microbiology, 2016, 7, 1553.	1.5	17
567	Extracting Conformational Ensembles of Small Molecules from Molecular Dynamics Simulations: Ampicillin as a Test Case. Computation, 2016, 4, 5.	1.0	17
568	Integrated Computational Approach for Virtual Hit Identification against Ebola Viral Proteins VP35 and VP40. International Journal of Molecular Sciences, 2016, 17, 1748.	1.8	37
569	Boronic Acid Group: A Cumbersome False Negative Case in the Process of Drug Design. Molecules, 2016, 21, 1185.	1.7	10
570	Multi-Layer Identification of Highly-Potent ABCA1 Up-Regulators Targeting LXRÎ² Using Multiple QSAR Modeling, Structural Similarity Analysis, and Molecular Docking. Molecules, 2016, 21, 1639.	1.7	7
571	Predicting Ligand Binding Sites on Protein Surfaces by 3-Dimensional Probability Density Distributions of Interacting Atoms. PLoS ONE, 2016, 11, e0160315.	1.1	17
572	Jump into a New Foldâ€"A Homology Based Model for the ABCG2/BCRP Multidrug Transporter. PLoS ONE, 2016, 11, e0164426.	1.1	45
573	Therapeutics Insight with Inclusive Immunopharmacology Explication of Human Rotavirus A for the Treatment of Diarrhea. Frontiers in Pharmacology, 2016, 7, 153.	1.6	6
574	Innovative Strategies to Develop Chemical Categories Using a Combination of Structural and Toxicological Properties. Frontiers in Pharmacology, 2016, 7, 321.	1.6	5
575	Combine multiple mass spectral similarity measures for compound identification. International Journal of Data Mining and Bioinformatics, 2016, 15, 84.	0.1	3
576	Conformational Dynamics of the Single Lipopolysaccharide Oâ€Antigen in Solution. ChemPhysChem, 2016, 17, 2839-2853.	1.0	6
577	Efficient determination of accurate atomic polarizabilities for polarizeable embedding calculations. Journal of Computational Chemistry, 2016, 37, 2052-2059.	1.5	8

#	Article	IF	Citations
578	Automatic molecular structure perception for the universal force field. Journal of Computational Chemistry, 2016, 37, 1191-1205.	1.5	20
579	Prediction of blood:air and fat:air partition coefficients of volatile organic compounds for the interpretation of data in breath gas analysis. Journal of Breath Research, 2016, 10, 017103.	1.5	15
580	A Software Package for Chemically Inspired Graph Transformation. Lecture Notes in Computer Science, 2016, , 73-88.	1.0	31
581	Toward the identification of molecular cogs. Journal of Computational Chemistry, 2016, 37, 848-860.	1.5	0
582	Electron tunneling in proteins program. Journal of Computational Chemistry, 2016, 37, 1388-1395.	1.5	3
583	ORBKIT: A modular python toolbox for crossâ€platform postprocessing of quantum chemical wavefunction data. Journal of Computational Chemistry, 2016, 37, 1511-1520.	1.5	88
584	Structural analysis of dihydrofolate reductases enables rationalization of antifolate binding affinities and suggests repurposing possibilities. FEBS Journal, 2016, 283, 1139-1167.	2.2	19
586	SM-TF: A structural database of small molecule-transcription factor complexes. Journal of Computational Chemistry, 2016, 37, 1559-1564.	1.5	4
587	In silico Prediction of Drug Induced Liver Toxicity Using Substructure Pattern Recognition Method. Molecular Informatics, 2016, 35, 136-144.	1.4	75
588	In silico design and screening of hypothetical MOF-74 analogs and their experimental synthesis. Chemical Science, 2016, 7, 6263-6272.	3.7	69
589	Hetero-annulated coumarins as new AChE/BuChE inhibitors: synthesis and biological evaluation. Medicinal Chemistry Research, 2016, 25, 1831-1841.	1.1	13
590	Theoretical investigation of electron structure and surface morphology of titanium dioxide anatase nano-particles. Computational and Theoretical Chemistry, 2016, 1091, 122-136.	1.1	18
591	SwissSimilarity: A Web Tool for Low to Ultra High Throughput Ligand-Based Virtual Screening. Journal of Chemical Information and Modeling, 2016, 56, 1399-1404.	2.5	229
592	Fragment-Based Analysis of Ligand Dockings Improves Classification of Actives. Journal of Chemical Information and Modeling, 2016, 56, 1597-1607.	2.5	4
593	Landscape of proteinâ€“small ligand binding modes. Protein Science, 2016, 25, 1659-1671.	3.1	3
594	Investigation of similarity and diversity threshold networks generated from diversity-oriented and focused chemical libraries. Journal of Mathematical Chemistry, 2016, 54, 1916-1941.	0.7	1
595	Clustered Low-Rank Tensor Format: Introduction and Application to Fast Construction of Hartreeâ€“Fock Exchange. Journal of Chemical Theory and Computation, 2016, 12, 5868-5880.	2.3	20
596	Impact of big data in healthcare: A survey. , 2016, , .		14

#	Article	IF	Citations
597	In silico profiling for secondary metabolites from Lepidium meyenii (maca) by the pharmacophore and ligand-shape-based joint approach. Chinese Medicine, 2016, 11, 42.	1.6	17
598	In silico identification of anti-cancer compounds and plants from traditional Chinese medicine database. Scientific Reports, 2016, 6, 25462.	1.6	39
599	Benchmarking platform for ligand-based virtual screening. , 2016, , .		4
600	Molecular docking approach to identify potential anticancer compounds from Begonia (Begonia sp). AIP Conference Proceedings, 2016, , .	0.3	10
601	Hyper-redundant Robots and bioinformatics: Modelling loops in RNA. , 2016, , .		3
602	DRABAL: novel method to mine large high-throughput screening assays using Bayesian active learning. Journal of Cheminformatics, 2016, 8, 64.	2.8	20
603	First-principles data set of 45,892 isolated and cation-coordinated conformers of 20 proteinogenic amino acids. Scientific Data, 2016, 3, 160009.	2.4	51
604	Salting-out effects by pressure-corrected 3D-RISM. Journal of Chemical Physics, 2016, 145, 194501.	1.2	14
605	RADER: a RApid DEcoy Retriever to facilitate decoy based assessment of virtual screening. Bioinformatics, 2017, 33, 1235-1237.	1.8	28
606	Efficient Identification of Tanimoto Nearest Neighbors. , 2016, , .		3
607	Multibody cofactor and substrate molecular recognition in the myo-inositol monophosphatase enzyme. Scientific Reports, 2016, 6, 30275.	1.6	17
608	PEPlife: A Repository of the Half-life of Peptides. Scientific Reports, 2016, 6, 36617.	1.6	108
609	Filtered circular fingerprints improve either prediction or runtime performance while retaining interpretability. Journal of Cheminformatics, 2016, 8, 60.	2.8	20
610	Large-scale calculations of gas phase thermochemistry: Enthalpy of formation, standard entropy, and heat capacity. Journal of Chemical Physics, 2016, 145, .	1.2	60
611	3D QSAR, pharmacophore and molecular docking studies of known inhibitors and designing of novel inhibitors for M18 aspartyl aminopeptidase of Plasmodium falciparum. BMC Structural Biology, 2016, 16, 12.	2.3	25
612	Substituted quinazolinones as kinase inhibitors endowed with anti-fibrotic properties. European Journal of Medicinal Chemistry, 2016, 115, 416-425.	2.6	12
613	Drug-induced adverse events prediction with the LINCS L1000 data. Bioinformatics, 2016, 32, 2338-2345.	1.8	155
614	Attracting cavities for docking. Replacing the rough energy landscape of the protein by a smooth attracting landscape. Journal of Computational Chemistry, 2016, 37, 437-447.	1.5	32

#	Article	IF	Citations
615	UNICON: A Powerful and Easy-to-Use Compound Library Converter. Journal of Chemical Information and Modeling, 2016, 56, 1105-1111.	2.5	26
616	Force Field Development from Periodic Density Functional Theory Calculations for Gas Separation Applications Using Metalâ€“Organic Frameworks. Journal of Physical Chemistry C, 2016, 120, 12590-12604.	1.5	95
617	Editor's Highlight: Analysis of the Effects of Cell Stress and Cytotoxicity onIn VitroAssay Activity Across a Diverse Chemical and Assay Space. Toxicological Sciences, 2016, 152, 323-339.	1.4	171
618	Computer modeling of ferrocene-substituted 3,7-diazabicyclo[3.3.1]nonanes as serine protease inhibitors. Mendeleev Communications, 2016, 26, 212-213.	0.6	10
619	Discovery of ERBB3 inhibitors for non-small cell lung cancer (NSCLC) via virtual screening. Journal of Molecular Modeling, 2016, 22, 135.	0.8	18
620	Exploring quantitative structureâ€“activity relationship (QSAR) models for some biologically active catechol structures using PC-LS-SVM and PC-ANFIS. Applied Biological Chemistry, 2016, 59, 433-441.	0.7	5
621	Development of a web-based tool for automated processing and cataloging of a unique combinatorial drug screen. Journal of Microbiological Methods, 2016, 126, 30-34.	0.7	5
622	Molecular docking and simulation studies to give insight of surfactin amyloid interaction for destabilizing Alzheimerâ€™s Aî²42 protofibrils. Medicinal Chemistry Research, 2016, 25, 1616-1622.	1.1	18
623	Synthesis and anticholinesterase activity of coumarin-3-carboxamides bearing tryptamine moiety. European Journal of Medicinal Chemistry, 2016, 121, 40-46.	2.6	88
624	RIFM fragrance ingredient safety assessment, Î±-Ionone, CAS Registry Number 127-41-3. Food and Chemical Toxicology, 2016, 97, S1-S10.	1.8	10
625	Synthesis, in vitro and in silico anti-proliferative activity of 4-aryl-4H-chromene derivatives. Medicinal Chemistry Research, 2016, 25, 1308-1315.	1.1	23
626	Impact of Binding Site Comparisons on Medicinal Chemistry and Rational Molecular Design. Journal of Medicinal Chemistry, 2016, 59, 4121-4151.	2.9	104
627	Comparative Ab-Initio Study of Substituted Norbornadiene-Quadricyclane Compounds for Solar Thermal Storage. Journal of Physical Chemistry C, 2016, 120, 3635-3645.	1.5	71
628	Combinatorial phenotypic screen uncovers unrecognized family of extended thiourea inhibitors with copper-dependent anti-staphylococcal activity. Metallomics, 2016, 8, 412-421.	1.0	18
629	ASDB: a resource for probing protein functions with small molecules. Bioinformatics, 2016, 32, 1752-1754.	1.8	8
630	Protective effect of Theobroma cacao on nitric oxide and endothelin-1 level in endothelial cells induced by plasma from preeclamptic patients: In silico and in vitro studies. European Journal of Integrative Medicine, 2016, 8, 73-78.	0.8	5
631	In silico methods for linking genes and secondary metabolites: The way forward. Synthetic and Systems Biotechnology, 2016, 1, 80-88.	1.8	35
632	Fragment oriented molecular shapes. Journal of Molecular Graphics and Modelling, 2016, 66, 143-154.	1.3	3

#	Article	IF	Citations
633	Design, Synthesis, and Binding Affinity Evaluation of Hoechst 33258 Derivatives for the Development of Sequence-Specific DNA-Based Asymmetric Catalysts. ACS Catalysis, 2016, 6, 3096-3105.	5.5	51
634	Peptide aptamer identified by molecular docking targeting translationally controlled tumor protein in leukemia cells. Investigational New Drugs, 2016, 34, 515-521.	1.2	18
635	Conformal Prediction Classification of a Large Data Set of Environmental Chemicals from ToxCast and Tox21 Estrogen Receptor Assays. Chemical Research in Toxicology, 2016, 29, 1003-1010.	1.7	43
636	Î±-Pinene Autoxidation Products May Not Have Extremely Low Saturation Vapor Pressures Despite High O:C Ratios. Journal of Physical Chemistry A, 2016, 120, 2569-2582.	1.1	95
637	Rosetta and the Design of Ligand Binding Sites. Methods in Molecular Biology, 2016, 1414, 47-62.	0.4	26
638	BIOPEP database of sensory peptides and amino acids. Food Research International, 2016, 85, 155-161.	2.9	116
639	Discovery of a potential lead compound for treating leprosy with dapsone resistance mutation in M. leprae folP1. Molecular BioSystems, 2016, 12, 2178-2188.	2.9	3
640	Pharmit: interactive exploration of chemical space. Nucleic Acids Research, 2016, 44, W442-W448.	6.5	219
641	Slow-binding inhibition of acetylcholinesterase by an alkylammonium derivative of 6-methyluracil: mechanism and possible advantages for myasthenia gravis treatment. Biochemical Journal, 2016, 473, 1225-1236.	1.7	39
642	Development of a credible 3D-QSAR CoMSIA model and docking studies for a series of triazoles and tetrazoles containing 11Î²-HSD1 inhibitors. SAR and QSAR in Environmental Research, 2016, 27, 265-292.	1.0	10
643	Rapid Discovery and Structureâ€“Activity Relationships of Pyrazolopyrimidines That Potently Suppress Breast Cancer Cell Growth via SRC Kinase Inhibition with Exceptional Selectivity over ABL Kinase. Journal of Medicinal Chemistry, 2016, 59, 4697-4710.	2.9	52
644	Curcumin Reduces the Motility of Salmonella enterica Serovar Typhimurium by Binding to the Flagella, Thereby Leading to Flagellar Fragility and Shedding. Journal of Bacteriology, 2016, 198, 1798-1811.	1.0	27
645	Improved metabolite identification with MIDAS and MAGMa through MS/MS spectral dataset-driven parameter optimization. Metabolomics, 2016, 12, 1.	1.4	35
646	Toxic effect of chemicals dumped in premises of UCIL, Bhopal leading to environmental pollution: An in silico approach. Asian Pacific Journal of Tropical Disease, 2016, 6, 284-290.	0.5	4
647	Predictive proteochemometric models for kinases derived from 3D protein field-based descriptors. MedChemComm, 2016, 7, 1007-1015.	3.5	12
648	SAMPL5: 3D-RISM partition coefficient calculations with partial molar volume corrections and solute conformational sampling. Journal of Computer-Aided Molecular Design, 2016, 30, 1115-1127.	1.3	29
649	Modeling, Synthesis, and Biological Evaluation of Potential Retinoid X Receptor (RXR)-Selective Agonists: Analogues of 4-[1-(3,5,5,8,8-Pentamethyl-5,6,7,8-tetrahydro-2-naphthyl)ethynyl]benzoic Acid (Bexarotene) and 6-(Ethyl(5,5,8,8-tetrahydronaphthalen-2-yl)amino)nicotinic Acid (NEt-TMN). Journal of Medicinal Chemistry, 2016, 59, 8924-8940.	2.9	14
650	Binding of Pollutants to Biomolecules: A Simulation Study. Chemical Research in Toxicology, 2016, 29, 1679-1688.	1.7	7

#	Article	IF	Citations
651	Anatomy of the SEAGrid Science Gateway. , 2016, , .		2
652	A D3R prospective evaluation of machine learning for protein-ligand scoring. Journal of Computer-Aided Molecular Design, 2016, 30, 761-771.	1.3	15
653	Chemogenomics knowledgebase and systems pharmacology for hallucinogen target identificationâ€"Salvinorin A as a case study. Journal of Molecular Graphics and Modelling, 2016, 70, 284-295.	1.3	18
654	Calculation of distribution coefficients in the SAMPL5 challenge from atomic solvation parameters and surface areas. Journal of Computer-Aided Molecular Design, 2016, 30, 1079-1086.	1.3	5
655	Prediction of compound-target interactions of natural products using large-scale drug and protein information. BMC Bioinformatics, 2016, 17, 219.	1.2	24
656	Optimal strategies for virtual screening of induced-fit and flexible target in the 2015 D3R Grand Challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 695-706.	1.3	20
657	Coupled molecular design diagrams to guide safer chemical design with reduced likelihood of perturbing the NRF2-ARE antioxidant pathway and inducing cytotoxicity. Green Chemistry, 2016, 18, 6387-6394.	4.6	7
658	Molecular dynamics simulation and quantum chemical studies on the investigation of aluminum nitride nanotube as phosgene gas sensor. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2016, 86, 305-322.	0.9	37
659	New Inhibitors of Indoleamine 2,3-Dioxygenase 1: Molecular Modeling Studies, Synthesis, and Biological Evaluation. Journal of Medicinal Chemistry, 2016, 59, 9760-9773.	2.9	35
660	Identification of potential inhibitor and enzyme-inhibitor complex on trypanothione reductase to control Chagas disease. Computational Biology and Chemistry, 2016, 65, 29-36.	1.1	19
661	Predicting binding poses and affinities for protein - ligand complexes in the 2015 D3R Grand Challenge using a physical model with a statistical parameter estimation. Journal of Computer-Aided Molecular Design, 2016, 30, 791-804.	1.3	11
662	Assessing the similarity of ligand binding conformations with the Contact Mode Score. Computational Biology and Chemistry, 2016, 64, 403-413.	1.1	45
663	A New Class of Allosteric HIV-1 Integrase Inhibitors Identified by Crystallographic Fragment Screening of the Catalytic Core Domain. Journal of Biological Chemistry, 2016, 291, 23569-23577.	1.6	20
664	Open source molecular modeling. Journal of Molecular Graphics and Modelling, 2016, 69, 127-143.	1.3	83
665	Effect of Substitution on the Aniline Moiety of the GPR88 Agonist 2-PCCA: Synthesis, Structureâ€"Activity Relationships, and Molecular Modeling Studies. ACS Chemical Neuroscience, 2016, 7, 1418-1432.	1.7	20
666	Interaction of small molecules with human tyrosinase: A surface plasmon resonance and molecular docking study. International Journal of Biological Macromolecules, 2016, 92, 1123-1129.	3.6	18
667	Evaluating Parametrization Protocols for Hydration Free Energy Calculations with the AMOEBA Polarizable Force Field. Journal of Chemical Theory and Computation, 2016, 12, 3871-3883.	2.3	27
668	The Rational Design, Synthesis, and Antimicrobial Properties of Thiophene Derivatives That Inhibit Bacterial Histidine Kinases. Journal of Medicinal Chemistry, 2016, 59, 8830-8847.	2.9	38

#	Article	IF	Citations
669	Azahar: a PyMOL plugin for construction, visualization and analysis of glycan molecules. Journal of Computer-Aided Molecular Design, 2016, 30, 619-624.	1.3	20
670	Quantitative structure-property relationship modelling of thermal decomposition temperatures of ionic liquids. Journal of Molecular Liquids, 2016, 223, 60-67.	2.3	35
671	Rational computing of energy levels for organic electronics: the case of 2-benzylidene-1,3-indandiones. RSC Advances, 2016, 6, 85242-85253.	1.7	2
672	Identification of compoundâ€“protein interactions through the analysis of gene ontology, KEGG enrichment for proteins and molecular fragments of compounds. Molecular Genetics and Genomics, 2016, 291, 2065-2079.	1.0	62
673	Simulation-Based Algorithm for Two-Dimensional Chemical Structure Diagram Generation of Complex Molecules and Ligandâ€“Protein Interactions. Journal of Chemical Information and Modeling, 2016, 56, 2320-2335.	2.5	2
674	Theoretical Investigation of Substituent Effects on the Dihydroazulene/Vinylheptafulvene Photoswitch: Increasing the Energy Storage Capacity. Journal of Physical Chemistry A, 2016, 120, 9782-9793.	1.1	39
675	A computationally identified compound antagonizes excess FGF-23 signaling in renal tubules and a mouse model of hypophosphatemia. Science Signaling, 2016, 9, ra113.	1.6	27
676	Using Science Gateways for Bridging the Differences between Research Infrastructures. Journal of Grid Computing, 2016, 14, 545-557.	2.5	12
677	Identifying enriched drug fragments as possible candidates for metabolic engineering. BMC Medical Genomics, 2016, 9, 46.	0.7	3
678	MOLS 2.0: software package for peptide modeling and proteinâ€“ligand docking. Journal of Molecular Modeling, 2016, 22, 239.	0.8	18
679	Targeting flavivirus RNA dependent RNA polymerase through a pyridobenzothiazole inhibitor. Antiviral Research, 2016, 134, 226-235.	1.9	49
680	StemCellCKB: An Integrated Stem Cell-Specific Chemogenomics KnowledgeBase for Target Identification and Systems-Pharmacology Research. Journal of Chemical Information and Modeling, 2016, 56, 1995-2004.	2.5	9
681	In silico prediction of chemical mechanism of action via an improved networkâ€based inference method. British Journal of Pharmacology, 2016, 173, 3372-3385.	2.7	73
682	HCK is a survival determinant transactivated by mutated MYD88, and a direct target of ibrutinib. Blood, 2016, 127, 3237-3252.	0.6	93
683	BioTriangle: a web-accessible platform for generating various molecular representations for chemicals, proteins, DNAs/RNAs and their interactions. Journal of Cheminformatics, 2016, 8, 34.	2.8	39
684	molSimplify: A toolkit for automating discovery in inorganic chemistry. Journal of Computational Chemistry, 2016, 37, 2106-2117.	1.5	127
685	Probabilistic diagram for designing chemicals with reduced potency to incur cytotoxicity. Green Chemistry, 2016, 18, 4461-4467.	4.6	11
686	Pharmacophore development and screening for discovery of potential inhibitors of ADAMTS-4 for osteoarthritis therapy. Journal of Molecular Modeling, 2016, 22, 178.	0.8	14

#	Article	IF	Citations
687	Anin silicoapproach predicted potential therapeutics that can confer protection from maximum pathogenic Hantaviruses. Future Virology, 2016, 11, 411-428.	0.9	3
688	Ocean acidification affects marine chemical communication by changing structure and function of peptide signalling molecules. Global Change Biology, 2016, 22, 3914-3926.	4.2	121
690	Gliptins in managing diabetes - Reviewing computational strategy. Life Sciences, 2016, 166, 108-120.	2.0	27
691	NEEMP: software for validation, accurate calculation and fast parameterization of EEM charges. Journal of Cheminformatics, 2016, 8, 57.	2.8	5
692	New one-pot synthesis of N-fused isoquinoline derivatives by palladium-catalyzed Câ€“H arylation: potent inhibitors of nucleotide pyrophosphatase-1 and -3. Organic and Biomolecular Chemistry, 2016, 14, 11402-11414.	1.5	42
693	Ligand-induced Epitope Masking. Journal of Biological Chemistry, 2016, 291, 20993-21007.	1.6	16
694	BATMAN-TCM: a Bioinformatics Analysis Tool for Molecular mechANism of Traditional Chinese Medicine. Scientific Reports, 2016, 6, 21146.	1.6	530
695	DockBench as docking selector tool: the lesson learned from D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 773-789.	1.3	13
696	MayaChemTools: An Open Source Package for Computational Drug Discovery. Journal of Chemical Information and Modeling, 2016, 56, 2292-2297.	2.5	65
697	Chemical Stabilization and Electrochemical Destabilization of the Iron Keggin Ion in Water. Inorganic Chemistry, 2016, 55, 11078-11088.	1.9	39
698	Synergies Between Quantum Mechanics and Machine Learning in Reaction Prediction. Journal of Chemical Information and Modeling, 2016, 56, 2125-2128.	2.5	43
699	Identification of Potential Therapeutics to Conquer Drug Resistance in Salmonella typhimurium: Drug Repurposing Strategy. BioDrugs, 2016, 30, 593-605.	2.2	17
700	Computer Simulation of Shallow Traps Created by Impurity Molecules in Anthracene Crystal. Journal of Physical Chemistry C, 2016, 120, 25189-25195.	1.5	0
701	The Harvard organic photovoltaic dataset. Scientific Data, 2016, 3, 160086.	2.4	85
702	System Prediction of Drug-Drug Interactions Through the Integration of Drug Phenotypic, Therapeutic, Structural, and Genomic Similarities. Lecture Notes in Computer Science, 2016, , 377-385.	1.0	0
703	The WEIZMASS spectral library for high-confidence metabolite identification. Nature Communications, 2016, 7, 12423.	5.8	95
704	Ligand-based virtual screening and inductive learning for identification of SIRT1 inhibitors in natural products. Scientific Reports, 2016, 6, 19312.	1.6	20
705	Comprehensive approach for predicting toxicological effects of ionic liquids on several biological systems using unified descriptors. Scientific Reports, 2016, 6, 33403.	1.6	35

#	Article	IF	Citations
706	Fast and accurate hybrid QM//MM approach for computing anharmonic corrections to vibrational frequencies. Journal of Molecular Modeling, 2016, 22, 285.	0.8	7
707	Interaction with specific HSP90 residues as a scoring function: validation in the D3R Grand Challenge 2015. Journal of Computer-Aided Molecular Design, 2016, 30, 731-742.	1.3	3
708	DPDR-CPI, a server that predicts Drug Positioning and Drug Repositioning via Chemical-Protein Interactome. Scientific Reports, 2016, 6, 35996.	1.6	27
709	Crystal structure of human interferon-Î³ receptor 2 reveals the structural basis for receptor specificity. Acta Crystallographica Section D: Structural Biology, 2016, 72, 1017-1025.	1.1	12
710	Technical Note: Development of chemoinformatic tools to enumerate functional groups in molecules for organic aerosol characterization. Atmospheric Chemistry and Physics, 2016, 16, 4401-4422.	1.9	19
711	Modelâ€“measurement comparison of functional group abundance in <i>Î±</i>-pinene and 1,3,5-trimethylbenzene secondary organic aerosol formation. Atmospheric Chemistry and Physics, 2016, 16, 8729-8747.	1.9	9
712	A functional NMR for membrane proteins: dynamics, ligand binding, and allosteric modulation. Protein Science, 2016, 25, 959-973.	3.1	14
713	Insights into regioselective metabolism of mefenamic acid by cytochrome <scp>P</scp>450 <scp>BM</scp>3 mutants through crystallography, docking, molecular dynamics, and free energy calculations. Proteins: Structure, Function and Bioinformatics, 2016, 84, 383-396.	1.5	29
714	Structure and Electrochemical Properties of Copper(Ii) Coordination Polymers with Ligands Containing Naphthyl and Anthracyl Fragments. Theoretical and Experimental Chemistry, 2016, 52, 111-118.	0.2	4
715	Impact of similarity threshold on the topology of molecular similarity networks and clustering outcomes. Journal of Cheminformatics, 2016, 8, 16.	2.8	15
716	Incorporating specificity into optimization: evaluation of SPA using CSAR 2014 and CASF 2013 benchmarks. Journal of Computer-Aided Molecular Design, 2016, 30, 219-227.	1.3	6
717	Optimizing Molecular Models Through Force-Field Parameterization via the Efficient Combination of Modular Program Packages. Molecular Modeling and Simulation, 2016, , 53-77.	0.2	11
718	MPInterfaces: A Materials Project based Python tool for high-throughput computational screening of interfacial systems. Computational Materials Science, 2016, 122, 183-190.	1.4	95
719	G-Proteinâ€“Coupled Receptor MrgD Is a Receptor for Angiotensin-(1â€“7) Involving Adenylyl Cyclase, cAMP, and Phosphokinase A. Hypertension, 2016, 68, 185-194.	1.3	109
720	Analysis of Ligandâ€“Receptor Association and Intermediate Transfer Rates in Multienzyme Nanostructures with All-Atom Brownian Dynamics Simulations. Journal of Physical Chemistry B, 2016, 120, 8518-8531.	1.2	11
721	Prediction of ¹⁹F NMR Chemical Shifts in Labeled Proteins: Computational Protocol and Case Study. Molecular Pharmaceutics, 2016, 13, 2376-2386.	2.3	23
722	StructMAn: annotation of single-nucleotide polymorphisms in the structural context. Nucleic Acids Research, 2016, 44, W463-W468.	6.5	32
723	Predicting Solvation Free Energies Using Parameter-Free Solvent Models. Journal of Physical Chemistry B, 2016, 120, 5724-5731.	1.2	30

#	Article	IF	Citations
724	Synthesis and evaluation of antibacterial and antioxidant activity of novel 2-phenyl-quinoline analogs derivatized at position 4 with aromatically substituted 4H-1,2,4-triazoles. Journal of Enzyme Inhibition and Medicinal Chemistry, 2016, 31, 104-110.	2.5	19
725	Interpretation of toxicological activity of ionic liquids to acetylcholinesterase inhibition via in silico modelling. Chemosphere, 2016, 159, 178-183.	4.2	21
726	A simple model predicts UGT-mediated metabolism. Bioinformatics, 2016, 32, 3183-3189.	1.8	51
727	Structure-based virtual screening of hypothetical inhibitors of the enzyme longiborneol synthaseâ€"a potential target to reduce Fusarium head blight disease. Journal of Molecular Modeling, 2016, 22, 163.	0.8	3
728	Structure-Based Drug Discovery for Prion Disease Using a Novel Binding Simulation. EBioMedicine, 2016, 9, 238-249.	2.7	34
729	Kekule.js: An Open Source JavaScript Chemoinformatics Toolkit. Journal of Chemical Information and Modeling, 2016, 56, 1132-1138.	2.5	29
730	Natural Product Anacardic Acid from Cashew Nut Shells Stimulates Neutrophil Extracellular Trap Production and Bactericidal Activity. Journal of Biological Chemistry, 2016, 291, 13964-13973.	1.6	50
731	Quantitative structure-(chromatographic) retention relationship models for dissociating compounds. Journal of Pharmaceutical and Biomedical Analysis, 2016, 127, 176-183.	1.4	20
732	Exploring neuroprotective potential of Withania somnifera phytochemicals by inhibition of GluN2B-containing NMDA receptors: An in silico study. Medical Hypotheses, 2016, 92, 35-43.	0.8	49
733	Examining the predictive accuracy of the novel 3D N-linear algebraic molecular codifications on benchmark datasets. Journal of Cheminformatics, 2016, 8, 10.	2.8	17
734	A graph-based approach to construct target-focused libraries for virtual screening. Journal of Cheminformatics, 2016, 8, 14.	2.8	23
735	Supercell program: a combinatorial structure-generation approach for the local-level modeling of atomic substitutions and partial occupancies in crystals. Journal of Cheminformatics, 2016, 8, 17.	2.8	292
736	The Glycome Analytics Platform: an integrative framework for glycobioinformatics. Bioinformatics, 2016, 32, 3005-3011.	1.8	5
737	ACFIS: a web server for fragment-based drug discovery. Nucleic Acids Research, 2016, 44, W550-W556.	6.5	111
738	Ligand cluster-based protein network and ePlatton, a multi-target ligand finder. Journal of Cheminformatics, 2016, 8, 23.	2.8	1
739	A Market-Basket Approach to Predict the Acute Aquatic Toxicity of Munitions and Energetic Materials. Bulletin of Environmental Contamination and Toxicology, 2016, 96, 779-783.	1.3	1
740	Machine learning optimization of cross docking accuracy. Computational Biology and Chemistry, 2016, 62, 133-144.	1.1	17
741	Proteome-wide covalent ligand discovery in native biological systems. Nature, 2016, 534, 570-574.	13.7	651

#	Article	IF	Citations
742	Flexible <scp>CDOCKER</scp>: Development and application of a pseudoâ€explicit structureâ€based docking method within <scp>CHARMM</scp>. Journal of Computational Chemistry, 2016, 37, 753-762.	1.5	88
743	Introduction to Cheminformatics. Current Protocols in Bioinformatics, 2016, 53, 14.1.1-14.1.21.	25.8	15
744	Molecular docking based virtual screening of natural compounds as potential BACE1 inhibitors: 3D QSAR pharmacophore mapping and molecular dynamics analysis. Journal of Biomolecular Structure and Dynamics, 2016, 34, 239-249.	2.0	44
745	DNA topoisomeraseâ€directed anticancerous alkaloids: ADMETâ€based screening, molecular docking, and dynamics simulation. Biotechnology and Applied Biochemistry, 2016, 63, 125-137.	1.4	22
746	Comprehensive curation and analysis of fungal biosynthetic gene clusters of published natural products. Fungal Genetics and Biology, 2016, 89, 18-28.	0.9	99
747	Model-Based Design of Tailor-Made Biofuels. Energy & Fuels, 2016, 30, 1109-1134.	2.5	70
748	TD-DFT based fine-tuning of molecular excitation energies using evolutionary algorithms. RSC Advances, 2016, 6, 3661-3670.	1.7	4
749	Discovery of novel phenoxazinone derivatives as DKK1/LRP6 interaction inhibitors: Synthesis, biological evaluation and structureâ€“activity relationships. Bioorganic and Medicinal Chemistry, 2016, 24, 1014-1022.	1.4	6
750	Discovery of novel dual inhibitors against Mdm2 and Mdmx proteins by in silico approaches and binding assay. Life Sciences, 2016, 145, 240-246.	2.0	17
751	Water-compatible imprinted pills for sensitive determination of cannabinoids in urine and oral fluid. Journal of Chromatography A, 2016, 1429, 53-64.	1.8	24
752	Attenuation of adhesion, quorum sensing and biofilm mediated virulence of carbapenem resistant Escherichia coli by selected natural plant products. Microbial Pathogenesis, 2016, 92, 76-85.	1.3	39
753	5-Benzylidene-hydantoin is a new scaffold for SIRT inhibition: From virtual screening to activity assays. European Journal of Pharmaceutical Sciences, 2016, 85, 59-67.	1.9	10
754	The 8-oxo-dGTP interaction with human DNA polymerase Î²: two patterns of ligand behavior. Structural Chemistry, 2016, 27, 175-183.	1.0	1
755	Synthesis of indoleâ€“quinolineâ€“oxadiazoles: their anticancer potential and computational tubulin binding studies. Research on Chemical Intermediates, 2016, 42, 5899-5914.	1.3	22
756	Predicting Binding Poses and Affinities in the CSAR 2013â€“2014 Docking Exercises Using the Knowledge-Based Convex-PL Potential. Journal of Chemical Information and Modeling, 2016, 56, 1053-1062.	2.5	8
757	Building a virtual ligand screening pipeline using free software: a survey. Briefings in Bioinformatics, 2016, 17, 352-366.	3.2	74
758	XtalOpt Âversion r9: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2016, 199, 178-179.	3.0	16
759	Evaluating enzymatic synthesis of small molecule drugs. Metabolic Engineering, 2016, 33, 138-147.	3.6	15

#	Article	IF	Citations
760	Secondary metabolites extracted from marine sponge associated Comamonas testosteroni and Citrobacter freundii as potential antimicrobials against MDR pathogens and hypothetical leads for VP40 matrix protein of Ebola virus: an in vitro and in silico investigation. Journal of Biomolecular Structure and Dynamics, 2016, 34, 1865-1883.	2.0	12
761	The Effect of Molecular Conformation on the Accuracy of Theoretical ¹H and ¹³C Chemical Shifts Calculated by Ab Initio Methods for Metabolic Mixture Analysis. Journal of Physical Chemistry B, 2016, 120, 3479-3487.	1.2	11
762	Isodesmic reaction for accurate theoretical pK_a calculations of amino acids and peptides. Physical Chemistry Chemical Physics, 2016, 18, 11202-11212.	1.3	35
763	One-pot synthesis, biological evaluation, and docking study of new chromeno-annulated thiopyrano[2,3-c]pyrazoles. Molecular Diversity, 2016, 20, 639-657.	2.1	6
764	Expanding DP4: application to drug compounds and automation. Organic and Biomolecular Chemistry, 2016, 14, 3943-3949.	1.5	40
765	Correlating toxicological effects of ionic liquids on Daphnia magna with in silico calculated linear free energy relationship descriptors. Chemosphere, 2016, 152, 207-213.	4.2	13
766	The selectivity and promiscuity of brain-neuroregenerative inhibitors between ROCK1 and ROCK2 isoforms: An integration of SB-QSSR modelling, QM/MM analysis andin vitrokinase assay. SAR and QSAR in Environmental Research, 2016, 27, 47-65.	1.0	6
767	Combined Approach of Patch-Surfer and PL-PatchSurfer for Proteinâ€“Ligand Binding Prediction in CSAR 2013 and 2014. Journal of Chemical Information and Modeling, 2016, 56, 1088-1099.	2.5	12
768	Following Ramachandran: exit vector plots (EVP) as a tool to navigate chemical space covered by 3D bifunctional scaffolds. The case of cycloalkanes. RSC Advances, 2016, 6, 17595-17605.	1.7	30
769	Discovery of Novel Nonactive Site Inhibitors of the Prothrombinase Enzyme Complex. Journal of Chemical Information and Modeling, 2016, 56, 535-547.	2.5	18
770	Predictions of the physicochemical properties of amino acid side chain analogs using molecular simulation. Physical Chemistry Chemical Physics, 2016, 18, 6559-6568.	1.3	7
771	Aquatic ecotoxicity of personal care products: QSAR models and ranking for prioritization and safer alternativesâ€™ design. Green Chemistry, 2016, 18, 4393-4406.	4.6	74
772	A designed DNA binding motif that recognizes extended sites and spans two adjacent major grooves. Chemical Science, 2016, 7, 3298-3303.	3.7	28
773	New basis set for the prediction of the specific rotation in flexible biological molecules. RSC Advances, 2016, 6, 19897-19902.	1.7	9
774	Prioritization of anti-malarial hits from nature: chemo-informatic profiling of natural products with in vitro antiplasmodial activities and currently registered anti-malarial drugs. Malaria Journal, 2016, 15, 50.	0.8	28
775	A comparative study on the druggability of Schiff bases and dithiocarbamate derivatives of chitosan. Polymer Bulletin, 2016, 73, 2165-2177.	1.7	3
776	Design and synthesis of novel chalcones as potent selective monoamine oxidase-B inhibitors. European Journal of Medicinal Chemistry, 2016, 114, 162-169.	2.6	77
777	CryptoSite: Expanding the Druggable Proteome by Characterization and Prediction of Cryptic Binding Sites. Journal of Molecular Biology, 2016, 428, 709-719.	2.0	190

#	Article	IF	Citations
778	High-throughput screening against $$sim $$ â^¼ 6.1 million structurally diverse, lead-like compounds to discover novel ROCK inhibitors for cerebral injury recovery. Molecular Diversity, 2016, 20, 537-549.	2.1	9
779	PBT assessment and prioritization of contaminants of emerging concern: Pharmaceuticals. Environmental Research, 2016, 147, 297-306.	3.7	75
780	Design, synthesis and biological evaluation of indazoleâ€“pyrimidine based derivatives as anticancer agents with anti-angiogenic and antiproliferative activities. MedChemComm, 2016, 7, 881-899.	3.5	27
781	Insight into Structure-Function Relationships and Inhibition of the Fatty Acyl-AMP Ligase (FadD32) Orthologs from Mycobacteria. Journal of Biological Chemistry, 2016, 291, 7973-7989.	1.6	22
782	Prevention of cardiac dysfunction, kidney fibrosis and lipid metabolic alterations in l-NAME hypertensive rats by sinapic acidâ€”Role of HMG-CoA reductase. European Journal of Pharmacology, 2016, 777, 113-123.	1.7	38
783	Docking and ADMET prediction of few GSK-3 inhibitors divulges 6-bromoindirubin-3-oxime as a potential inhibitor. Journal of Molecular Graphics and Modelling, 2016, 65, 100-107.	1.3	75
784	Efficient preparation and analysis of membrane and membrane protein systems. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2468-2482.	1.4	33
785	Theobroma cacao increases cells viability and reduces IL-6 and sVCAM-1 level in endothelial cells induced by plasma from preeclamptic patients. Pregnancy Hypertension, 2016, 6, 42-46.	0.6	9
786	An Automated Strategy for Binding-Pose Selection and Docking Assessment in Structure-Based Drug Design. Journal of Chemical Information and Modeling, 2016, 56, 54-72.	2.5	46
787	Design and Synthesis of Simplified Largazole Analogues as Isoform-Selective Human Lysine Deacetylase Inhibitors. Journal of Medicinal Chemistry, 2016, 59, 1613-1633.	2.9	26
788	Structural Basis of Stereospecificity in the Bacterial Enzymatic Cleavage of Î²-Aryl Ether Bonds in Lignin. Journal of Biological Chemistry, 2016, 291, 5234-5246.	1.6	40
789	Probing the biophysical interaction between Neocarzinostatin toxin and EpCAM RNA aptamer. Biochemical and Biophysical Research Communications, 2016, 469, 257-262.	1.0	7
790	Theoretical analysis of a high performance protein imprint on a nanosensor. Sensing and Bio-Sensing Research, 2016, 7, 12-19.	2.2	5
791	Application of an Artificial Neural Network to the Prediction of OH Radical Reaction Rate Constants for Evaluating Global Warming Potential. Journal of Physical Chemistry B, 2016, 120, 1854-1863.	1.2	16
792	Unraveling the origin of splice switching activity of hemoglobin Î²-globin gene modulators via QSAR modeling. Chemometrics and Intelligent Laboratory Systems, 2016, 151, 51-60.	1.8	9
793	Novel triazolothiadiazines act as potent anticancer agents in liver cancer cells through Akt and ASK-1 proteins. Bioorganic and Medicinal Chemistry, 2016, 24, 858-872.	1.4	31
794	Molecular Dynamics Simulations of Sulfobetaine-Type Zwitterionic Surfactant at the Decane/Water Interface. Journal of Dispersion Science and Technology, 2016, 37, 1480-1485.	1.3	15
795	An overview of molecular fingerprint similarity search in virtual screening. Expert Opinion on Drug Discovery, 2016, 11, 137-148.	2.5	158

#	Article	IF	Citations
796	Identification of new highly selective inhibitors of the human ADP/ATP carriers by molecular docking and in vitro transport assays. Biochemical Pharmacology, 2016, 100, 112-132.	2.0	41
797	Structural modeling of the ExuR and UxuR transcription factors ofE. coli: search for the ligands affecting their regulatory properties. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2296-2304.	2.0	8
798	Molecular Dynamics Study ofN-Dodecyl-N,N-Dimethyl-3-Ammonio-1-Propanesulfonate Mono-Layer Adsorbed at the Air/Water Interface. Journal of Dispersion Science and Technology, 2016, 37, 1067-1075.	1.3	9
799	Synthesis and evaluation of gallocyanine dyes as potential agents for the treatment of Alzheimer's disease and related neurodegenerative tauopathies. European Journal of Medicinal Chemistry, 2016, 108, 28-38.	2.6	17
800	Choosing the Optimal Rigid Receptor for Docking and Scoring in the CSAR 2013/2014 Experiment. Journal of Chemical Information and Modeling, 2016, 56, 1004-1012.	2.5	19
801	ccmGDB: a database for cancer cell metabolism genes. Nucleic Acids Research, 2016, 44, D959-D968.	6.5	41
802	Analysis of non-peptidic compounds as potential malarial inhibitors against Plasmodial cysteine proteases via integrated virtual screening workflow. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2084-2101.	2.0	25
803	OpenGrowth: An Automated and Rational Algorithm for Finding New Protein Ligands. Journal of Medicinal Chemistry, 2016, 59, 4171-4188.	2.9	53
804	Wild Roman chamomile extracts and phenolic compounds: enzymatic assays and molecular modelling studies with VEGFR-2 tyrosine kinase. Food and Function, 2016, 7, 79-83.	2.1	19
805	CSAR Benchmark of Flexible MedusaDock in Affinity Prediction and Nativelike Binding Pose Selection. Journal of Chemical Information and Modeling, 2016, 56, 1042-1052.	2.5	20
806	Evaluation of potential flavonoid inhibitors of glyoxalase-I based on virtual screening andin vitrostudies. Journal of Biomolecular Structure and Dynamics, 2016, 34, 993-1007.	2.0	22
807	Current status and prospects of computational resources for natural product dereplication: a review. Briefings in Bioinformatics, 2016, 17, 309-321.	3.2	43
808	Molecular insight into amyloid oligomer destabilizing mechanism of flavonoid derivative 2-(4â€²) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 2 Journal of Biomolecular Structure and Dynamics, 2016, 34, 1252-1263.	2.0	37
809	Fingerprints of polycyclic aromatic hydrocarbons (PAHs) in infrared absorption spectroscopy. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 152, 134-148.	2.0	48
810	Interaction of Quercetin of Onion with Axon Guidance Protein Receptor, NRP-1 Plays Important Role in Cancer Treatment: An In Silico Approach. Interdisciplinary Sciences, Computational Life Sciences, 2017, 9, 184-191.	2.2	11
811	Exploration and analysis of drug modes of action through feature integration. Molecular BioSystems, 2017, 13, 425-431.	2.9	0
812	RIFM fragrance ingredient safety assessment, 5-Ethylidenebicyclo[2.2.1]hept-2-yl propionate, CAS Registry Number 73347-77-0. Food and Chemical Toxicology, 2017, 110, S22-S29.	1.8	0
813	Common Hits Approach: Combining Pharmacophore Modeling and Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2017, 57, 365-385.	2.5	59

#	Article	IF	Citations
814	A surface site interaction point methodology for macromolecules and huge molecular databases. Journal of Computational Chemistry, 2017, 38, 419-426.	1.5	2
815	Piceatannol, a natural trans-stilbene compound, inhibits human glyoxalase I. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 1169-1174.	1.0	20
816	Open Source Chemoinformatics Software including KNIME Analytics. , 2017, , 2201-2230.		3
817	Identification of Inhibitors of CD36-Amyloid Beta Binding as Potential Agents for Alzheimerâ€™s Disease. ACS Chemical Neuroscience, 2017, 8, 1232-1241.	1.7	35
818	The binding of free and copper-complexed fluoroquinolones to OmpF porins: an experimental and molecular docking study. RSC Advances, 2017, 7, 10009-10019.	1.7	14
819	Successes and pitfalls in automated dereplication strategy using liquid chromatography coupled to mass spectrometry data: A CASMI 2016 experience. Phytochemistry Letters, 2017, 21, 297-305.	0.6	8
820	3D-e-Chem-VM: Structural Cheminformatics Research Infrastructure in a Freely Available Virtual Machine. Journal of Chemical Information and Modeling, 2017, 57, 115-121.	2.5	21
821	Identification of novel inhibitors of the translationally controlled tumor protein (TCTP): insights from molecular dynamics. Molecular BioSystems, 2017, 13, 510-524.	2.9	23
822	S2RSLDB: a comprehensive manually curated, internet-accessible database of the sigma-2 receptor selective ligands. Journal of Cheminformatics, 2017, 9, 3.	2.8	27
823	Prediction of acute toxicity of emerging contaminants on the water flea Daphnia magna by Ant Colony Optimizationâ€“Support Vector Machine QSTR models. Environmental Sciences: Processes and Impacts, 2017, 19, 438-448.	1.7	62
824	aRMSD: A Comprehensive Tool for Structural Analysis. Journal of Chemical Information and Modeling, 2017, 57, 428-438.	2.5	15
825	A Hybrid Knowledge-Based and Empirical Scoring Function for Proteinâ€“Ligand Interaction: SMoG2016. Journal of Chemical Information and Modeling, 2017, 57, 584-593.	2.5	29
826	High-Quality Dataset of Protein-Bound Ligand Conformations and Its Application to Benchmarking Conformer Ensemble Generators. Journal of Chemical Information and Modeling, 2017, 57, 529-539.	2.5	57
827	Structural insights of SmKDAC8 inhibitors: Targeting Schistosoma epigenetics through a combined structure-based 3D QSAR, in vitro and synthesis strategy. Bioorganic and Medicinal Chemistry, 2017, 25, 2105-2132.	1.4	12
828	The Crystal Structure of Cytochrome P450 4B1 (CYP4B1) Monooxygenase Complexed with Octane Discloses Several Structural Adaptations for Ï‰-Hydroxylation. Journal of Biological Chemistry, 2017, 292, 5610-5621.	1.6	43
829	Structural Isosteres of Phosphate Groups in the Protein Data Bank. Journal of Chemical Information and Modeling, 2017, 57, 499-516.	2.5	23
830	Combined powder X-ray diffraction data and quantum-chemical calculations in EXPO2014. Powder Diffraction, 2017, 32, S123-S128.	0.4	7
831	Photoswitching of Azobenzene-Based Reverse Micelles above and at Subzero Temperatures As Studied by NMR and Molecular Dynamics Simulations. Langmuir, 2017, 33, 2306-2317.	1.6	10

#	Article	IF	Citations
832	Creating the New from the Old: Combinatorial Libraries Generation with Machine-Learning-Based Compound Structure Optimization. Journal of Chemical Information and Modeling, 2017, 57, 133-147.	2.5	12
833	Quantifying the equilibrium partitioning of substituted polycyclic aromatic hydrocarbons in aerosols and clouds using COSMOtherm. Environmental Sciences: Processes and Impacts, 2017, 19, 288-299.	1.7	6
834	Methyl and p-Bromobenzyl Esters of Hydrogenated Kaurenoic Acid for Controlling Anthracnose in Common Bean Plants. Journal of Agricultural and Food Chemistry, 2017, 65, 1489-1495.	2.4	10
835	Ginsenoside F1 attenuates lipid accumulation and triglycerides content in 3T3-L1 adipocytes with the modulation of reactive oxygen species (ROS) production through PPAR-Î³/JAK2 signaling responses. Medicinal Chemistry Research, 2017, 26, 1042-1051.	1.1	4
836	SwissADME: a free web tool to evaluate pharmacokinetics, drug-likeness and medicinal chemistry friendliness of small molecules. Scientific Reports, 2017, 7, 42717.	1.6	7,635
837	Chemical Space Mimicry for Drug Discovery. Journal of Chemical Information and Modeling, 2017, 57, 875-882.	2.5	63
838	Improved Quantum Chemical NMR Chemical Shift Prediction of Metabolites in Aqueous Solution toward the Validation of Unknowns. Journal of Physical Chemistry A, 2017, 121, 3071-3078.	1.1	29
839	Photoaffinity labeling with cholesterol analogues precisely maps a cholesterol-binding site in voltage-dependent anion channel-1. Journal of Biological Chemistry, 2017, 292, 9294-9304.	1.6	54
840	A tabu-search based strategy for modeling molecular aggregates and binary reactions. Computational and Theoretical Chemistry, 2017, 1111, 69-81.	1.1	24
841	Targeting on poly(ADPâ€ribose) polymerase activity with DNAâ€damaging hybrid lactamâ€steroid alkylators in wildâ€type and BRCA1â€mutated ovarian cancer cells. Chemical Biology and Drug Design, 2017, 90, 854-866.	1.5	7
842	Polypharmacological in Silico Bioactivity Profiling and Experimental Validation Uncovers Sedative-Hypnotic Effects of Approved and Experimental Drugs in Rat. ACS Chemical Biology, 2017, 12, 1593-1602.	1.6	9
843	PubChemQC Project: A Large-Scale First-Principles Electronic Structure Database for Data-Driven Chemistry. Journal of Chemical Information and Modeling, 2017, 57, 1300-1308.	2.5	132
844	Evaluation of Different Methods for Identification of Structural Alerts Using Chemical Ames Mutagenicity Data Set as a Benchmark. Chemical Research in Toxicology, 2017, 30, 1355-1364.	1.7	53
845	Bayesian molecular design with a chemical language model. Journal of Computer-Aided Molecular Design, 2017, 31, 379-391.	1.3	102
846	Assessment of several machine learning methods towards reliable prediction of hormone receptor binding affinity. Chemical Data Collections, 2017, 9-10, 114-124.	1.1	6
847	Berberine Induces Toxicity in HeLa Cells through Perturbation of Microtubule Polymerization by Binding to Tubulin at a Unique Site. Biochemistry, 2017, 56, 2594-2611.	1.2	32
848	Biodegradation of phthalic acid esters (PAEs) and in silico structural characterization of mono-2-ethylhexyl phthalate (MEHP) hydrolase on the basis of close structural homolog. Journal of Hazardous Materials, 2017, 338, 11-22.	6.5	96
849	Antiplasmodial Sesquiterpenoid Lactones from Trichospira verticillata: Structure Elucidation by Spectroscopic Methods and Comparison of Experimental and Calculated ECD Data. Journal of Natural Products, 2017, 80, 1639-1647.	1.5	23

#	Article	IF	Citations
850	SBSPKSv2: structure-based sequence analysis of polyketide synthases and non-ribosomal peptide synthetases. Nucleic Acids Research, 2017, 45, W72-W79.	6.5	47
851	ArbAlign: A Tool for Optimal Alignment of Arbitrarily Ordered Isomers Using the Kuhnâ€“Munkres Algorithm. Journal of Chemical Information and Modeling, 2017, 57, 1045-1054.	2.5	48
852	ADMETNet: The knowledge base of pharmacokinetics and toxicology network. Journal of Genetics and Genomics, 2017, 44, 273-276.	1.7	6
853	Performance of machine-learning scoring functions in structure-based virtual screening. Scientific Reports, 2017, 7, 46710.	1.6	243
854	Use of in silico models for prioritization of heat-induced food contaminants in mutagenicity and carcinogenicity testing. Archives of Toxicology, 2017, 91, 3157-3174.	1.9	31
855	Computerâ€aided Dereplication and Structure Elucidation of Natural Products at the University of Reims. Molecular Informatics, 2017, 36, 1700027.	1.4	11
856	G-LoSA for Prediction of Protein-Ligand Binding Sites and Structures. Methods in Molecular Biology, 2017, 1611, 97-108.	0.4	15
857	Multiobjective Feature Selection Approach to Quantitative Structure Property Relationship Models for Predicting the Octane Number of Compounds Found in Gasoline. Energy & Fuels, 2017, 31, 5828-5839.	2.5	8
858	When Does Chemical Elaboration Induce a Ligand To Change Its Binding Mode?. Journal of Medicinal Chemistry, 2017, 60, 128-145.	2.9	37
859	From theoretical energy barriers to decomposition temperatures of organic peroxides. Journal of Thermal Analysis and Calorimetry, 2017, 129, 323-337.	2.0	10
860	Photofragmentation of Tetranitromethane: Spin-Unrestricted Time-Dependent Excited-State Molecular Dynamics. Journal of Physical Chemistry Letters, 2017, 8, 3185-3192.	2.1	21
861	Searching for stereoisomerism in crystallographic databases: algorithm, analysis and chiral curiosities. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2017, 73, 453-465.	0.5	7
862	Documenting and harnessing the biological potential of molecules in Distributed Drug Discovery (D3) virtual catalogs. Chemical Biology and Drug Design, 2017, 90, 909-918.	1.5	6
863	Evolutionary conservation of influenza A PB2 sequences reveals potential target sites for small molecule inhibitors. Virology, 2017, 509, 112-120.	1.1	16
864	Predicting electronic structure properties of transition metal complexes with neural networks. Chemical Science, 2017, 8, 5137-5152.	3.7	152
865	High conductance values in Ï€-folded molecular junctions. Nature Communications, 2017, 8, 15195.	5.8	54
866	Structural insight into the active site of mushroom tyrosinase using phenylbenzoic acid derivatives. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 2868-2872.	1.0	12
867	RiPPMiner: a bioinformatics resource for deciphering chemical structures of RiPPs based on prediction of cleavage and cross-links. Nucleic Acids Research, 2017, 45, W80-W88.	6.5	100

#	Article	IF	Citations
868	ExcelAutomat: a tool for systematic processing of files as applied to quantum chemical calculations. Journal of Computer-Aided Molecular Design, 2017, 31, 667-673.	1.3	14
869	TCM-Mesh: The database and analytical system for network pharmacology analysis for TCM preparations. Scientific Reports, 2017, 7, 2821.	1.6	168
870	Discovery of ^{wt}RET and ^{V804M}RET Inhibitors: From Hit to Lead. ChemMedChem, 2017, 12, 1390-1398.	1.6	7
871	NANPDB: A Resource for Natural Products from Northern African Sources. Journal of Natural Products, 2017, 80, 2067-2076.	1.5	103
872	Collision cross section predictions using 2-dimensional molecular descriptors. Chemical Communications, 2017, 53, 7624-7627.	2.2	42
874	Towards the Revival of Interpretable QSAR Models. Challenges and Advances in Computational Chemistry and Physics, 2017, , 3-55.	0.6	17
875	PrimaDORAC: A Free Web Interface for the Assignment of Partial Charges, Chemical Topology, and Bonded Parameters in Organic or Drug Molecules. Journal of Chemical Information and Modeling, 2017, 57, 1240-1245.	2.5	39
876	Synthesis, docking study and neuroprotective effects of some novel pyrano[3,2- c]chromene derivatives bearing morpholine/phenylpiperazine moiety. Bioorganic and Medicinal Chemistry, 2017, 25, 3980-3988.	1.4	33
877	Direct Binding of the Corrector VX-809 to Human CFTR NBD1: Evidence of an Allosteric Coupling between the Binding Site and the NBD1:CL4 Interface. Molecular Pharmacology, 2017, 92, 124-135.	1.0	85
878	Structural basis for the potent inhibition of the HIV integrase-LEDGF/p75 proteinâ€“protein interaction. Journal of Molecular Graphics and Modelling, 2017, 75, 189-198.	1.3	1
879	Unique identifiers for small molecules enable rigorous labeling of their atoms. Scientific Data, 2017, 4, 170073.	2.4	30
880	Recent advances in the prediction of nonâ€<scp>CYP450</scp>â€mediated drug metabolism. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1323.	6.2	22
881	Assessing therapeutic potential of molecules: molecular property diagnostic suite for tuberculosis $$(mathbf{MPDS}^{mathbf{TB}})$$ (MPDS TB). Journal of Chemical Sciences, 2017, 129, 515-531.	0.7	20
882	Blocking of Single Î± -Hemolysin Pore by Rhodamine Derivatives. Biophysical Journal, 2017, 112, 2327-2335.	0.2	9
883	Searching for bioactive conformations of drug-like ligands with current force fields: how good are we?. Journal of Cheminformatics, 2017, 9, 29.	2.8	25
884	WatAA: Atlas of Protein Hydration. Exploring synergies between data mining and ab initio calculations. Physical Chemistry Chemical Physics, 2017, 19, 17094-17102.	1.3	8
885	Oxabicycloheptene Sulfonate Protects Against Î²-Amyloid-induced Toxicity by Activation of PI3K/Akt and ERK Signaling Pathways Via GPER1 in C6 Cells. Neurochemical Research, 2017, 42, 2246-2256.	1.6	9
886	Resolving protein structureâ€functionâ€binding site relationships from a binding site similarity network perspective. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1319-1335.	1.5	14

#	Article	IF	Citations
887	High-Throughput in Silico Structure Validation and Revision of Halogenated Natural Products Is Enabled by Parametric Corrections to DFT-Computed ¹³C NMR Chemical Shifts and Spinâ€“Spin Coupling Constants. Journal of Organic Chemistry, 2017, 82, 3368-3381.	1.7	121
888	Insights into a key sulfite scavenger enzyme sulfite oxidase (SOX) gene in plants. Physiology and Molecular Biology of Plants, 2017, 23, 385-395.	1.4	7
889	Upon the Shoulders of Giants: Open-Source Hardware and Software in Analytical Chemistry. Analytical Chemistry, 2017, 89, 4330-4338.	3.2	67
890	Proteinâ€“Ligand Scoring with Convolutional Neural Networks. Journal of Chemical Information and Modeling, 2017, 57, 942-957.	2.5	578
891	Assessment of model chemistries for hydrofluoropolyethers: A DFT/M08â€HX benchmark study. International Journal of Quantum Chemistry, 2017, 117, e25381.	1.0	8
892	Leveraging Cheminformatics Strategies for Inorganic Discovery: Application to Redox Potential Design. Industrial & Engineering Chemistry Research, 2017, 56, 4898-4910.	1.8	45
893	Cî€Ć/Bâ€“N substitution in five membered heterocycles. A computational analysis. New Journal of Chemistry, 2017, 41, 3619-3633.	1.4	11
894	Break Down in Order To Build Up: Decomposing Small Molecules for Fragment-Based Drug Design with eMolFrag. Journal of Chemical Information and Modeling, 2017, 57, 627-631.	2.5	42
895	Identification of small molecule inhibitors of Interleukin-18. Scientific Reports, 2017, 7, 483.	1.6	18
896	Modern Approaches to Chemical Image Recognition. The Kluwer International Series on Information Retrieval, 2017, , 369-389.	1.0	4
897	In silico prediction of chemical subcellular localization via multi-classification methods. MedChemComm, 2017, 8, 1225-1234.	3.5	15
898	Synthesis, characterization, cytotoxicity and computational studies of new phosphineâ€•and carbodithioateâ€based palladium(II) complexes. Applied Organometallic Chemistry, 2017, 31, e3771.	1.7	15
899	Structural and Sequence Similarity Makes a Significant Impact on Machine-Learning-Based Scoring Functions for Proteinâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2017, 57, 1007-1012.	2.5	67
900	Monte Carlo method based QSAR modelling of natural lipase inhibitors using hybrid optimal descriptors. SAR and QSAR in Environmental Research, 2017, 28, 179-197.	1.0	32
901	MOST: most-similar ligand based approach to target prediction. BMC Bioinformatics, 2017, 18, 165.	1.2	43
902	Molecular dynamics simulations and molecular flooding studies of the retinoid X-receptor ligand binding domain. Journal of Molecular Modeling, 2017, 23, 98.	0.8	12
903	Systems Pharmacology-Based Discovery of Natural Products for Precision Oncology Through Targeting Cancer Mutated Genes. CPT: Pharmacometrics and Systems Pharmacology, 2017, 6, 177-187.	1.3	49
904	Tensile strength of commercial polymer materials for fused filament fabrication 3D printing. Additive Manufacturing, 2017, 15, 40-47.	1.7	172

#	Article	IF	Citations
905	On-the-Fly QM/MM Docking with Attracting Cavities. Journal of Chemical Information and Modeling, 2017, 57, 73-84.	2.5	42
906	Design and synthesis of emodin derivatives as novel inhibitors of ATP-citrate lyase. European Journal of Medicinal Chemistry, 2017, 126, 920-928.	2.6	60
907	Sequence Effects in Donorâ€“Acceptor Oligomeric Semiconductors Comprising Benzothiadiazole and Phenylenevinylene Monomers. Macromolecules, 2017, 50, 151-161.	2.2	33
908	Integrating ion mobility spectrometry into mass spectrometry-based exposome measurements: what can it add and how far can it go?. Bioanalysis, 2017, 9, 81-98.	0.6	66
909	Split-Charge Equilibration Parameters for Generating Rapid Partial Atomic Charges in Metalâ€“Organic Frameworks and Porous Polymer Networks for High-Throughput Screening. Journal of Physical Chemistry C, 2017, 121, 903-910.	1.5	12
910	Network pharmacology-based virtual screening of natural products from Clerodendrum species for identification of novel anti-cancer therapeutics. Molecular BioSystems, 2017, 13, 406-416.	2.9	34
911	In silico design and bioevaluation of selective benzotriazepine <scp>BRD</scp>4 inhibitors with potent antiosteoclastogenic activity. Chemical Biology and Drug Design, 2017, 90, 97-111.	1.5	8
912	Screening for Novel Small-Molecule Inhibitors Targeting the Assembly of Influenza Virus Polymerase Complex by a Bimolecular Luminescence Complementation-Based Reporter System. Journal of Virology, 2017, 91, .	1.5	12
913	Small Molecule-Based Pattern Recognition To Classify RNA Structure. Journal of the American Chemical Society, 2017, 139, 409-416.	6.6	47
914	Rational Design of Novel Highly Potent and Selective Phosphatidylinositol 4-Kinase IIIÎ² (PI4KB) Inhibitors as Broad-Spectrum Antiviral Agents and Tools for Chemical Biology. Journal of Medicinal Chemistry, 2017, 60, 100-118.	2.9	50
915	Arpeggio: A Web Server for Calculating and Visualising Interatomic Interactions in Protein Structures. Journal of Molecular Biology, 2017, 429, 365-371.	2.0	340
916	Assessment of a novel device for onsite integrative large-volume solid phase extraction of water samples to enable a comprehensive chemical and effect-based analysis. Science of the Total Environment, 2017, 581-582, 350-358.	3.9	63
917	Using <scp>PyMOL</scp> as a platform for computational drug design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1298.	6.2	348
918	Design and synthesis of benzodiazepine analogs as isoform-selective human lysine deacetylase inhibitors. European Journal of Medicinal Chemistry, 2017, 127, 531-553.	2.6	17
919	Density functional theory for modelling large molecular adsorbateâ€“surface interactions: a mini-review and worked example. Molecular Simulation, 2017, 43, 327-345.	0.9	39
920	1 H NMR-based kinetic and theoretical studies of the simultaneous formation of two discrete rotameric systems of a novel difenchyl sulfite ester. Tetrahedron, 2017, 73, 6922-6931.	1.0	0
921	Hydroxyethylamine derivatives as HIV-1 protease inhibitors: a predictive QSAR modelling study based on Monte Carlo optimization. SAR and QSAR in Environmental Research, 2017, 28, 973-990.	1.0	23
922	Endogenous retinoid X receptor ligands in mouse hematopoietic cells. Science Signaling, 2017, 10, .	1.6	18

#	Article	IF	Citations
923	Discovery of novel non-competitive inhibitors of mammalian neutral M1 aminopeptidase (APN). Biochimie, 2017, 142, 216-225.	1.3	13
924	Observation of giant conductance fluctuations in a protein. Nano Futures, 2017, 1, 035002.	1.0	27
925	Drug repurposing in idiopathic pulmonary fibrosis filtered by a bioinformatics-derived composite score. Scientific Reports, 2017, 7, 12569.	1.6	27
926	Overlapping CD8 + and CD4 + T-cell epitopes identification for the progression of epitope-based peptide vaccine from nucleocapsid and glycoprotein of emerging Rift Valley fever virus using immunoinformatics approach. Infection, Genetics and Evolution, 2017, 56, 75-91.	1.0	41
927	Isomer activation controls stereospecificity of class I fructose-1,6-bisphosphate aldolases. Journal of Biological Chemistry, 2017, 292, 19849-19860.	1.6	5
928	Solid Aluminum Borohydrides for Prospective Hydrogen Storage. ChemSusChem, 2017, 10, 4725-4734.	3.6	24
929	Chemical Reactant Recommendation Using a Network of Organic Chemistry. , 2017, , .		11
930	Biochemical efficacy, molecular docking and inhibitory effect of 2, 3-dimethylmaleic anhydride on insect acetylcholinesterase. Scientific Reports, 2017, 7, 12483.	1.6	26
931	Expression and Functional Characterization of Breast Cancer-Associated Cytochrome P450 4Z1 inSaccharomyces cerevisiae. Drug Metabolism and Disposition, 2017, 45, 1364-1371.	1.7	35
932	Quantitative and Systems Pharmacology. 1. In Silico Prediction of Drugâ€“Target Interactions of Natural Products Enables New Targeted Cancer Therapy. Journal of Chemical Information and Modeling, 2017, 57, 2657-2671.	2.5	76
933	Predicting novel substrates for enzymes with minimal experimental effort with active learning. Metabolic Engineering, 2017, 44, 171-181.	3.6	31
934	Diminazene Is a Slow Pore Blocker of Acid-Sensing Ion Channel 1a (ASIC1a). Molecular Pharmacology, 2017, 92, 665-675.	1.0	42
935	Rotamer Libraries for the High-Resolution Design of Î²-Amino Acid Foldamers. Structure, 2017, 25, 1771-1780.e3.	1.6	13
936	Cheminformatics Approaches in Modern Drug Discovery. , 2017, , 135-148.		4
937	Arjunolic acid, a peroxisome proliferator-activated receptor Î± agonist, regresses cardiac fibrosis by inhibiting non-canonical TGF-Î² signaling. Journal of Biological Chemistry, 2017, 292, 16440-16462.	1.6	50
938	Exploring putative inhibitors of Death Associated Protein Kinase 1 (DAPK1) via targeting Gly- Glu -Leu (G) Tj ETQq1 1 0.784314 rgBT /Ov Modelling, 2017, 77, 153-167.	1.3	11
939	New heterometallic pivalates with Fe III and Zn II ions: Synthesis, structures, magnetic, thermal properties. Polyhedron, 2017, 137, 165-175.	1.0	21
940	doGlycansâ€“Tools for Preparing Carbohydrate Structures for Atomistic Simulations of Glycoproteins, Glycolipids, and Carbohydrate Polymers for GROMACS. Journal of Chemical Information and Modeling, 2017, 57, 2401-2406.	2.5	71

#	Article	IF	Citations
941	Inhibition of Wnt/Î²-Catenin pathway and Histone acetyltransferase activity by Rimonabant: a therapeutic target for colon cancer. Scientific Reports, 2017, 7, 11678.	1.6	57
942	Spectral studies, crystal structure, molecular docking and Hirshfeld surfaces computational studies of 3-(3-Bromophenyl)-5-(4- methoxyphenyl) isoxazole. Chemical Data Collections, 2017, 11-12, 131-138.	1.1	5
943	Synthesis, biological evaluation and quantitative structure-active relationships of 1,3-thiazolidin-4-one derivatives. A promising chemical scaffold endowed with high antifungal potency and low cytotoxicity. European Journal of Medicinal Chemistry, 2017, 140, 274-292.	2.6	21
944	Prediction Errors of Molecular Machine Learning Models Lower than Hybrid DFT Error. Journal of Chemical Theory and Computation, 2017, 13, 5255-5264.	2.3	435
945	Spectroscopic investigations (FT-IR, UV, 1 H and 13 C NMR) and DFT/TD-DFT calculations of potential analgesic drug 2-[2-(dimethylamino)ethyl]-6-methoxy-4-(pyridin-2-yl)-1(2 H)-phthalazinone. Journal of Molecular Structure, 2017, 1150, 614-628.	1.8	4
946	Quick Way to Port Existing C/C++ Chemoinformatics Toolkits to the Web Using Emscripten. Journal of Chemical Information and Modeling, 2017, 57, 2407-2412.	2.5	8
947	An iterative compound screening contest method for identifying target protein inhibitors using the tyrosine-protein kinase Yes. Scientific Reports, 2017, 7, 12038.	1.6	28
948	Customizable de novo design strategies for DOCK: Application to HIVgp41 and other therapeutic targets. Journal of Computational Chemistry, 2017, 38, 2641-2663.	1.5	25
949	A novel approach for the prediction of species-specific biotransformation of xenobiotic/drug molecules by the human gut microbiota. Scientific Reports, 2017, 7, 9751.	1.6	54
950	Comparative analyses of enzymatic activity, structural study and docking of fungal cellulases. Gene Reports, 2017, 9, 54-60.	0.4	12
951	Discovery of Inhibitors of Four Bromodomains by Fragment-Anchored Ligand Docking. Journal of Chemical Information and Modeling, 2017, 57, 2584-2597.	2.5	21
952	Structure-based drug discovery for combating influenza virus by targeting the PAâ€“PB1 interaction. Scientific Reports, 2017, 7, 9500.	1.6	27
953	Automation of route identification and optimisation based on data-mining and chemical intuition. Faraday Discussions, 2017, 202, 483-496.	1.6	23
954	The Binding Mode of N-Hydroxyamidines to Indoleamine 2,3-Dioxygenase 1 (IDO1). Biochemistry, 2017, 56, 4323-4325.	1.2	17
955	Comparison of the Predictive Performance and Interpretability of Random Forest and Linear Models on Benchmark Data Sets. Journal of Chemical Information and Modeling, 2017, 57, 1773-1792.	2.5	88
956	Study of new interactions of glitazoneâ€™s stereoisomers and the endogenous ligand 15d-PGJ2 on six different PPAR gamma proteins. Biochemical Pharmacology, 2017, 142, 168-193.	2.0	18
957	Explicit treatment of hydrogen bonds in the universal force field: Validation and application for metal-organic frameworks, hydrates, and host-guest complexes. Journal of Chemical Physics, 2017, 147, 161705.	1.2	10
958	Role of Protein Dimeric Interface in Allosteric Inhibition of N-Acetyl-Aspartate Hydrolysis by Human Aspartoacylase. Journal of Chemical Information and Modeling, 2017, 57, 1999-2008.	2.5	18

#	Article	IF	Citations
959	Functional annotation of chemical libraries across diverse biological processes. Nature Chemical Biology, 2017, 13, 982-993.	3.9	76
960	Investigation of naphthofuran moiety as potential dual inhibitor against BACE-1 and GSK-3Î²: molecular dynamics simulations, binding energy, and network analysis to identify first-in-class dual inhibitors against Alzheimerâ€™s disease. Journal of Molecular Modeling, 2017, 23, 239.	0.8	20
961	Predicting CO2 capture of ionic liquids using machine learning. Journal of CO2 Utilization, 2017, 21, 162-168.	3.3	70
962	Effects of flexibility and electrostatic interactions on the coupled bindingâ€“folding mechanisms of Chz.core and H2A.zâ€“H2B. Molecular BioSystems, 2017, 13, 2152-2159.	2.9	4
963	New anthrarobin acyl derivatives as butyrylcholinesterase inhibitors: synthesis, in vitro and in silico studies. Heliyon, 2017, 3, e00350.	1.4	3
964	Pocket detection and interaction-weighted ligand-similarity search yields novel high-affinity binders for Myocilin-OLF, a protein implicated in glaucoma. Bioorganic and Medicinal Chemistry Letters, 2017, 27, 4133-4139.	1.0	2
965	Screening-level exposure-based prioritization to identify potential POPs, vPvBs and planetary boundary threats among Arctic contaminants. Emerging Contaminants, 2017, 3, 85-94.	2.2	22
966	Cyclooxygenase-2 identified as a potential target for novel radiomodulator scopolamine methyl bromide: An in silico study. Informatics in Medicine Unlocked, 2017, 9, 18-25.	1.9	3
967	An in silico strategy for identification of novel drug targets against Plasmodium falciparum. Parasitology Research, 2017, 116, 2539-2559.	0.6	7
968	In silico identification of milk antihypertensive di- and tripeptides involved in angiotensin Iâ€“converting enzyme inhibitory activity. Nutrition Research, 2017, 46, 22-30.	1.3	26
969	Targeting of dopamine transporter to filopodia requires an outward-facing conformation of the transporter. Scientific Reports, 2017, 7, 5399.	1.6	16
970	NuBBEDB: an updated database to uncover chemical and biological information from Brazilian biodiversity. Scientific Reports, 2017, 7, 7215.	1.6	139
971	New racemic annulated pyrazolo[1,2-b]phthalazines as tacrine-like AChE inhibitors with potential use in Alzheimer's disease. European Journal of Medicinal Chemistry, 2017, 139, 280-289.	2.6	45
972	Identification and functionality prediction of pathogenesisâ€related protein 1 from legume family. Proteins: Structure, Function and Bioinformatics, 2017, 85, 2066-2080.	1.5	10
973	RealityConvert: a tool for preparing 3D models of biochemical structures for augmented and virtual reality. Bioinformatics, 2017, 33, 3816-3818.	1.8	27
974	The octet rule in chemical space: generating virtual molecules. Molecular Diversity, 2017, 21, 769-778.	2.1	0
975	An integrative study to identify novel scaffolds for sphingosine kinase 1 inhibitors. European Journal of Medicinal Chemistry, 2017, 139, 461-481.	2.6	33
976	Location of Organic Structure-Directing Agents in Zeolites Using Diffraction Techniques. Structure and Bonding, 2017, , 43-73.	1.0	2

#	Article	IF	Citations
977	Statistical Profiling of One Promiscuous Protein Binding Site: Illustrated by Urokinase Catalytic Domain. Molecular Informatics, 2017, 36, 1700040.	1.4	4
978	Rational Design of Membraneâ€Poreâ€Forming Peptides. Small, 2017, 13, 1701316.	5.2	24
979	Endocannabinoid Transport Proteins. Methods in Enzymology, 2017, 593, 99-121.	0.4	20
980	Structure-based prediction of ligandâ€“protein interactions on a genome-wide scale. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 13685-13690.	3.3	44
981	Machine learning unifies the modeling of materials and molecules. Science Advances, 2017, 3, e1701816.	4.7	488
982	A Next Generation Connectivity Map: L1000 Platform and the First 1,000,000 Profiles. Cell, 2017, 171, 1437-1452.e17.	13.5	2,281
983	Comparative computational assessment of the pathogenicity of mutations in the Aspartoacylase enzyme. Metabolic Brain Disease, 2017, 32, 2105-2118.	1.4	34
984	Design Principles and Top Non-Fullerene Acceptor Candidates for Organic Photovoltaics. Joule, 2017, 1, 857-870.	11.7	157
985	RosÃ© Wine Fining Using Polyvinylpolypyrrolidone: Colorimetry, Targeted Polyphenomics, and Molecular Dynamics Simulations. Journal of Agricultural and Food Chemistry, 2017, 65, 10591-10597.	2.4	31
986	Receptor structure-based discovery of non-metabolite agonists for the succinate receptor GPR91. Molecular Metabolism, 2017, 6, 1585-1596.	3.0	40
987	Heat shock protein 90 and serine/threonine kinase B-Raf inhibitors have overlapping chemical space. RSC Advances, 2017, 7, 31069-31074.	1.7	17
988	In vitroefficacy andin silicoanalysis of cefixime-ofloxacin combination forSalmonellaTyphi from bloodstream infection. Journal of Applied Microbiology, 2017, 123, 615-624.	1.4	6
989	High-temperature decomposition of the cellulose molecule: a stochastic molecular dynamics study. Cellulose, 2017, 24, 2713-2725.	2.4	63
990	Virtual Screening, pharmacophore development and structure based similarity search to identify inhibitors against IdeR, a transcription factor of Mycobacterium tuberculosis. Scientific Reports, 2017, 7, 4653.	1.6	40
991	Identification of flavanones from Boesenbergia rotunda as potential antioxidants and monoamine oxidase B inhibitors. Chemical Papers, 2017, 71, 2473-2483.	1.0	5
992	LigQ: A Webserver to Select and Prepare Ligands for Virtual Screening. Journal of Chemical Information and Modeling, 2017, 57, 1741-1746.	2.5	5
993	Study of intraâ€“inter species proteinâ€“protein interactions for potential drug targets identification and subsequent drug design for Escherichia coli O104:H4 C277-11. In Silico Pharmacology, 2017, 5, 1.	1.8	13
994	Exhaustive conformational search for transition states: the case of catechol O -methyltransferase active site. Mendeleev Communications, 2017, 27, 224-227.	0.6	23

#	Article	IF	Citations
995	Inhibition of Alzheimer's amyloid-beta aggregation in-vitro by carbenoxolone: Insight into mechanism of action. Neurochemistry International, 2017, 108, 481-493.	1.9	34
996	HybridSim-VS: a web server for large-scale ligand-based virtual screening using hybrid similarity recognition techniques. Bioinformatics, 2017, 33, 3480-3481.	1.8	26
997	Predicting anatomic therapeutic chemical classification codes using tiered learning. BMC Bioinformatics, 2017, 18, 266.	1.2	11
998	A metadata-driven approach to data repository design. Journal of Cheminformatics, 2017, 9, 4.	2.8	17
999	Technical implications of new IUPAC elements in cheminformatics. Journal of Cheminformatics, 2017, 9, 10.	2.8	1
1000	Critical Assessment of Small Molecule Identification 2016: automated methods. Journal of Cheminformatics, 2017, 9, 22.	2.8	122
1001	ChemSAR: an online pipelining platform for molecular SAR modeling. Journal of Cheminformatics, 2017, 9, 27.	2.8	45
1002	Comparative evaluation of atom mapping algorithms for balanced metabolic reactions: application to Recon 3D. Journal of Cheminformatics, 2017, 9, 39.	2.8	23
1003	chemalot and chemalot_knime: Command line programs as workflow tools for drug discovery. Journal of Cheminformatics, 2017, 9, 38.	2.8	14
1004	Tetracyclines as a potential antiviral therapy against Crimean Congo hemorrhagic fever virus: Docking and molecular dynamic studies. Computational Biology and Chemistry, 2017, 70, 1-6.	1.1	14
1005	In vitroandin silicointeraction of porcine Î±-amylase withVicia fabacrude seed extract and evaluation of antidiabetic activity. Bioengineered, 2017, 8, 393-403.	1.4	20
1006	Structural-conformational aspects of tRNA complexation with chloroethyl nitrosourea derivatives: A molecular modeling and spectroscopic investigation. Journal of Photochemistry and Photobiology B: Biology, 2017, 166, 1-11.	1.7	6
1007	Improvement of thermostability and halostability of Î²-1,3-1,4-glucanase by substituting hydrophobic residue for Lys 48. International Journal of Biological Macromolecules, 2017, 94, 594-602.	3.6	23
1008	Structure and Function of a Câ€“C Bond Cleaving Oxygenase in Atypical Angucycline Biosynthesis. ACS Chemical Biology, 2017, 12, 142-152.	1.6	17
1009	Computer-Aided Drug Design Methods. Methods in Molecular Biology, 2017, 1520, 85-106.	0.4	317
1010	Novel non-Î²-lactam inhibitor of Î²-lactamase TEM-171 based on acylated phenoxyaniline. Biochimie, 2017, 132, 45-53.	1.3	26
1011	Protein Data Bank Japan (PDBj): updated user interfaces, resource description framework, analysis tools for large structures. Nucleic Acids Research, 2017, 45, D282-D288.	6.5	108
1012	An integrated approach of network-based systems biology, molecular docking, and molecular dynamics approach to unravel the role of existing antiviral molecules against AIDS-associated cancer. Journal of Biomolecular Structure and Dynamics, 2017, 35, 1547-1558.	2.0	6

#	Article	IF	Citations
1013	Characterization of MymA protein as a flavinâ€containing monooxygenase and as a target of isoniazid. Chemical Biology and Drug Design, 2017, 89, 152-160.	1.5	5
1014	Structureâ€based discovery of novel US28 small molecule ligands with different modes of action. Chemical Biology and Drug Design, 2017, 89, 289-296.	1.5	10
1015	Role of E542 and E545 missense mutations of PIK3CA in breast cancer: a comparative computational approach. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2745-2757.	2.0	33
1016	Surface charge modification increases firefly luciferase rigidity without alteration in bioluminescence spectra. Enzyme and Microbial Technology, 2017, 96, 47-59.	1.6	16
1017	A computational investigation on the structure, global parameters and antioxidant capacity of a polyphenol, Gallic acid. Food Chemistry, 2017, 220, 93-99.	4.2	141
1018	Structural characterization of the yeast CF IA complex through a combination of mass spectrometry approaches. International Journal of Mass Spectrometry, 2017, 420, 57-66.	0.7	5
1019	Conformer and pharmacophore based identification of peptidomimetic inhibitors of chikungunya virus nsP2 protease. Journal of Biomolecular Structure and Dynamics, 2017, 35, 3522-3539.	2.0	15
1020	Induced fit of the peptidyl-transferase center of the ribosome and conformational freedom of the esterified amino acids. Rna, 2017, 23, 229-239.	1.6	15
1021	Strategies for dereplication of natural compounds using high-resolution tandem mass spectrometry. Phytochemistry Letters, 2017, 21, 313-319.	0.6	26
1022	On the importance of composite protein multiple ligand interactions in protein pockets. Journal of Computational Chemistry, 2017, 38, 1252-1259.	1.5	10
1023	Quercetin derivatives as non-nucleoside inhibitors for dengue polymerase: molecular docking, molecular dynamics simulation, and binding free energy calculation. Journal of Biomolecular Structure and Dynamics, 2017, 35, 2895-2909.	2.0	34
1024	Identification of novel microsomal prostaglandin E2 synthase-1 (mPGES-1) lead inhibitors from Fragment Virtual Screening. European Journal of Medicinal Chemistry, 2017, 125, 278-287.	2.6	19
1025	mutLBSgeneDB: mutated ligand binding site gene DataBase. Nucleic Acids Research, 2017, 45, D256-D263.	6.5	21
1026	Swarming behaviour of salps algorithm for predicting chemical compound activities. , 2017, , .		65
1027	Energy calculation of MMFF94 force field on GPU (Special session on array computing systems and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5 0		
1028	Molecular docking analysis of curcumin analogues against kinase domain of ALK5. In Silico Pharmacology, 2017, 5, 15.	1.8	32
1029	The ChEMBL database in 2017. Nucleic Acids Research, 2017, 45, D945-D954.	6.5	1,718
1030	Molecular property diagnostic suite (MPDS): Development of disease-specific open source web portals for drug discovery. SAR and QSAR in Environmental Research, 2017, 28, 913-926.	1.0	11

#	Article	IF	Citations
1031	Synthesis, Biological Evaluation and Molecular Docking of Avicequinone C Analogues as Potential Steroid 5Î±-Reductase Inhibitors. Chemical and Pharmaceutical Bulletin, 2017, 65, 253-260.	0.6	14
1032	Open chemistry: RESTful web APIs, JSON, NWChem and the modern web application. Journal of Cheminformatics, 2017, 9, 55.	2.8	16
1033	Molecular characterization, modeling, in silico analysis of equine pituitary gonadotropin alpha subunit and docking interaction studies with ganirelix. In Silico Pharmacology, 2017, 5, 5.	1.8	1
1034	Parallelization of Large-Scale Drug-Protein Binding Experiments. , 2017, , .		1
1035	Virtual Screening for Dual Hsp90/B-Raf Inhibitors. Methods in Pharmacology and Toxicology, 2017, , 355-365.	0.1	0
1036	Crystal Structure of 17Î±-Dihydroequilin, C18H22O2, from Synchrotron Powder Diffraction Data and Density Functional Theory. Crystals, 2017, 7, 218.	1.0	0
1037	STRAPS v1.0: evaluating a methodology for predicting electron impact ionisation mass spectra for the aerosol mass spectrometer. Geoscientific Model Development, 2017, 10, 2365-2377.	1.3	1
1038	BETWEEN ARTEMISININ AND DERIVATIVES WITH NEURAMINIDASE: A DOCKING STUDY INSIGHT. Asian Journal of Pharmaceutical and Clinical Research, 2017, 10, 304.	0.3	6
1039	VIRTUAL SCREENING OF INDONESIAN HERBAL DATABASE FOR DNA METHYLTRANSFERASE INHIBITORS. Asian Journal of Pharmaceutical and Clinical Research, 2017, 10, 153.	0.3	0
1040	In silico Approach for Anti-Thrombosis Drug Discovery: P2Y1R Structure-Based TCMs Screening. Frontiers in Pharmacology, 2016, 7, 531.	1.6	28
1041	Nano-Lazar: Read across Predictions for Nanoparticle Toxicities with Calculated and Measured Properties. Frontiers in Pharmacology, 2017, 8, 377.	1.6	26
1042	Quantitative and Systems Pharmacology 3. Network-Based Identification of New Targets for Natural Products Enables Potential Uses in Aging-Associated Disorders. Frontiers in Pharmacology, 2017, 8, 747.	1.6	38
1043	Novel Tacrine-Scutellarin Hybrids as Multipotent Anti-Alzheimerâ€™s Agents: Design, Synthesis and Biological Evaluation. Molecules, 2017, 22, 1006.	1.7	32
1044	DeCAFâ€”Discrimination, Comparison, Alignment Tool for 2D PHarmacophores. Molecules, 2017, 22, 1128.	1.7	5
1045	Development of 2-Methoxyhuprine as Novel Lead for Alzheimerâ€™s Disease Therapy. Molecules, 2017, 22, 1265.	1.7	26
1046	Study on the Anticoagulant or Procoagulant Activities of Type II Phenolic Acid Derivatives. Molecules, 2017, 22, 2047.	1.7	14
1047	Annotation of Peptide Structures Using SMILES and Other Chemical Codesâ€“Practical Solutions. Molecules, 2017, 22, 2075.	1.7	11
1048	Chemical Data Formats, Fingerprints, and Other Molecular Descriptions for Database Analysis and Searching. , 2017, , 329-378.		27

#	Article	IF	Citations
1049	A QSTR-Based Expert System to Predict Sweetness of Molecules. Frontiers in Chemistry, 2017, 5, 53.	1.8	41
1050	Angular Phenozaxine Ethers as Potent Multi-microbial Targets Inhibitors: Design, Synthesis, and Molecular Docking Studies. Frontiers in Chemistry, 2017, 5, 107.	1.8	19
1051	Structural Insights into the Cytotoxic Mechanism of Vibrio parahaemolyticus PirAvp and PirBvp Toxins. Marine Drugs, 2017, 15, 373.	2.2	45
1052	Towards a critical evaluation of an empirical and volume-based solvation function for ligand docking. PLoS ONE, 2017, 12, e0174336.	1.1	11
1053	Rational design of drug-like compounds targeting Mycobacterium marinum MelF protein. PLoS ONE, 2017, 12, e0183060.	1.1	13
1054	A conformational switch high-throughput screening assay and allosteric inhibition of the flavivirus NS2B-NS3 protease. PLoS Pathogens, 2017, 13, e1006411.	2.1	116
1055	Leishmania infantum 5â€™-Methylthioadenosine Phosphorylase presents relevant structural divergence to constitute a potential drug target. BMC Structural Biology, 2017, 17, 9.	2.3	2
1056	Predicting drug-disease interactions by semi-supervised graph cut algorithm and three-layer data integration. BMC Medical Genomics, 2017, 10, 79.	0.7	23
1057	eTOX ALLIES: an automated pipeLine for linear interaction energy-based simulations. Journal of Cheminformatics, 2017, 9, 58.	2.8	7
1058	Consensus queries in ligand-based virtual screening experiments. Journal of Cheminformatics, 2017, 9, 60.	2.8	12
1059	Utilizing random Forest QSAR models with optimized parameters for target identification and its application to target-fishing server. BMC Bioinformatics, 2017, 18, 567.	1.2	44
1060	Aqueous-phase photooxygenation of enes, amines, sulfides and polycyclic aromatics by singlet (a1Î”g) oxygen: prediction of rate constants using orbital energies, substituent factors and quantitative structureâ€“property relationships. Environmental Chemistry, 2017, 14, 442.	0.7	13
1061	IN VITRO AND IN SILICO ANTIMICROBIAL STUDY OF STANNANE OF PYRIDOXAL 5-PHOSPHATE. International Journal of Pharmacy and Pharmaceutical Sciences, 2017, 9, 145.	0.3	5
1062	The cornucopia of meaningful leads: Applying deep adversarial autoencoders for new molecule development in oncology. Oncotarget, 2017, 8, 10883-10890.	0.8	249
1063	Comparative Study on the Binding Affinity of Methimazole and Propylthiouracil to Thyroid Peroxidase as an Anti-Thyroid Drug: An Insilico Approach. Journal of Molecular Imaging & Dynamics, 2017, 07, .	0.2	3
1064	BINARY QUANTITATIVE STRUCTURE-ACTIVITY RELATIONSHIP ANALYSIS IN RETROSPECTIVE STRUCTURE-BASED VIRTUAL SCREENING CAMPAIGNS TARGETING ESTROGEN RECEPTOR ALPHA. Asian Journal of Pharmaceutical and Clinical Research, 2017, 10, 206.	0.3	7
1065	Repositioning of amprenavir as a novel extracellular signal-regulated kinase-2 inhibitor and apoptosis inducer in MCF-7 human breast cancer. International Journal of Oncology, 2017, 50, 823-834.	1.4	6
1066	Virtual Screening of potential inhibitors from Herbs for the treatment of Breast Cancer. Asian Journal of Pharmaceutical and Clinical Research, 2017, 10, 62.	0.3	1

#	Article	IF	Citations
1067	Synthesis, bioactivity, 3D-QSAR studies of novel dibenzofuran derivatives as PTP-MEG2 inhibitors. Oncotarget, 2017, 8, 38466-38481.	0.8	4
1068	In silico pharmacodynamics, toxicity profile and biological activities of the Saharan medicinal plant Limoniastrum feei. Brazilian Journal of Pharmaceutical Sciences, 2017, 53, .	1.2	10
1069	Application of an advanced and wide scope non-target screening workflow with LC-ESI-QTOF-MS and chemometrics for the classification of the Greek olive oil varieties. Food Chemistry, 2018, 256, 53-61.	4.2	63
1070	Low-resolution SAXS and comparative modeling based structure analysis of endo-Î²-1,4-xylanase a family 10 glycoside hydrolase from Pseudopedobacter saltans comb. nov.. International Journal of Biological Macromolecules, 2018, 112, 1104-1114.	3.6	19
1071	POAP: A GNU parallel based multithreaded pipeline of open babel and AutoDock suite for boosted high throughput virtual screening. Computational Biology and Chemistry, 2018, 74, 39-48.	1.1	60
1072	ESIgen: Electronic Supporting Information Generator for Computational Chemistry Publications. Journal of Chemical Information and Modeling, 2018, 58, 561-564.	2.5	19
1073	Structure-based discovery of glycomimetic FmlH ligands as inhibitors of bacterial adhesion during urinary tract infection. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E2819-E2828.	3.3	63
1074	Virtual target screening reveals rosmarinic acid and salvianolic acid A inhibiting metallo- and serine-Î²-lactamases. Bioorganic and Medicinal Chemistry Letters, 2018, 28, 1037-1042.	1.0	21
1075	Mapping two neurosteroid-modulatory sites in the prototypic pentameric ligand-gated ion channel GLIC. Journal of Biological Chemistry, 2018, 293, 3013-3027.	1.6	28
1076	MARSI: metabolite analogues for rational strain improvement. Bioinformatics, 2018, 34, 2319-2321.	1.8	7
1077	LS-align: an atom-level, flexible ligand structural alignment algorithm for high-throughput virtual screening. Bioinformatics, 2018, 34, 2209-2218.	1.8	62
1078	NPASS: natural product activity and species source database for natural product research, discovery and tool development. Nucleic Acids Research, 2018, 46, D1217-D1222.	6.5	177
1079	The quest for determining one-electron redox potentials of azulene-1-carbonitriles by calculation. Physical Chemistry Chemical Physics, 2018, 20, 7438-7446.	1.3	12
1080	An Augmented Pocketome: Detection and Analysis of Small-Molecule Binding Pockets in Proteins of Known 3D Structure. Structure, 2018, 26, 499-512.e2.	1.6	38
1081	Highly Potent, Stable, and Selective Dimeric Hetarylpropylguanidine-Type Histamine H₂ Receptor Agonists. ACS Omega, 2018, 3, 2865-2882.	1.6	24
1082	A Comprehensive Analysis of Anionâ€“Quadrupole Interactions in Protein Structures. Biochemistry, 2018, 57, 1852-1867.	1.2	29
1083	Electronic and optical properties of chromophores from bacterial cellulose. Cellulose, 2018, 25, 2191-2203.	2.4	28
1084	Uncovering reaction sequences on surfaces through graphical methods. Physical Chemistry Chemical Physics, 2018, 20, 7721-7729.	1.3	10

#	Article	IF	Citations
1085	Computational prediction of chemical reactions: current status and outlook. Drug Discovery Today, 2018, 23, 1203-1218.	3.2	126
1086	In-silico study of toxicokinetics and disease association of chemicals present in smokeless tobacco products. Regulatory Toxicology and Pharmacology, 2018, 95, 8-16.	1.3	7
1087	Diclofenac Identified as a Kynurenine 3-Monooxygenase Binder and Inhibitor by Molecular Similarity Techniques. ACS Omega, 2018, 3, 2564-2568.	1.6	11
1088	Semiconductor color-center structure and excitation spectra: Equation-of-motion coupled-cluster description of vacancy and transition-metal defect photoluminescence. Physical Review B, 2018, 97, .	1.1	3
1089	Machine-Learning Energy Gaps of Porphyrins with Molecular Graph Representations. Journal of Physical Chemistry A, 2018, 122, 4571-4578.	1.1	40
1090	Computational Analysis for the Rational Design of Anti-Amyloid Beta (AÎ²) Antibodies. Journal of Physical Chemistry B, 2018, 122, 4521-4536.	1.2	8
1091	Improving classical scoring functions using random forest: The nonâ€additivity of free energy termsâ€™ contributions in binding. Chemical Biology and Drug Design, 2018, 92, 1429-1434.	1.5	26
1092	Resolving Confined ⁷Li Dynamics of Uranyl Peroxide Capsule U₂₄. Inorganic Chemistry, 2018, 57, 5514-5525.	1.9	10
1093	Ultrafast Trap State-Mediated Electron Transfer for Quantum Dot Redox Sensing. Journal of Physical Chemistry C, 2018, 122, 10173-10180.	1.5	22
1094	Computational Analysis of Solvent Inclusion in Docking Studies of Proteinâ€“Glycosaminoglycan Systems. Methods in Molecular Biology, 2018, 1762, 445-454.	0.4	3
1095	Virtual Ligand Screening Using PL-PatchSurfer2, a Molecular Surface-Based Proteinâ€“Ligand Docking Method. Methods in Molecular Biology, 2018, 1762, 105-121.	0.4	6
1096	Identification of Non-Zinc Binding Inhibitors of MMP-2 Through Virtual Screening and Subsequent Rescoring. Drug Research, 2018, 68, 529-535.	0.7	4
1097	Lifting the Curse of Dimensionality on Enhanced Sampling of Reaction Networks with Parallel Bias Metadynamics. Journal of Chemical Theory and Computation, 2018, 14, 2516-2525.	2.3	24
1098	Benchmarking tripletâ€“triplet annihilation photon upconversion schemes. Physical Chemistry Chemical Physics, 2018, 20, 12182-12192.	1.3	19
1099	The dye-sensitized solar cell database. Journal of Cheminformatics, 2018, 10, 18.	2.8	47
1100	The Alexandria library, a quantum-chemical database of molecular properties for force field development. Scientific Data, 2018, 5, 180062.	2.4	45
1101	Validation and updating of QSAR models for partitioning coefficients of ionic liquids in octanol-water and development of a new LFER model. Science of the Total Environment, 2018, 633, 920-928.	3.9	17
1102	Novel Insights for Inhibiting Mutant Heterodimer IDH1wt-R132H in Cancer: An In-Silico Approach. Molecular Diagnosis and Therapy, 2018, 22, 369-380.	1.6	2

#	Article	IF	Citations
1103	New selective cyclooxygenase-2 inhibitors from cyclocoumarol: Synthesis, characterization, biological evaluation and molecular modeling. European Journal of Medicinal Chemistry, 2018, 146, 577-587.	2.6	13
1104	Ab-initio and experimental study of pentose sugar dehydration mechanism in the gas phase. Carbohydrate Research, 2018, 458-459, 19-28.	1.1	11
1105	GCâ€“MS determination of phthalate esters in human urine: A potential biomarker for phthalate bio-monitoring. Journal of Chromatography B: Analytical Technologies in the Biomedical and Life Sciences, 2018, 1079, 15-24.	1.2	22
1106	ChemDistiller: an engine for metabolite annotation in mass spectrometry. Bioinformatics, 2018, 34, 2096-2102.	1.8	43
1107	Identification of cisapride as new inhibitor of putrescine uptake in Trypanosoma cruzi by combined ligand- and structure-based virtual screening. European Journal of Medicinal Chemistry, 2018, 149, 22-29.	2.6	15
1108	Computationally Assessing the Bioactivation of Drugs by N-Dealkylation. Chemical Research in Toxicology, 2018, 31, 68-80.	1.7	30
1109	Performance of combined fragmentation and retention prediction for the identification of organic micropollutants by LC-HRMS. Analytical and Bioanalytical Chemistry, 2018, 410, 1931-1941.	1.9	22
1110	3Dâ€eâ€Chem: Structural Cheminformatics Workflows for Computerâ€Aided Drug Discovery. ChemMedChem, 2018, 13, 614-626.	1.6	17
1111	Disruptor of telomeric silencing 1-like (DOT1L): disclosing a new class of non-nucleoside inhibitors by means of ligand-based and structure-based approaches. Journal of Computer-Aided Molecular Design, 2018, 32, 435-458.	1.3	15
1112	Analysis of the HIV-2 proteaseâ€™s adaptation to various ligands: characterization of backbone asymmetry using a structural alphabet. Scientific Reports, 2018, 8, 710.	1.6	8
1113	Multipole models of sulphur for accurate anisotropic electrostatic interactions within force fields. SAR and QSAR in Environmental Research, 2018, 29, 21-42.	1.0	5
1114	Guanosine monophosphate reductase 1 is a potential therapeutic target for Alzheimerâ€™s disease. Scientific Reports, 2018, 8, 2759.	1.6	24
1115	An integrated structure- and pharmacophore-based MMP-12 virtual screening. Molecular Diversity, 2018, 22, 383-395.	2.1	9
1116	Understanding the Influence of the Electrochemical Behavior of Potassium Hexacyanoferrate(II/III) on Acetonitrile/Water Binary Mixtures: An Experimental and Molecular Dynamics Study. Journal of Physical Chemistry C, 2018, 122, 2717-2725.	1.5	5
1117	Crystal structure of methylprednisolone acetate form II, C24H32O6. Powder Diffraction, 2018, 33, 44-48.	0.4	0
1118	The PEG-responding desiccome of the alder microsymbiont Frankia alni. Scientific Reports, 2018, 8, 759.	1.6	14
1119	In silico identification, synthesis and biological evaluation of novel tetrazole inhibitors of MurB. Chemical Biology and Drug Design, 2018, 91, 1101-1112.	1.5	10
1120	Discovery of novel bacterial topoisomerase I inhibitors by use of in silico docking and in vitro assays. Scientific Reports, 2018, 8, 1437.	1.6	21

#	Article	IF	Citations
1121	Congestion game scheduling for virtual drug screening optimization. Journal of Computer-Aided Molecular Design, 2018, 32, 363-374.	1.3	8
1122	C2x: A tool for visualisation and input preparation for Castep and other electronic structure codes. Computer Physics Communications, 2018, 225, 174-179.	3.0	45
1123	Locating Large, Flexible Ligands on Proteins. Journal of Chemical Information and Modeling, 2018, 58, 315-327.	2.5	6
1124	Introducing Membrane Transport Energy into the Design of Sustainable Chemicals against Cytotoxicity. ACS Sustainable Chemistry and Engineering, 2018, 6, 2055-2061.	3.2	2
1125	Structure-based virtual screening identifies a small-molecule inhibitor of the profilin 1â€“actin interaction. Journal of Biological Chemistry, 2018, 293, 2606-2616.	1.6	15
1126	Synthesis and anticancer activity of novel water soluble benzimidazole carbamates. European Journal of Medicinal Chemistry, 2018, 144, 372-385.	2.6	79
1127	Unimolecular Reaction Pathways of a Î³-Ketohydroperoxide from Combined Application of Automated Reaction Discovery Methods. Journal of the American Chemical Society, 2018, 140, 1035-1048.	6.6	82
1128	FilTer BaSe: A web accessible chemical database for small compound libraries. Journal of Molecular Graphics and Modelling, 2018, 80, 95-103.	1.3	6
1129	Oneâ€pot synthesis of anilides, herbicidal activity and molecular docking study. Pest Management Science, 2018, 74, 1637-1645.	1.7	9
1130	Binding free energy predictions of farnesoid X receptor (FXR) agonists using a linear interaction energy (LIE) approach with reliability estimation: application to the D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 239-249.	1.3	19
1131	Learning a Local-Variable Model of Aromatic and Conjugated Systems. ACS Central Science, 2018, 4, 52-62.	5.3	18
1132	A program for automatically predicting supramolecular aggregates and its application to urea and porphin. Journal of Computational Chemistry, 2018, 39, 763-772.	1.5	9
1133	Systematic analyses of drugs and disease indications in RepurposeDB reveal pharmacological, biological and epidemiological factors influencing drug repositioning. Briefings in Bioinformatics, 2018, 19, 656-678.	3.2	81
1134	DeepSynergy: predicting anti-cancer drug synergy with Deep Learning. Bioinformatics, 2018, 34, 1538-1546.	1.8	341
1135	PAMDB: a comprehensive Pseudomonas aeruginosa metabolome database. Nucleic Acids Research, 2018, 46, D575-D580.	6.5	45
1136	Novel 3-phenylcoumarinâ€“lipoic acid conjugates as multi-functional agents for potential treatment of Alzheimer's disease. Bioorganic Chemistry, 2018, 79, 223-234.	2.0	34
1137	A combined computational and experimental study on selective flucloxacillin hydroxylation by cytochrome P450 BM3 variants. Journal of Inorganic Biochemistry, 2018, 184, 115-122.	1.5	14
1138	Two inhibitors of yeast plasma membrane ATPase 1 (ScPma1p): toward the development of novel antifungal therapies. Journal of Cheminformatics, 2018, 10, 6.	2.8	17

#	Article	IF	Citations
1139	Crius: A novel fragmentâ€based algorithm of de novo substrate prediction for enzymes. Protein Science, 2018, 27, 1526-1534.	3.1	0
1140	Design, synthesis and evaluation of novel multi-target-directed ligands for treatment of Alzheimer's disease based on coumarin and lipoic acid scaffolds. European Journal of Medicinal Chemistry, 2018, 152, 600-614.	2.6	59
1141	In Silico Pharmacoepidemiologic Evaluation of Drug-Induced Cardiovascular Complications Using Combined Classifiers. Journal of Chemical Information and Modeling, 2018, 58, 943-956.	2.5	37
1142	Identification of novel therapeutic candidates inCryptosporidium parvum: anin silicoapproach. Parasitology, 2018, 145, 1907-1916.	0.7	4
1143	Understanding the mode of binding mechanism of doripenem to human serum albumin: Spectroscopic and molecular docking approaches. Journal of Molecular Recognition, 2018, 31, e2710.	1.1	7
1144	Practices in Molecular Docking and Structure-Based Virtual Screening. Methods in Molecular Biology, 2018, 1762, 31-50.	0.4	34
1145	Interface mechanics of carbon fibers with radially-grown carbon nanotubes. Carbon, 2018, 134, 123-133.	5.4	22
1146	Predicting ionic liquid melting points using machine learning. Journal of Molecular Liquids, 2018, 264, 318-326.	2.3	64
1147	Virtual Screening of Novel and Selective Inhibitors of Protein Tyrosine Phosphatase 1B over T-Cell Protein Tyrosine Phosphatase Using a Bidentate Inhibition Strategy. Journal of Chemical Information and Modeling, 2018, 58, 837-847.	2.5	17
1148	Novel 2-pheynlbenzofuran derivatives as selective butyrylcholinesterase inhibitors for Alzheimerâ€™s disease. Scientific Reports, 2018, 8, 4424.	1.6	71
1149	Active Site Flexibility as a Hallmark for Efficient PET Degradation by I.Âsakaiensis PETase. Biophysical Journal, 2018, 114, 1302-1312.	0.2	190
1150	Combining first-principles and data modeling for the accurate prediction of the refractive index of organic polymers. Journal of Chemical Physics, 2018, 148, 241712.	1.2	33
1151	Identification and Characterization of Novel Receptor-Interacting Serine/Threonineâ€Protein Kinase 2 Inhibitors Using Structural Similarity Analysis. Journal of Pharmacology and Experimental Therapeutics, 2018, 365, 354-367.	1.3	22
1152	Synergistic in-vitro effects of combining an antiglycolytic, 3-bromopyruvate, and a bromodomain-4 inhibitor on U937 myeloid leukemia cells. Anti-Cancer Drugs, 2018, 29, 429-439.	0.7	4
1153	Investigation of the binding mode of a novel cruzain inhibitor by docking, molecular dynamics, ab initio and MM/PBSA calculations. Journal of Computer-Aided Molecular Design, 2018, 32, 591-605.	1.3	18
1154	Quantitative Structureâ€“Activity Relationship Models for Predicting Risk of Drug-Induced Liver Injury in Humans. Methods in Pharmacology and Toxicology, 2018, , 77-100.	0.1	16
1155	Structural changes at the myrtenol backbone reverse its positive allosteric potential into inhibitory GABA_A receptor modulation. Biological Chemistry, 2018, 399, 549-563.	1.2	6
1156	Deciphering metabonomics biomarkers-targets interactions for psoriasis vulgaris by network pharmacology. Annals of Medicine, 2018, 50, 323-332.	1.5	10

#	Article	IF	Citations
1157	Non-covalent interactions across organic and biological subsets of chemical space: Physics-based potentials parametrized from machine learning. Journal of Chemical Physics, 2018, 148, 241706.	1.2	136
1158	Large-scale computational drug repositioning to find treatments for rare diseases. Npj Systems Biology and Applications, 2018, 4, 13.	1.4	40
1159	IMPPAT: A curated database of Indian Medicinal Plants, Phytochemistry And Therapeutics. Scientific Reports, 2018, 8, 4329.	1.6	306
1160	Association of CTH variant with sinusoidal obstruction syndrome in children receiving intravenous busulfan and cyclophosphamide before hematopoietic stem cell transplantation. Pharmacogenomics Journal, 2018, 18, 64-69.	0.9	13
1161	Inhibition of Gelatinases (MMP-2 and MMP-9) by Withania somnifera Phytochemicals Confers Neuroprotection in Stroke: An In Silico Analysis. Interdisciplinary Sciences, Computational Life Sciences, 2018, 10, 722-733.	2.2	23
1162	Exploring pyrazolo[3,4-d]pyrimidine phosphodiesterase 1 (PDE1) inhibitors: a predictive approach combining comparative validated multiple molecular modelling techniques. Journal of Biomolecular Structure and Dynamics, 2018, 36, 590-608.	2.0	52
1163	Development of human biotransformation QSARs and application for PBT assessment refinement. Food and Chemical Toxicology, 2018, 112, 535-543.	1.8	27
1164	Mapping the scientific research on open data: A bibliometric review. Learned Publishing, 2018, 31, 95-106.	0.8	26
1165	Drug repurposing: An approach to tackle drug resistance in S. typhimurium. Journal of Cellular Biochemistry, 2018, 119, 2818-2831.	1.2	3
1166	Prediction of binding poses to FXR using multi-targeted docking combined with molecular dynamics and enhanced sampling. Journal of Computer-Aided Molecular Design, 2018, 32, 59-73.	1.3	6
1167	Proteinâ€“protein interaction specificity is captured by contact preferences and interface composition. Bioinformatics, 2018, 34, 459-468.	1.8	29
1168	RandiÄ‡ index and information. AKCE International Journal of Graphs and Combinatorics, 2018, 15, 307-312.	0.4	59
1169	Râ€based Tool for a Pairwise Structureâ€activity Relationship Analysis. Molecular Informatics, 2018, 37, e1700094.	1.4	4
1170	Monte Carlo Method Based QSAR Studies of Mer Kinase Inhibitors in Compliance with OECD Principles. Drug Research, 2018, 68, 189-195.	0.7	37
1171	A systematic method to estimate and validate enthalpies of formation using error-cancelling balanced reactions. Combustion and Flame, 2018, 187, 105-121.	2.8	15
1172	A sobering assessment of smallâ€molecule force field methods for low energy conformer predictions. International Journal of Quantum Chemistry, 2018, 118, e25512.	1.0	43
1173	Glandular hair constituents of Mallotus philippinensis Muell. fruit act as tyrosinase inhibitors: Insights from enzyme kinetics and simulation study. International Journal of Biological Macromolecules, 2018, 107, 1675-1682.	3.6	17
1174	Ensemble docking to difficult targets in earlyâ€stage drug discovery: Methodology and application to fibroblast growth factor 23. Chemical Biology and Drug Design, 2018, 91, 491-504.	1.5	25

#	Article	IF	Citations
1175	Network pharmacology analysis of the anti-cancer pharmacological mechanisms of Ganoderma lucidum extract with experimental support using Hepa1-6-bearing C57 BL/6 mice. Journal of Ethnopharmacology, 2018, 210, 287-295.	2.0	67
1176	Understanding the molecular mechanism of improved proliferation and osteogenic potential of human mesenchymal stem cells grown on a polyelectrolyte complex derived from non-mulberry silk fibroin and chitosan. Biomedical Materials (Bristol), 2018, 13, 015011.	1.7	25
1177	Aromatic interactions at the ligandâ€“protein interface: Implications for the development of docking scoring functions. Chemical Biology and Drug Design, 2018, 91, 380-390.	1.5	72
1178	Optimal affinity ranking for automated virtual screening validated in prospective D3R grand challenges. Journal of Computer-Aided Molecular Design, 2018, 32, 287-297.	1.3	14
1179	Predicting the affinity of Farnesoid X Receptor ligands through a hierarchical ranking protocol: a D3R Grand Challenge 2 case study. Journal of Computer-Aided Molecular Design, 2018, 32, 231-238.	1.3	14
1180	Docking of small molecules to farnesoid X receptors using AutoDock Vina with the Convex-PL potential: lessons learned from D3R Grand Challenge 2. Journal of Computer-Aided Molecular Design, 2018, 32, 151-162.	1.3	15
1181	Extended Metabolic Space Modeling. Methods in Molecular Biology, 2018, 1671, 83-96.	0.4	1
1182	Molecular Modeling of Multidrug Properties of Resistance Nodulation Division (RND) Transporters. Methods in Molecular Biology, 2018, 1700, 179-219.	0.4	6
1183	PLHINT: A knowledge-driven computational approach based on the intermolecular H bond interactions at the protein-ligand interface from docking solutions. Journal of Molecular Graphics and Modelling, 2018, 79, 194-212.	1.3	9
1184	Methamidophos removal from aqueous solutions using a super adsorbent based on crosslinked poly(vinyl alcohol) hydrogel. Journal of Applied Polymer Science, 2018, 135, 45964.	1.3	23
1185	Efficient prediction of reaction paths through molecular graph and reaction network analysis. Chemical Science, 2018, 9, 825-835.	3.7	82
1186	Bonding of Butylparaben, Bis(2-ethylhexyl)-phthalate, and Perfluorooctanesulfonic Acid to DNA: Comparison with Benzo[a]pyrene Shows Low Probability for Strong Noncovalent DNA Intercalation. Chemical Research in Toxicology, 2018, 31, 22-36.	1.7	3
1187	Cinnamomum burmanini Blume increases bone turnover marker and induces tibia's granule formation in ovariectomized rats. Journal of Ayurveda and Integrative Medicine, 2018, 9, 20-26.	0.9	11
1188	Experimental and density functional theory studies on benzalkonium ibuprofenate, a double active pharmaceutical ingredient. Computational Biology and Chemistry, 2018, 72, 113-121.	1.1	21
1189	Discovery and structure-activity relationship of novel 4-hydroxy-thiazolidine-2-thione derivatives as tumor cell specific pyruvate kinase M2 activators. European Journal of Medicinal Chemistry, 2018, 143, 48-65.	2.6	15
1190	Automated Training of ReaxFF Reactive Force Fields for Energetics of Enzymatic Reactions. Journal of Chemical Theory and Computation, 2018, 14, 291-302.	2.3	28
1191	A retention index-based QSPR model for the quality control of rice. Journal of Cereal Science, 2018, 79, 303-310.	1.8	4
1192	Fast and accurate prediction of the regioselectivity of electrophilic aromatic substitution reactions. Chemical Science, 2018, 9, 660-665.	3.7	59

#	Article	IF	Citations
1193	Structureâ€based discovery of new selective smallâ€molecule sirtuin 5 inhibitors. Chemical Biology and Drug Design, 2018, 91, 257-268.	1.5	23
1194	Applicability of in silico tools for the prediction of dermal absorption for pesticides. EFSA Supporting Publications, 2018, 15, 1493E.	0.3	3
1195	Regression Models and Ranking Method for p53 Inhibitor Candidates Using Machine Learning. , 2018, , .		3
1196	CHEMICAL STRUCTURE OPTIMIZATION OF LUPEOL AS ER-Î' AND HER2 INHIBITOR. Asian Journal of Pharmaceutical and Clinical Research, 2018, 11, 298.	0.3	4
1197	Modeling of Structure-Property Relationships of Polymerizable Surfactants with Antimicrobial Activity. Applied Sciences (Switzerland), 2018, 8, 1972.	1.3	5
1198	GCDB: a glaucomatous chemogenomics database forin silicodrug discovery. Database: the Journal of Biological Databases and Curation, 2018, 2018, .	1.4	2
1199	A strategy to find novel candidate anti-Alzheimerâ€™s disease drugs by constructing interaction networks between drug targets and natural compounds in medical plants. PeerJ, 2018, 6, e4756.	0.9	8
1200	Environmental Concerns Regarding Ionic Liquids in Biotechnological Applications. Advances in Biochemical Engineering/Biotechnology, 2018, 168, 241-328.	0.6	3
1201	Molecular Docking for Active Compounds of Scurrula Atropurpurea as Anti-inflammatory Candidate in Endometriosis. Acta Informatica Medica, 2018, 26, 254.	0.5	19
1202	Systematic polypharmacology and drug repurposing via an integrated L1000-based Connectivity Map database mining. Royal Society Open Science, 2018, 5, 181321.	1.1	36
1203	Anti-flavi: A Web Platform to Predict Inhibitors of Flaviviruses Using QSAR and Peptidomimetic Approaches. Frontiers in Microbiology, 2018, 9, 3121.	1.5	19
1204	STRUCTURE-BASED DRUG DESIGNING STUDIES TOWARDS EXPLORING THE POTENTIAL ANTICANCER ACTIVITY OF SELECTED PHYTOCOMPOUNDS AGAINST HISTONE DEACETYLASE 10 PROTEIN. Asian Journal of Pharmaceutical and Clinical Research, 2018, 11, 262.	0.3	0
1205	Computational insights into the inhibition of Î²-haematin crystallization by antimalarial drugs. Dalton Transactions, 2018, 47, 15364-15381.	1.6	3
1206	A probabilistic molecular fingerprint for big data settings. Journal of Cheminformatics, 2018, 10, 66.	2.8	71
1207	Studies of 4-arylthiazolylhydrazones derived from 1-indanones as Trypanosoma cruzi squalene epoxidase inhibitors by molecular simulations. Organic and Biomolecular Chemistry, 2018, 16, 8525-8536.	1.5	2
1208	Simulation of Peptide Docking with Terminal Post-Translational Modifications. , 2018, , .		0
1209	Pranlukast; An Alternative Potential Leptin Stimulator: Structure-Based Virtual Screening Study. Immunochemistry & Immunopathology, 2018, 04, .	0.4	0
1210	INHIBITION OF Î±-AMYLASE AND Î±-GLUCOSIDASE BY (6RS)-22-HYDROXY-23,24,25,26,27-PENTANOR-VITAMIN-D3-6,19-SULFUR DIOXIDE-ADDUCT, MANOALIDE AND 5Î²-CHOLESTANE-3Î±,7Î±,12Î±,24,25,26-HEXOL ISOLATED FROM ACETONE EXTRACT OF HELIANTHUS ANNUUS L. SEEDS. International Journal of Pharmacy and Pharmaceutical Sciences, 2018, 10, 39.	0.3	5

#	Article	IF	Citations
1211	In silico assessment of new progesterone receptor inhibitors using molecular dynamics: a new insight into breast cancer treatment. Journal of Molecular Modeling, 2018, 24, 337.	0.8	20
1212	Exploring the Reactivity of Hydrofluoropolyethers toward OH through a Cost-Effective Protocol for Calculating Multiconformer Transition State Theory Rate Constants. Journal of Physical Chemistry A, 2018, 122, 9721-9732.	1.1	17
1213	Open-source sensor for measuring oxygen partial pressures below 100 microbars. PLoS ONE, 2018, 13, e0206678.	1.1	6
1214	Improved understanding of aqueous solubility modeling through topological data analysis. Journal of Cheminformatics, 2018, 10, 54.	2.8	14
1215	An integrated approach towards the development of novel antifungal agents containing thiadiazole: synthesis and a combined similarity search, homology modelling, molecular dynamics and molecular docking study. Chemistry Central Journal, 2018, 12, 121.	2.6	18
1216	A Robust and Costâ€Efficient Scheme for Accurate Conformational Energies of Organic Molecules. ChemPhysChem, 2019, 20, 92-102.	1.0	27
1217	Characterization of Keto and Enol Forms of Indoline-2,3-dione-3-oxime using Avogadro software Tool (A Theoretical Study). Oriental Journal of Chemistry, 2018, 34, 1270-1277.	0.1	3
1218	Target-specific toxicity knowledgebase (TsTKb): a novel toolkit for in silico predictive toxicology. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2018, 36, 219-236.	2.9	6
1219	ANTIBACTERIAL ACTIVITY OF AKAR KUNING (ARCANGELISIA FLAVA) SECONDARY METABOLITES: MOLECULAR DOCKING APPROACH. Asian Journal of Pharmaceutical and Clinical Research, 2018, 11, 447.	0.3	8
1220	Integrating Strategies of Herbal Metabolomics, Network Pharmacology, and Experiment Validation to Investigate Frankincense Processing Effects. Frontiers in Pharmacology, 2018, 9, 1482.	1.6	23
1221	A review on machine learning methods forin silicotoxicity prediction. Journal of Environmental Science and Health, Part C: Environmental Carcinogenesis and Ecotoxicology Reviews, 2018, 36, 169-191.	2.9	91
1222	Prediction of Drug-Likeness Using Deep Autoencoder Neural Networks. Frontiers in Genetics, 2018, 9, 585.	1.1	43
1223	Molecular Recipe for Î³-Secretase Modulation from Computational Analysis of 60 Active Compounds. ACS Omega, 2018, 3, 18078-18088.	1.6	19
1224	Visualization and Simulation of Carbon Structures with Higher Genus. , 2018, , .		0
1225	Evaluating apoenzymeâ€“coenzymeâ€“substrate interactions of methane monooxygenase with an engineered active site for electron harvesting: a computational study. Journal of Molecular Modeling, 2018, 24, 347.	0.8	2
1226	Dibutyltin(IV) Complexes Derived from L-DOPA: Synthesis, Molecular Docking, Cytotoxic and Antifungal Activity. Chemical and Pharmaceutical Bulletin, 2018, 66, 1104-1113.	0.6	10
1227	Structural properties of a haemophore facilitate targeted elimination of the pathogen Porphyromonas gingivalis. Nature Communications, 2018, 9, 4097.	5.8	31
1228	Prediction of Antimicrobial Potential of a Chemically Modified Peptide From Its Tertiary Structure. Frontiers in Microbiology, 2018, 9, 2551.	1.5	38

#	Article	IF	Citations
1229	Steroids-specific target library for steroids target prediction. Steroids, 2018, 140, 83-91.	0.8	4
1230	Strategies and Software for Machine Learning Accelerated Discovery in Transition Metal Chemistry. Industrial & Engineering Chemistry Research, 2018, 57, 13973-13986.	1.8	104
1231	Antifungal activity of Cardiospermum halicacabum L. (Sapindaceae) against Trichophyton rubrum occurs through molecular interaction with fungal Hsp90. Drug Design, Development and Therapy, 2018, Volume 12, 2185-2193.	2.0	27
1232	ADMETopt: A Web Server for ADMET Optimization in Drug Design via Scaffold Hopping. Journal of Chemical Information and Modeling, 2018, 58, 2051-2056.	2.5	60
1233	Predicting Fraction Unbound in Human Plasma from Chemical Structure: Improved Accuracy in the Low Value Ranges. Molecular Pharmaceutics, 2018, 15, 5302-5311.	2.3	95
1234	Identification of (4-(9H-fluoren-9-yl) piperazin-1-yl) methanone derivatives as falcipain 2 inhibitors active against Plasmodium falciparum cultures. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 2911-2923.	1.1	6
1235	Activity of oxygen-versus sulfur-containing analogs of the Flex-Het anticancer agent SHetA2. European Journal of Medicinal Chemistry, 2018, 158, 720-732.	2.6	12
1236	Polarizable Drude Model with s-Type Gaussian or Slater Charge Density for General Molecular Mechanics Force Fields. Journal of Chemical Theory and Computation, 2018, 14, 5553-5566.	2.3	27
1237	New phosphorus ylide palladacyclic: Synthesis, characterization, X-Ray crystal structure, biomolecular interaction studies, molecular docking and inÂvitro cytotoxicity evaluations. Journal of Organometallic Chemistry, 2018, 878, 60-76.	0.8	12
1238	The ReFRAME library as a comprehensive drug repurposing library and its application to the treatment of cryptosporidiosis. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10750-10755.	3.3	165
1239	The Rational Discovery of a Tau Aggregation Inhibitor. Biochemistry, 2018, 57, 6099-6107.	1.2	22
1240	Formation of hierarchically-ordered nanoporous silver foam and its electrocatalytic properties in reductive dehalogenation of organic compounds. New Journal of Chemistry, 2018, 42, 17499-17512.	1.4	6
1241	Low dose dimethyl sulfoxide driven gross molecular changes have the potential to interfere with various cellular processes. Scientific Reports, 2018, 8, 14828.	1.6	72
1242	Escaping Atom Types in Force Fields Using Direct Chemical Perception. Journal of Chemical Theory and Computation, 2018, 14, 6076-6092.	2.3	110
1243	Network-Based Methods for Prediction of Drug-Target Interactions. Frontiers in Pharmacology, 2018, 9, 1134.	1.6	131
1244	Targeting DNA Binding for NF-ÎºB as an Anticancer Approach in Hepatocellular Carcinoma. Cells, 2018, 7, 177.	1.8	11
1245	Triazole-linked transition state analogs as selective inhibitors against V. cholerae sialidase. Bioorganic and Medicinal Chemistry, 2018, 26, 5751-5757.	1.4	14
1246	DNA Targeting Long-Chain Alkoxy Appended Tin(IV) Porphyrin Scaffolds: Photophysical and Antimicrobial PDT Investigations. ACS Applied Bio Materials, 2018, 1, 1705-1716.	2.3	37

#	Article	IF	Citations
1247	Could the presence of sodium ion influence the accuracy and precision of the ligand-posing in the human A2A adenosine receptor orthosteric binding site using a molecular docking approach? Insights from Dockbench. Journal of Computer-Aided Molecular Design, 2018, 32, 1337-1346.	1.3	9
1248	Synthesis, Molecular Docking and in Vitro Screening of Some Newly Synthesized Triazolopyridine, Pyridotriazine and Pyridineâ€“Pyrazole Hybrid Derivatives. Molecules, 2018, 23, 2548.	1.7	27
1249	An automated framework for NMR chemical shift calculations of small organic molecules. Journal of Cheminformatics, 2018, 10, 52.	2.8	37
1250	Use of quantum-chemical descriptors to analyse reaction rate constants between organic chemicals and superoxide/hydroperoxyl (O₂^{â€¢â”}/HO₂^{â€¢}). Free Radical Research, 2018, 52, 1118-1131.	1.5	19
1251	Comprehensive assessment of nine docking programs on type II kinase inhibitors: prediction accuracy of sampling power, scoring power and screening power. Briefings in Bioinformatics, 2018, , .	3.2	16
1252	Glaulactams Aâ€“C, daphniphyllum alkaloids from Daphniphyllum glaucescens. Scientific Reports, 2018, 8, 15417.	1.6	6
1253	Noncovalent Inhibitors of Mosquito Acetylcholinesterase 1 with Resistance-Breaking Potency. Journal of Medicinal Chemistry, 2018, 61, 10545-10557.	2.9	14
1254	MBâ€Ìsoster: A software for bioisosterism simulation. Journal of Computational Chemistry, 2018, 39, 2481-2487.	1.5	7
1255	Impact of Molecular Descriptors on Computational Models. Methods in Molecular Biology, 2018, 1825, 171-209.	0.4	34
1256	Analysis of Isocratic-Chromatographic-Retention Data using Bayesian Multilevel Modeling. Analytical Chemistry, 2018, 90, 13670-13679.	3.2	6
1257	Online structure-based screening of purchasable approved drugs and natural compounds: retrospective examples of drug repositioning on cancer targets. Oncotarget, 2018, 9, 32346-32361.	0.8	25
1258	Receptor pharmacophore ensemble (REPHARMBLE): a probabilistic pharmacophore modeling approach using multiple protein-ligand complexes. Journal of Molecular Modeling, 2018, 24, 282.	0.8	11
1259	Structural, Mechanistic, and Ultradilute Catalysis Portrayal of Substrate Inhibition in the TAMLâ€“Hydrogen Peroxide Catalytic Oxidation of the Persistent Drug and Micropollutant, Propranolol. Journal of the American Chemical Society, 2018, 140, 12280-12289.	6.6	21
1260	Molecular Docking Analysis of Pyrimethamine Derivatives with Plasmodium falciparum Dihydrofolate Reductase. Bioinformation, 2018, 14, 232-235.	0.2	13
1261	In Silico Identification of JMJD3 Demethylase Inhibitors. Journal of Chemical Information and Modeling, 2018, 58, 2151-2163.	2.5	10
1262	Combining (Non)linear Optical and Fluorescence Analysis of DiD To Enhance Lipid Phase Recognition. Journal of Chemical Theory and Computation, 2018, 14, 5350-5359.	2.3	11
1263	Predicting Thermodynamic Properties of Alkanes by High-Throughput Force Field Simulation and Machine Learning. Journal of Chemical Information and Modeling, 2018, 58, 2502-2516.	2.5	23
1264	Structure-Based Discovery and Synthesis of Potential Transketolase Inhibitors. Molecules, 2018, 23, 2116.	1.7	18

#	Article	IF	Citations
1265	Tinker 8: Software Tools for Molecular Design. Journal of Chemical Theory and Computation, 2018, 14, 5273-5289.	2.3	403
1266	Enzyme Discovery: Enzyme Selection and Pathway Design. Methods in Enzymology, 2018, 608, 3-27.	0.4	2
1267	Machine Learning based Prediction of Anatomical Therapeutic Chemical (ATC) Class of Drug Like Molecule. , 2018, , .		2
1268	Prediction of binding potential of natural leads against the prioritized drug targets of chikungunya and dengue viruses by computational screening. 3 Biotech, 2018, 8, 274.	1.1	12
1269	Perturbation Theory/Machine Learning Model of ChEMBL Data for Dopamine Targets: Docking, Synthesis, and Assay of New <scp>l</scp>-Prolyl-<scp>l</scp>-leucyl-glycinamide Peptidomimetics. ACS Chemical Neuroscience, 2018, 9, 2572-2587.	1.7	38
1270	Building and deploying a cyberinfrastructure for the data-driven design of chemical systems and the exploration of chemical space. Molecular Simulation, 2018, 44, 921-929.	0.9	28
1271	Identification of small molecule compounds targeting the interaction of HIV-1 Vif and human APOBEC3G by virtual screening and biological evaluation. Scientific Reports, 2018, 8, 8067.	1.6	22
1272	Neural network for prediction of ¹³C NMR chemical shifts of fullerene C₆₀ monoâ€adducts. Journal of Chemometrics, 2018, 32, e3037.	0.7	2
1273	Computational discovery of potent drugs to improve the treatment of pyrazinamide resistant Mycobacterium tuberculosis mutants. Journal of Cellular Biochemistry, 2018, 119, 7328-7338.	1.2	3
1274	Prediction of Human Cytochrome P450 Inhibition Using a Multitask Deep Autoencoder Neural Network. Molecular Pharmaceutics, 2018, 15, 4336-4345.	2.3	85
1275	In silico prediction and experimental verification of ionic liquid refractive indices. Journal of Molecular Liquids, 2018, 264, 563-570.	2.3	17
1276	Identification of novel phosphatidic acid binding domain on sphingosine kinase 1 of Arabidopsis thaliana. Plant Physiology and Biochemistry, 2018, 128, 178-184.	2.8	23
1277	Putative vaccine candidates and drug targets identified by reverse vaccinology and subtractive genomics approaches to control Haemophilus ducreyi , the causative agent of chancroid. Journal of the Royal Society Interface, 2018, 15, 20180032.	1.5	11
1278	Synthesis, docking study, and biological evaluation of novel umbellipherone/hymecromone derivatives as acetylcholinesterase/butyrylcholinesterase inhibitors. Medicinal Chemistry Research, 2018, 27, 1741-1747.	1.1	16
1279	Synthesis and evaluation of a series of caffeic acid derivatives as anticancer agents. Future Journal of Pharmaceutical Sciences, 2018, 4, 124-130.	1.1	10
1280	Temperature Transferability of Force Field Parameters for Dispersion Interactions. Journal of Chemical Theory and Computation, 2018, 14, 3595-3602.	2.3	14
1281	Double Precision Is Not Needed for Many-Body Calculations: Emergent Conventional Wisdom. Journal of Chemical Theory and Computation, 2018, 14, 4088-4096.	2.3	38
1282	Synthesis, Anti-Inflammatory Activity, and In Silico Study of Novel Diclofenac and Isatin Conjugates. International Journal of Medicinal Chemistry, 2018, 2018, 1-11.	2.2	10

#	Article	IF	Citations
1283	Kinetic, spectroscopic and computational docking study of the inhibitory effect of the pesticides 2,4,5-T, 2,4-D and glyphosate on the diphenolase activity of mushroom tyrosinase. International Journal of Biological Macromolecules, 2018, 118, 427-434.	3.6	17
1284	Development of a High-Throughput, In Vivo Selection Platform for NADPH-Dependent Reactions Based on Redox Balance Principles. ACS Synthetic Biology, 2018, 7, 1715-1721.	1.9	33
1285	Antiplasmodial activity of hydroxyethylamine analogs: Synthesis, biological activity and structure activity relationship of plasmepsin inhibitors. Bioorganic and Medicinal Chemistry, 2018, 26, 3837-3844.	1.4	17
1286	Virtual Screening of Hole Transport, Electron Transport, and Host Layers for Effective OLED Design. Journal of Chemical Information and Modeling, 2018, 58, 2440-2449.	2.5	22
1287	Chemoinformatic Approach to Assess Toxicity of Ionic Liquids. Methods in Molecular Biology, 2018, 1800, 559-571.	0.4	4
1288	Designing Algorithms To Aid Discovery by Chemical Robots. ACS Central Science, 2018, 4, 793-804.	5.3	64
1289	Evaluation of the reactive molecular dynamics method for Research on flame retardants: ATH-filled polyethylene. Computational Materials Science, 2018, 153, 103-112.	1.4	24
1290	Fully Automated Molecular Design with Atomic Resolution for Desired Thermophysical Properties. Industrial & Engineering Chemistry Research, 2018, 57, 9683-9692.	1.8	5
1291	Molecular Descriptors for Structureâ€“Activity Applications: A Hands-On Approach. Methods in Molecular Biology, 2018, 1800, 3-53.	0.4	28
1292	SIMPLE: Sparse Interaction Model over Peaks of moLEcules for fast, interpretable metabolite identification from tandem mass spectra. Bioinformatics, 2018, 34, i323-i332.	1.8	26
1293	Computational prediction of cellulose solubilities in ionic liquids based on COSMO-RS. Fluid Phase Equilibria, 2018, 475, 25-36.	1.4	27
1294	Molecular design, synthesis and biological evaluation of cage compound-based inhibitors of hepatitis C virus p7 ion channels. European Journal of Medicinal Chemistry, 2018, 158, 214-235.	2.6	32
1295	Modeling Chronic Toxicity: A Comparison of Experimental Variability With (Q)SAR/Read-Across Predictions. Frontiers in Pharmacology, 2018, 9, 413.	1.6	12
1296	A Computational Systems Pharmacology Approach to Investigate Molecular Mechanisms of Herbal Formula Tian-Ma-Gou-Teng-Yin for Treatment of Alzheimerâ€™s Disease. Frontiers in Pharmacology, 2018, 9, 668.	1.6	43
1297	Fatty-acylation target sequence in the ligand-binding domain of vertebrate steroid receptors demarcates evolution from estrogen-related receptors. Journal of Steroid Biochemistry and Molecular Biology, 2018, 184, 20-28.	1.2	3
1298	Development and Validation of Molecular Overlays Derived from Three-Dimensional Hydrophobic Similarity with PharmScreen. Journal of Chemical Information and Modeling, 2018, 58, 1596-1609.	2.5	14
1299	An Immunopharmacoinformatics Approach in Development of Vaccine and Drug Candidates for West Nile Virus. Frontiers in Chemistry, 2018, 6, 246.	1.8	16
1300	Use of Simplified Molecular Input Line Entry System and molecular graph based descriptors in prediction and design of pancreatic lipase inhibitors. Future Medicinal Chemistry, 2018, 10, 1603-1622.	1.1	25

#	Article	IF	Citations
1301	Protein-Ligand Docking in Drug Design: Performance Assessment and Binding-Pose Selection. Methods in Molecular Biology, 2018, 1824, 67-88.	0.4	14
1302	Identification of Natural Compounds against Neurodegenerative Diseases Using In Silico Techniques. Molecules, 2018, 23, 1847.	1.7	14
1303	From in silico to in vitro: a trip to reveal flavonoid binding on the Rattus norvegicus Kir6.1 ATP-sensitive inward rectifier potassium channel. PeerJ, 2018, 6, e4680.	0.9	14
1304	Prediction of Cell-Penetrating Potential of Modified Peptides Containing Natural and Chemically Modified Residues. Frontiers in Microbiology, 2018, 9, 725.	1.5	58
1305	VSpipe, an Integrated Resource for Virtual Screening and Hit Selection: Applications to Protein Tyrosine Phospahatase Inhibition. Molecules, 2018, 23, 353.	1.7	11
1306	Virtual Screening of Small Molecular Inhibitors against DprE1. Molecules, 2018, 23, 524.	1.7	18
1307	Synthesis, Molecular Docking, and Antimycotic Evaluation of Some 3-Acyl Imidazo[1,2-a]pyrimidines. Molecules, 2018, 23, 599.	1.7	22
1308	Identfication of Potent LXRÎ²-Selective Agonists without LXRÎ± Activation by In Silico Approaches. Molecules, 2018, 23, 1349.	1.7	3
1309	In Silico Screening of Isocitrate Lyase for Novel Anti-Buruli Ulcer Natural Products Originating from Africa. Molecules, 2018, 23, 1550.	1.7	29
1310	In-Silico Design, Synthesis and Evaluation of a Nanostructured Hydrogel as a Dimethoate Removal Agent. Nanomaterials, 2018, 8, 23.	1.9	12
1311	Changing Trends in Computational Drug Repositioning. Pharmaceuticals, 2018, 11, 57.	1.7	127
1312	Rational Design, Synthesis and Evaluation of Î³-CD-Containing Cross-Linked Polyvinyl Alcohol Hydrogel as a Prednisone Delivery Platform. Pharmaceutics, 2018, 10, 30.	2.0	19
1313	Designing High-Refractive Index Polymers Using Materials Informatics. Polymers, 2018, 10, 103.	2.0	31
1314	4,5-Dimethoxy-2-nitrobenzohydrazides and 1-(1-Benzylpiperidin-4-yl)ethan-1-ones as Potential Antioxidant/Cholinergic Endowed Small Molecule Leads. Scientia Pharmaceutica, 2018, 86, 2.	0.7	3
1315	Synthesis, Anti-Proliferative Activity Evaluation and 3D-QSAR Study of Naphthoquinone Derivatives as Potential Anti-Colorectal Cancer Agents. Molecules, 2018, 23, 186.	1.7	10
1316	The cardenolides strophanthidin, digoxigenin and dihydroouabain act as activators of the human RORÎ³/RORÎ³T receptors. Toxicology Letters, 2018, 295, 314-324.	0.4	24
1317	Evaluation of AutoDock and AutoDock Vina on the CASF-2013 Benchmark. Journal of Chemical Information and Modeling, 2018, 58, 1697-1706.	2.5	238
1318	Machine learning meets volcano plots: computational discovery of cross-coupling catalysts. Chemical Science, 2018, 9, 7069-7077.	3.7	154

#	Article	IF	Citations
1319	OChemDb: the free online Open Chemistry Database portal for searching and analysing crystal structure information. Journal of Applied Crystallography, 2018, 51, 1229-1236.	1.9	10
1320	3,20-Dihydroxy-13Î±-19-norpregna-1,3,5(10)-trienes. Synthesis, structures, and cytotoxic, estrogenic, and antiestrogenic effects. Steroids, 2018, 137, 1-13.	0.8	5
1321	Molecular docking studies of human MCT8 protein with soy isoflavones in Allan-Herndon-Dudley syndrome (AHDS). Journal of Pharmaceutical Analysis, 2018, 8, 318-323.	2.4	10
1322	In Silico Prediction of Chemical Toxicity for Drug Design Using Machine Learning Methods and Structural Alerts. Frontiers in Chemistry, 2018, 6, 30.	1.8	152
1323	e-Bitter: Bitterant Prediction by the Consensus Voting From the Machine-Learning Methods. Frontiers in Chemistry, 2018, 6, 82.	1.8	43
1324	The Mu.Ta.Lig. Chemotheca: A Community-Populated Molecular Database for Multi-Target Ligands Identification and Compound-Repurposing. Frontiers in Chemistry, 2018, 6, 130.	1.8	13
1325	Comparative assessment of strategies to identify similar ligand-binding pockets in proteins. BMC Bioinformatics, 2018, 19, 91.	1.2	40
1326	Targeting matrix metalloproteinases with novel diazepine substituted cinnamic acid derivatives: design, synthesis, in vitro and in silico studies. Chemistry Central Journal, 2018, 12, 41.	2.6	13
1327	Spectrophores as one-dimensional descriptors calculated from three-dimensional atomic properties: applications ranging from scaffold hopping to multi-target virtual screening. Journal of Cheminformatics, 2018, 10, 9.	2.8	13
1328	Determining the Relative Binding Affinity of Ricin Toxin A Inhibitors by Using Molecular Docking and Nonequilibrium Work. Journal of Chemical Information and Modeling, 2018, 58, 1205-1213.	2.5	10
1329	Development and evaluation of a deep learning model for proteinâ€“ligand binding affinity prediction. Bioinformatics, 2018, 34, 3666-3674.	1.8	368
1330	HIVprotI: an integrated web based platform for prediction and design of HIV proteins inhibitors. Journal of Cheminformatics, 2018, 10, 12.	2.8	25
1331	Mordred: a molecular descriptor calculator. Journal of Cheminformatics, 2018, 10, 4.	2.8	622
1332	An Integrated Study on the Antitumor Effect and Mechanism of Triphala Against Gynecological Cancers Based on Network Pharmacological Prediction and In Vitro Experimental Validation. Integrative Cancer Therapies, 2018, 17, 894-901.	0.8	18
1333	Prediction and Optimization of Pharmacokinetic and Toxicity Properties of the Ligand. Methods in Molecular Biology, 2018, 1762, 271-284.	0.4	42
1334	An EPR Investigation of Binding Environments by N-Donor Chelating Exchange Resins for Cu Extraction from Aqueous Media. Inorganic Chemistry, 2018, 57, 10857-10866.	1.9	8
1335	Computerâ€aided identification of a novel pyruvate kinase M2 activator compound. Cell Proliferation, 2018, 51, e12509.	2.4	12
1336	Sachem: a chemical cartridge for high-performance substructure search. Journal of Cheminformatics, 2018, 10, 27.	2.8	18

#	Article	IF	Citations
1337	Using SMILES strings for the description of chemical connectivity in the Crystallography Open Database. Journal of Cheminformatics, 2018, 10, 23.	2.8	126
1338	ChemFrag: Chemically meaningful annotation of fragment ion mass spectra. Journal of Mass Spectrometry, 2018, 53, 1104-1115.	0.7	14
1339	In silico and in vivo characterization of cabralealactone, solasodin and salvadorin in a rat model: potential anti-inflammatory agents. Drug Design, Development and Therapy, 2018, Volume 12, 1431-1443.	2.0	11
1340	In Silico Prediction of Bloodâ€“Brain Barrier Permeability of Compounds by Machine Learning and Resampling Methods. ChemMedChem, 2018, 13, 2189-2201.	1.6	111
1341	Investigation of the anti-TB potential of selected propolis constituents using a molecular docking approach. Scientific Reports, 2018, 8, 12238.	1.6	22
1342	Small moleculeâ€“based targeting of TTD-A dimerization to control TFIIH transcriptional activity represents a potential strategy for anticancer therapy. Journal of Biological Chemistry, 2018, 293, 14974-14988.	1.6	12
1343	Theoretical investigation of cyromazine tautomerism using density functional theory and MÃ¸llerâ€“Plesset perturbation theory methods. Molecular Simulation, 2018, 44, 1344-1352.	0.9	0
1344	Absolute and relative pKa predictions via a DFT approach applied to the SAMPL6 blind challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1179-1189.	1.3	25
1345	Analysis of the Frequency and Diversity of 1,3-Dialkylimidazolium Ionic Liquids Appearing in the Literature. Industrial & Engineering Chemistry Research, 2018, 57, 15971-15981.	1.8	24
1346	Monte Carlo based modelling approach for designing and predicting cytotoxicity of 2-phenylindole derivatives against breast cancer cell line MCF7. Toxicology in Vitro, 2018, 52, 23-32.	1.1	21
1347	Toward a unified scoring function for native state discrimination and drug-binding pocket recognition. Physical Chemistry Chemical Physics, 2018, 20, 17148-17155.	1.3	5
1348	Identification of potential drug targets and inhibitor of the pathogenic bacteria Shigella flexneri 2a through the subtractive genomic approach. In Silico Pharmacology, 2018, 6, 11.	1.8	7
1349	Searching for New Leads To Treat Epilepsy: Target-Based Virtual Screening for the Discovery of Anticonvulsant Agents. Journal of Chemical Information and Modeling, 2018, 58, 1331-1342.	2.5	11
1350	In silico identification of AChE and PARP-1 dual-targeted inhibitors of Alzheimerâ€™s disease. Journal of Molecular Modeling, 2018, 24, 151.	0.8	13
1351	Myeloid Cell Leukemia 1 Inhibition: An in Silico Study Using Non-equilibrium Fast Double Annihilation Technology. Journal of Chemical Theory and Computation, 2018, 14, 3890-3902.	2.3	13
1352	Automated Chemical Kinetic Modeling via Hybrid Reactive Molecular Dynamics and Quantum Chemistry Simulations. Journal of Chemical Information and Modeling, 2018, 58, 1343-1355.	2.5	25
1353	Applying machine learning techniques to predict the properties of energetic materials. Scientific Reports, 2018, 8, 9059.	1.6	166
1354	Identification of allosteric inhibitors of the ecto-5'-nucleotidase (CD73) targeting the dimer interface. PLoS Computational Biology, 2018, 14, e1005943.	1.5	25

#	Article	IF	Citations
1355	Role of Trace Elements as Cofactor: An Efficient Strategy toward Enhanced Biobutanol Production. ACS Sustainable Chemistry and Engineering, 2018, 6, 9304-9313.	3.2	31
1356	Synthesis, docking and anticancer activity of azo-linked hybrids of 1,3,4-thia-/oxadiazoles with cyclic imides. Molecular Diversity, 2018, 22, 827-840.	2.1	10
1357	Machine learning-based screening of complex molecules for polymer solar cells. Journal of Chemical Physics, 2018, 148, 241735.	1.2	94
1358	DPubChem: a web tool for QSAR modeling and high-throughput virtual screening. Scientific Reports, 2018, 8, 9110.	1.6	40
1359	Genome scale metabolic models as tools for drug design and personalized medicine. PLoS ONE, 2018, 13, e0190636.	1.1	35
1360	Identification of Nontoxic Substructures: A New Strategy to Avoid Potential Toxicity Risk. Toxicological Sciences, 2018, 165, 396-407.	1.4	16
1361	Addressing the Challenges of Structure Elucidation in Natural Products Possessing the Oxirane Moiety. Journal of Organic Chemistry, 2018, 83, 8341-8352.	1.7	37
1362	Design and Amberlyst-15 mediated synthesis of novel thienyl-pyrazole carboxamides that potently inhibit Phospholipase A2 by binding to an allosteric site on the enzyme. Bioorganic Chemistry, 2018, 80, 444-452.	2.0	14
1363	Structure investigation, enrichment analysis and structure-based repurposing of FDA-approved drugs as inhibitors of BET-BRD4. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3048-3057.	2.0	13
1364	Mono(2â€ethylhexyl) phthalate (MEHP) and mono(2â€ethylâ€5â€oxohexyl) phthalate (MEOHP) but not di(2â€ethylhexyl) phthalate (DEHP) bind productively to the peroxisome proliferatorâ€activated receptor Î³. Rapid Communications in Mass Spectrometry, 2019, 33, 75-85.	0.7	26
1365	Recent applications of deep learning and machine intelligence on in silico drug discovery: methods, tools and databases. Briefings in Bioinformatics, 2019, 20, 1878-1912.	3.2	310
1366	QSAR Models for Nitrogen Containing Monophosphonate and Bisphosphonate Derivatives as Human Farnesyl Pyrophosphate Synthase Inhibitors Based on Monte Carlo Method. Drug Research, 2019, 69, 159-167.	0.7	43
1367	Rational Structure-Based Drug Design. , 2019, , 585-600.		3
1368	Capturing aromaticity in automatic mechanism generation software. Proceedings of the Combustion Institute, 2019, 37, 575-581.	2.4	9
1369	Evaluation of pyrrole-2,3-dicarboxylate derivatives: Synthesis, DFT analysis, molecular docking, virtual screening and inÂvitro anti-hepatic cancer study. Journal of Molecular Structure, 2019, 1176, 314-334.	1.8	24
1370	In silicodiscovery of potential drug molecules to improve the treatment of isoniazid-resistantMycobacterium tuberculosis. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3388-3398.	2.0	14
1371	Mathematical deep learning for pose and binding affinity prediction and ranking in D3R Grand Challenges. Journal of Computer-Aided Molecular Design, 2019, 33, 71-82.	1.3	106
1372	Identification of molecular features necessary for selective inhibition of B cell lymphoma proteins using machine learning techniques. Molecular Diversity, 2019, 23, 55-73.	2.1	5

#	Article	IF	Citations
1373	Convolutional neural network scoring and minimization in the D3R 2017 community challenge. Journal of Computer-Aided Molecular Design, 2019, 33, 19-34.	1.3	37
1374	Improving ensemble docking for drug discovery by machine learning. Journal of Theoretical and Computational Chemistry, 2019, 18, 1920001.	1.8	7
1375	Rapid, comprehensive screening of ionic liquids towards sustainable applications. Sustainable Energy and Fuels, 2019, 3, 2798-2808.	2.5	35
1376	Computational study of antioxidant activity and bioavailability of papua red fruit (Pandanus) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf Proceedings, 2019, , .	0.3	5
1377	Deep Learning-Based Structure-Activity Relationship Modeling for Multi-Category Toxicity Classification: A Case Study of 10K Tox21 Chemicals With High-Throughput Cell-Based Androgen Receptor Bioassay Data. Frontiers in Physiology, 2019, 10, 1044.	1.3	52
1378	Homology Modelling and Molecular Docking Studies of Selected Substituted Lyase Receptor. Bioinformatics and Biology Insights, 2019, 13, 117793221986553.	1.0	35
1379	Development of 3,5-Dinitrophenyl-Containing 1,2,4-Triazoles and Their Trifluoromethyl Analogues as Highly Efficient Antitubercular Agents Inhibiting Decaprenylphosphoryl-Î²-<scp>d</scp>-ribofuranose 2â€²-Oxidase. Journal of Medicinal Chemistry, 2019, 62, 8115-8139.	2.9	37
1380	New Data Structure for Computational Molecular Design with Atomic or Fragment Resolution. Journal of Chemical Information and Modeling, 2019, 59, 3703-3713.	2.5	2
1381	Fast, efficient fragment-based coordinate generation for Open Babel. Journal of Cheminformatics, 2019, 11, 49.	2.8	43
1382	Elucidation of the role of in silico methodologies in approaches to studying bioactive peptides derived from foods. Journal of Functional Foods, 2019, 61, 103486.	1.6	52
1383	Reverse vaccinology and subtractive genomics reveal new therapeutic targets against Mycoplasma pneumoniae : a causative agent of pneumonia. Royal Society Open Science, 2019, 6, 190907.	1.1	42
1384	Exploring Novel N-Myristoyltransferase Inhibitors: A Molecular Dynamics Simulation Approach. ACS Omega, 2019, 4, 13658-13670.	1.6	11
1385	Synthesis of novel benzopyran-connected pyrimidine and pyrazole derivatives via a green method using Cu(<scp>ii</scp>)-tyrosinase enzyme catalyst as potential larvicidal, antifeedant activities. RSC Advances, 2019, 9, 25533-25543.	1.7	13
1386	Exploring Chemical and Biological Space of Terpenoids. Journal of Chemical Information and Modeling, 2019, 59, 3667-3678.	2.5	19
1387	A cell-based screening system for RNA polymerase I inhibitors. MedChemComm, 2019, 10, 1765-1774.	3.5	4
1388	ETM-DB: integrated Ethiopian traditional herbal medicine and phytochemicals database. BMC Complementary and Alternative Medicine, 2019, 19, 212.	3.7	26
1389	The Topology of the Contacts of Potential Ligands for the UxuR Transcription Factor of Escherichia coli as Revealed by Flexible Molecular Docking. Biophysics (Russian Federation), 2019, 64, 49-56.	0.2	4
1390	Derivatisation of parthenolide to address chemoresistant chronic lymphocytic leukaemia. MedChemComm, 2019, 10, 1379-1390.	3.5	15

#	Article	IF	Citations
1391	Norbornadieneâ€“dihydroazulene conjugates. Organic and Biomolecular Chemistry, 2019, 17, 7735-7746.	1.5	25
1392	In silico study: the antiglycation potency of aloin on the protein surface of human serum albumin. IOP Conference Series: Materials Science and Engineering, 2019, 509, 012087.	0.3	0
1393	Antibacterial Activity and Molecular Docking Studies of a Selected Series of Hydroxy-3-arylcoumarins. Molecules, 2019, 24, 2815.	1.7	69
1394	Cosolvent-Based Protein Pharmacophore for Ligand Enrichment in Virtual Screening. Journal of Chemical Information and Modeling, 2019, 59, 3572-3583.	2.5	21
1395	A systems pharmacology approach to investigate the mechanism of Oryeong-san formula for the treatment of hypertension. Journal of Ethnopharmacology, 2019, 244, 112129.	2.0	38
1396	Learning To Predict Reaction Conditions: Relationships between Solvent, Molecular Structure, and Catalyst. Journal of Chemical Information and Modeling, 2019, 59, 3645-3654.	2.5	36
1397	Robocrystallographer: automated crystal structure text descriptions and analysis. MRS Communications, 2019, 9, 874-881.	0.8	30
1398	Pressure-viscosity relation of 2,2,4-trimethylhexane predicted using all-atom TEAM force field. Fluid Phase Equilibria, 2019, 497, 64-70.	1.4	7
1399	Development of Dual Chitinase Inhibitors as Potential New Treatment for Respiratory System Diseases. Journal of Medicinal Chemistry, 2019, 62, 7126-7145.	2.9	22
1400	A quantitative uncertainty metric controls error in neural network-driven chemical discovery. Chemical Science, 2019, 10, 7913-7922.	3.7	129
1401	Searching new structural scaffolds for BRAF inhibitors. An integrative study using theoretical and experimental techniques. Bioorganic Chemistry, 2019, 91, 103125.	2.0	9
1402	Getting Docking into Shape Using Negative Image-Based Rescoring. Journal of Chemical Information and Modeling, 2019, 59, 3584-3599.	2.5	22
1403	Evaluation of in silico designed inhibitors targeting MelF (Rv1936) against Mycobacterium marinum within macrophages. Scientific Reports, 2019, 9, 10084.	1.6	1
1404	Converting SMILES to Stacking Interaction Energies. Journal of Chemical Information and Modeling, 2019, 59, 3413-3421.	2.5	11
1405	Phytosterols and triterpenes from Morinda lucida Benth (Rubiaceae) as potential inhibitors of anti-apoptotic BCL-XL, BCL-2, and MCL-1: an in-silico study. Journal of Receptor and Signal Transduction Research, 2019, 39, 87-97.	1.3	14
1406	Recent Advances in the Machine Learning-Based Drug-Target Interaction Prediction. Current Drug Metabolism, 2019, 20, 194-202.	0.7	48
1407	Insights into the transport side of the human SLC38A9 transceptor. Biochimica Et Biophysica Acta - Biomembranes, 2019, 1861, 1558-1567.	1.4	24
1408	A deep neural network model for packing density predictions and its application in the study of 1.5 million organic molecules. Chemical Science, 2019, 10, 8374-8383.	3.7	30

#	Article	IF	Citations
1409	Classification of alkaloids according to the starting substances of their biosynthetic pathways using graph convolutional neural networks. BMC Bioinformatics, 2019, 20, 380.	1.2	45
1410	Insights about multi-targeting and synergistic neuromodulators in Ayurvedic herbs against epilepsy: integrated computational studies on drug-target and protein-protein interaction networks. Scientific Reports, 2019, 9, 10565.	1.6	31
1411	Potent and selective inhibitors for M32 metallocarboxypeptidases identified from high-throughput screening of anti-kinetoplastid chemical boxes. PLoS Neglected Tropical Diseases, 2019, 13, e0007560.	1.3	3
1412	Elastic interphase properties of nanoparticle/epoxy nanocomposites: A molecular dynamics study. Composites Part B: Engineering, 2019, 176, 107211.	5.9	33
1413	The role of conserved residues in the catalytic activity of NDM-1: an approach involving site directed mutagenesis and molecular dynamics. Physical Chemistry Chemical Physics, 2019, 21, 17821-17835.	1.3	14
1414	In silico screening of anticholinesterase alkaloids for cyclooxygenase-2 (COX-2) and matrix metalloproteinase 8 (MMP-8) inhibitory potentials as multi-target inhibitors of Alzheimerâ€™s disease. Medicinal Chemistry Research, 2019, 28, 1704-1717.	1.1	6
1415	Cardiolipin-Dependent Properties of Model Mitochondrial Membranes from Molecular Simulations. Biophysical Journal, 2019, 117, 429-444.	0.2	36
1416	A curated knowledgebase on endocrine disrupting chemicals and their biological systems-level perturbations. Science of the Total Environment, 2019, 692, 281-296.	3.9	67
1417	Structural Analysis of a Nitrogenase Iron Protein from Methanosarcina acetivorans: Implications for CO ₂ Capture by a Surface-Exposed [Fe ₄ S ₄] Cluster. MBio, 2019, 10, .	1.8	10
1418	Preparation, characterization, inÂvitro and inÂvivo evaluation of metronidazoleâ€“gallic acid cocrystal: A combined experimental and theoretical investigation. Journal of Molecular Structure, 2019, 1197, 727-735.	1.8	17
1419	Reverse Engineering of an Aspirin-Responsive Transcriptional Regulator in Escherichia coli. ACS Synthetic Biology, 2019, 8, 1890-1900.	1.9	13
1420	Combined Ensemble Docking and Machine Learning in Identification of Therapeutic Agents with Potential Inhibitory Effect on Human CES1. Molecules, 2019, 24, 2747.	1.7	6
1421	Bulbine frutescens Phytochemicals as a Promising Anti-cancer Drug Discovery Source: A Computational Study. , 2019, , 491-510.		1
1422	Cyclooxygenase-2 Inhibitory Compounds from the Leaves of Glycosmis pentaphylla (Retz.) A. DC.: Chemical and in silico Studies. Asian Journal of Chemistry, 2019, 31, 1260-1264.	0.1	7
1423	Theoretical exploration of 2,2â€²-bipyridines as electro-active compounds in flow batteries. Physical Chemistry Chemical Physics, 2019, 21, 15823-15832.	1.3	8
1424	Repurposing an Ancient Protein Core Structure: Structural Studies on FmtA, a Novel Esterase of Staphylococcus aureus. Journal of Molecular Biology, 2019, 431, 3107-3123.	2.0	51
1425	In-silico Prediction of Synergistic Anti-Cancer Drug Combinations Using Multi-omics Data. Scientific Reports, 2019, 9, 8949.	1.6	66
1426	Computational elucidation of the binding mechanisms of curcumin analogues as bacterial RecA inhibitors. RSC Advances, 2019, 9, 19869-19881.	1.7	5

#	Article	IF	Citations
1427	A procedure combining molecular docking and semiempirical method PM7 for identification of selective Shp2 inhibitors. Biopolymers, 2019, 110, e23320.	1.2	5
1428	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. Structure, 2019, 27, 1326-1335.e4.	1.6	39
1429	Structure and product relationship analysis of acyl homoserine lactone synthases among Ensifer adhaerens reveals distinct chromosome and plasmid origins. Biochemical and Biophysical Research Communications, 2019, 516, 907-913.	1.0	5
1430	Structurally Modified Cyclopenta[b]benzofuran Analogues Isolated from Aglaia perviridis. Journal of Natural Products, 2019, 82, 2870-2877.	1.5	11
1431	A computational study targeting the mutated L321F of ERG11 gene in C.Âalbicans, associated with fluconazole resistance with bioactive compounds from Acacia nilotica. Journal De Mycologie Medicale, 2019, 29, 303-309.	0.7	14
1432	Characterization of the Impact of Drug Metabolism on the Gas-Phase Structures of Drugs Using Ion Mobility-Mass Spectrometry. Analytical Chemistry, 2019, 91, 14498-14507.	3.2	14
1433	Pharmacoinformatics-based identification of anti-bacterial catalase-peroxidase enzyme inhibitors. Computational Biology and Chemistry, 2019, 83, 107136.	1.1	15
1434	STS-NLSP: A Network-Based Label Space Partition Method for Predicting the Specificity of Membrane Transporter Substrates Using a Hybrid Feature of Structural and Semantic Similarity. Frontiers in Bioengineering and Biotechnology, 2019, 7, 306.	2.0	17
1435	Data of small peptides in SMILES and three-dimensional formats for virtual screening campaigns. Data in Brief, 2019, 27, 104607.	0.5	9
1436	Exploring T & B-cell epitopes and designing multi-epitope subunit vaccine targeting integration step of HIV-1 lifecycle using immunoinformatics approach. Microbial Pathogenesis, 2019, 137, 103791.	1.3	31
1437	Prediction of ligands to universally conserved binding sites of the influenza a virus nuclear export protein. Virology, 2019, 537, 97-103.	1.1	8
1438	Protein Preparation Automatic Protocol for High-Throughput Inverse Virtual Screening: Accelerating the Target Identification by Computational Methods. Journal of Chemical Information and Modeling, 2019, 59, 4678-4690.	2.5	13
1439	Comparison of Carbohydrate Force Fields Using Gaussian Accelerated Molecular Dynamics Simulations and Development of Force Field Parameters for Heparin-Analogue Pentasaccharides. Journal of Chemical Information and Modeling, 2019, 59, 4855-4867.	2.5	20
1440	Computational methods for NMR and MS for structure elucidation II: database resources and advanced methods. Physical Sciences Reviews, 2019, 4, .	0.8	6
1441	Application of the 3D-RISM-KH molecular solvation theory for DMSO as solvent. Journal of Computer-Aided Molecular Design, 2019, 33, 905-912.	1.3	5
1442	PEPCONF, a diverse data set of peptide conformational energies. Scientific Data, 2019, 6, 180310.	2.4	23
1443	Automated evaluation of consistency within the PubChem Compound database. Scientific Data, 2019, 6, 190023.	2.4	15
1445	FlavoDb: a web-based chemical repository of flavonoid compounds. 3 Biotech, 2019, 9, 431.	1.1	3

#	Article	IF	Citations
1446	Machine-Learning-Based Predictive Modeling of Glass Transition Temperatures: A Case of Polyhydroxyalkanoate Homopolymers and Copolymers. Journal of Chemical Information and Modeling, 2019, 59, 5013-5025.	2.5	85
1447	Machine learningâ€“assisted molecular design and efficiency prediction for high-performance organic photovoltaic materials. Science Advances, 2019, 5, eaay4275.	4.7	181
1448	Enhanced uptake, high selective and microtubule disrupting activity of carbohydrate fused pyrano-pyranones derived from natural coumarins attributes to its anti-malarial potential. Malaria Journal, 2019, 18, 346.	0.8	9
1449	ANTIMICROBIAL INVESTIGATION AND BINDING MODE ANALYSIS OF SOME NEWLY SYNTHESIZED 4-AMINO-5-((ARYL SUBSTITUTED)-4H-1, 2, 4-TRIAZOLE-3-YL)-THIO LINKED HYDROXAMIC ACID DERIVATIVES. Asian Journal of Pharmaceutical and Clinical Research, 0, , 469-479.	0.3	2
1450	ContraDRG: Automatic Partial Charge Prediction by Machine Learning. Frontiers in Genetics, 2019, 10, 990.	1.1	12
1451	Convolutional Neural Networks for the Design and Analysis of Non-Fullerene Acceptors. Journal of Chemical Information and Modeling, 2019, 59, 4993-5001.	2.5	29
1452	Methods of Metabolite Identification Using MS/MS Data. Journal of Computer Information Systems, 2019, , 1-7.	2.0	3
1453	TDR Targets 6: driving drug discovery for human pathogens through intensive chemogenomic data integration. Nucleic Acids Research, 2020, 48, D992-D1005.	6.5	26
1454	Comparison of affinity ranking using AutoDock-GPU and MM-GBSA scores for BACE-1 inhibitors in the D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2019, 33, 1011-1020.	1.3	50
1455	D3R Grand Challenge 4: prospective pose prediction of BACE1 ligands with AutoDock-GPU. Journal of Computer-Aided Molecular Design, 2019, 33, 1071-1081.	1.3	21
1456	A Chemosensory GPCR as a Potential Target to Control the Root-Knot Nematode Meloidogyne incognita Parasitism in Plants. Molecules, 2019, 24, 3798.	1.7	11
1457	Enhancing thermal tolerance of a fungal GH11 xylanase guided by B-factor analysis and multiple sequence alignment. Enzyme and Microbial Technology, 2019, 131, 109422.	1.6	18
1458	The Grouping and Assessment Strategy for Organic Pigments (GRAPE): Scientific evidence to facilitate regulatory decision-making. Regulatory Toxicology and Pharmacology, 2019, 109, 104501.	1.3	4
1459	Method for Predicting Dipole Moments of Complex Molecules for Use in Thermophysical Property Estimation. Industrial & Engineering Chemistry Research, 2019, 58, 19263-19270.	1.8	4
1460	Oxamniquine resistance alleles are widespread in Old World Schistosoma mansoni and predate drug deployment. PLoS Pathogens, 2019, 15, e1007881.	2.1	28
1461	Molecular Insights into Destabilization of Alzheimerâ€™s AÎ² Protofibril by Arginine Containing Short Peptides: A Molecular Modeling Approach. ACS Omega, 2019, 4, 892-903.	1.6	38
1462	Exploration in the Mechanism of Action of Licorice by Network Pharmacology. Molecules, 2019, 24, 2959.	1.7	23
1463	Integrated Targetâ€Based and Phenotypic Screening Approaches for the Identification of Antiâ€Tubercular Agents That Bind to the Mycobacterial Adenylating Enzyme MbtA. ChemMedChem, 2019, 14, 1735-1741.	1.6	9

#	Article	IF	Citations
1464	Simulation of the Adsorption of Polychlorinated Aromatic Hydrocarbons on Graphitized Thermal Carbon Black for Predicting Chromatographic Retention Values. Journal of Analytical Chemistry, 2019, 74, 47-51.	0.4	4
1465	Comparative Assessment of Seven Docking Programs on a Nonredundant Metalloprotein Subset of the PDBbind Refined. Journal of Chemical Information and Modeling, 2019, 59, 3846-3859.	2.5	35
1466	Characterization of Entamoeba histolytica adenosine 5â€²-phosphosulfate (APS) kinase; validation as a target and provision of leads for the development of new drugs against amoebiasis. PLoS Neglected Tropical Diseases, 2019, 13, e0007633.	1.3	15
1467	Implementation of Microservices Architecture for Application of Cyclooxygenase-2 Inhibitors Identifier. Journal of Physics: Conference Series, 2019, 1235, 012053.	0.3	0
1468	EK-DRD: A Comprehensive Database for Drug Repositioning Inspired by Experimental Knowledge. Journal of Chemical Information and Modeling, 2019, 59, 3619-3624.	2.5	4
1469	MeLAD: an integrated resource for metalloenzyme-ligand associations. Bioinformatics, 2020, 36, 904-909.	1.8	23
1470	Machine learning prediction of accurate atomization energies of organic molecules from low-fidelity quantum chemical calculations. MRS Communications, 2019, 9, 891-899.	0.8	38
1471	Identification of adaptive inhibitors of Cryptosporidium parvum fatty acyl-coenzyme A synthetase isoforms by virtual screening. Parasitology Research, 2019, 118, 3159-3171.	0.6	6
1472	Î²-Carotene: A Natural Compound Improves Cognitive Impairment and Oxidative Stress in a Mouse Model of Streptozotocin-Induced Alzheimerâ€™s Disease. Biomolecules, 2019, 9, 441.	1.8	70
1473	Computational Drug Repurposing Algorithm Targeting TRPA1 Calcium Channel as a Potential Therapeutic Solution for Multiple Sclerosis. Pharmaceutics, 2019, 11, 446.	2.0	21
1474	Computational Assessment of the Pharmacological Profiles of Degradation Products of Chitosan. Frontiers in Bioengineering and Biotechnology, 2019, 7, 214.	2.0	35
1475	Can we predict trends in tribo-charging of pharmaceutical materials from first principles?. Powder Technology, 2019, 356, 892-898.	2.1	5
1476	Crystal structure of cloxacillin sodium monohydrate, C19H17ClN3O5SNa(H2O). Powder Diffraction, 2019, 34, 374-378.	0.4	3
1477	Development linear and non-linear QSAR models for predicting AXL kinase inhibitory activity of N-[4-(quinolin-4-yloxy)phenyl]benzenesulfonamides. Journal of Receptor and Signal Transduction Research, 2019, 39, 264-275.	1.3	2
1478	Exploring chemical space in the search for improved azoheteroarene-based photoswitches. Physical Chemistry Chemical Physics, 2019, 21, 20782-20790.	1.3	10
1479	Tracing Potential Covalent Inhibitors of an E3 Ubiquitin Ligase through Target-Focused Modelling. Molecules, 2019, 24, 3125.	1.7	4
1480	A Fragmenting Protocol with Explicit Hydration for Calculation of Binding Enthalpies of Target-Ligand Complexes at a Quantum Mechanical Level. International Journal of Molecular Sciences, 2019, 20, 4384.	1.8	11
1481	Predicting binding poses and affinity ranking in D3R Grand Challenge using PL-PatchSurfer2.0. Journal of Computer-Aided Molecular Design, 2019, 33, 1083-1094.	1.3	3

#	Article	IF	Citations
1482	One Among Millions: The Chemical Space of Nucleic Acid-Like Molecules. Journal of Chemical Information and Modeling, 2019, 59, 4266-4277.	2.5	25
1483	BigSMILES: A Structurally-Based Line Notation for Describing Macromolecules. ACS Central Science, 2019, 5, 1523-1531.	5.3	134
1484	New oxadiazoles with selective-COX-2 and EGFR dual inhibitory activity: Design, synthesis, cytotoxicity evaluation and in silico studies. European Journal of Medicinal Chemistry, 2019, 183, 111693.	2.6	44
1485	Establishing Predictive Models for Solvatochromic Parameters of Ionic Liquids. Frontiers in Chemistry, 2019, 7, 605.	1.8	9
1486	Effect of piceatannol-rich passion fruit seed extract on human glyoxalase Iâ€“mediated cancer cell growth. Biochemistry and Biophysics Reports, 2019, 20, 100684.	0.7	13
1487	Genome-Wide Analysis and Expression Profiling of Rice Hybrid Proline-Rich Proteins in Response to Biotic and Abiotic Stresses, and Hormone Treatment. Plants, 2019, 8, 343.	1.6	13
1488	Identification Schemes for Metalâ€“Organic Frameworks To Enable Rapid Search and Cheminformatics Analysis. Crystal Growth and Design, 2019, 19, 6682-6697.	1.4	123
1489	A Simple Method to Predict and Interpret the Formation of Azeotropes in Binary Systems Using Conventional Solvation Free Energy Calculations. Industrial & Engineering Chemistry Research, 2019, 58, 22626-22632.	1.8	11
1490	Synthesis, Biological Activities and Docking Studies of Novel 4-(Arylaminomethyl)benzamide Derivatives as Potential Tyrosine Kinase Inhibitors. Molecules, 2019, 24, 3543.	1.7	11
1491	The metaRbolomics Toolbox in Bioconductor and beyond. Metabolites, 2019, 9, 200.	1.3	64
1492	Identification of Functional and Druggable Sites in Aspergillus fumigatus Essential Phosphatases by Virtual Screening. International Journal of Molecular Sciences, 2019, 20, 4636.	1.8	6
1493	A new steroid glycoside from Begonia sp.: cytotoxic activity and docking studies. Natural Product Research, 2019, 35, 1-8.	1.0	4
1494	A Free Web-Based Protocol to Assist Structure-Based Virtual Screening Experiments. International Journal of Molecular Sciences, 2019, 20, 4648.	1.8	16
1495	Tacroximes: novel unique compounds for the recovery of organophosphorus-inhibited acetylcholinesterase. Future Medicinal Chemistry, 2019, 11, 2625-2634.	1.1	6
1496	HybridMolDB: A Manually Curated Database Dedicated to Hybrid Molecules for Chemical Biology and Drug Discovery. Journal of Chemical Information and Modeling, 2019, 59, 4063-4069.	2.5	5
1497	Application of the SwissDrugDesign Online Resources in Virtual Screening. International Journal of Molecular Sciences, 2019, 20, 4612.	1.8	58
1498	In vitro antitumor activity, ADME-Tox and 3D-QSAR of synthesized and selected natural styryl lactones. Computational Biology and Chemistry, 2019, 83, 107112.	1.1	6
1499	Potential off-target effects of beta-blockers on gut hormone receptors: In silico study including GUT-DOCKâ€”A web service for small-molecule docking. PLoS ONE, 2019, 14, e0210705.	1.1	12

#	Article	IF	Citations
1500	Identifying Protein Features Responsible for Improved Drug Repurposing Accuracies Using the CANDO Platform: Implications for Drug Design. Molecules, 2019, 24, 167.	1.7	24
1501	Design, Synthesis, and Biological Evaluation of 3,5â€Disubstituted 2â€Pyrazineamide Derivatives as Antitubercular Agents. Journal of Heterocyclic Chemistry, 2019, 56, 1117-1126.	1.4	2
1502	Systematic domain-based aggregation of protein structures highlights DNA-, RNA- and other ligand-binding positions. Nucleic Acids Research, 2019, 47, 582-593.	6.5	16
1503	Comprehensive anticancer drug response prediction based on a simple cell line-drug complex network model. BMC Bioinformatics, 2019, 20, 44.	1.2	43
1504	Homology models of mouse and rat estrogen receptor-Î± ligand-binding domain created by in silico mutagenesis of a human template: Molecular docking with 17Î²-estradiol, diethylstilbestrol, and paraben analogs. Computational Toxicology, 2019, 10, 1-16.	1.8	18
1505	Examining pharmacodynamic and pharmacokinetic properties of eleven analogues of saquinavir for HIV protease inhibition. Archives of Virology, 2019, 164, 949-960.	0.9	4
1506	Assessment of GAFF2 and OPLS-AA General Force Fields in Combination with the Water Models TIP3P, SPCE, and OPC3 for the Solvation Free Energy of Druglike Organic Molecules. Journal of Chemical Theory and Computation, 2019, 15, 1983-1995.	2.3	131
1507	Isoquinoline Alkaloids from Berberis vulgaris as Potential Lead Compounds for the Treatment of Alzheimerâ€™s Disease. Journal of Natural Products, 2019, 82, 239-248.	1.5	55
1508	Benchmarking DFT approaches for the calculation of polarizability inputs for refractive index predictions in organic polymers. Physical Chemistry Chemical Physics, 2019, 21, 4452-4460.	1.3	24
1509	Discovering highly selective and diverse PPAR-delta agonists by ligand based machine learning and structural modeling. Scientific Reports, 2019, 9, 1106.	1.6	36
1510	Toxin Î¶ Reduces the ATP and Modulates the Uridine Diphosphate-N-acetylglucosamine Pool. Toxins, 2019, 11, 29.	1.5	6
1511	Synthesis, characterisation, molecular docking, biomolecular interaction and cytotoxicity studies of novel ruthenium(<scp>ii</scp>)â€“arene-2-heteroarylbenzoxazole complexes. New Journal of Chemistry, 2019, 43, 3291-3302.	1.4	31
1512	MoDoop: An Automated Computational Approach for COSMO-RS Prediction of Biopolymer Solubilities in Ionic Liquids. ACS Omega, 2019, 4, 2337-2343.	1.6	25
1513	Propolis Components from Stingless Bees Collected on South Sulawesi, Indonesia, and Their Xanthine Oxidase Inhibitory Activity. Journal of Natural Products, 2019, 82, 205-210.	1.5	30
1514	Chalcone analogues: Synthesis, activity against Meloidogyne incognita, and in silico interaction with cytochrome P450. Journal of Phytopathology, 2019, 167, 197-208.	0.5	10
1515	Thein silicoandin vivoevaluation of puerarin against Alzheimer's disease. Food and Function, 2019, 10, 799-813.	2.1	36
1516	Donorâ€“Acceptor Sequence Engineering in Ï€-Conjugated Polymers for Enhanced Hole Transport and Photocurrent. Journal of Physical Chemistry C, 2019, 123, 14253-14260.	1.5	4
1517	Gypsum-DL: an open-source program for preparing small-molecule libraries for structure-based virtual screening. Journal of Cheminformatics, 2019, 11, 34.	2.8	45

#	Article	IF	Citations
1518	Exploring the Potential of Spherical Harmonics and PCVM for Compounds Activity Prediction. International Journal of Molecular Sciences, 2019, 20, 2175.	1.8	2
1519	Analysis and Comparison of Vector Space and Metric Space Representations in QSAR Modeling. Molecules, 2019, 24, 1698.	1.7	17
1520	Inhibitory Effects of Phenylpropanoid Derivatives from Oenanthe javanica on Antigen-Stimulated Degranulation in RBL-2H3 Cells. Journal of Natural Products, 2019, 82, 1518-1526.	1.5	6
1521	Insights into the pH-dependent catalytic mechanism of Sulfolobus solfataricus Î²-glycosidase: A molecular dynamics study. Carbohydrate Research, 2019, 480, 42-53.	1.1	7
1522	iCOX2: An open source and offline graphical-user-interface application to identify cyclooxygenase-2 inhibitors. AIP Conference Proceedings, 2019, , .	0.3	0
1523	Caver Web 1.0: identification of tunnels and channels in proteins and analysis of ligand transport. Nucleic Acids Research, 2019, 47, W414-W422.	6.5	138
1524	Association of HLA-C*03:02 with methimazole-induced liver injury in Gravesâ€™ disease patients. Biomedicine and Pharmacotherapy, 2019, 117, 109095.	2.5	23
1525	Autoignition Characteristics of Ethers Blended with Low Cetane Distillates. Energy & Fuels, 2019, 33, 6775-6787.	2.5	10
1526	DockRMSD: an open-source tool for atom mapping and RMSD calculation of symmetric molecules through graph isomorphism. Journal of Cheminformatics, 2019, 11, 40.	2.8	174
1527	The dataset of covalent bond lengths resulting from the first-principle calculations. Computational and Theoretical Chemistry, 2019, 1163, 112508.	1.1	7
1528	Melting Temperature Estimation of Imidazole Ionic Liquids with Clustering Methods. Journal of Chemical Information and Modeling, 2019, 59, 3144-3153.	2.5	12
1529	A Complete Assessment of Dopamine Receptor- Ligand Interactions through Computational Methods. Molecules, 2019, 24, 1196.	1.7	23
1530	A Practical Perspective: The Effect of Ligand Conformers on the Negative Image-Based Screening. International Journal of Molecular Sciences, 2019, 20, 2779.	1.8	9
1531	Computational Opportunities and Challenges in Finding Cyclic Peptide Modulators of Proteinâ€“Protein Interactions. Methods in Molecular Biology, 2019, 2001, 73-95.	0.4	7
1532	A Systems Pharmacology Approach Uncovers Wogonoside as an Angiogenesis Inhibitor of Triple-Negative Breast Cancer by Targeting Hedgehog Signaling. Cell Chemical Biology, 2019, 26, 1143-1158.e6.	2.5	53
1533	Cocrystals in the Cambridge Structural Database: a network approach. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2019, 75, 371-383.	0.5	25
1534	Tackling Halogenated Species with PBSA: Effect of Emulating the Ï*f*-Hole. Journal of Chemical Theory and Computation, 2019, 15, 4241-4251.	2.3	15
1535	BitterSweet: Building machine learning models for predicting the bitter and sweet taste of small molecules. Scientific Reports, 2019, 9, 7155.	1.6	37

#	Article	IF	Citations
1536	Drug repositioning of herbal compounds via a machine-learning approach. BMC Bioinformatics, 2019, 20, 247.	1.2	37
1537	Implementation of the Molecular Electrostatic Potential over Graphics Processing Units. Journal of Chemical Information and Modeling, 2019, 59, 3120-3127.	2.5	16
1538	Elucidation of Scavenging Properties of Nanoparticles in the Prevention of Carcinogenicity Induced by Cigarette Smoke Carcinogens: An In Silico Study. Environmental Science and Engineering, 2019, , 171-183.	0.1	1
1539	The molecular determinants of neurosteroid binding in the GABA(A) receptor. Journal of Steroid Biochemistry and Molecular Biology, 2019, 192, 105383.	1.2	14
1540	Large-Scale Target Identification of Herbal Medicine Using a Reverse Docking Approach. ACS Omega, 2019, 4, 9710-9719.	1.6	16
1541	Computational prediction of chiroptical properties in structure elucidation of natural products. Natural Product Reports, 2019, 36, 1005-1030.	5.2	66
1542	Chemical synthesis and characterization of a new quinazolinedione competitive antagonist for strigolactone receptors with an unexpected binding mode. Biochemical Journal, 2019, 476, 1843-1856.	1.7	5
1543	Ligands and Receptors with Broad Binding Capabilities Have Common Structural Characteristics: An Antibiotic Design Perspective. Journal of Medicinal Chemistry, 2019, 62, 9357-9374.	2.9	9
1544	Exploration of interaction scoring criteria in the CANDO platform. BMC Research Notes, 2019, 12, 318.	0.6	18
1545	The Selective Rat Toxicant Norbormide Blocks KATP Channels in Smooth Muscle Cells But Not in Insulin-Secreting Cells. Frontiers in Pharmacology, 2019, 10, 598.	1.6	6
1546	Structural insights into EntamoebaÂhistolytica arginase and structureâ€based identification of novel nonâ€amino acid based inhibitors as potential antiamoebic molecules. FEBS Journal, 2019, 286, 4135-4155.	2.2	39
1547	Towards creating an extended metabolic model (EMM) for E. coli using enzyme promiscuity prediction and metabolomics data. Microbial Cell Factories, 2019, 18, 109.	1.9	14
1548	A Deep Learning Approach for Molecular Crystallinity Prediction. Advances in Intelligent Systems and Computing, 2019, , 219-225.	0.5	0
1549	Deep learning for molecular designâ€"a review of the state of the art. Molecular Systems Design and Engineering, 2019, 4, 828-849.	1.7	379
1550	SwissTargetPrediction: updated data and new features for efficient prediction of protein targets of small molecules. Nucleic Acids Research, 2019, 47, W357-W364.	6.5	1,634
1551	Bayesian optimization for conformer generation. Journal of Cheminformatics, 2019, 11, 32.	2.8	37
1552	Enhancing Acute Oral Toxicity Predictions by using Consensus Modeling and Algebraic Form-Based 0D-to-2D Molecular Encodes. Chemical Research in Toxicology, 2019, 32, 1178-1192.	1.7	19
1553	In silico identification of genetic mutations conferring resistance to acetohydroxyacid synthase inhibitors: A case study of Kochia scoparia. PLoS ONE, 2019, 14, e0216116.	1.1	6

#	Article	IF	Citations
1554	SLTChemDB: A database of chemical compounds present in Smokeless tobacco products. Scientific Reports, 2019, 9, 7142.	1.6	9
1555	BRUSELAS: HPC Generic and Customizable Software Architecture for 3D Ligand-Based Virtual Screening of Large Molecular Databases. Journal of Chemical Information and Modeling, 2019, 59, 2805-2817.	2.5	12
1556	A Universal Quantitative Descriptor of the Dispersion Interaction Potential. Angewandte Chemie - International Edition, 2019, 58, 9758-9769.	7.2	41
1557	An integrative bioinformatics pipeline to demonstrate the alteration of the interaction between the ALDH2*2 allele with NAD + and Disulfiram. Journal of Cellular Biochemistry, 2019, 120, 17030-17041.	1.2	0
1558	CGRtools: Python Library for Molecule, Reaction, and Condensed Graph of Reaction Processing. Journal of Chemical Information and Modeling, 2019, 59, 2516-2521.	2.5	34
1559	Revealing Drug-Target Interactions with Computational Models and Algorithms. Molecules, 2019, 24, 1714.	1.7	42
1560	Accelerated Discovery of High-Refractive-Index Polyimides via First-Principles Molecular Modeling, Virtual High-Throughput Screening, and Data Mining. Journal of Physical Chemistry C, 2019, 123, 14610-14618.	1.5	36
1561	Ellagic Acid, Kaempferol, and Quercetin from Acacia nilotica: Promising Combined Drug With Multiple Mechanisms of Action. Current Pharmacology Reports, 2019, 5, 255-280.	1.5	37
1562	Highly tunable thiosulfonates as a novel class of cysteine protease inhibitors with anti-parasitic activity against Schistosoma mansoni. Bioorganic and Medicinal Chemistry, 2019, 27, 2857-2870.	1.4	3
1563	Structural aspects of 4-aminoquinolines as reversible inhibitors of human acetylcholinesterase and butyrylcholinesterase. Chemico-Biological Interactions, 2019, 308, 101-109.	1.7	26
1564	Predicting skin permeability using the 3D-RISM-KH theory based solvation energy descriptors for a diverse class of compounds. Journal of Computer-Aided Molecular Design, 2019, 33, 605-611.	1.3	4
1565	Structural basis of ligand recognition at the human MT1 melatonin receptor. Nature, 2019, 569, 284-288.	13.7	140
1566	Middle-way flexible docking: Pose prediction using mixed-resolution Monte Carlo in estrogen receptor Î±. PLoS ONE, 2019, 14, e0215694.	1.1	6
1567	Some Functional Properties of khambir, an Ethnic Fermented Cereal-Based Food of Western Himalayas. Frontiers in Microbiology, 2019, 10, 730.	1.5	11
1568	A Molecular Dynamics Approach to Explore the Intramolecular Signal Transduction of PPAR-Î±. International Journal of Molecular Sciences, 2019, 20, 1666.	1.8	29
1569	Extension of TEAM Force-Field Database to Ionic Liquids. Journal of Chemical & Engineering Data, 2019, 64, 3718-3730.	1.0	10
1570	A Machine Learning Approach to Zeolite Synthesis Enabled by Automatic Literature Data Extraction. ACS Central Science, 2019, 5, 892-899.	5.3	176
1571	Ligand-Binding-Site Structure Shapes Allosteric Signal Transduction and the Evolution of Allostery in Protein Complexes. Molecular Biology and Evolution, 2019, 36, 1711-1727.	3.5	33

#	Article	IF	Citations
1572	Insights into mechanisms and severity of drug-induced liver injury via computational systems toxicology approach. Toxicology Letters, 2019, 312, 22-33.	0.4	13
1573	Search for aglycone isoflavone from soybean as candidate for pelvic organ prolapse treatment: In silico study of TGF-Î²1, Hsp70, and Bcl-xl signals. Clinical Nutrition Experimental, 2019, 23, 15-22.	2.0	0
1574	Energy Landscapes of Ligand Motion Inside the Tunnel-Like Cavity of Lipid Transfer Proteins: The Case of the Pru p 3 Allergen. International Journal of Molecular Sciences, 2019, 20, 1432.	1.8	9
1575	Performance of 3D-RISM-KH in Predicting Hydration Free Energy: Effect of Solute Parameters. Journal of Physical Chemistry A, 2019, 123, 4087-4093.	1.1	26
1576	DNAmod: the DNA modification database. Journal of Cheminformatics, 2019, 11, 30.	2.8	53
1577	Structure-Based Virtual Screening and In Vitro Evaluation of New Trypanosoma cruzi Cruzain Inhibitors. International Journal of Molecular Sciences, 2019, 20, 1742.	1.8	22
1578	Herbicidal activity of isobenzofuranones and in silico identification of their enzyme target. Pest Management Science, 2019, 75, 3331-3339.	1.7	8
1579	Training Neural Nets To Learn Reactive Potential Energy Surfaces Using Interactive Quantum Chemistry in Virtual Reality. Journal of Physical Chemistry A, 2019, 123, 4486-4499.	1.1	65
1580	Phenolic Compounds Inhibit 3T3-L1 Adipogenesis Depending on the Stage of Differentiation and Their Binding Affinity to PPARÎ³. Molecules, 2019, 24, 1045.	1.7	61
1581	New factor Xa inhibitors based on 1,2,3,4-tetrahydroquinoline developed by molecular modelling. Journal of Molecular Graphics and Modelling, 2019, 89, 215-224.	1.3	19
1582	Development of a virtual reality platform for effective communication of structural data in drug discovery. Journal of Molecular Graphics and Modelling, 2019, 89, 234-241.	1.3	46
1583	Learning from Failure: Predicting Electronic Structure Calculation Outcomes with Machine Learning Models. Journal of Chemical Theory and Computation, 2019, 15, 2331-2345.	2.3	66
1584	Electronic and optical properties of chromophores from hexeneuronic acids. Cellulose, 2019, 26, 1489-1501.	2.4	13
1585	3D-QSAR for binding constants of Î²-cyclodextrin host-guest complexes by utilising spectrophores as molecular descriptors. Chemosphere, 2019, 225, 135-138.	4.2	12
1586	Parallelization of large-scale drugâ€“protein binding experiments. Future Generation Computer Systems, 2019, 97, 492-502.	4.9	0
1587	Thalidomide and Its Analogs Differentially Target Fibroblast Growth Factor Receptors: Thalidomide Suppresses FGFR Gene Expression while Pomalidomide Dampens FGFR2 Activity. Chemical Research in Toxicology, 2019, 32, 589-602.	1.7	9
1588	Designing in the Face of Uncertainty: Exploiting Electronic Structure and Machine Learning Models for Discovery in Inorganic Chemistry. Inorganic Chemistry, 2019, 58, 10592-10606.	1.9	79
1589	Effects of phosphorylation on the NLRP3 inflammasome. Archives of Biochemistry and Biophysics, 2019, 670, 43-57.	1.4	23

#	Article	IF	Citations
1590	Identification of the Criegee intermediate reaction network in ethylene ozonolysis: impact on energy conversion strategies and atmospheric chemistry. Physical Chemistry Chemical Physics, 2019, 21, 7341-7357.	1.3	29
1591	Pareto Optimality Explanation of the Glycolytic Alternatives in Nature. Scientific Reports, 2019, 9, 2633.	1.6	16
1592	Stalis : A Computational Method for Templateâ€Based Ab Initio Ligand Design. Journal of Computational Chemistry, 2019, 40, 1622-1632.	1.5	4
1593	In Silico Repurposing of Cell Cycle Modulators for Cancer Treatment. , 2019, , 255-279.		0
1594	Experimental and theoretical study on cetylpyridinium dipicrylamide â€“ A promising ion-exchanger for cetylpyridinium selective electrodes. Journal of Molecular Structure, 2019, 1187, 77-85.	1.8	28
1595	Enzyme annotation for orphan and novel reactions using knowledge of substrate reactive sites. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 7298-7307.	3.3	65
1596	Bridging the Homogeneous-Heterogeneous Divide: Modeling Spin for Reactivity in Single Atom Catalysis. Frontiers in Chemistry, 2019, 7, 219.	1.8	34
1597	<scp>Valence</scp>: A Massively Parallel Implementation of the Variational Subspace Valence Bond Method. Journal of Computational Chemistry, 2019, 40, 1664-1673.	1.5	3
1598	In silico study of M18 aspartyl amino peptidase (M18AAP) of Plasmodium vivax as an antimalarial drug target. Bioorganic and Medicinal Chemistry, 2019, 27, 2553-2571.	1.4	11
1599	Chemoinformatics and structural bioinformatics in OCaml. Journal of Cheminformatics, 2019, 11, 10.	2.8	5
1600	Towards Unraveling the Histone Code by Fragment Blind Docking. International Journal of Molecular Sciences, 2019, 20, 422.	1.8	8
1601	Insights into the antineoplastic mechanism of Chelidonium majus via systems pharmacology approach. Quantitative Biology, 2019, 7, 42-53.	0.3	1
1602	A new Mycobacterium leprae dihydropteroate synthase variant (V39I) from Papua, Indonesia. Heliyon, 2019, 5, e01279.	1.4	7
1603	Insights into Substrate and Inhibitor Selectivity among Human GLUT Transporters through Comparative Modeling and Molecular Docking. ACS Omega, 2019, 4, 4748-4760.	1.6	7
1604	Quantum chemical investigation of the detection properties of alternariol and alternariol monomethyl ether. Structural Chemistry, 2019, 30, 1749-1759.	1.0	7
1605	A small molecule Nec-1 directly induces amyloid clearance in the brains of aged APP/PS1 mice. Scientific Reports, 2019, 9, 4183.	1.6	27
1606	Machine Learning Approach for Determining the Formation of Î²-Lactam Antibiotic Complexes with Cyclodextrins Using Multispectral Analysis. Molecules, 2019, 24, 743.	1.7	6
1607	Structure-function relationship of a citrus salicylate methylesterase and role of salicylic acid in citrus canker resistance. Scientific Reports, 2019, 9, 3901.	1.6	15

#	Article	IF	Citations
1608	In Silico Screening to Identify Inhibitors of Growth Factor Receptor 2â€“Focal Adhesion Kinase Interaction for Therapeutic Treatment of Pathological Cardiac Hypertrophy. Assay and Drug Development Technologies, 2019, 17, 58-67.	0.6	3
1609	CSgator: an integrated web platform for compound set analysis. Journal of Cheminformatics, 2019, 11, 17.	2.8	7
1610	Network-based prediction of drug combinations. Nature Communications, 2019, 10, 1197.	5.8	437
1611	LipidII interaction with specific residues of Mycobacterium tuberculosis PknB extracytoplasmic domain governs its optimal activation. Nature Communications, 2019, 10, 1231.	5.8	42
1612	DAKB-GPCRs: An Integrated Computational Platform for Drug Abuse Related GPCRs. Journal of Chemical Information and Modeling, 2019, 59, 1283-1289.	2.5	23
1613	Development of a nano-QSPR model to predict band gaps of spherical metal oxide nanoparticles. RSC Advances, 2019, 9, 8426-8434.	1.7	9
1614	Synthesis, biological evaluation, and molecular docking of dihydroflavonol derivatives as anti-inflammatory agents. Medicinal Chemistry Research, 2019, 28, 863-872.	1.1	0
1615	Structural bases of peptidoglycan recognition by lysostaphin SH3b domain. Scientific Reports, 2019, 9, 5965.	1.6	54
1616	A Bayesian framework that integrates multi-omics data and gene networks predicts risk genes from schizophrenia GWAS data. Nature Neuroscience, 2019, 22, 691-699.	7.1	118
1617	Methodology of aiQSAR: a group-specific approach to QSAR modelling. Journal of Cheminformatics, 2019, 11, 27.	2.8	16
1618	Derivatives of the Î²-Crinane Amaryllidaceae Alkaloid Haemanthamine as Multi-Target Directed Ligands for Alzheimerâ€™s Disease. Molecules, 2019, 24, 1307.	1.7	22
1619	Optimized GPU implementation of Merck Molecular Force Field and Universal Force Field. Journal of Molecular Structure, 2019, 1188, 227-233.	1.8	20
1620	Prediction of drug-disease associations based on ensemble meta paths and singular value decomposition. BMC Bioinformatics, 2019, 20, 134.	1.2	24
1621	Active-site differences between substrate-free and ritonavir-bound cytochrome P450 (CYP) 3A5 reveal plasticity differences between CYP3A5 and CYP3A4. Journal of Biological Chemistry, 2019, 294, 8015-8022.	1.6	32
1622	A comprehensive review of feature based methods for drug target interaction prediction. Journal of Biomedical Informatics, 2019, 93, 103159.	2.5	104
1623	Exponential consensus ranking improves the outcome in docking and receptor ensemble docking. Scientific Reports, 2019, 9, 5142.	1.6	89
1624	Effects of ladder structure on the electronic properties and field-effect transistor performance of Poly(benzobisimidazobenzophenanthroline). Organic Electronics, 2019, 69, 301-307.	1.4	25
1625	Prediction of Hemolytic Toxicity for Saponins by Machine-Learning Methods. Chemical Research in Toxicology, 2019, 32, 1014-1026.	1.7	14

#	Article	IF	Citations
1626	Inhibition of Oncogenic Kinases: An In Vitro Validated Computational Approach Identified Potential Multi-Target Anticancer Compounds. Biomolecules, 2019, 9, 124.	1.8	26
1627	Exploration of Chemical Compound, Conformer, and Reaction Space with Meta-Dynamics Simulations Based on Tight-Binding Quantum Chemical Calculations. Journal of Chemical Theory and Computation, 2019, 15, 2847-2862.	2.3	551
1628	Molecular Dynamics Insights for Screening the Ability of Polymers to Remove Pesticides from Water. ChemistryOpen, 2019, 8, 438-446.	0.9	8
1629	Bioprospection of antiâ€inflammatory phytochemicals suggests rutaecarpine and quinine as promising 15â€lipoxygenase inhibitors. Journal of Cellular Biochemistry, 2019, 120, 13598-13613.	1.2	4
1630	Docking software performance in protein-glycosaminoglycan systems. Journal of Molecular Graphics and Modelling, 2019, 90, 42-50.	1.3	31
1631	Antioxidant activity and antibacterial evaluation of new thiazolin-4-one derivatives as potential tryptophanyl-tRNA synthetase inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2019, 34, 898-908.	2.5	16
1632	Discovery of novel triazolo[4,3-b]pyridazin-3-yl-quinoline derivatives as PIM inhibitors. European Journal of Medicinal Chemistry, 2019, 168, 87-109.	2.6	21
1633	e-Sweet: A Machine-Learning Based Platform for the Prediction of Sweetener and Its Relative Sweetness. Frontiers in Chemistry, 2019, 7, 35.	1.8	29
1634	Identification of an indol-based multi-target kinase inhibitor through phenotype screening and target fishing using inverse virtual screening approach. European Journal of Medicinal Chemistry, 2019, 167, 61-75.	2.6	20
1635	Implementing cheminformatics. Journal of Cheminformatics, 2019, 11, 12.	2.8	0
1636	A natural anticancer pigment,Pheophytin a,from a seagrass acts as a high affinity human mitochondrial translocator protein (TSPO) ligand, in silico, to reduce mitochondrial membrane Potential (âˆ†Ïˆ) in adenocarcinomic A549 cells.. Phytomedicine, 2019, 61, 152858.	2.3	16
1637	DeepDrug3D: Classification of ligand-binding pockets in proteins with a convolutional neural network. PLoS Computational Biology, 2019, 15, e1006718.	1.5	85
1638	A cell-free platform for the prenylation of natural products and application to cannabinoid production. Nature Communications, 2019, 10, 565.	5.8	82
1639	Mycobacterium tuberculosis metC(Rv3340) derived hydrogen sulphide conferring bacteria stress survival. Journal of Drug Targeting, 2019, 27, 1004-1016.	2.1	15
1640	Small Molecule Docking of DNA Repair Proteins Associated with Cancer Survival Following PCNA Metagene Adjustment: A Potential Novel Class of Repair Inhibitors. Molecules, 2019, 24, 645.	1.7	7
1641	Beta-Cryptoxanthin Inhibits Lipopolysaccharide-Induced Osteoclast Differentiation and Bone Resorption via the Suppression of Inhibitor of NF-ÎºB Kinase Activity. Nutrients, 2019, 11, 368.	1.7	28
1642	ImmunoSPdb: an archive of immunosuppressive peptides. Database: the Journal of Biological Databases and Curation, 2019, 2019, .	1.4	2
1643	ISiCLE: A Quantum Chemistry Pipeline for Establishing in Silico Collision Cross Section Libraries. Analytical Chemistry, 2019, 91, 4346-4356.	3.2	74

#	Article	IF	Citations
1644	A primer on natural product-based virtual screening. Physical Sciences Reviews, 2019, 4, .	0.8	7
1645	Graph Theory Approach to High-Throughput Surface Adsorption Structure Generation. Journal of Physical Chemistry A, 2019, 123, 2281-2285.	1.1	61
1646	Computational Identification of Inhibitors Using QSAR Approach Against Nipah Virus. Frontiers in Pharmacology, 2019, 10, 71.	1.6	19
1647	Predicting Bloodâ€“Brain Partitioning of Small Molecules Using a Novel Minimalistic Descriptor-Based Approach via the 3D-RISM-KH Molecular Solvation Theory. ACS Omega, 2019, 4, 3055-3060.	1.6	12
1648	Anti-oxidant and anti-inflammatory effects of cinnamaldehyde and eugenol on mononuclear cells of rheumatoid arthritis patients. European Journal of Pharmacology, 2019, 852, 14-24.	1.7	88
1649	Dimorphite-DL: an open-source program for enumerating the ionization states of drug-like small molecules. Journal of Cheminformatics, 2019, 11, 14.	2.8	34
1650	Molecular modelling of epoxy resin crosslinking experimentally validated by near-infrared spectroscopy. Computational Materials Science, 2019, 161, 223-235.	1.4	41
1651	Shooting three inflammatory targets with a single bullet: Novel multi-targeting anti-inflammatory glitazones. European Journal of Medicinal Chemistry, 2019, 167, 562-582.	2.6	33
1652	Selective recognition of c-MYC Pu22 G-quadruplex by a fluorescent probe. Nucleic Acids Research, 2019, 47, 2190-2204.	6.5	66
1653	DeepChemStable: Chemical Stability Prediction with an Attention-Based Graph Convolution Network. Journal of Chemical Information and Modeling, 2019, 59, 1044-1049.	2.5	58
1654	Phytosterols and triterpenes from Morinda lucida Benth. exhibit binding tendency against class I HDAC and HDAC7 isoforms. Molecular Biology Reports, 2019, 46, 2307-2325.	1.0	13
1655	The impact of feature selection methods on machine learning-based docking prediction of Indonesian medicinal plant compounds and HIV-1 protease. , 2019, , .		0
1656	Document Domain Adaptation with Generative Adversarial Networks. , 2019, , .		4
1657	The chemfp project. Journal of Cheminformatics, 2019, 11, 76.	2.8	24
1658	Urological cancer: molecular docking of the active compound Scurrula atropurpurea against nuclear factor erythroid2-related factor2 (Nrf2). Journal of Physics: Conference Series, 2019, 1374, 012055.	0.3	0
1659	Predicting Drug-Disease Treatment Associations Based on Topological Similarity and Singular Value Decomposition. , 2019, , .		4
1660	Chemical Structure Recognition (CSR) System: Automatic Analysis of 2D Chemical Structures in Document Images. , 2019, , .		4
1661	Molecular docking of the active compound Garcinia mangostana on the RANKL/RANK/OPG system. Journal of Physics: Conference Series, 2019, 1374, 012054.	0.3	1

#	Article	IF	Citations
1662	Metabolite Identification Using Artificial Neural Network. , 2019, , .		6
1663	CyBy2: a strongly typed, purely functional framework for chemical data management. Journal of Cheminformatics, 2019, 11, 80.	2.8	0
1664	Anti-Acetylcholinesterase Activities of Mono-Herbal Extracts and Exhibited Synergistic Effects of the Phytoconstituents: A Biochemical and Computational Study. Molecules, 2019, 24, 4175.	1.7	39
1665	Epigenetic drug discovery: systematic assessment of chemical space. Future Medicinal Chemistry, 2019, 11, 2803-2819.	1.1	4
1666	Targeting Inflammation with Conjugated Cinnamic Amides, Ethers and Esters. Letters in Drug Design and Discovery, 2019, 17, 3-11.	0.4	4
1667	Comparative dataset of experimental and computational attributes of UV/vis absorption spectra. Scientific Data, 2019, 6, 307.	2.4	63
1668	A prospective compound screening contest identified broader inhibitors for Sirtuin 1. Scientific Reports, 2019, 9, 19585.	1.6	15
1669	ADMET properties of novel 5-O-benzoylpinostrobin derivatives. Journal of Basic and Clinical Physiology and Pharmacology, 2019, 30, .	0.7	20
1670	ACID: a free tool for drug repurposing using consensus inverse docking strategy. Journal of Cheminformatics, 2019, 11, 73.	2.8	52
1671	A Universal Quantitative Descriptor of the Dispersion Interaction Potential. Angewandte Chemie, 2019, 131, 9860-9871.	1.6	8
1672	BIOPEP-UWM Database of Bioactive Peptides: Current Opportunities. International Journal of Molecular Sciences, 2019, 20, 5978.	1.8	454
1673	Model Optimization and In Silico Analysis of Potential Dipeptidyl Peptidase IV Antagonists from GC-MS Identified Compounds in Nauclea latifolia Leaf Extracts. International Journal of Molecular Sciences, 2019, 20, 5913.	1.8	11
1674	Network inference with ensembles of bi-clustering trees. BMC Bioinformatics, 2019, 20, 525.	1.2	12
1675	Predicting Meridian in Chinese traditional medicine using machine learning approaches. PLoS Computational Biology, 2019, 15, e1007249.	1.5	41
1676	Structureâ€“Activity Relationships for CYP4B1 Bioactivation of 4-Ipomeanol Congeners: Direct Correlation between Cytotoxicity and Trapped Reactive Intermediates. Chemical Research in Toxicology, 2019, 32, 2488-2498.	1.7	7
1677	Deep learning long-range information in undirected graphs with wave networks. , 2019, , .		8
1678	Molecular docking of novel 5-O-benzoylpinostrobin derivatives as wild type and L858R/T790M/V948R mutant EGFR inhibitor. Journal of Basic and Clinical Physiology and Pharmacology, 2019, 30, .	0.7	8
1679	Datasetâ€™s chemical diversity limits the generalizability of machine learning predictions. Journal of Cheminformatics, 2019, 11, 69.	2.8	57

#	Article	IF	Citations
1680	ChemScanner: extraction and re-use(ability) of chemical information from common scientific documents containing ChemDraw files. Journal of Cheminformatics, 2019, 11, 77.	2.8	7
1681	Evaluation of New Benzimidazole Derivatives as Cysticidal Agents: <i>In Vitro</i>, <i>in Vivo</i> and Docking Studies. Chemical and Pharmaceutical Bulletin, 2019, 67, 1293-1300.	0.6	1
1683	Design of organic structure directing agents to control the synthesis of zeolites for carbon capture and storage. RSC Advances, 2019, 9, 41934-41942.	1.7	1
1684	Comparative comprehension on the anti-rheumatic Chinese herbal medicine Siegesbeckiae Herba: Combined computational predictions and experimental investigations. Journal of Ethnopharmacology, 2019, 228, 200-209.	2.0	22
1685	Application of molecular framework-based data-mining method in the search for beta-secretase 1 inhibitors through drug repurposing. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3674-3685.	2.0	13
1686	Quadrupole Correction: From Molecular Electrostatic Potential to Free Energies of Halogen Bonding. Journal of Chemical Theory and Computation, 2019, 15, 1159-1167.	2.3	13
1687	Predicting drug-target interactions using Lasso with random forest based on evolutionary information and chemical structure. Genomics, 2019, 111, 1839-1852.	1.3	145
1688	Affinity Calculations of Cyclodextrin Hostâ€“Guest Complexes: Assessment of Strengths and Weaknesses of End-Point Free Energy Methods. Journal of Chemical Information and Modeling, 2019, 59, 421-440.	2.5	17
1689	Lone pairs vs. covalent bonds: conformational effects in bicyclo[3.3.1]nonane derivatives. Structural Chemistry, 2019, 30, 509-522.	1.0	7
1690	Synthesis, computational evaluation and pharmacological assessment of acetylsalicylic esters as anti-inflammatory agents. Medicinal Chemistry Research, 2019, 28, 292-299.	1.1	0
1691	Discovery of Potent Inhibitors for the Large Neutral Amino Acid Transporter 1 (LAT1) by Structure-Based Methods. International Journal of Molecular Sciences, 2019, 20, 27.	1.8	38
1692	Structural insights into the substrate binding mechanism of novel ArgA from Mycobacterium tuberculosis. International Journal of Biological Macromolecules, 2019, 125, 970-978.	3.6	4
1693	A Distance-Based Boolean Applicability Domain for Classification of High Throughput Screening Data. Journal of Chemical Information and Modeling, 2019, 59, 463-476.	2.5	13
1694	Similarity-based machine learning support vector machine predictor of drug-drug interactions with improved accuracies. Journal of Clinical Pharmacy and Therapeutics, 2019, 44, 268-275.	0.7	38
1695	ezCADD: A Rapid 2D/3D Visualization-Enabled Web Modeling Environment for Democratizing Computer-Aided Drug Design. Journal of Chemical Information and Modeling, 2019, 59, 18-24.	2.5	47
1696	Common binding sites for cholesterol and neurosteroids on a pentameric ligand-gated ion channel. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2019, 1864, 128-136.	1.2	18
1697	Electrophilic fatty acids impair RAD51 function and potentiate the effects of DNA-damaging agents on growth of triple-negative breast cells. Journal of Biological Chemistry, 2019, 294, 397-404.	1.6	16
1698	Chlorogenic acid attenuates virulence factors and pathogenicity of Pseudomonas aeruginosa by regulating quorum sensing. Applied Microbiology and Biotechnology, 2019, 103, 903-915.	1.7	60

#	Article	IF	Citations
1699	Mitochondrial disfunction and ROS production are essential for anti-Trypanosoma cruzi activity of Î²-lapachone-derived naphthoimidazoles. Free Radical Biology and Medicine, 2019, 130, 408-418.	1.3	32
1700	Evaluating Charge Equilibration Methods To Generate Electrostatic Fields in Nanoporous Materials. Journal of Chemical Theory and Computation, 2019, 15, 382-401.	2.3	70
1701	Antinociceptive properties of 25â€methoxy hispidol A, a triterpinoid isolated from Poncirus trifoliata (Rutaceae) through inhibition of NFâ€ÎºB signalling in mice. Phytotherapy Research, 2019, 33, 327-341.	2.8	43
1702	Molecular Solar Thermal Energy Storage Systems with Long Discharge Times Based on the Dihydroazulene/Vinylheptafulvene Couple. European Journal of Organic Chemistry, 2019, 2019, 1986-1993.	1.2	28
1703	A new chlorinated diphenyl ether and a new sesquilignan from the stems of Mappianthus tomentosus. Phytochemistry Letters, 2019, 30, 49-52.	0.6	5
1704	CoII Complexes with a Tripyridine Ligand, Containing a 2,6-Di-tert-butylphenolic Fragment: Synthesis, Structure, and Formation of Stable Radicals. ACS Omega, 2019, 4, 203-213.	1.6	3
1705	SUV39H1 Represses the Expression of Cytotoxic T-Lymphocyte Effector Genes to Promote Colon Tumor Immune Evasion. Cancer Immunology Research, 2019, 7, 414-427.	1.6	40
1706	PeptoGridâ€"Rescoring Function for AutoDock Vina to Identify New Bioactive Molecules from Short Peptide Libraries. Molecules, 2019, 24, 277.	1.7	14
1707	eToxPred: a machine learning-based approach to estimate the toxicity of drug candidates. BMC Pharmacology & Toxicology, 2019, 20, 2.	1.0	97
1708	FABP4 inhibitors 3D-QSAR model and isosteric replacement of BMS309403 datasets. Data in Brief, 2019, 22, 471-483.	0.5	19
1709	Finding the Right Bricks for Molecular Legos: A Data Mining Approach to Organic Semiconductor Design. Chemistry of Materials, 2019, 31, 969-978.	3.2	38
1710	CycloMolder software: building theoretical cyclodextrin derivatives models and evaluating their host:guest interactions. Journal of Inclusion Phenomena and Macrocyclic Chemistry, 2019, 93, 301-308.	0.9	9
1711	Potential Anti-Cancer Flavonoids Isolated From Caesalpinia bonduc Young Twigs and Leaves: Molecular Docking and In Silico Studies. Bioinformatics and Biology Insights, 2019, 13, 117793221882137.	1.0	40
1712	farPPI: a webserver for accurate prediction of protein-ligand binding structures for small-molecule PPI inhibitors by MM/PB(GB)SA methods. Bioinformatics, 2019, 35, 1777-1779.	1.8	59
1713	Computational Prediction of a New ADMET Endpoint for Small Molecules: Anticommensal Effect on Human Gut Microbiota. Journal of Chemical Information and Modeling, 2019, 59, 1215-1220.	2.5	8
1714	Phloroglucinols from the Roots of Garcinia dauphinensis and Their Antiproliferative and Antiplasmodial Activities. Journal of Natural Products, 2019, 82, 431-439.	1.5	16
1715	TANGO: A high throughâ€put conformation generation and semiempirical methodâ€based optimization tool for ligand molecules. Journal of Computational Chemistry, 2019, 40, 900-909.	1.5	2
1716	In silico analysis of plasmodium falciparum CDPK5 protein through molecular modeling, docking and dynamics. Journal of Theoretical Biology, 2019, 461, 254-267.	0.8	14

#	Article	IF	Citations
1717	Elucidation of the mechanism of complexation between oncocalyxone A and cyclodextrins by isothermal titration calorimetry and molecular modeling. Journal of Molecular Liquids, 2019, 274, 165-172.	2.3	17
1718	Computational Approach to Molecular Catalysis by 3d Transition Metals: Challenges and Opportunities. Chemical Reviews, 2019, 119, 2453-2523.	23.0	260
1719	In Silico Oncology Drug Repositioning and Polypharmacology. Methods in Molecular Biology, 2019, 1878, 243-261.	0.4	48
1720	Effects of Phenothiazines on Aldehyde Oxidase Activity Towards Aldehydes and N-Heterocycles: an In Vitro and In Silico Study. European Journal of Drug Metabolism and Pharmacokinetics, 2019, 44, 275-286.	0.6	4
1721	Design, synthesis and anti-Alzheimerâ€™s activity of novel 1,2,3-triazole-chromenone carboxamide derivatives. Bioorganic Chemistry, 2019, 83, 391-401.	2.0	77
1722	In Silico-Directed Evolution Using CADEE. Methods in Molecular Biology, 2019, 1851, 381-415.	0.4	8
1723	Quantitative and systems pharmacology 4. Network-based analysis of drug pleiotropy on coronary artery disease. European Journal of Medicinal Chemistry, 2019, 161, 192-204.	2.6	25
1724	Computational Methods for Modeling Metalloproteins. Methods in Molecular Biology, 2019, 1876, 245-266.	0.4	5
1725	Extended first-principles thermochemistry for the oxidation of titanium tetrachloride. Combustion and Flame, 2019, 199, 441-450.	2.8	5
1726	Generalized molecular solvation in non-aqueous solutions by a single parameter implicit solvation scheme. Journal of Chemical Physics, 2019, 150, 041710.	1.2	31
1727	A comparative study of the efficiency of HCV NS3/4A protease drugs against different HCV genotypes using in silico approaches. Life Sciences, 2019, 217, 176-184.	2.0	7
1728	Application of anisotropic NMR parameters to the confirmation of molecular structure. Nature Protocols, 2019, 14, 217-247.	5.5	101
1729	Performing an In Silico Repurposing of Existing Drugs by Combining Virtual Screening and Molecular Dynamics Simulation. Methods in Molecular Biology, 2019, 1903, 23-43.	0.4	27
1730	An Application of Computational Drug Repurposing Based on Transcriptomic Signatures. Methods in Molecular Biology, 2019, 1903, 149-177.	0.4	12
1731	Designâ€toâ€Device Approach Affords Panchromatic Coâ€Sensitized Solar Cells. Advanced Energy Materials, 2019, 9, 1802820.	10.2	40
1732	Design of new CD38 inhibitors based on CoMFA modelling and molecular docking analysis of 4â€amino-8-quinoline carboxamides and 2,4-diamino-8-quinazoline carboxamides. SAR and QSAR in Environmental Research, 2019, 30, 21-38.	1.0	6
1733	Isolation and in silico prediction of potential drug-like compounds from Anethum sowa L. root extracts targeted towards cancer therapy. Computational Biology and Chemistry, 2019, 78, 242-259.	1.1	14
1734	Metronidazole aryloxy, carboxy and azole derivatives: Synthesis, anti-tumor activity, QSAR, molecular docking and dynamics studies. Bioorganic and Medicinal Chemistry, 2019, 27, 305-314.	1.4	8

#	Article	IF	Citations
1735	XtalOptÂVersion r12: An open-source evolutionary algorithm for crystal structure prediction. Computer Physics Communications, 2019, 237, 274-275.	3.0	37
1736	Structural characterization of synthetic peptides using electrospray ion mobility spectrometry and molecular dynamics simulations. International Journal of Mass Spectrometry, 2019, 436, 108-117.	0.7	3
1737	Molecular characteristics, proton dissociation properties, and metal binding properties of soil organic matter: A theoretical study. Science of the Total Environment, 2019, 656, 521-530.	3.9	29
1738	Design of antimalarial transmission blocking agents: Pharmacophore mapping of ligands active against stage-V mature gametocytes of Plasmodium falciparum. Journal of Biomolecular Structure and Dynamics, 2019, 37, 3660-3673.	2.0	3
1739	High-Throughput Reconstruction of Ancestral Protein Sequence, Structure, and Molecular Function. Methods in Molecular Biology, 2019, 1851, 135-170.	0.4	15
1740	A novel silver (I) complex of Î±-keto phosphorus ylide: Synthesis, characterization, crystal structure, biomolecular interaction studies, molecular docking and inÂvitro cytotoxic evaluation. Journal of Molecular Structure, 2019, 1177, 430-443.	1.8	14
1741	Characterisation and identification of antibacterial compound from marine actinobacteria: In vitro and in silico analysis. Journal of Infection and Public Health, 2019, 12, 83-89.	1.9	20
1742	Hacking events: Project development practices and technology use at hackathons. Convergence, 2019, 25, 1000-1026.	1.6	26
1743	Web-based drug repurposing tools: a survey. Briefings in Bioinformatics, 2019, 20, 299-316.	3.2	38
1744	An Approach to Reveal the Possible Underlying Mechanisms Inherent to Oecophylla smaragdina as a Biocontrol Agent. Proceedings of the National Academy of Sciences India Section B - Biological Sciences, 2019, 89, 313-319.	0.4	0
1745	Identification of Ideal Multi-targeting Bioactive Compounds Against Mur Ligases of Enterobacter aerogenes and Its Binding Mechanism in Comparison with Chemical Inhibitors. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 135-144.	2.2	5
1746	Computational prediction of drugâ€“target interactions using chemogenomic approaches: an empirical survey. Briefings in Bioinformatics, 2019, 20, 1337-1357.	3.2	182
1747	Homology Modeling of 5-alpha-Reductase 2 Using Available Experimental Data. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 475-484.	2.2	5
1748	Orthosteric and benzodiazepine cavities of the Î±1Î²2Î³2 GABAA receptor: insights from experimentally validated in silico methods. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1597-1615.	2.0	11
1749	Dechlorination of polychlorobiphenyl degradation metabolites by a recombinant glutathione Sâ€transferase from Acidovorax sp. <scp>KKS</scp>102. FEBS Open Bio, 2019, 9, 408-419.	1.0	10
1750	Docking, molecular dynamics, binding energy-MM-PBSA studies of naphthofuran derivatives to identify potential dual inhibitors against BACE-1 and GSK-3Î². Journal of Biomolecular Structure and Dynamics, 2019, 37, 275-290.	2.0	37
1751	Structural basis of flavonoids as dengue polymerase inhibitors: insights from QSAR and docking studies. Journal of Biomolecular Structure and Dynamics, 2019, 37, 104-115.	2.0	24
1752	Identifying potential GluN2B subunit containing N-Methyl-D-aspartate receptor inhibitors: an integrative in silico and molecular modeling approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2533-2545.	2.0	20

#	Article	IF	Citations
1753	In Silico Prediction of Hemolytic Toxicity on the Human Erythrocytes for Small Molecules by Machine-Learning and Genetic Algorithm. Journal of Medicinal Chemistry, 2020, 63, 6499-6512.	2.9	13
1754	Identification of the potential biological target of N-benzenesulfonyl-1,2,3,4-tetrahydroquinoline compounds active against gram-positive and gram-negative bacteria. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2412-2421.	2.0	6
1755	Identification of new DNA gyrase inhibitors based on bioactive compounds from streptomyces: structure-based virtual screening and molecular dynamics simulations approaches. Journal of Biomolecular Structure and Dynamics, 2020, 38, 791-806.	2.0	15
1756	Associating 197ÂChinese herbal medicine with drug targets and diseases using the similarity ensemble approach. Acta Pharmacologica Sinica, 2020, 41, 432-438.	2.8	15
1757	Vibrational spectra, hydrogen bonding analysis and herbicidal activity study of mefenacet: A DFT approach. Journal of Molecular Structure, 2020, 1201, 127203.	1.8	12
1758	Synthesis of cytotoxic urs-12-ene- and 28-norurs-12-ene- type conjugates with amino- and mercapto-1,3,4-oxadiazoles and mercapto-1,2,4-triazoles. Steroids, 2020, 153, 108524.	0.8	16
1759	6-Cinnamoyl-4-arylaminothienopyrimidines as highly potent cytotoxic agents: Design, synthesis and structure-activity relationship studies. European Journal of Medicinal Chemistry, 2020, 185, 111786.	2.6	33
1760	In Vitro Activation of Cytochrome P450 46A1 (CYP46A1) by Efavirenz-Related Compounds. Journal of Medicinal Chemistry, 2020, 63, 6477-6488.	2.9	28
1761	Evaluation of the inhibitory effect of caffeic acid and gallic acid on tetR and tetM efflux pumps mediating tetracycline resistance in Streptococcus sp., using computational approach. Journal of King Saud University - Science, 2020, 32, 904-909.	1.6	11
1762	Mitogen activated protein kinase-1 and cell division control protein-42 are putative targets for the binding of novel natural lead molecules: a therapeutic intervention against Candida albicans. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4584-4599.	2.0	10
1763	Gas-phase structures and thermochemical properties of protonated 5-HMF isomers. International Journal of Mass Spectrometry, 2020, 447, 116237.	0.7	4
1764	A platform for target prediction of phenotypic screening hit molecules. Journal of Molecular Graphics and Modelling, 2020, 95, 107485.	1.3	1
1765	In silico analysis of codon usage and rare codon clusters in the halophilic bacteria L-asparaginase. Biologia (Poland), 2020, 75, 151-160.	0.8	5
1766	Making machine learning a useful tool in the accelerated discovery of transition metal complexes. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1439.	6.2	34
1767	Computational prediction and experimental validation of the activator function of C2-Î²-D-glucopyranosyl-1,3,6,7-tetrahydroxyxanthone on pancreatic and hepatic hexokinase. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2976-2987.	2.0	3
1768	A systematic computational analysis of human matrix metalloproteinase 13 (MMP-13) crystal structures and structure-based identification of prospective drug candidates as MMP-13 inhibitors repurposable for osteoarthritis. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3074-3086.	2.0	3
1769	Potential novel inhibitors against emerging zoonotic pathogen Nipah virus: a virtual screening and molecular dynamics approach. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3225-3234.	2.0	16
1770	Molecular docking and dynamics studies on novel benzene sulfonamide substituted pyrazole-pyrazoline analogues as potent inhibitors of Plasmodium falciparum Histo aspartic protease. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3235-3245.	2.0	20

#	Article	IF	Citations
1771	CB-Dock: a web server for cavity detection-guided proteinâ€“ligand blind docking. Acta Pharmacologica Sinica, 2020, 41, 138-144.	2.8	377
1772	Structure Based Screening for Inhibitory Therapeutics of CTLA-4 Unveiled New Insights About Biology of ACTH. International Journal of Peptide Research and Therapeutics, 2020, 26, 849-859.	0.9	8
1773	Repurposing of FDA-approved drugs to target MurB and MurE enzymes in Mycobacterium tuberculosis. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2521-2532.	2.0	26
1774	Targeting ROS overgeneration by N-benzyl-2-nitro-1-imidazole-acetamide as a potential therapeutic reposition approach for cancer therapy. Investigational New Drugs, 2020, 38, 785-799.	1.2	5
1775	Towards accurate high-throughput ligand affinity prediction by exploiting structural ensembles, docking metrics and ligand similarity. Bioinformatics, 2020, 36, 160-168.	1.8	19
1776	Survey of ribose ring pucker of signaling nucleosides and nucleotides. Nucleosides, Nucleotides and Nucleic Acids, 2020, 39, 322-341.	0.4	4
1777	In vivo antiulcer activity, phytochemical exploration, and molecular modelling of the polyphenolic-rich fraction of Crepis sancta extract. Inflammopharmacology, 2020, 28, 321-331.	1.9	22
1778	In silico screening of anti-inflammatory compounds from Lichen by targeting cyclooxygenase-2. Journal of Biomolecular Structure and Dynamics, 2020, 38, 3544-3562.	2.0	31
1779	The crystal structure and insight into the substrate specificity of the Î±-L rhamnosidase RHA-P from Novosphingobium sp. PP1Y. Archives of Biochemistry and Biophysics, 2020, 679, 108189.	1.4	6
1780	Density Functional Studies of Coenzyme NADPH and Its Oxidized Form NADP+: Structures, UVâ€“Vis Spectra, and the Oxidation Mechanism of NADPH. Journal of Computational Chemistry, 2020, 41, 305-316.	1.5	13
1781	Characterization, inhibitory activity and mechanism of polyphenols from faba bean (gallic-acid and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 Biochemistry and Biotechnology, 2020, 50, 123-132.	1.0	18
1782	Structure-based screening and molecular dynamics simulation studies for the identification of potential acetylcholinesterase inhibitors. Molecular Simulation, 2020, 46, 169-185.	0.9	25
1783	In Silico Identification of Potential Inhibitors of the Wnt Signaling Pathway in Human Breast Cancer. Journal of Computational Biology, 2020, 27, 999-1010.	0.8	6
1784	Quercetin pentaacetate inhibits in vitro human respiratory syncytial virus adhesion. Virus Research, 2020, 276, 197805.	1.1	40
1785	Crossâ€docking benchmark for automated pose and ranking prediction of ligand binding. Protein Science, 2020, 29, 298-305.	3.1	31
1786	Radiation mitigation of the intestinal acute radiation injury in mice by 1â€[(4â€nitrophenyl)sulfonyl]â€4â€phenylpiperazine. Stem Cells Translational Medicine, 2020, 9, 106-119.	1.6	16
1787	Steroid identification via deep learning retention time predictions and two-dimensional gas chromatography-high resolution mass spectrometry. Journal of Chromatography A, 2020, 1612, 460661.	1.8	19
1788	Human CYP1A1 inhibition by flavonoids. Toxicology in Vitro, 2020, 62, 104681.	1.1	20

#	Article	IF	Citations
1789	Deep neural network affinity model for BACE inhibitors in D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 201-217.	1.3	7
1790	Benzimidazole Containing Acetamide Derivatives Attenuate Neuroinflammation and Oxidative Stress in Ethanol-Induced Neurodegeneration. Biomolecules, 2020, 10, 108.	1.8	34
1791	Highly Flexible Ligand Docking: Benchmarking of the DockThor Program on the LEADS-PEP Proteinâ€“Peptide Data Set. Journal of Chemical Information and Modeling, 2020, 60, 667-683.	2.5	144
1792	Computational insights into mechanism of AIM4-mediated inhibition of aggregation of TDP-43 protein implicated in ALS and evidence for in vitro inhibition of liquid-liquid phase separation (LLPS) of TDP-432C-A315T by AIM4. International Journal of Biological Macromolecules, 2020, 147, 117-130.	3.6	22
1793	Toxicities of 4,5-Dihydroisoxazoles Against Root-Knot Nematodes and in Silico Studies of Their Modes of Action. Journal of Agricultural and Food Chemistry, 2020, 68, 523-529.	2.4	11
1794	ReacNetGenerator: an automatic reaction network generator for reactive molecular dynamics simulations. Physical Chemistry Chemical Physics, 2020, 22, 683-691.	1.3	54
1795	IMPRESSION â€“ prediction of NMR parameters for 3-dimensional chemical structures using machine learning with near quantum chemical accuracy. Chemical Science, 2020, 11, 508-515.	3.7	66
1796	Cytotoxic and non-cytotoxic cardiac glycosides isolated from the combined flowers, leaves, and twigs of Streblus asper. Bioorganic and Medicinal Chemistry, 2020, 28, 115301.	1.4	14
1797	The Cap-Snatching SFTSV Endonuclease Domain Is an Antiviral Target. Cell Reports, 2020, 30, 153-163.e5.	2.9	31
1798	Substitution Effects on the Optoelectronic Properties of Coumarin Derivatives. Applied Sciences (Switzerland), 2020, 10, 144.	1.3	17
1799	Archaeal cyclopentane fragment in a surfactant's hydrophobic tail decreases the Krafft point. Soft Matter, 2020, 16, 1333-1341.	1.2	2
1800	DFT study of [Pt(Cl)2L] complex (LÂ=Ârubeanic acid) and its derived compounds with DNA purine bases. Chemical Physics, 2020, 530, 110646.	0.9	3
1801	Rationalization of a traditional liver medicine using systems biology approach and its evaluation in preclinical trial. Computational Biology and Chemistry, 2020, 84, 107196.	1.1	9
1802	ClusPro LigTBM: Automated Template-based Small Molecule Docking. Journal of Molecular Biology, 2020, 432, 3404-3410.	2.0	17
1803	Computational screening of promising beta-secretase 1 inhibitors through multi-step molecular docking and molecular dynamics simulations - Pharmacoinformatics approach. Journal of Molecular Structure, 2020, 1205, 127660.	1.8	22
1804	Computational network biology: Data, models, and applications. Physics Reports, 2020, 846, 1-66.	10.3	126
1805	Identification of a C2-symmetric diol based human immunodeficiency virus protease inhibitor targeting Zika virus NS2B-NS3 protease. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5526-5536.	2.0	9
1806	A non-conformational QSAR study for plant-derived larvicides against Zika Aedes aegypti L. vector. Environmental Science and Pollution Research, 2020, 27, 6205-6214.	2.7	6

#	Article	IF	Citations
1807	Discovery of novel nonpeptide small-molecule NRP1 antagonists: Virtual screening, molecular simulation and structural modification. Bioorganic and Medicinal Chemistry, 2020, 28, 115183.	1.4	7
1808	[1,2,4]Triazolo[1,5-a]pyrimidine derivative (Mol-5) is a new NS5-RdRp inhibitor of DENV2 proliferation and DENV2-induced inflammation. Acta Pharmacologica Sinica, 2020, 41, 706-718.	2.8	18
1809	A novel class of small molecule inhibitors with radioprotective properties. European Journal of Medicinal Chemistry, 2020, 187, 111606.	2.6	7
1810	Combined Linear Interaction Energy and Alchemical Solvation Free-Energy Approach for Protein-Binding Affinity Computation. Journal of Chemical Theory and Computation, 2020, 16, 1300-1310.	2.3	12
1811	Inhibitor discovery for the E. coli meningitis virulence factor IbeA from homology modeling and virtual screening. Journal of Computer-Aided Molecular Design, 2020, 34, 11-25.	1.3	3
1812	Tetrahydroquinoline units in flexible heteroarotinoids (Flex-Hets) convey anti-cancer properties in A2780 ovarian cancer cells. Bioorganic and Medicinal Chemistry, 2020, 28, 115244.	1.4	5
1813	A physicochemical and conformational study of co-solvent effect on the molecular interactions between similarly charged protein surfactant (BSA-SDBS) system. Journal of Chemical Thermodynamics, 2020, 142, 106022.	1.0	32
1814	A Pharmacological Chaperone Therapy for Acute Intermittent Porphyria. Molecular Therapy, 2020, 28, 677-689.	3.7	10
1815	DStruBTarget: Integrating Binding Affinity with Structure Similarity for Ligand-Binding Protein Prediction. Journal of Chemical Information and Modeling, 2020, 60, 400-409.	2.5	5
1816	Benchmarking Electronic Structure Methods for Accurate Fixed-Charge Electrostatic Models. Journal of Chemical Information and Modeling, 2020, 60, 249-258.	2.5	12
1817	Design and synthesis of benzodiazepine-1,2,3-triazole hybrid derivatives as selective butyrylcholinesterase inhibitors. Molecular Diversity, 2020, 24, 997-1013.	2.1	17
1818	Use of three-dimensional descriptors in molecular design for biologically active compounds. Current Opinion in Chemical Engineering, 2020, 27, 60-64.	3.8	8
1819	Novel structured diacylglycerol (DAG) rich oleo formulations activate the Nrf2 pathway and impedes NF-Îº B translocation to mitigate pre-clinical conditions of hypertension. Journal of Functional Foods, 2020, 64, 103650.	1.6	1
1820	Deep learning of pharmacogenomics resources: moving towards precision oncology. Briefings in Bioinformatics, 2020, 21, 2066-2083.	3.2	43
1821	The index of ideality of correlation: A statistical yardstick for better QSAR modeling of glucokinase activators. Structural Chemistry, 2020, 31, 831-839.	1.0	33
1822	Machine Learning Enabled Tailor-Made Design of Application-Specific Metalâ€“Organic Frameworks. ACS Applied Materials & Interfaces, 2020, 12, 734-743.	4.0	42
1823	Implementation of permeation rules leads to a FabI inhibitor with activity against Gram-negative pathogens. Nature Microbiology, 2020, 5, 67-75.	5.9	87
1824	Mutation studies and structure-based identification of potential inhibitor molecules against periplasmic amino acid binding protein of Candidatus Liberibacter asiaticus (CLasTcyA). International Journal of Biological Macromolecules, 2020, 147, 1228-1238.	3.6	23

#	Article	IF	Citations
1825	Development of classification models for identification of important structural features of isoform-selective histone deacetylase inhibitors (class I). Molecular Diversity, 2020, 24, 1077-1094.	2.1	4
1826	The mechanism of high affinity pentasaccharide binding to antithrombin, insights from Gaussian accelerated molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2020, 38, 4718-4732.	2.0	10
1827	In silico drug repurposing for the identification of potential candidate molecules against arboviruses infection. Antiviral Research, 2020, 173, 104668.	1.9	19
1828	A novel hybrid Harris hawks optimization and support vector machines for drug design and discovery. Computers and Chemical Engineering, 2020, 133, 106656.	2.0	161
1829	Identifying potential entry inhibitors for emerging Nipah virus by molecular docking and chemical-protein interaction network. Journal of Biomolecular Structure and Dynamics, 2020, 38, 5108-5125.	2.0	15
1830	Discovery of 5-aryl-3-thiophen-2-yl-1H-pyrazoles as a new class of Hsp90 inhibitors in hepatocellular carcinoma. Bioorganic Chemistry, 2020, 94, 103433.	2.0	8
1831	Identification of Potential Carbonic Anhydrase Inhibitors for Glaucoma Treatment Through an In-Silico Approach. International Journal of Peptide Research and Therapeutics, 2020, 26, 2147-2154.	0.9	7
1832	Novel cyclohexanone compound as a potential ligand against SARS-CoV-2 main-protease. Microbial Pathogenesis, 2020, 149, 104546.	1.3	30
1833	Structural Basis for the Inhibitor and Substrate Specificity of the Unique Fph Serine Hydrolases of Staphylococcus aureus. ACS Infectious Diseases, 2020, 6, 2771-2782.	1.8	14
1834	Predicting binding sites from unbound versus bound protein structures. Scientific Reports, 2020, 10, 15856.	1.6	17
1835	Data-powered augmented volcano plots for homogeneous catalysis. Chemical Science, 2020, 11, 12070-12080.	3.7	23
1836	Stochastic simulation of nonequilibrium heat conduction in extended molecular junctions. Journal of Chemical Physics, 2020, 153, 144113.	1.2	11
1837	Pain Chemogenomics Knowledgebase (Pain-CKB) for Systems Pharmacology Target Mapping and Physiologically Based Pharmacokinetic Modeling Investigation of Opioid Drugâ€“Drug Interactions. ACS Chemical Neuroscience, 2020, 11, 3245-3258.	1.7	2
1838	Molecular force fields with gradient-domain machine learning (GDML): Comparison and synergies with classical force fields. Journal of Chemical Physics, 2020, 153, 124109.	1.2	25
1839	Machine Learning Models of Vibrating H₂CO: Comparing Reproducing Kernels, FCHL, and PhysNet. Journal of Physical Chemistry A, 2020, 124, 8853-8865.	1.1	24
1840	An immersive journey to the molecular structure of SARS-CoV-2: Virtual reality in COVID-19. Computational and Structural Biotechnology Journal, 2020, 18, 2621-2628.	1.9	16
1841	Identification and validation of a novel anti-virulent that binds to pyoverdine and inhibits its function. Virulence, 2020, 11, 1293-1309.	1.8	11
1842	Detergent Properties of Coconut Oil Derived N-Acyl Prolinate Surfactant and the In silico Studies on its Effectiveness Against SARS-CoV-2 (COVID-19). Tenside, Surfactants, Detergents, 2020, 57, 361-374.	0.5	6

#	Article	IF	Citations
1843	Discovery of human coronaviruses pan-papain-like protease inhibitors using computational approaches. Journal of Pharmaceutical Analysis, 2020, 10, 546-559.	2.4	67
1844	Design of novel viral attachment inhibitors of the spike glycoprotein (S) of severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2) through virtual screening and dynamics. International Journal of Antimicrobial Agents, 2020, 56, 106177.	1.1	21
1845	Using Chouâ€™s 5-steps rule to study pharmacophore-based virtual screening of SARS-CoV-2 Mpro inhibitors. Molecular Diversity, 2021, 25, 1731-1744.	2.1	12
1846	Structural basis for the inhibition of SARS-CoV2 main protease by Indian medicinal plant-derived antiviral compounds. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1970-1978.	2.0	30
1847	Performance of Force-Field- and Machine Learning-Based Scoring Functions in Ranking MAO-B Proteinâ€“Inhibitor Complexes in Relevance to Developing Parkinsonâ€™s Therapeutics. International Journal of Molecular Sciences, 2020, 21, 7648.	1.8	9
1848	Design, synthesis, molecular docking study, and antibacterial evaluation of some new fluoroquinolone analogues bearing a quinazolinone moiety. DARU, Journal of Pharmaceutical Sciences, 2020, 28, 661-672.	0.9	16
1849	Targeting the 3CLpro and RdRp of SARS-CoV-2 with phytochemicals from medicinal plants of the Andean Region: molecular docking and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2010-2023.	2.0	48
1850	Regioisomerization of Antimalarial Drug WR99210 Explains the Inactivity of a Commercial Stock. Antimicrobial Agents and Chemotherapy, 2020, 65, .	1.4	3
1851	Finding potent inhibitors for COVID-19 main protease (M^{pro}): anin silicoapproach using SARS-CoV-3CL protease inhibitors for combating CORONA. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1534-1545.	2.0	22
1852	Structural-based virtual screening and in vitro assays for small molecules inhibiting the feline coronavirus 3CL protease as a surrogate platform for coronaviruses. Antiviral Research, 2020, 182, 104927.	1.9	9
1853	An in silico approach to identify potential medicinal plants for treating Alzheimer disease: a case study with acetylcholinesterase. Journal of Biomolecular Structure and Dynamics, 2020, , 1-13.	2.0	9
1854	Computational studies of the properties and activities of selected trisubstituted benzimidazoles as potential antitubercular drugs inhibiting MTB-FtsZ polymerization. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1558-1570.	2.0	9
1855	Maximum common property: a new approach for molecular similarity. Journal of Cheminformatics, 2020, 12, 61.	2.8	3
1856	Antibacterial of Dibenzo-p-Dioxi-2,8-Dicarboxylic Acid Against Pathogenic Oral Bacteria E. faecalis ATCC 29212 Peptide Pheromones: Quorum Sensing of in vitro and in silico Study . Drug Design, Development and Therapy, 2020, Volume 14, 3079-3086.	2.0	1
1857	Novel 3,4-diarylpyrazole as prospective anti-cancerous agents. Heliyon, 2020, 6, e04397.	1.4	2
1858	Evaluation of Assay Central Machine Learning Models for Rat Acute Oral Toxicity Prediction. ACS Sustainable Chemistry and Engineering, 2020, 8, 16020-16027.	3.2	15
1859	In silico toxicity evaluation of Salubrinal and its analogues. European Journal of Pharmaceutical Sciences, 2020, 155, 105538.	1.9	12
1860	Leveraging Uncertainty in Machine Learning Accelerates Biological Discovery and Design. Cell Systems, 2020, 11, 461-477.e9.	2.9	92

#	Article	IF	Citations
1861	Antidiabetic and cytotoxic polyhydroxylated oleanane and ursane type triterpenoids from Salvia grossheimii. Bioorganic Chemistry, 2020, 104, 104297.	2.0	13
1862	In silico identification of novel PrfA inhibitors to fight listeriosis: A virtual screening and molecular dynamics studies. Journal of Molecular Graphics and Modelling, 2020, 101, 107728.	1.3	1
1863	Piceatannol reduces resistance to statins in hypercholesterolemia by reducing PCSK9 expression through p300 acetyltransferase inhibition. Pharmacological Research, 2020, 161, 105205.	3.1	8
1864	Synthesis, structural characterization, Hirshfeld surface and DFT based reactivity, UV filter and NLO studies of Schiff base analogue of 4-aminoantipyrine. Results in Chemistry, 2020, 2, 100062.	0.9	17
1865	In silico exploration of small-molecule Î±-helix mimetics as inhibitors of SARS-COV-2 attachment to ACE2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1546-1557.	2.0	7
1866	Exploration of the mechanism of traditional Chinese medicine by AI approach using unsupervised machine learning for cellular functional similarity of compounds in heterogeneous networks, XiaoErFuPi granules as an example. Pharmacological Research, 2020, 160, 105077.	3.1	21
1867	Comparison of umbrella sampling and steered molecular dynamics methods for computing free energy profiles of aromatic substrates through phospholipid bilayers. Journal of Chemical Physics, 2020, 153, 034115.	1.2	15
1868	NetInfer: A Web Server for Prediction of Targets and Therapeutic and Adverse Effects via Network-Based Inference Methods. Journal of Chemical Information and Modeling, 2020, 60, 3687-3691.	2.5	23
1869	Design and Synthesis of a Highly Selective and In Vivo-Capable Inhibitor of the Second Bromodomain of the Bromodomain and Extra Terminal Domain Family of Proteins. Journal of Medicinal Chemistry, 2020, 63, 9070-9092.	2.9	40
1870	Quantum chemical calculations for over 200,000 organic radical species and 40,000 associated closed-shell molecules. Scientific Data, 2020, 7, 244.	2.4	49
1871	Cyanobacterial metabolites as promising drug leads against the M^{pro}and PL^{pro}of SARS-CoV-2: anin silicoanalysis. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6218-6230.	2.0	35
1872	COVID-19 Docking Server: a meta server for docking small molecules, peptides and antibodies against potential targets of COVID-19. Bioinformatics, 2020, 36, 5109-5111.	1.8	122
1873	Predicting phosphirane air stability using density functional theory. Journal of Physical Organic Chemistry, 2020, 33, e4110.	0.9	0
1874	Proposed model of the Dictyostelium cAMP receptors bound to cAMP. Journal of Molecular Graphics and Modelling, 2020, 100, 107662.	1.3	4
1875	Evolving geographic diversity in SARS-CoV2 and in silico analysis of replicating enzyme 3CLpro targeting repurposed drug candidates. Journal of Translational Medicine, 2020, 18, 278.	1.8	29
1876	A simple open source bioinformatic methodology for initial exploration of GPCR ligandsâ€™ agonistic/antagonistic properties. Pharmacology Research and Perspectives, 2020, 8, e00600.	1.1	7
1877	Designing Singlet Fission Candidates from Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2020, 32, 6515-6524.	3.2	27
1878	Highly selective and potent anti-cancer agents based on 2,9-substituted-1,10-phenanthroline derivatives. Inorganic Chemistry Communication, 2020, 119, 108085.	1.8	2

#	Article	IF	Citations
1879	Spectroscopic and molecular structure investigation of Propachlor herbicide: A combined experimental and theoretical study. Journal of Molecular Structure, 2020, 1221, 128866.	1.8	6
1880	Design, synthesis, in vitro evaluation and molecular docking study of N'-Arylidene imidazo [1,2-a] pyridine -2-carbohydrazide derivatives as novel Tyrosinase inhibitors. Journal of Molecular Structure, 2020, 1222, 128876.	1.8	12
1881	Toward a Computational Ecotoxicity Assay. Journal of Chemical Information and Modeling, 2020, 60, 3792-3803.	2.5	5
1882	Computer-aided screening for potential TMPRSS2 inhibitors: a combination of pharmacophore modeling, molecular docking and molecular dynamics simulation approaches. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5638-5656.	2.0	55
1883	Integration of modern computational chemistry and <scp>ASPEN PLUS</scp> for chemical process design. AICHE Journal, 2020, 66, e16987.	1.8	6
1884	Artificial Intelligence-Based Drug Design and Discovery. , 2020, , .		6
1885	Probabilistic identification of saccharide moieties in biomolecules and their protein complexes. Scientific Data, 2020, 7, 210.	2.4	4
1886	Challenges and opportunities of automated proteinâ€protein docking: HDOCK server vs human predictions in CAPRI <scp>Rounds</scp> 38â€46. Proteins: Structure, Function and Bioinformatics, 2020, 88, 1055-1069.	1.5	10
1887	Self-Learning Molecular Design for High Lithium-Ion Conductive Ionic Liquids using Maze Game. Journal of Chemical Information and Modeling, 2020, 60, 4904-4911.	2.5	4
1888	Identification of Small Moleculeâ€“miRNA Associations with Graph Regularization Techniques in Heterogeneous Networks. Journal of Chemical Information and Modeling, 2020, 60, 6709-6721.	2.5	11
1889	LigGrep: a tool for filtering docked poses to improve virtual-screening hit rates. Journal of Cheminformatics, 2020, 12, 69.	2.8	16
1890	Virtual screening and molecular simulation study of natural products database for lead identification of novel coronavirus main protease inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3655-3667.	2.0	29
1891	MetaADEDB 2.0: a comprehensive database on adverse drug events. Bioinformatics, 2021, 37, 2221-2222.	1.8	8
1892	Target-Centered Drug Repurposing Predictions of Human Angiotensin-Converting Enzyme 2 (ACE2) and Transmembrane Protease Serine Subtype 2 (TMPRSS2) Interacting Approved Drugs for Coronavirus Disease 2019 (COVID-19) Treatment through a Drug-Target Interaction Deep Learning Model. Viruses, 2020, 12, 1325.	1.5	24
1893	Ilimaquinone (marine sponge metabolite) as a novel inhibitor of SARS-CoV-2 key target proteins in comparison with suggested COVID-19 drugs: designing, docking and molecular dynamics simulation study. RSC Advances, 2020, 10, 37707-37720.	1.7	57
1894	Virtual screening of anti-HIV1 compounds against SARS-CoV-2: machine learning modeling, chemoinformatics and molecular dynamics simulation based analysis. Scientific Reports, 2020, 10, 20397.	1.6	41
1895	Targeting the GRP78-Dependant SARS-CoV-2 Cell Entry by Peptides and Small Molecules. Bioinformatics and Biology Insights, 2020, 14, 117793222096550.	1.0	45
1896	Molecular docking studies of phytocompounds ofRheum emodiWall with proteins responsible for antibiotic resistance in bacterial and fungal pathogens:in silicoapproach to enhance the bio-availability of antibiotics. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3789-3803.	2.0	24

#	Article	IF	Citations
1897	Interaction of Chloramphenicol Cationic Peptide Analogues with the Ribosome. Biochemistry (Moscow), 2020, 85, 1443-1457.	0.7	2
1898	The active site of magnesium chelatase. Nature Plants, 2020, 6, 1491-1502.	4.7	27
1899	Retention of antibiotic activity against resistant bacteria harbouring aminoglycoside-N-acetyltransferase enzyme by adjuvants: a combination of in-silico and in-vitro study. Scientific Reports, 2020, 10, 19381.	1.6	14
1900	Role of cardiac drugs and flavonoids on the IRE1â€“JNK pathway as revealed by re-ranked molecular docking scores, MM/PBSA and umbrella sampling. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3428-3450.	2.0	2
1901	Carfilzomib as a potential inhibitor of NADH-dependent enoyl-acyl carrier protein reductases ofKlebsiella pneumoniaeandMycobacterium tuberculosisas a drug target enzyme: insights from molecular docking and molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4021-4037.	2.0	8
1902	Supporting SARS-CoV-2 Papain-Like Protease Drug Discovery: In silico Methods and Benchmarking. Frontiers in Chemistry, 2020, 8, 592289.	1.8	33
1903	N-(Pyrimidin-2-yl)-1,2,3,4-tetrahydroisoquinolin-6-amine Derivatives as Selective Janus Kinase 2 Inhibitors for the Treatment of Myeloproliferative Neoplasms. Journal of Medicinal Chemistry, 2020, 63, 14921-14936.	2.9	12
1904	In-silico drug repurposing for targeting SARS-CoV-2 main protease (M^{pro}). Journal of Biomolecular Structure and Dynamics, 2022, 40, 3003-3010.	2.0	31
1905	Raltegravir, Indinavir, Tipranavir, Dolutegravir, and Etravirine against main protease and RNA-dependent RNA polymerase of SARS-CoV-2: A molecular docking and drug repurposing approach. Journal of Infection and Public Health, 2020, 13, 1856-1861.	1.9	44
1906	Screening of Human CYP1A2 and CYP3A4 Inhibitors from Seaweed In Silico and In Vitro. Marine Drugs, 2020, 18, 603.	2.2	21
1907	Interaction between the Lentil Lipid Transfer Protein Lc-LTP2 and Its Novel Signal Ligand PI(4,5)P2. Membranes, 2020, 10, 357.	1.4	6
1908	FragRep: A Web Server for Structure-Based Drug Design by Fragment Replacement. Journal of Chemical Information and Modeling, 2020, 60, 5900-5906.	2.5	16
1909	Computational guided identification of novel potent inhibitors of N-terminal domain of nucleocapsid protein of severe acute respiratory syndrome coronavirus 2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4084-4099.	2.0	31
1910	Developing a Kinase-Specific Target Selection Method Using a Structure-Based Machine Learning Approach . Advances and Applications in Bioinformatics and Chemistry, 2020, Volume 13, 27-40.	1.6	2
1911	Structural characterization and in vitro lipid binding studies of non-specific lipid transfer protein 1 (nsLTP1) from fennel (Foeniculum vulgare) seeds. Scientific Reports, 2020, 10, 21243.	1.6	13
1912	Predicting multi-enzyme inhibition in the arachidonic acid metabolic network by Heritiera fomes extracts. Journal of Biomolecular Structure and Dynamics, 2020, , 1-14.	2.0	1
1913	Complex reaction processes in combustion unraveled by neural network-based molecular dynamics simulation. Nature Communications, 2020, 11, 5713.	5.8	111
1914	Epitope-Based Immunoinformatics Approach on Nucleocapsid Protein of Severe Acute Respiratory Syndrome-Coronavirus-2. Molecules, 2020, 25, 5088.	1.7	33

#	Article	IF	Citations
1915	Extreme Low-Temperature Combustion Chemistry: Ozone-Initiated Oxidation of Methyl Hexanoate. Journal of Physical Chemistry A, 2020, 124, 9897-9914.	1.1	13
1916	Identification of natural inhibitors against prime targets of SARS-CoV-2 using molecular docking, molecular dynamics simulation and MM-PBSA approaches. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3296-3311.	2.0	31
1917	LigMate: A Multifeature Integration Algorithm for Ligand-Similarity-Based Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 6044-6053.	2.5	8
1918	Trapping conformational states of a flavin-dependent N-monooxygenase in crystallo reveals protein and flavin dynamics. Journal of Biological Chemistry, 2020, 295, 13239-13249.	1.6	13
1919	A comprehensivein silicoexploration of pharmacological properties, bioactivities and COX-2 inhibitory potential of eleutheroside B fromEleutherococcus senticosus(Rupr. & Maxim.) Maxim.. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6553-6566.	2.0	19
1920	Elucidation of phytomedicinal efficacies of Clerodendrum inerme (L.) Gaertn. (Wild Jasmine). South African Journal of Botany, 2021, 140, 356-364.	1.2	2
1921	Classifying disease-associated variants using measures of protein activity and stability. , 2020, , 91-107.		21
1922	Structure-based virtual screening and molecular dynamics of phytochemicals derived from Saudi medicinal plants to identify potential COVID-19 therapeutics. Arabian Journal of Chemistry, 2020, 13, 7224-7234.	2.3	43
1923	Anti-HCV and anti-malaria agent, potential candidates to repurpose for coronavirus infection: Virtual screening, molecular docking, and molecular dynamics simulation study. Life Sciences, 2020, 258, 118205.	2.0	69
1924	The Literature of Chemoinformatics: 1978â€“2018. International Journal of Molecular Sciences, 2020, 21, 5576.	1.8	9
1925	Enantioselective sensing of (S)-Thalidomide in blood plasma with a chiral naphthalene diimide derivative. Biosensors and Bioelectronics, 2020, 167, 112446.	5.3	10
1926	Identification of SARS-CoV-2 Cell Entry Inhibitors by Drug Repurposing Using in silico Structure-Based Virtual Screening Approach. Frontiers in Immunology, 2020, 11, 1664.	2.2	163
1927	Preparation and characterization of spiro-acridine derivative and 2-hydroxypropyl-Î²-cyclodextrin inclusion complex. Journal of Molecular Structure, 2020, 1222, 128945.	1.8	9
1928	PyPLIF HIPPOS: A Molecular Interaction Fingerprinting Tool for Docking Results of AutoDock Vina and PLANTS. Journal of Chemical Information and Modeling, 2020, 60, 3697-3702.	2.5	14
1929	Potential mechanism prediction of Cold-Damp Plague Formula against COVID-19 via network pharmacology analysis and molecular docking. Chinese Medicine, 2020, 15, 78.	1.6	24
1930	Structure-based virtual screening of phytochemicals and repurposing of FDA approved antiviral drugs unravels lead molecules as potential inhibitors of coronavirus 3C-like protease enzyme. Journal of King Saud University - Science, 2020, 32, 2845-2853.	1.6	30
1931	Reactive Molecular Dynamics Study on the Effect of H₂O on the Thermal Decomposition of Ammonium Dinitramide. Propellants, Explosives, Pyrotechnics, 2020, 45, 1590-1599.	1.0	7
1932	In silico methods predict new blood-brain barrier permeable structure for the inhibition of kynurenine 3-monooxygenase. Journal of Molecular Graphics and Modelling, 2020, 100, 107701.	1.3	3

#	Article	IF	Citations
1933	Chemical space and diversity of seaweed metabolite database (SWMD): A cheminformatics study. Journal of Molecular Graphics and Modelling, 2020, 100, 107702.	1.3	8
1934	DUBS: A Framework for Developing <u>D</u>irectory of <u>U</u>seful <u>B</u>enchmarking <u>S</u>ets for Virtual Screening. Journal of Chemical Information and Modeling, 2020, 60, 4137-4143.	2.5	2
1935	Molecular dynamics simulation for screening phytochemicals as Î±-amylase inhibitors from medicinal plants. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6524-6538.	2.0	31
1936	In silico drug design and molecular docking studies targeting Art1 (RAC-alpha) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 6 investigation of CYP (cytochrome P450) inhibitors against MAOB (monoamine oxidase B) for OSCC (oral squamous cell carcinoma) treatment. Journal of Biomolecular Structure and Dynamics, 2021, 39, 6467-6479.	2.0	19
1937	Modeling and simulation study to identify threonine synthase as possible drug target in Leishmania major. Molecular Diversity, 2021, 25, 1679-1700.	2.1	5
1938	Evaluation of the gastrointestinal anti-motility effect of Anacardium occidentale stem bark extract: A mechanistic study of antidiarrheal activity. Journal of Pharmaceutical Analysis, 2021, 11, 776-782.	2.4	3
1939	Bioactive Conformational Ensemble Server and Database. A Public Framework to Speed Up In Silico Drug Discovery. Journal of Chemical Theory and Computation, 2020, 16, 6586-6597.	2.3	10
1940	Analytical Model of Electron Density and Its Machine Learning Inference. Journal of Chemical Information and Modeling, 2020, 60, 3831-3842.	2.5	17
1941	Large-scale comparison of 3d and 4d transition metal complexes illuminates the reduced effect of exchange on second-row spin-state energetics. Physical Chemistry Chemical Physics, 2020, 22, 19326-19341.	1.3	20
1942	Immunoinformatics-guided design of an epitope-based vaccine against severe acute respiratory syndrome coronavirus 2 spike glycoprotein. Computers in Biology and Medicine, 2020, 124, 103967.	3.9	62
1943	Are In Silico Approaches Applicable As a First Step for the Prediction of e-Liquid Toxicity in e-Cigarettes?. Chemical Research in Toxicology, 2020, 33, 2381-2389.	1.7	1
1944	Exploring the Conformational Landscape of Bioactive Small Molecules. Journal of Chemical Theory and Computation, 2020, 16, 6575-6585.	2.3	17
1945	Understanding the diversity of the metal-organic framework ecosystem. Nature Communications, 2020, 11, 4068.	5.8	282
1946	Understanding the role of galectin inhibitors as potential candidates for SARS-CoV-2 spike protein: in silico studies. RSC Advances, 2020, 10, 29873-29884.	1.7	23
1947	In silico exploration of the fingerprints triggering modulation of glutaminyl cyclase inhibition for the treatment of Alzheimerâ€™s disease using SMILES based attributes in Monte Carlo optimization. Journal of Biomolecular Structure and Dynamics, 2021, 39, 7181-7193.	2.0	10
1948	Laser irradiated phenothiazines: New potential treatment for COVID-19 explored by molecular docking. Journal of Photochemistry and Photobiology B: Biology, 2020, 211, 111997.	1.7	28
1949	Identification of a repurposed drug as an inhibitor of Spike protein of human coronavirus SARS-CoV-2 by computational methods. Journal of Biosciences, 2020, 45, 1.	0.5	40
1950	Structure elucidation of small organic molecules by contemporary computational chemistry methods. Archives of Pharmacal Research, 2020, 43, 1114-1127.	2.7	18

#	Article	IF	Citations
1951	Chemical analysis and in silico anticancer and anti-inflammatory potentials of bioactive compounds from Moringaoleifera seed oil. Advances in Traditional Medicine, 2022, 22, 59-74.	1.0	4
1952	Gastroprotective activity of Hypericum perforatum extract in ethanol-induced gastric mucosal injury in Wistar rats: A possible involvement of H+/K+ ATPase Î± inhibition. Heliyon, 2020, 6, e05249.	1.4	9
1953	GridSolvate: A Web Server for the Prediction of Biomolecular Hydration Properties. Journal of Chemical Information and Modeling, 2020, 60, 5907-5911.	2.5	2
1954	Anin-silicoanalysis of ivermectin interaction with potential SARS-CoV-2 targets and host nuclear importin Î±. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2851-2864.	2.0	33
1955	Cloud 3D-QSAR: a web tool for the development of quantitative structureâ€“activity relationship models in drug discovery. Briefings in Bioinformatics, 2021, 22, .	3.2	36
1956	Polyphenolic rich extract of Oroxylum indicum alleviate Î²-glucuronidase activity via down-regulate oxidative stress: Experimental and computational studies. Biocatalysis and Agricultural Biotechnology, 2020, 29, 101804.	1.5	8
1957	PubChemQC PM6: Data Sets of 221 Million Molecules with Optimized Molecular Geometries and Electronic Properties. Journal of Chemical Information and Modeling, 2020, 60, 5891-5899.	2.5	36
1958	Antagonistic interaction between TTA-A2 and paclitaxel for anti-cancer effects by complex formation with T-type calcium channel. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2395-2406.	2.0	19
1959	Predicting target profiles with confidence as a service using docking scores. Journal of Cheminformatics, 2020, 12, .	2.8	2
1960	Virtual Double-System Single-Box: A Nonequilibrium Alchemical Technique for Absolute Binding Free Energy Calculations: Application to Ligands of the SARS-CoV-2 Main Protease. Journal of Chemical Theory and Computation, 2020, 16, 7160-7172.	2.3	27
1961	Prevention of SARS-CoV-2 cell entry: insight fromin silicointeraction of drug-like alkaloids with spike glycoprotein, human ACE2, and TMPRSS2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2121-2145.	2.0	39
1962	TMLRpred: A machine learning classification model to distinguish reversible EGFR double mutant inhibitors. Chemical Biology and Drug Design, 2020, 96, 921-930.	1.5	6
1963	High-throughput virtual screening of drug databanks for potential inhibitors of SARS-CoV-2 spike glycoprotein. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2099-2112.	2.0	28
1964	Binding mechanism and structural insights into the identified protein target of COVID-19 and importin-Î± within-vitroeffective drug ivermectin. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2217-2226.	2.0	44
1965	InstaDock: A single-click graphical user interface for molecular docking-based virtual high-throughput screening. Briefings in Bioinformatics, 2021, 22, .	3.2	127
1966	Profiling SARS-CoV-2 Main Protease (M^{PRO}) Binding to Repurposed Drugs Using Molecular Dynamics Simulations in Classical and Neural Network-Trained Force Fields. ACS Combinatorial Science, 2020, 22, 826-832.	3.8	29
1967	In silico analysis of the interactions of certain flavonoids with the receptor-binding domain of 2019 novel coronavirus and cellular proteases and their pharmacokinetic properties. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2460-2474.	2.0	22
1968	The pathogenic S688Y mutation in the ligand-binding domain of the GluN1 subunit regulates the properties of NMDA receptors. Scientific Reports, 2020, 10, 18576.	1.6	13

#	Article	IF	Citations
1969	Anti-staphylococcal activity and mode of action of thioridazine photoproducts. Scientific Reports, 2020, 10, 18043.	1.6	21
1970	Training atomic neural networks using fragment-based data generated in virtual reality. Journal of Chemical Physics, 2020, 153, 154105.	1.2	16
1971	Energetic and thermodynamical aspects of the cyclodextrins-cannabidiol complex in aqueous solution: a molecular-dynamics study. European Biophysics Journal, 2020, 49, 571-589.	1.2	8
1972	An open source chemical structure curation pipeline using RDKit. Journal of Cheminformatics, 2020, 12, 51.	2.8	166
1973	Pharmacoinformatics and hypothetical studies on allicin, curcumin, and gingerol as potential candidates against COVID-19-associated proteases. Journal of Biomolecular Structure and Dynamics, 2022, 40, 389-400.	2.0	40
1974	Extending the identification of structural features responsible for anti-SARS-CoV activity of peptide-type compounds using QSAR modelling. SAR and QSAR in Environmental Research, 2020, 31, 643-654.	1.0	24
1975	TAML- and Buffer-Catalyzed Oxidation of Picric Acid by H2O2: Products, Kinetics, DFT, and the Mechanism of Dual Catalysis. Inorganic Chemistry, 2020, 59, 13223-13232.	1.9	4
1976	Discovery of an Inhibitor for the TREK-1 Channel Targeting an Intermediate Transition State of Channel Gating. Journal of Medicinal Chemistry, 2020, 63, 10972-10983.	2.9	6
1977	Structural Comparison of Diverse HIV-1 Subtypes using Molecular Modelling and Docking Analyses of Integrase Inhibitors. Viruses, 2020, 12, 936.	1.5	8
1978	Structure-based inhibitors targeting the alpha-helical domain of the Spiroplasma melliferum histone-like HU protein. Scientific Reports, 2020, 10, 15128.	1.6	11
1979	Pharmacoinformatic Investigation of Medicinal Plants from East Africa. Molecular Informatics, 2020, 39, e2000163.	1.4	28
1980	Dissecting Molecular Principles of the Hsp90 Chaperone Regulation by Allosteric Modulators Using a Hierarchical Simulation Approach and Network Modeling of Allosteric Interactions: Conformational Selection Dictates the Diversity of Protein Responses and Ligand-Specific Functional Mechanisms. Journal of Chemical Theory and Computation, 2020, 16, 6656-6677.	2.3	3
1981	Repurposing of the approved small molecule drugs in order to inhibit SARS-CoV-2â€‰S protein and human ACE2 interaction through virtual screening approaches. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1299-1315.	2.0	38
1982	Computer-Aided Analysis of Multiple SARS-CoV-2 Therapeutic Targets: Identification of Potent Molecules from African Medicinal Plants. Scientifica, 2020, 2020, 1-25.	0.6	8
1983	In silico Prediction of New Drug Candidates Against the Multidrug-Resistant and Potentially Zoonotic Fish Pathogen Serotype III Streptococcus agalactiae. Frontiers in Genetics, 2020, 11, 1024.	1.1	3
1984	In silico structure modelling of SARS-CoV-2 Nsp13 helicase and Nsp14 and repurposing of FDA approved antiviral drugs as dual inhibitors. Gene Reports, 2020, 21, 100860.	0.4	55
1985	Computational insights into the binding mode of curcumin analogues against EP300 HAT domain as potent acetyltransferase inhibitors. Journal of Molecular Graphics and Modelling, 2020, 101, 107756.	1.3	2
1986	A dynamic simulation study of FDA drug from zinc database against COVID-19 main protease receptor. Journal of Biomolecular Structure and Dynamics, 2022, 40, 1084-1100.	2.0	18

#	Article	IF	Citations
1987	AMDock: a versatile graphical tool for assisting molecular docking with Autodock Vina and Autodock4. Biology Direct, 2020, 15, 12.	1.9	119
1988	Synthesis and Structureâ€“Activity Relationship of Dual-Stage Antimalarial Pyrazolo[3,4-b]pyridines. Journal of Medicinal Chemistry, 2020, 63, 11902-11919.	2.9	20
1989	Identification of a nanomolar affinity Î±-synuclein fibril imaging probe by ultra-high throughput in silico screening. Chemical Science, 2020, 11, 12746-12754.	3.7	30
1990	Short-chain dehydrogenase/reductase, PsDeHase, from opium poppy: putative involvement in papaverine biosynthesis. Plant Cell, Tissue and Organ Culture, 2020, 143, 431-440.	1.2	3
1991	Discovery of potent inhibitors for SARS-CoV-2's main protease by ligand-based/structure-based virtual screening, MD simulations, and binding energy calculations. Physical Chemistry Chemical Physics, 2020, 22, 23099-23106.	1.3	29
1992	In vitro and in silico Determination of the Interaction of Artemisinin with Human Serum Albumin. Molecular Biology, 2020, 54, 586-598.	0.4	4
1993	Blood pressure-lowering effects of a Bowman-Birk inhibitor and its derived peptides in normotensive and hypertensive rats. Scientific Reports, 2020, 10, 11680.	1.6	9
1994	In Silico Identification of Potential Natural Product Inhibitors of Human Proteases Key to SARS-CoV-2 Infection. Molecules, 2020, 25, 3822.	1.7	51
1995	Targeting homologous recombination (HR) repair mechanism for cancer treatment: discovery of new potential UCHL-3 inhibitors via virtual screening, molecular dynamics and binding mode analysis. Journal of Biomolecular Structure and Dynamics, 2022, 40, 276-289.	2.0	4
1996	In silico discovery and biological validation of ligands of FAD synthase, a promising new antimicrobial target. PLoS Computational Biology, 2020, 16, e1007898.	1.5	11
1997	Kinetic Properties of Aqueous Organic Redox Flow Battery Anolytes Using the Marcusâ€“Hush Theory. ACS Applied Energy Materials, 2020, 3, 8833-8841.	2.5	12
1998	Imprinted Contact Lenses for Ocular Administration of Antiviral Drugs. Polymers, 2020, 12, 2026.	2.0	24
1999	Intuitive, reproducible high-throughput molecular dynamics in Galaxy: a tutorial. Journal of Cheminformatics, 2020, 12, 54.	2.8	13
2000	Atom Identifiers Generated by a Neighborhood-Specific Graph Coloring Method Enable Compound Harmonization across Metabolic Databases. Metabolites, 2020, 10, 368.	1.3	6
2001	The ChemicalToolbox: reproducible, user-friendly cheminformatics analysis on the Galaxy platform. Journal of Cheminformatics, 2020, 12, 40.	2.8	21
2002	Hijacking SARS-CoV-2/ACE2 Receptor Interaction by Natural and Semi-synthetic Steroidal Agents Acting on Functional Pockets on the Receptor Binding Domain. Frontiers in Chemistry, 2020, 8, 572885.	1.8	76
2003	Crystal structure and X-ray absorption spectroscopy of trimethylarsine oxide dihydrate, (CH3)3AsOâ‹…2H2O. Powder Diffraction, 2020, 35, 190-196.	0.4	1
2004	In-silico screening of plant-derived antivirals against main protease, 3CL^{pro} and endoribonuclease, NSP15 proteins of SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 86-100.	2.0	26

#	Article	IF	Citations
2005	Thiocolchicoside and Colchicine Induced Apoptosis in Breast Cancer (MCF-7) Cells Via Up-regulated Expression of p53 Tumor Suppressor Protein Gene: An In vitro and In silico Docking Approaches. Journal of Biologically Active Products From Nature, 2020, 10, 264-274.	0.1	0
2006	Effects of Moringa oleifera Leaf Extract on Diabetes-Induced Alterations in Paraoxonase 1 and Catalase in Rats Analyzed through Progress Kinetic and Blind Docking. Antioxidants, 2020, 9, 840.	2.2	9
2007	Targeting the Initiator Protease of the Classical Pathway of Complement Using Fragment-Based Drug Discovery. Molecules, 2020, 25, 4016.	1.7	9
2008	Metabolic Forest: Predicting the Diverse Structures of Drug Metabolites. Journal of Chemical Information and Modeling, 2020, 60, 4702-4716.	2.5	11
2009	Pain-CKB, A Pain-Domain-Specific Chemogenomics Knowledgebase for Target Identification and Systems Pharmacology Research. Journal of Chemical Information and Modeling, 2020, 60, 4429-4435.	2.5	3
2010	An integrated drug repurposing strategy for the rapid identification of potential SARS-CoV-2 viral inhibitors. Scientific Reports, 2020, 10, 13866.	1.6	90
2011	Exploring Cocrystallized Aromatic Cage Binders to Target Histone Methylation Reader Proteins. Journal of Chemical Information and Modeling, 2020, 60, 5225-5233.	2.5	7
2012	Semi-supervised Machine Learning Enables the Robust Detection of Multireference Character at Low Cost. Journal of Physical Chemistry Letters, 2020, 11, 6640-6648.	2.1	27
2013	QSAR Study of Fusidic Acid Derivative as Anti-Malaria Agents by using Artificial Neural Network-Genetic Algorithm. , 2020, , .		7
2014	Repositioning of Ligands That Target the Spike Glycoprotein as Potential Drugs for SARS-CoV-2 in an In Silico Study. Molecules, 2020, 25, 5615.	1.7	15
2015	DockingApp RF: A State-of-the-Art Novel Scoring Function for Molecular Docking in a User-Friendly Interface to AutoDock Vina. International Journal of Molecular Sciences, 2020, 21, 9548.	1.8	21
2016	A Computer-Aided Drug Design Approach to Predict Marine Drug-Like Leads for SARS-CoV-2 Main Protease Inhibition. Marine Drugs, 2020, 18, 633.	2.2	25
2017	An In-Silico Pipeline for Rapid Screening of DNA Aptamers against Mycotoxins: The Case-Study of Fumonisin B1, Aflatoxin B1 and Ochratoxin A. Polymers, 2020, 12, 2983.	2.0	10
2018	In Silico Identification of New Targets for Diagnosis, Vaccine, and Drug Candidates against Trypanosoma cruzi. Disease Markers, 2020, 2020, 1-15.	0.6	6
2019	Identification of the Interactions Interference Between the PH and START Domain of CERT by Limonoid and HPA Inhibitors. Frontiers in Molecular Biosciences, 2020, 7, 603983.	1.6	2
2020	Why Conventional Design Rules for Câ€“H Activation Fail for Open-Shell Transition-Metal Catalysts. ACS Catalysis, 2020, 10, 15033-15047.	5.5	30
2021	HuskinDB, a database for skin permeation of xenobiotics. Scientific Data, 2020, 7, 426.	2.4	18
2022	ITScore-NL: An Iterative Knowledge-Based Scoring Function for Nucleic Acidâ€“Ligand Interactions. Journal of Chemical Information and Modeling, 2020, 60, 6698-6708.	2.5	25

#	Article	IF	Citations
2023	Understanding the biological role of PqqB in Pseudomonas stutzeri using molecular dynamics simulation approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4237-4249.	2.0	10
2024	Anisotine and amarogentin as promising inhibitory candidates against SARS-CoV-2 proteins: a computational investigation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4532-4542.	2.0	35
2025	Chespa: Streamlining Expansive Chemical Space Evaluation of Molecular Sets. Journal of Chemical Information and Modeling, 2020, 60, 6251-6257.	2.5	2
2026	Inhibition analysis of aflatoxin by in silico targeting the thioesterase domain of polyketide synthase enzyme in Aspergillus ssp. Journal of Biomolecular Structure and Dynamics, 2022, 40, 4328-4340.	2.0	11
2027	A Multi-Pronged Computational Pipeline for Prioritizing Drug Target Strategies for Latent Tuberculosis. Frontiers in Chemistry, 2020, 8, 593497.	1.8	9
2028	Permeation of Î²-Lactamase Inhibitors through the General Porins of Gram-Negative Bacteria. Molecules, 2020, 25, 5747.	1.7	8
2029	Identification of natural inhibitors against Mpro of SARS-CoV-2 by molecular docking, molecular dynamics simulation, and MM/PBSA methods. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2757-2768.	2.0	25
2030	Predicting in silico electron ionization mass spectra using quantum chemistry. Journal of Cheminformatics, 2020, 12, 63.	2.8	20
2031	Interaction of Cucurbit[7]uril with Oxime K027, Atropine, and Paraoxon: Risky or Advantageous Delivery System?. International Journal of Molecular Sciences, 2020, 21, 7883.	1.8	8
2032	Predicting ionic liquid melting points using machine learning. Journal of Molecular Liquids, 2020, , 114686.	2.3	2
2033	Machine learning property prediction for organic photovoltaic devices. Npj Computational Materials, 2020, 6, .	3.5	55
2034	Pathway enrichment analysis of virus-host interactome and prioritization of novel compounds targeting the spike glycoprotein receptor binding domainâ€“human angiotensin-converting enzyme 2 interface to combat SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2701-2714.	2.0	9
2035	Traditional medicinal plants against replication, maturation and transmission targets of SARS-CoV-2: computational investigation. Journal of Biomolecular Structure and Dynamics, 2022, 40, 2715-2732.	2.0	11
2036	Baicalin inhibits inflammation caused by coinfection of Mycoplasma gallisepticum and Escherichia coli involving IL-17 signaling pathway. Poultry Science, 2020, 99, 5472-5480.	1.5	16
2037	Design, synthesis and pharmacological evaluation of ester-based quercetin derivatives as selective vascular KCa1.1 channel stimulators. Bioorganic Chemistry, 2020, 105, 104404.	2.0	17
2038	Human Biotransformation Pathway of Temephos Using an In Silico Approach. Chemical Research in Toxicology, 2020, 33, 2765-2774.	1.7	3
2039	Description of Chiral Complexes within Functional-Group Symmetry-Adapted PerturbationÂTheoryâ€”The Case ofÂ(S/R)-Carvone with Derivatives of (â^')-Menthol. Journal of Physical Chemistry A, 2020, 124, 7735-7748.	1.1	2
2040	QSIdb: quorum sensing interference molecules. Briefings in Bioinformatics, 2021, 22, .	3.2	6

#	Article	IF	Citations
2041	2-D chemical structure image-based in silico model to predict agonist activity for androgen receptor. BMC Bioinformatics, 2020, 21, 245.	1.2	4
2042	Quantitative Prediction of Hemolytic Toxicity for Small Molecules and Their Potential Hemolytic Fragments by Machine Learning and Recursive Fragmentation Methods. Journal of Chemical Information and Modeling, 2020, 60, 3231-3245.	2.5	9
2043	Potential inhibitors of coronavirus 3-chymotrypsin-like protease (3CL^{pro}): an in silico screening of alkaloids and terpenoids from African medicinal plants. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1-13.	2.0	153
2044	A theoretical study of chemical bonding and topological and electrostatic properties of the anti-leprosy drug dapsone. Journal of Molecular Modeling, 2020, 26, 138.	0.8	7
2045	PLIDflow: an open-source workflow for the online analysis of proteinâ€“ligand docking using galaxy. Bioinformatics, 2020, 36, 4203-4205.	1.8	2
2046	Ecotoxicological Modeling of Organic Chemicals for Their Acute Toxicity in Algae Using Classification and Toxicophore-Based Approaches. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 17-72.	1.1	4
2047	KinomeRun: An interactive utility for kinome target screening and interaction fingerprint analysis towards holistic visualization on kinome tree. Chemical Biology and Drug Design, 2020, 96, 1162-1175.	1.5	2
2048	The ANI-1ccx and ANI-1x data sets, coupled-cluster and density functional theory properties for molecules. Scientific Data, 2020, 7, 134.	2.4	104
2049	Antimicrobial Isoflavones and Derivatives from Erythrina (Fabaceae): Structure Activity Perspective (Sar & Qsar) on Experimental and Mined Values Against Staphylococcus aureus. Antibiotics, 2020, 9, 223.	1.5	19
2050	Link Prediction Only With Interaction Data and its Application on Drug Repositioning. IEEE Transactions on Nanobioscience, 2020, 19, 547-555.	2.2	10
2051	Potential antiâ€SARSâ€CoVâ€2 drug candidates identified through virtual screening of the ChEMBL database for compounds that target the main coronavirus protease. FEBS Open Bio, 2020, 10, 995-1004.	1.0	49
2052	Metadynamics as a Postprocessing Method for Virtual Screening with Application to the Pseudokinase Domain of JAK2. Journal of Chemical Information and Modeling, 2020, 60, 4403-4415.	2.5	12
2053	Repurposing of chloroquine and some clinically approved antiviral drugs as effective therapeutics to prevent cellular entry and replication of coronavirus. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-11.	2.0	66
2054	Accelerated CDOCKER with GPUs, Parallel Simulated Annealing, and Fast Fourier Transforms. Journal of Chemical Theory and Computation, 2020, 16, 3910-3919.	2.3	36
2055	Retip: Retention Time Prediction for Compound Annotation in Untargeted Metabolomics. Analytical Chemistry, 2020, 92, 7515-7522.	3.2	128
2056	GalaxySagittarius: Structure- and Similarity-Based Prediction of Protein Targets for Druglike Compounds. Journal of Chemical Information and Modeling, 2020, 60, 3246-3254.	2.5	27
2057	Reactants, products, and transition states of elementary chemical reactions based on quantum chemistry. Scientific Data, 2020, 7, 137.	2.4	71
2058	Prospects of Indole derivatives as methyl transfer inhibitors: antimicrobial resistance managers. BMC Pharmacology & Toxicology, 2020, 21, 33.	1.0	4

#	Article	IF	Citations
2059	Development of highly potent Arene-Ru (II)-ninhydrin complexes for inhibition of cancer cell growth. Inorganica Chimica Acta, 2020, 508, 119641.	1.2	8
2060	Macromolecular modeling and design in Rosetta: recent methods and frameworks. Nature Methods, 2020, 17, 665-680.	9.0	513
2061	Identification of potential natural inhibitors of SARS-CoV2 main protease by molecular docking and simulation studies. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4334-4345.	2.0	129
2062	Amaryllidaceae Alkaloids of Belladine-Type from Narcissus pseudonarcissus cv. Carlton as New Selective Inhibitors of Butyrylcholinesterase. Biomolecules, 2020, 10, 800.	1.8	21
2063	New bioactive Cu(I) thiourea derivatives with triphenylphosphine; synthesis, structure and molecular docking studies. Journal of Coordination Chemistry, 2020, 73, 1191-1207.	0.8	10
2064	Effect of Adiantum philippense Extract on Biofilm Formation, Adhesion With Its Antibacterial Activities Against Foodborne Pathogens, and Characterization of Bioactive Metabolites: An in vitro-in silico Approach. Frontiers in Microbiology, 2020, 11, 823.	1.5	71
2065	Computational Methods for the Identification of Molecular Targets of Toxic Food Additives. Butylated Hydroxytoluene as a Case Study. Molecules, 2020, 25, 2229.	1.7	11
2066	TURBOMOLE: Modular program suite for ab initio quantum-chemical and condensed-matter simulations. Journal of Chemical Physics, 2020, 152, 184107.	1.2	616
2067	Structureâ€“Activity Relationship Study Reveals the Molecular Basis for Specific Sensing of Hydrophobic Amino Acids by the Campylobacter jejuni Chemoreceptor Tlp3. Biomolecules, 2020, 10, 744.	1.8	14
2068	Olfactory marker protein directly buffers cAMP to avoid depolarization-induced silencing of olfactory receptor neurons. Nature Communications, 2020, 11, 2188.	5.8	23
2069	Monte Carlo simulations of hydrogen adsorption in fullerene pillared graphene nanocomposites. Molecular Simulation, 2020, 46, 650-659.	0.9	22
2070	Synthesis, biological evaluation and modeling of hybrids from tetrahydro-1H-pyrazolo[3,4-b]quinolines as dual cholinestrase and COX-2 inhibitors. Bioorganic Chemistry, 2020, 100, 103895.	2.0	22
2071	Atomic Charge Calculator II: web-based tool for the calculation of partial atomic charges. Nucleic Acids Research, 2020, 48, W591-W596.	6.5	26
2072	FTIR, Raman and DFT studies on 2-[4-(4-ethylbenzamido)phenyl]benzothiazole and 2-[4-(4-nitrobenzamido)phenyl]benzothiazole supported by differential scanning calorimetry. Journal of Molecular Structure, 2020, 1218, 128454.	1.8	8
2073	Data-Driven Advancement of Homogeneous Nickel Catalyst Activity for Aryl Ether Cleavage. ACS Catalysis, 2020, 10, 7021-7031.	5.5	40
2074	Design of organic structure directing agents to guide the synthesis of zeolites for the separation of ethyleneâ€“ethane mixtures. RSC Advances, 2020, 10, 20313-20321.	1.7	1
2075	Network Pharmacological Screening of the Active Ingredients and Hypoglycemic Effect of Isodon rubescens in the Treatment of Diabetes. Planta Medica, 2020, 86, 556-564.	0.7	5
2076	Flexibilities of wavelets as a computational basis set for large-scale electronic structure calculations. Journal of Chemical Physics, 2020, 152, 194110.	1.2	60

#	Article	IF	Citations
2077	DeepCDA: deep cross-domain compoundâ€“protein affinity prediction through LSTM and convolutional neural networks. Bioinformatics, 2020, 36, 4633-4642.	1.8	110
2078	Using human in vitro transcriptome analysis to build trustworthy machine learning models for prediction of animal drug toxicity. Scientific Reports, 2020, 10, 9522.	1.6	16
2079	Side chain virtual screening of matched molecular pairs: a PDB-wide and ChEMBL-wide analysis. Journal of Computer-Aided Molecular Design, 2020, 34, 953-963.	1.3	2
2080	XenoNet: Inference and Likelihood of Intermediate Metabolite Formation. Journal of Chemical Information and Modeling, 2020, 60, 3431-3449.	2.5	14
2081	Comparative Dynamics and Functional Mechanisms of the CYP17A1 Tunnels Regulated by Ligand Binding. Journal of Chemical Information and Modeling, 2020, 60, 3632-3647.	2.5	17
2082	Quantitative Structureâ€“Activity Relationship Models for Predicting Inflammatory Potential of Metal Oxide Nanoparticles. Environmental Health Perspectives, 2020, 128, 67010.	2.8	58
2083	Screening and druggability analysis of some plant metabolites against SARS-CoV-2: An integrative computational approach. Informatics in Medicine Unlocked, 2020, 20, 100367.	1.9	46
2084	The potential of halogenated olefins as working fluids for organic Rankine cycle technology. Journal of Molecular Liquids, 2020, 310, 112971.	2.3	4
2085	Data-Driven Approaches Can Overcome the Costâ€“Accuracy Trade-Off in Multireference Diagnostics. Journal of Chemical Theory and Computation, 2020, 16, 4373-4387.	2.3	28
2086	Computational investigation on Andrographis paniculata phytochemicals to evaluate their potency against SARS-CoV-2 in comparison to known antiviral compounds in drug trials. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4415-4426.	2.0	73
2087	In silicoidentification of potential inhibitors fromCinnamonagainst main protease and spike glycoprotein of SARS CoV-2. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4618-4632.	2.0	108
2088	In silico identification of natural fungicide from Melia azedarach against isocitrate lyase of Fusarium graminearum. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4816-4834.	2.0	9
2089	A Haloalkane Dehalogenase from Saccharomonospora viridis Strain DSM 43017, a Compost Bacterium with Unusual Catalytic Residues, Unique (S)-Enantiopreference, and High Thermostability. Applied and Environmental Microbiology, 2020, 86, .	1.4	7
2090	Novel Noncompetitive Type Three Secretion System ATPase Inhibitors Shut Down Shigella Effector Secretion. Biochemistry, 2020, 59, 2667-2678.	1.2	2
2091	Uncovering Alternate Pathways to Nafion Membrane Degradation in Fuel Cells with First-Principles Modeling. Journal of Physical Chemistry C, 2020, 124, 15094-15106.	1.5	6
2092	A computational approach to validate novel drug targets of gentianine from Swertiya chirayita in Plasmodium falciparum. BioSystems, 2020, 196, 104175.	0.9	3
2093	DFT studies on vibrational and electronic spectra, HOMOâ€“LUMO, MEP, HOMA, NBO and molecular docking analysis of benzyl-3-N-(2,4,5-trimethoxyphenylmethylene)hydrazinecarbodithioate. Journal of Molecular Structure, 2020, 1220, 128715.	1.8	167
2094	Teaching and Learning Computational Drug Design: Student Investigations of 3D Quantitative Structureâ€“Activity Relationships through Web Applications. Journal of Chemical Education, 2020, 97, 1922-1930.	1.1	27

#	Article	IF	Citations
2095	Pharmacoinformatics and molecular dynamics simulation studies reveal potential covalent and FDA-approved inhibitors of SARS-CoV-2 main protease 3CL^{pro}. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4936-4948.	2.0	103
2096	Identification of luteolin -7-glucoside and epicatechin gallate from Vernonia cinerea, as novel EGFR L858R kinase inhibitors against lung cancer: Docking and simulation-based study. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5048-5057.	2.0	11
2097	Preparation and DFT Studies of Î²2C,N-Hypercoordinated Oxazoline Organotins: Monomer Constructs for Stable Polystannanes. Inorganics, 2020, 8, 35.	1.2	2
2098	Ethaninidothioic acid (R5421) is not a selective inhibitor of platelet phospholipid scramblase activity. British Journal of Pharmacology, 2020, 177, 4007-4020.	2.7	8
2099	Aromatic clusters in proteinâ€“protein and proteinâ€“drug complexes. Journal of Cheminformatics, 2020, 12, 30.	2.8	38
2100	An integrated biophysical approach to discovering mechanisms of NDM-1 inhibition for several thiol-containing drugs. Journal of Biological Inorganic Chemistry, 2020, 25, 717-727.	1.1	6
2101	Revealing the Strong Relationships between Ligand Conformers and Activation Barriers: A Case Study of Bisphosphine Reductive Elimination. ACS Catalysis, 2020, 10, 7136-7145.	5.5	25
2102	Index of ideality of correlation and correlation contradiction index: a confluent perusal on acetylcholinesterase inhibitors. Molecular Simulation, 2020, 46, 777-786.	0.9	11
2103	Identification of novel class I and class IIb histone deacetylase inhibitor for Alzheimer's disease therapeutics. Life Sciences, 2020, 256, 117912.	2.0	13
2104	Planning new Trypanosoma cruzi CYP51 inhibitors using QSAR studies. Molecular Diversity, 2020, 25, 2219-2235.	2.1	2
2105	Predicting a Molecular Fingerprint from an Electron Ionization Mass Spectrum with Deep Neural Networks. Analytical Chemistry, 2020, 92, 8649-8653.	3.2	59
2106	Extending the Applicability of the ANI Deep Learning Molecular Potential to Sulfur and Halogens. Journal of Chemical Theory and Computation, 2020, 16, 4192-4202.	2.3	160
2107	Identification of structural fingerprints for ABCG2 inhibition by using Monte Carlo optimization, Bayesian classification, and structural and physicochemical interpretation (SPCI) analysis. SAR and QSAR in Environmental Research, 2020, 31, 439-455.	1.0	10
2108	Implementation of ensemble methods on QSAR Study of NS3 inhibitor activity as anti-dengue agent. SAR and QSAR in Environmental Research, 2020, 31, 477-492.	1.0	10
2109	Use of Graph Based Descriptors for Determination of Structural Features Causing Modulation of Fructose-1,6-Bisphosphatase. Drug Research, 2020, 70, 226-232.	0.7	5
2110	Natural compounds fromClerodendrumspp. as possible therapeutic candidates against SARS-CoV-2: Anin silicoinvestigation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4774-4785.	2.0	57
2111	Computational Drug Repositioning for Chagas Disease Using Protein-Ligand Interaction Profiling. International Journal of Molecular Sciences, 2020, 21, 4270.	1.8	16
2112	Enhancing NMR Quantum Computation by Exploring Heavy Metal Complexes as Multiqubit Systems: A Theoretical Investigation. Journal of Physical Chemistry A, 2020, 124, 4946-4955.	1.1	12

#	Article	IF	Citations
2113	Software tools for toxicology and risk assessment. , 2020, , 791-812.		1
2114	Personalized Mapping of Drug Metabolism by the Human Gut Microbiome. Cell, 2020, 181, 1661-1679.e22.	13.5	239
2115	Homology Modeling of Leishmanolysin (gp63) from Leishmania panamensis and Molecular Docking of Flavonoids. ACS Omega, 2020, 5, 14741-14749.	1.6	26
2116	Assessment of the SM12, SM8, and SMD Solvation Models for Predicting Limiting Activity Coefficients at 298.15 K. Processes, 2020, 8, 623.	1.3	7
2117	Kinetic study of depolymerization of polyurethanes: A experimental and computational insight for chemical recycling. International Journal of Chemical Kinetics, 2020, 52, 611-619.	1.0	2
2118	Synthesis, Cytotoxic Activity and Molecular Docking Studies of New Condensed Thieno[2,3-d]Pyrimidines as Antitumor Agents. Pharmaceutical Chemistry Journal, 2020, 54, 258-267.	0.3	4
2119	In silico screening of FDA approved drugs reveals ergotamine and dihydroergotamine as potential coronavirus main protease enzyme inhibitors. Saudi Journal of Biological Sciences, 2020, 27, 2674-2682.	1.8	18
2120	Basic Limonoid modulates Chaperone-mediated Proteostasis and dissolve Tau fibrils. Scientific Reports, 2020, 10, 4023.	1.6	17
2121	OntoQSAR: an Ontology for Interpreting Chemical and Biological Data in Quantitative Structure-Activity Relationship Studies. , 2020, , .		2
2122	Pharmacoinformatics and molecular dynamic simulation studies to identify potential small-molecule inhibitors of WNK-SPAK/OSR1 signaling that mimic the RFQV motifs of WNK kinases. Arabian Journal of Chemistry, 2020, 13, 5107-5117.	2.3	18
2123	Virtual screening of small-molecule libraries. , 2020, , 103-125.		3
2124	A Method for Predicting Hemolytic Potency of Chemically Modified Peptides From Its Structure. Frontiers in Pharmacology, 2020, 11, 54.	1.6	19
2125	Accurate Multiobjective Design in a Space of Millions of Transition Metal Complexes with Neural-Network-Driven Efficient Global Optimization. ACS Central Science, 2020, 6, 513-524.	5.3	114
2126	Predictions of High-Order Electric Properties of Molecules: Can We Benefit from Machine Learning?. ACS Omega, 2020, 5, 5318-5325.	1.6	8
2127	Prediction of Side Effects Using Comprehensive Similarity Measures. BioMed Research International, 2020, 2020, 1-10.	0.9	12
2128	Towards a Treatment for Gulf War Illness: A Consensus Docking Approach. Military Medicine, 2020, 185, 554-561.	0.4	1
2129	Computational design of substrate selective inhibition. PLoS Computational Biology, 2020, 16, e1007713.	1.5	4
2130	Small molecule inhibitors of IÎºB kinase Î²: A chip-based screening and molecular docking simulation. Bioorganic and Medicinal Chemistry, 2020, 28, 115440.	1.4	5

#	Article	IF	Citations
2131	Linking reaction mechanisms and quantum chemistry: An ontological approach. Computers and Chemical Engineering, 2020, 137, 106813.	2.0	20
2132	The covalent radii derived from the first-principle data. Molecular Physics, 2020, 118, e1742937.	0.8	2
2133	Transformer-CNN: Swiss knife for QSAR modeling and interpretation. Journal of Cheminformatics, 2020, 12, 17.	2.8	134
2134	In-Silico-Generated Library for Sensitive Detection of 2-Dimethylaminoethylamine Derivatized FAHFA Lipids Using High-Resolution Tandem Mass Spectrometry. Analytical Chemistry, 2020, 92, 5960-5968.	3.2	23
2135	Molecular Architect: A User-Friendly Workflow for Virtual Screening. ACS Omega, 2020, 5, 6628-6640.	1.6	26
2136	Complexity Reduction in Density Functional Theory Calculations of Large Systems: System Partitioning and Fragment Embedding. Journal of Chemical Theory and Computation, 2020, 16, 2952-2964.	2.3	19
2137	Molecule Identification with Rotational Spectroscopy and Probabilistic Deep Learning. Journal of Physical Chemistry A, 2020, 124, 3002-3017.	1.1	21
2138	Catalyst-Free Three-Component Synthesis, Antibacterial, Antifungal, and Docking Studies of Spiroindoline Derivatives. Polycyclic Aromatic Compounds, 2022, 42, 517-533.	1.4	2
2139	Improving Protein-Ligand Docking Results with High-Throughput Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2020, 60, 2189-2198.	2.5	152
2140	Cov_FB3D: A De Novo Covalent Drug Design Protocol Integrating the BA-SAMP Strategy and Machine-Learning-Based Synthetic Tractability Evaluation. Journal of Chemical Information and Modeling, 2020, 60, 4388-4402.	2.5	12
2141	Insights into structures of imidazo oxazines as potent polyketide synthase XIII inhibitors using molecular modeling techniques. Journal of Receptor and Signal Transduction Research, 2020, 40, 313-323.	1.3	11
2142	Self-Consistent Component Increment Theory for Predicting Enthalpy of Formation. Journal of Chemical Information and Modeling, 2020, 60, 2199-2207.	2.5	11
2143	Succinamide Derivatives Ameliorate Neuroinflammation and Oxidative Stress in Scopolamine-Induced Neurodegeneration. Biomolecules, 2020, 10, 443.	1.8	47
2144	In silico Screening of Flavones and its Derivatives as Potential Inhibitors of Quorum-Sensing Regulator LasR of Pseudomonas aeruginosa. Molecular Biology, 2020, 54, 134-143.	0.4	13
2145	Improved Prediction of Aqueous Solubility of Novel Compounds by Going Deeper With Deep Learning. Frontiers in Oncology, 2020, 10, 121.	1.3	49
2146	Stereochemical revision of xylogranatin F by GIAO and DU8+ NMR calculations. Chirality, 2020, 32, 515-523.	1.3	14
2147	Discovery of 9-phenylacridinediones as highly selective butyrylcholinesterase inhibitors through structure-based virtual screening. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127075.	1.0	11
2148	Looking for new xanthine oxidase inhibitors: 3-Phenylcoumarins versus 2-phenylbenzofurans. International Journal of Biological Macromolecules, 2020, 162, 774-780.	3.6	19

#	Article	IF	Citations
2149	Estimation of a stronger heparin binding locus in fibronectin domain III¹⁴using thermodynamics and molecular dynamics. RSC Advances, 2020, 10, 20288-20301.	1.7	9
2150	De novo design based identification of potential HIV-1 integrase inhibitors: A pharmacoinformatics study. Computational Biology and Chemistry, 2020, 88, 107319.	1.1	8
2151	Molecular profiling of lamellar ichthyosis pathogenic missense mutations on the structural and stability aspects of TGM1 protein. Journal of Biomolecular Structure and Dynamics, 2021, 39, 4962-4972.	2.0	6
2152	Molecular insights into benzene sulphonamide substituted diarylpyrazoles as cyclooxygenase-2 inhibitor and its structural modifications. Journal of Biomolecular Structure and Dynamics, 2021, 39, 5093-5104.	2.0	4
2153	Structure-Based Discovery of Dual-Target Hits for Acetylcholinesterase and the Î±7 Nicotinic Acetylcholine Receptors: In Silico Studies and In Vitro Confirmation. Molecules, 2020, 25, 2872.	1.7	9
2154	Construction of pioneering quantitative structure activity relationship screening models for abuse potential of designer drugs using index of ideality of correlation in monte carlo optimization. Archives of Toxicology, 2020, 94, 3069-3086.	1.9	22
2155	The Cyclopropane Ring as a Reporter of Radical Leaving-Group Reactivity for Ni-Catalyzed C(sp³)â€“O Arylation. Journal of the American Chemical Society, 2020, 142, 13246-13254.	6.6	34
2156	PhyteByte: identification of foods containing compounds with specific pharmacological properties. BMC Bioinformatics, 2020, 21, 238.	1.2	6
2157	Artificial Intelligence Algorithms for Discovering New Active Compounds Targeting TRPA1 Pain Receptors. AI, 2020, 1, 276-285.	2.1	4
2158	A review of mathematical representations of biomolecular data. Physical Chemistry Chemical Physics, 2020, 22, 4343-4367.	1.3	56
2159	M<scp>olassembler</scp>: Molecular Graph Construction, Modification, and Conformer Generation for Inorganic and Organic Molecules. Journal of Chemical Information and Modeling, 2020, 60, 3884-3900.	2.5	36
2160	Deep learning and knowledge-based methods for computer-aided molecular designâ€”toward a unified approach: State-of-the-art and future directions. Computers and Chemical Engineering, 2020, 141, 107005.	2.0	67
2161	Computational evaluation of major components from plant essential oils as potent inhibitors of SARS-CoV-2 spike protein. Journal of Molecular Structure, 2020, 1221, 128823.	1.8	125
2162	Parameterization of Unnatural Amino Acids with Azido and Alkynyl R-Groups for Use in Molecular Simulations. Journal of Physical Chemistry A, 2020, 124, 6246-6253.	1.1	7
2163	In-silico analysis of Calcium Dependent Protein Kinase 6 of Cryptosporidium parvum through molecular modeling, docking, and dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2020, 39, 1-10.	2.0	3
2164	Thymus musilii Velen. as a promising source of potent bioactive compounds with its pharmacological properties: In vitro and in silico analysis. Arabian Journal of Chemistry, 2020, 13, 6782-6801.	2.3	54
2165	Structure of the Brain N-Acetylaspartate Biosynthetic Enzyme NAT8L Revealed by Computer Modeling. ACS Chemical Neuroscience, 2020, 11, 2296-2302.	1.7	4
2166	Molecular docking and machine learning analysis of Abemaciclib in colon cancer. BMC Molecular and Cell Biology, 2020, 21, 52.	1.0	20

#	Article	IF	Citations
2167	Identification of a Broad-Spectrum Viral Inhibitor Targeting a Novel Allosteric Site in the RNA-Dependent RNA Polymerases of Dengue Virus and Norovirus. Frontiers in Microbiology, 2020, 11, 1440.	1.5	14
2168	In silico rationalisation of selectivity and reactivity in Pd-catalysed Câ€“H activation reactions. Beilstein Journal of Organic Chemistry, 2020, 16, 1465-1475.	1.3	2
2169	DREAM-in-CDM Approach and Identification of a New Generation of Anti-inflammatory Drugs Targeting mPGES-1. Scientific Reports, 2020, 10, 10187.	1.6	13
2170	Repurposing drugs against the main protease of SARS-CoV-2: mechanism-based insights supported by available laboratory and clinical data. Molecular Omics, 2020, 16, 474-491.	1.4	33
2171	Ogre: A Python package for molecular crystal surface generation with applications to surface energy and crystal habit prediction. Journal of Chemical Physics, 2020, 152, 244122.	1.2	15
2172	Aqueous Dielsâ€“Alder reactions for thermochemical storage and heat transfer fluids identified using density functional theory. Journal of Computational Chemistry, 2020, 41, 2137-2150.	1.5	4
2173	Deeper inside the specificity of lysozyme when degrading chitosan. A structural bioinformatics study. Journal of Molecular Graphics and Modelling, 2020, 100, 107676.	1.3	15
2174	Computational Investigation of Correlations in Adsorbate Entropy for Pure-Silica Zeolite Adsorbents. Journal of Physical Chemistry C, 2020, 124, 16350-16361.	1.5	4
2175	3DStructGen: an interactive web-based 3D structure generation for non-periodic molecule and crystal. Journal of Cheminformatics, 2020, 12, 7.	2.8	7
2176	In silico screening of GMQ-like compounds reveals guanabenz and sephin1 as new allosteric modulators of acid-sensing ion channel 3. Biochemical Pharmacology, 2020, 174, 113834.	2.0	12
2177	Incorporating Clinical, Chemical and Biological Information for Predicting Small Molecule-microRNA Associations Based on Non-Negative Matrix Factorization. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2021, 18, 2535-2545.	1.9	13
2178	Druggability Assessment in TRAPP Using Machine Learning Approaches. Journal of Chemical Information and Modeling, 2020, 60, 1685-1699.	2.5	29
2179	Elucidating the multiple roles of hydration for accurate protein-ligand binding prediction via deep learning. Communications Chemistry, 2020, 3, .	2.0	41
2180	TheoDORE: A toolbox for a detailed and automated analysis of electronic excited state computations. Journal of Chemical Physics, 2020, 152, 084108.	1.2	209
2181	Chemical promenades: Exploring potentialâ€energy surfaces with immersive virtual reality. Journal of Computational Chemistry, 2020, 41, 1310-1323.	1.5	21
2182	Structureâ€guided screening of chemical database to identify NS3â€NS2B inhibitors for effective therapeutic application in dengue infection. Journal of Molecular Recognition, 2020, 33, e2838.	1.1	23
2183	Quantum chemical predictions of waterâ€“octanol partition coefficients applied to the SAMPL6 logP blind challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 485-493.	1.3	13
2184	Anti-influenza virus phytochemicals from Radix Paeoniae Alba and characterization of their neuraminidase inhibitory activities. Journal of Ethnopharmacology, 2020, 253, 112671.	2.0	21

#	Article	IF	Citations
2185	Allosteric Activation of PI3KÎ± Results in Dynamic Access to Catalytically Competent Conformations. Structure, 2020, 28, 465-474.e5.	1.6	13
2186	Matingâ€based regulation and ligand binding of an odorantâ€binding protein support the inverse sexual communication of the greater wax moth, Galleria mellonella (Lepidoptera: Pyralidae). Insect Molecular Biology, 2020, 29, 337-351.	1.0	7
2187	Atomic structures and orbital energies of 61,489 crystal-forming organic molecules. Scientific Data, 2020, 7, 58.	2.4	52
2188	Correcting Rate Constants from Anharmonic Molecular Dynamics for Quantum Effects. ACS Omega, 2020, 5, 2242-2253.	1.6	9
2189	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of waterâ€“octanol partition coefficients in the SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 471-483.	1.3	7
2190	Crystal structure of O-Acetylserine sulfhydralase (OASS) isoform 3 from Entamoeba histolytica: Pharmacophore-based virtual screening and validation of novel inhibitors. European Journal of Medicinal Chemistry, 2020, 192, 112157.	2.6	9
2191	Discovery of sulfone-resistant dihydropteroate synthase (DHPS) as a target enzyme for kaempferol, a natural flavanoid. Heliyon, 2020, 6, e03378.	1.4	7
2192	CANDOCK: Chemical Atomic Network-Based Hierarchical Flexible Docking Algorithm Using Generalized Statistical Potentials. Journal of Chemical Information and Modeling, 2020, 60, 1509-1527.	2.5	36
2193	ProtoCaller: Robust Automation of Binding Free Energy Calculations. Journal of Chemical Information and Modeling, 2020, 60, 1917-1921.	2.5	18
2194	Ameliorative effect of a standardized polyherbal combination in methotrexate-induced nephrotoxicity in the rat. Pharmaceutical Biology, 2020, 58, 184-199.	1.3	21
2195	Multi-spectroscopic, conformational, and computational atomic-level insights into the interaction of Î²-lactoglobulin with apigenin at different pH levels. Food Hydrocolloids, 2020, 105, 105810.	5.6	42
2196	Design and synthesis of dansyl-labeled inhibitors of steroid sulfatase for optical imaging. Bioorganic and Medicinal Chemistry, 2020, 28, 115368.	1.4	9
2197	The rcdk and cluster R packages applied to drug candidate selection. Journal of Cheminformatics, 2020, 12, 3.	2.8	32
2198	The Metabolic Rainbow: Deep Learning Phase I Metabolism in Five Colors. Journal of Chemical Information and Modeling, 2020, 60, 1146-1164.	2.5	26
2199	BOKEI: Bayesian optimization using knowledge of correlated torsions and expected improvement for conformer generation. Physical Chemistry Chemical Physics, 2020, 22, 5211-5219.	1.3	14
2200	Green synthesis, molecular docking and anticancer activity of novel 1,4-dihydropyridine-3,5-Dicarbohydrazones under grind-stone chemistry. Green Chemistry Letters and Reviews, 2020, 13, 6-17.	2.1	46
2201	Covalent Complex of DNA and Bacterial Topoisomerase: Implications in Antibacterial Drug Development. ChemMedChem, 2020, 15, 623-631.	1.6	7
2202	Target identification among known drugs by deep learning from heterogeneous networks. Chemical Science, 2020, 11, 1775-1797.	3.7	193

#	Article	IF	Citations
2203	Clonorchis sinensis MF6p/HDM (CsMF6p/HDM) induces pro-inflammatory immune response in RAW 264.7 macrophage cells via NF-ÎºB-dependent MAPK pathways. Parasites and Vectors, 2020, 13, 20.	1.0	11
2204	Machine-Learning-Assisted De Novo Design of Organic Molecules and Polymers: Opportunities and Challenges. Polymers, 2020, 12, 163.	2.0	95
2205	D3R grand challenge 4: blind prediction of proteinâ€“ligand poses, affinity rankings, and relative binding free energies. Journal of Computer-Aided Molecular Design, 2020, 34, 99-119.	1.3	81
2206	The role of human in the loop: lessons from D3R challenge 4. Journal of Computer-Aided Molecular Design, 2020, 34, 121-130.	1.3	9
2207	Self-Parametrizing System-Focused Atomistic Models. Journal of Chemical Theory and Computation, 2020, 16, 1646-1665.	2.3	22
2208	QSPR study of the Henryâ€™s law constant for heterogeneous compounds. Chemical Engineering Research and Design, 2020, 154, 115-121.	2.7	16
2209	METADOCK 2: a high-throughput parallel metaheuristic scheme for molecular docking. Bioinformatics, 2021, 37, 1515-1520.	1.8	10
2210	LogP prediction performance with the SMD solvation model and the M06 density functional family for SAMPL6 blind prediction challenge molecules. Journal of Computer-Aided Molecular Design, 2020, 34, 511-522.	1.3	19
2211	Effect of ion exchange capacity and water uptake on hydroxide transport in PSU-TMA membranes: A DFT and molecular dynamics study. Journal of Membrane Science, 2020, 599, 117837.	4.1	31
2212	Modulation of lymphocyte-mediated tissue repair by rational design of heterocyclic aryl hydrocarbon receptor agonists. Science Advances, 2020, 6, eaay8230.	4.7	31
2213	Binding of adenosine derivatives to carrier proteins may reduce their antiplatelet activity. Biochemical Pharmacology, 2020, 174, 113827.	2.0	6
2214	Bayesian Analysis of Theoretical Rotational Constants from Low-Cost Electronic Structure Methods. Journal of Physical Chemistry A, 2020, 124, 898-910.	1.1	22
2215	The synergistic effect of biosynthesized silver nanoparticles from a combined extract of parsley, corn silk, and gum arabic: in vivo antioxidant, anti-inflammatory and antimicrobial activities. Materials Research Express, 2020, 7, 025002.	0.8	17
2216	Synthesis, in vitro biological evaluation and in silico docking studies of new quinazolinâ€2,4â€dione analogues as possible anticarcinoma agents. Journal of Heterocyclic Chemistry, 2020, 57, 1637-1654.	1.4	23
2217	Quinazoline Ligands Induce Cancer Cell Death through Selective STAT3 Inhibition and G-Quadruplex Stabilization. Journal of the American Chemical Society, 2020, 142, 2876-2888.	6.6	47
2218	Design and novel synthetic approach supported with molecular docking and biological evidence for naphthoquinone-hydrazinotriazolothiadiazine analogs as potential anticancer inhibiting topoisomerase-IIB. Bioorganic Chemistry, 2020, 96, 103641.	2.0	20
2219	ChemML: A machine learning and informatics program package for the analysis, mining, and modeling of chemical and materials data. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2020, 10, e1458.	6.2	41
2220	Computational approach to target USP28 for regulating Myc. Computational Biology and Chemistry, 2020, 85, 107208.	1.1	5

#	Article	IF	Citations
2221	Mutational landscape screening of methylene tetrahydrofolate reductase to predict homocystinuria associated variants: An integrative computational approach. Mutation Research - Fundamental and Molecular Mechanisms of Mutagenesis, 2020, 819-820, 111687.	0.4	11
2222	Structure-based discovery of novel inhibitors of Mycobacterium tuberculosis CYP121 from Indonesian natural products. Computational Biology and Chemistry, 2020, 85, 107205.	1.1	11
2223	Reveal the interaction mechanism of five old drugs targeting VEGFR2 through computational simulations. Journal of Molecular Graphics and Modelling, 2020, 96, 107538.	1.3	4
2224	Effect of Structural Descriptors on the Design of Cyclin Dependent Kinase Inhibitors Using Similarityâ€based Molecular Evolution. Molecular Informatics, 2020, 39, 1900126.	1.4	5
2225	Effects of network structure on the mechanical and thermal responses of liquid crystal elastomers. Multifunctional Materials, 2020, 3, 015002.	2.4	4
2226	Novel 3â€arylâ€5â€substitutedâ€coumarin analogues: Synthesis and bioactivity profile. Drug Development Research, 2020, 81, 456-469.	1.4	11
2227	MoSDeF, a Python Framework Enabling Large-Scale Computational Screening of Soft Matter: Application to Chemistry-Property Relationships in Lubricating Monolayer Films. Journal of Chemical Theory and Computation, 2020, 16, 1779-1793.	2.3	22
2228	Predicting octanol/water partition coefficients for the SAMPL6 challenge using the SM12, SM8, and SMD solvation models. Journal of Computer-Aided Molecular Design, 2020, 34, 575-588.	1.3	12
2229	Substituted Piperazines as Novel Potential Radioprotective Agents. Molecules, 2020, 25, 532.	1.7	4
2230	A comparative chemogenic analysis for predicting Drug-Target Pair via Machine Learning Approaches. Scientific Reports, 2020, 10, 6870.	1.6	12
2231	Brain-targeting by optimized ^{99m}Tc-olanzapine: inÂvivo and in silico studies. International Journal of Radiation Biology, 2020, 96, 1017-1027.	1.0	5
2232	Molecular Perception for Visualization and Computation: The Proxima Library. Journal of Chemical Information and Modeling, 2020, 60, 2668-2672.	2.5	24
2233	ProteinVR: Web-based molecular visualization in virtual reality. PLoS Computational Biology, 2020, 16, e1007747.	1.5	46
2234	Predicting commercially available antiviral drugs that may act on the novel coronavirus (SARS-CoV-2) through a drug-target interaction deep learning model. Computational and Structural Biotechnology Journal, 2020, 18, 784-790.	1.9	568
2235	Metabolic profiling, histopathological anti-ulcer study, molecular docking and molecular dynamics of ursolic acid isolated from Ocimum forskolei Benth. (family Lamiaceae). South African Journal of Botany, 2020, 131, 311-319.	1.2	16
2236	Are 2D fingerprints still valuable for drug discovery?. Physical Chemistry Chemical Physics, 2020, 22, 8373-8390.	1.3	77
2237	Multitarget Approach to Drug Candidates against Alzheimerâ€™s Disease Related to AChE, SERT, BACE1 and GSK3Î² Protein Targets. Molecules, 2020, 25, 1846.	1.7	10
2238	Molecular Investigation of SARSâ€“CoV-2 Proteins and Their Interactions with Antiviral Drugs. Viruses, 2020, 12, 445.	1.5	102

#	Article	IF	Citations
2239	Synthesis, antifungal activity and potential mechanism of fusidic acid derivatives possessing amino-terminal groups. Future Medicinal Chemistry, 2020, 12, 763-774.	1.1	8
2240	Design of fluorophore-loaded human serum albumin nanoparticles for specific targeting of NIH:OVCAR3 ovarian cancer cells. Nanotechnology, 2020, 31, 315102.	1.3	8
2241	Synthesis, Docking, and In Vitro Anticoagulant Activity Assay of Hybrid Derivatives of Pyrrolo[3,2,1-ij]Quinolin-2(1H)-one as New Inhibitors of Factor Xa and Factor XIa. Molecules, 2020, 25, 1889.	1.7	21
2242	FDA-Approved Drugs Efavirenz, Tipranavir, and Dasabuvir Inhibit Replication of Multiple Flaviviruses in Vero Cells. Microorganisms, 2020, 8, 599.	1.6	17
2243	Kinetic Characterization of Tyrosinase-catalyzed Oxidation of Four Polyphenols. Current Medical Science, 2020, 40, 239-248.	0.7	6
2244	Screening and analysis of bioactive food compounds for modulating the CDK2 protein for cell cycle arrest: Multi-cheminformatics approaches for anticancer therapeutics. Journal of Molecular Structure, 2020, 1216, 128316.	1.8	24
2245	Pre-Clinical Pharmacokinetics, Tissue Distribution and Physicochemical Studies of CLBQ14, a Novel Methionine Aminopeptidase Inhibitor for the Treatment of Infectious Diseases . Drug Design, Development and Therapy, 2020, Volume 14, 1263-1277.	2.0	9
2246	Systems Pharmacology Approach to Investigate the Mechanism of Kai-Xin-San in Alzheimerâ€™s Disease. Frontiers in Pharmacology, 2020, 11, 381.	1.6	27
2247	Synthesis, Crystal Structure and Computational Investigation of New 4â€Phenylâ€decahydroâ€1‹i›H‹/i›â€1,5â€benzodiazepinâ€2â€one as Potent Inhibitor of Muâ€opioid Receptor. ChemistrySelect, 2020, 5, 4601-4607.	0.7	7
2248	Identifying GPCR-drug interaction based on wordbook learning from sequences. BMC Bioinformatics, 2020, 21, 150.	1.2	10
2249	An open-source drug discovery platform enables ultra-large virtual screens. Nature, 2020, 580, 663-668.	13.7	345
2250	D3Targets-2019-nCoV: a webserver for predicting drug targets and for multi-target and multi-site based virtual screening against COVID-19. Acta Pharmaceutica Sinica B, 2020, 10, 1239-1248.	5.7	65
2251	Fast Identification of Possible Drug Treatment of Coronavirus Disease-19 (COVID-19) through Computational Drug Repurposing Study. Journal of Chemical Information and Modeling, 2020, 60, 3277-3286.	2.5	373
2252	Prediction of Soil Adsorption Coefficient in Pesticides Using Physicochemical Properties and Molecular Descriptors by Machine Learning Models. Environmental Toxicology and Chemistry, 2020, 39, 1451-1459.	2.2	16
2253	TeraChem Cloud: A High-Performance Computing Service for Scalable Distributed GPU-Accelerated Electronic Structure Calculations. Journal of Chemical Information and Modeling, 2020, 60, 2126-2137.	2.5	21
2254	Computational studies of drug repurposing and synergism of lopinavir, oseltamivir and ritonavir binding with SARS-CoV-2 protease against COVID-19. Journal of Biomolecular Structure and Dynamics, 2021, 39, 2673-2678.	2.0	325
2255	Drug repositioning by prediction of drugâ€™s anatomical therapeutic chemical code via network-based inference approaches. Briefings in Bioinformatics, 2021, 22, 2058-2072.	3.2	25
2256	Pharmacophore modeling of pretomanid (PA-824) derivatives for antitubercular potency against replicating and non-replicating Mycobacterium tuberculosis. Journal of Biomolecular Structure and Dynamics, 2021, 39, 889-900.	2.0	1

#	Article	IF	Citations
2257	Machine learning approaches and databases for prediction of drugâ€“target interaction: a survey paper. Briefings in Bioinformatics, 2021, 22, 247-269.	3.2	217
2258	Computational investigation on the effect of Oleuropein aglycone on the Î±-synuclein aggregation. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1259-1270.	2.0	14
2259	Understanding structure-based dynamic interactions of antihypertensive peptides extracted from food sources. Journal of Biomolecular Structure and Dynamics, 2021, 39, 635-649.	2.0	9
2260	Novel quinolinoneâ€“pyrazoline hybrids: synthesis and evaluation of antioxidant and lipoxygenase inhibitory activity. Molecular Diversity, 2021, 25, 723-740.	2.1	20
2261	Homology modeling, structural insights and in-silico screening for selective inhibitors of mycobacterial CysE. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1547-1560.	2.0	2
2262	Understanding the mechanism of amygdalinâ€™s multifunctional anti-cancer action using computational approach. Journal of Biomolecular Structure and Dynamics, 2021, 39, 1600-1610.	2.0	14
2263	Culinary spice bioactives as potential therapeutics against SARS-CoV-2: Computational investigation. Computers in Biology and Medicine, 2021, 128, 104102.	3.9	36
2264	Automated theoretical chemical kinetics: Predicting the kinetics for the initial stages of pyrolysis. Proceedings of the Combustion Institute, 2021, 38, 375-384.	2.4	28
2265	A binding mode hypothesis for prothioconazole binding to CYP51 derived from first principles quantum chemistry. Journal of Computer-Aided Molecular Design, 2021, 35, 493-503.	1.3	4
2266	Recent advances in user-friendly computational tools to engineer protein function. Briefings in Bioinformatics, 2021, 22, .	3.2	41
2267	Antiviral activity of puerarin as potent inhibitor of influenza virus neuraminidase. Phytotherapy Research, 2021, 35, 324-336.	2.8	31
2268	Finding distinctions between oral cancer and periodontitis using saliva metabolites and machine learning. Oral Diseases, 2021, 27, 484-493.	1.5	32
2269	MolAICal: a soft tool for 3D drug design of protein targets by artificial intelligence and classical algorithm. Briefings in Bioinformatics, 2021, 22, .	3.2	163
2270	Virus-CKB: an integrated bioinformatics platform and analysis resource for COVID-19 research. Briefings in Bioinformatics, 2021, 22, 882-895.	3.2	28
2271	Lead optimization of 4-(thio)-chromenone 6-O-sulfamate analogs using QSAR, molecular docking and DFT â€“ a combined approach as steroidal sulfatase inhibitors. Journal of Receptor and Signal Transduction Research, 2021, 41, 123-137.	1.3	7
2272	Assessing conformer energies using electronic structure and machine learning methods. International Journal of Quantum Chemistry, 2021, 121, e26381.	1.0	40
2273	New insights into antiviral and cytotoxic potential of quercetin and its derivatives â€“ A biochemical perspective. Food Chemistry, 2021, 334, 127508.	4.2	35
2274	Synthesis, spectroscopic and molecular docking studies of novel 10-heterylazo-9-anthrone derivatives as potential antimicrobial and anticancer agents. Journal of Molecular Structure, 2021, 1226, 129359.	1.8	7

#	Article	IF	Citations
2275	Pyrimido[1,2-b]indazole derivatives: Selective inhibitors of human monoamine oxidase B with neuroprotective activity. European Journal of Medicinal Chemistry, 2021, 209, 112911.	2.6	23
2276	DockCoV2: a drug database against SARS-CoV-2. Nucleic Acids Research, 2021, 49, D1152-D1159.	6.5	42
2277	Li-doped fullerene pillared graphene nanocomposites for enhancing hydrogen storage: A computational study. Computational Materials Science, 2021, 186, 110023.	1.4	25
2278	Pentacoordinated diorganotin(IV) complexes resulting from tridentate (NOO) donor Schiff bases: Synthesis, characterization, inÂvitro antioxidant, antimicrobial activities, and QSAR studies. Phosphorus, Sulfur and Silicon and the Related Elements, 2021, 196, 119-132.	0.8	9
2279	The ModelSEED Biochemistry Database for the integration of metabolic annotations and the reconstruction, comparison and analysis of metabolic models for plants, fungi and microbes. Nucleic Acids Research, 2021, 49, D575-D588.	6.5	119
2280	Attenuation of Acinetobacter baumannii virulence by inhibition of polyphosphate kinase 1 with repurposed drugs. Microbiological Research, 2021, 242, 126627.	2.5	13
2281	Design, synthesis, biological activity evaluation of 3-(4-phenyl-1H-imidazol-2-yl)-1H-pyrazole derivatives as potent JAK 2/3 and aurora A/B kinases multi-targeted inhibitors. European Journal of Medicinal Chemistry, 2021, 209, 112934.	2.6	14
2282	Antitrichomonal activity and docking analysis of thiazole derivatives as TvMP50 protease inhibitors. Parasitology Research, 2021, 120, 233-241.	0.6	0
2283	Assessing the biological potential of new symmetrical ferrocene based bisthiourea analogues. Bioorganic Chemistry, 2021, 106, 104180.	2.0	14
2284	On the alleged importance of the molecular electron-donating ability and the HOMOâ€“LUMO gap in corrosion inhibition studies. Corrosion Science, 2021, 180, 109016.	3.0	50
2285	Antileishmanial and pharmacophore modeling of abietane-type diterpenoids extracted from the roots of Salvia hydrangea. Journal of Molecular Structure, 2021, 1228, 129447.	1.8	7
2286	Systematic design of biomolecular force fields. Current Opinion in Structural Biology, 2021, 67, 18-24.	2.6	30
2287	Synthesis, spectroscopy, crystal structure, TGA/DTA study, DFT and molecular docking investigations of (E)-4-(4-methylbenzyl)-6-styrylpyridazin-3(2H)-one. Journal of Molecular Structure, 2021, 1228, 129435.	1.8	55
2288	Modulation of IR as a therapeutic target to prevent NASH using NRF from Diceratella elliptica (DC.) jonsell. Strong Nrf2 and leptin inducer as well as NF-kB inhibitor. Phytomedicine, 2021, 80, 153388.	2.3	3
2289	Selection of low-toxic and highly efficient ionic liquids for the separation of palladium and platinum in acidic solution, and prediction of the metal affinity of ionic liquids. Separation and Purification Technology, 2021, 258, 118019.	3.9	7
2290	Design and in Vitro Characterization of Tricyclic Benzodiazepine Derivatives as Potent and Selective Antileukemic Agents. Chemistry and Biodiversity, 2021, 18, e2000733.	1.0	3
2291	Bile acid biosynthesis in Smith-Lemli-Opitz syndrome bypassing cholesterol: Potential importance of pathway intermediates. Journal of Steroid Biochemistry and Molecular Biology, 2021, 206, 105794.	1.2	12
2292	The XtalOpt Evolutionary Algorithm for Crystal Structure Prediction. Journal of Physical Chemistry C, 2021, 125, 1601-1620.	1.5	42

#	Article	IF	Citations
2293	Drug designing against NSP15 of SARS-COV2 via high throughput computational screening and structural dynamics approach. European Journal of Pharmacology, 2021, 892, 173779.	1.7	11
2294	The potential of Paritaprevir and Emetine as inhibitors of SARS-CoV-2 RdRp. Saudi Journal of Biological Sciences, 2021, 28, 1426-1432.	1.8	11
2295	Improvement in the screening performance of potential aryl hydrocarbon receptor ligands by using supervised machine learning. Chemosphere, 2021, 265, 129099.	4.2	15
2296	In Silico Models to Predict the Perturbation of Molecular Initiating Events Related to Thyroid Hormone Homeostasis. Chemical Research in Toxicology, 2021, 34, 396-411.	1.7	20
2297	Structural insight into the novel ironâ€coordination and domain interactions of transferrinâ€1 from a model insect, Manduca sexta. Protein Science, 2021, 30, 408-422.	3.1	9
2298	Solution structures of the Shewanella woodyi<scp>Hâ€NOX</scp> protein in the presence and absence of soluble guanylyl cyclase stimulator <scp>IWP</scp>â€051. Protein Science, 2021, 30, 448-463.	3.1	4
2299	Antiquorum Sensing Activity of Copper Nanoparticle in Pseudomonas aeruginosa: An In Silico Approach. Proceedings of the National Academy of Sciences India Section B - Biological Sciences, 2021, 91, 29-36.	0.4	7
2300	Analyses of structural dynamics revealed flexible binding mechanism for the <scp>Agrilus mali</scp> odorant binding protein 8 towards plant volatiles. Pest Management Science, 2021, 77, 1642-1653.	1.7	15
2301	Kinetic inequivalence between Î± and Î² subunits of ligand dissociation from ferrous nitrosylated human haptoglobin:hemoglobin complexes. A comparison with O2 and CO dissociation. Journal of Inorganic Biochemistry, 2021, 214, 111272.	1.5	0
2302	Discovery, development, chemical diversity and design of isoxazoline-based insecticides. Bioorganic and Medicinal Chemistry, 2021, 30, 115934.	1.4	22
2303	Comparisons of different force fields in conformational analysis and searching of organic molecules: A review. Tetrahedron, 2021, 79, 131865.	1.0	34
2304	Essential interpretations of bioinformatics in COVID-19 pandemic. Meta Gene, 2021, 27, 100844.	0.3	15
2305	Artificial intelligence in the early stages of drug discovery. Archives of Biochemistry and Biophysics, 2021, 698, 108730.	1.4	33
2306	Alkaloids of Zephyranthes citrina (Amaryllidaceae) and their implication to Alzheimer's disease: Isolation, structural elucidation and biological activity. Bioorganic Chemistry, 2021, 107, 104567.	2.0	20
2307	Insights into the Molecular Mechanisms of Liuwei Dihuang Decoction via Network Pharmacology. Chemical Research in Toxicology, 2021, 34, 91-102.	1.7	8
2308	Next-generation computational tools and resources for coronavirus research: From detection to vaccine discovery. Computers in Biology and Medicine, 2021, 128, 104158.	3.9	14
2309	BCL::Conf: Improved Open-Source Knowledge-Based Conformation Sampling Using the Crystallography Open Database. Journal of Chemical Information and Modeling, 2021, 61, 189-201.	2.5	17
2310	Are losartan and imatinib effective against SARS-CoV2 pathogenesis? A pathophysiologic-based in silico study. In Silico Pharmacology, 2021, 9, 1.	1.8	40

#	Article	IF	Citations
2311	Selection of a new peptide homing SKâ€BRâ€3 breast cancer cells. Chemical Biology and Drug Design, 2021, 97, 893-903.	1.5	2
2312	Towards a universal digital chemical space for pure component properties prediction. Fluid Phase Equilibria, 2021, 527, 112829.	1.4	2
2313	MASI: microbiotaâ€"active substance interactions database. Nucleic Acids Research, 2021, 49, D776-D782.	6.5	28
2314	Structure-Based Design of Novel Peptidomimetics Targeting the SARS-CoV-2 Spike Protein. Cellular and Molecular Bioengineering, 2021, 14, 177-185.	1.0	17
2315	The influence of lipid membranes on fluorescent probes' optical properties. Biochimica Et Biophysica Acta - Biomembranes, 2021, 1863, 183494.	1.4	11
2316	In-silico screening of database for finding potential sweet molecules: A combined data and structure based modeling approach. Food Chemistry, 2021, 343, 128538.	4.2	12
2317	ChemVA: Interactive Visual Analysis of Chemical Compound Similarity in Virtual Screening. IEEE Transactions on Visualization and Computer Graphics, 2021, 27, 891-901.	2.9	6
2318	Machine learningâ€based atom contribution method for the prediction of surface charge density profiles and solvent design. AICHE Journal, 2021, 67, e17110.	1.8	30
2319	Supervised molecular dynamics for exploring the druggability of the SARS-CoV-2 spike protein. Journal of Computer-Aided Molecular Design, 2021, 35, 195-207.	1.3	41
2320	Effect of thiophene-based Ï€-spacers on N-arylphenothiazine dyes for dye-sensitized solar cells. Dyes and Pigments, 2021, 185, 108951.	2.0	27
2321	Identification of good and bad fragments of tricyclic triazinone analogues as potential PKC-Î¸ inhibitors through SMILESâ€"based QSAR and molecular docking. Structural Chemistry, 2021, 32, 149-165.	1.0	18
2322	LCâ€"QTOF-MS Presumptive Identification of Synthetic Cannabinoids without Reference Chromatographic Retention/Mass Spectral Information. II. Evaluation of a Computational Approach for Predicting and Identifying Unknown High-Resolution Product Ion Mass Spectra. Journal of Analytical Toxicology, 2021, 45, 440-461.	1.7	9
2323	Synthesis of 1,2,3-triazolyl nucleoside analogues and their antiviral activity. Molecular Diversity, 2021, 25, 473-490.	2.1	23
2324	A DFT/machineâ€learning hybrid method for the prediction of ³J_{HCCH} couplings. Magnetic Resonance in Chemistry, 2021, 59, 414-422.	1.1	4
2325	Molecular modeling of a series of dehydroquinate dehydratase type II inhibitors of Mycobacterium tuberculosis and design of new binders. Molecular Diversity, 2021, 25, 1-12.	2.1	3
2326	In-silico profiling and structural insights into the impact of nSNPs in the P. falciparum acetyl-CoA transporter gene to understand the mechanism of drug resistance in malaria. Journal of Biomolecular Structure and Dynamics, 2021, 39, 558-569.	2.0	2
2327	AromTool: predicting aromatic stacking energy using an atomic neural network model. Physical Chemistry Chemical Physics, 2021, 23, 16044-16052.	1.3	0
2328	The iPPI-DB initiative: a community-centered database of proteinâ€"protein interaction modulators. Bioinformatics, 2021, 37, 89-96.	1.8	24

#	Article	IF	Citations
2329	Performance of protein-ligand docking with CDK4/6 inhibitors: a case study. Mathematical Biosciences and Engineering, 2021, 18, 456-470.	1.0	2
2330	Derivatives of Tenuazonic Acid as Potential New Multi-Target Anti-Alzheimerâ€™s Disease Agents. Biomolecules, 2021, 11, 111.	1.8	17
2331	Monte-Carlo method-based QSAR model to discover phytochemical urease inhibitors using SMILES and GRAPH descriptors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5090-5099.	2.0	11
2332	Advances in structure-based drug design. , 2021, , 55-103.		9
2333	Short- and Long-Range Particle-Matrix Interphases. Research Topics in Aerospace, 2021, , 143-178.	0.6	1
2334	Response of Human Glioblastoma Cells to Vitamin B12 Deficiency: A Study Using the Non-Toxic Cobalamin Antagonist. Biology, 2021, 10, 69.	1.3	4
2335	Feature Based Method for Predicting Pharmacological Interaction. International Journal of Recent Technology and Engineering, 2021, 9, 125-129.	0.2	0
2336	Structural insights and inhibition mechanism of TMPRSS2 by experimentally known inhibitors Camostat mesylate, Nafamostat and Bromhexine hydrochloride to control SARS-coronavirus-2: A molecular modeling approach. Informatics in Medicine Unlocked, 2021, 24, 100597.	1.9	32
2337	Conservation of binding properties in protein models. Computational and Structural Biotechnology Journal, 2021, 19, 2549-2566.	1.9	2
2338	Dual targeting of 3CLpro and PLpro of SARS-CoV-2: A novel structure-based design approach to treat COVID-19. Current Research in Structural Biology, 2021, 3, 9-18.	1.1	46
2339	A comprehensive drug repurposing study for COVID19 treatment: novel putative dihydroorotate dehydrogenase inhibitors show association to serotoninâ€“dopamine receptors. Briefings in Bioinformatics, 2021, 22, 1023-1037.	3.2	14
2340	Accelerating A<scp>uto</scp>D<scp>ock</scp>4 with GPUs and Gradient-Based Local Search. Journal of Chemical Theory and Computation, 2021, 17, 1060-1073.	2.3	128
2341	Association of CYP1A1 and CYP1B1 inhibition in <i>in vitro</i> assays with drug-induced liver injury. Journal of Toxicological Sciences, 2021, 46, 167-176.	0.7	9
2342	Bypassing the requirement for aminoacyl-tRNA by a cyclodipeptide synthase enzyme. RSC Chemical Biology, 2021, 2, 230-240.	2.0	5
2343	Deciphering the interaction of flavones with calf thymus DNA and octamer DNA sequence (CCAATTGG)₂. RSC Advances, 2021, 11, 29354-29371.	1.7	12
2344	Spiro-Î²-lactam BSS-730A Displays Potent Activity against HIV and Plasmodium. ACS Infectious Diseases, 2021, 7, 421-434.	1.8	11
2345	SAMPL7 blind predictions using nonequilibrium alchemical approaches. Journal of Computer-Aided Molecular Design, 2021, 35, 37-47.	1.3	16
2346	Alternative pathways utilize or circumvent putrescine for biosynthesis of putrescine-containing rhizoferrin. Journal of Biological Chemistry, 2021, 296, 100146.	1.6	8

#	Article	IF	Citations
2349	Investigative studies on the inhibition of amyloid-like fibrils formation by the extracts of Vernonia amygdalina Del. leaf. Advances in Traditional Medicine, 2022, 22, 163-176.	1.0	2
2350	Washingtonia filifera seed extracts inhibit the islet amyloid polypeptide fibrils formations and Î±-amylase and Î±-glucosidase activity. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 517-524.	2.5	11
2352	Effects of side chain length of 10-methyl-aplog-1, a simplified analog of debromoaplysiatoxin, on PKC binding, anti-proliferative, and pro-inflammatory activities. Bioscience, Biotechnology and Biochemistry, 2021, 85, 168-180.	0.6	6
2353	Corilagin and 1,3,6-Tri-O-galloy-Î²-d-glucose: potential inhibitors of SARS-CoV-2 variants. Physical Chemistry Chemical Physics, 2021, 23, 14873-14888.	1.3	12
2354	In vitro and in silico evaluation of antifungal activity of cassia (CinnamomumÂcassia) and holy basil (Ocimum tenuiflorum) essential oils for the control of anthracnose and crown-rot postharvest diseases of banana fruits. Chemical Papers, 2021, 75, 2043-2057.	1.0	7
2355	Molecular Modeling of Epoxy Resin Crosslinking Experimentally Validated by Near-Infrared Spectroscopy. Research Topics in Aerospace, 2021, , 325-349.	0.6	1
2356	Evaluation of certain medicinal plants compounds as new potential inhibitors of novel corona virus (COVID-19) using molecular docking analysis. In Silico Pharmacology, 2021, 9, 10.	1.8	41
2357	In-silico predictions of deleterious SNPs in human ephrin type-A receptor 3 (EPHA3) gene. Informatics in Medicine Unlocked, 2021, 26, 100728.	1.9	0
2358	Computational molecular docking and virtual screening revealed promising SARS-CoV-2 drugs. Precision Clinical Medicine, 2021, 4, 1-16.	1.3	66
2359	Dynamic Docking Using Multicanonical Molecular Dynamics: Simulating Complex Formation at the Atomistic Level. Methods in Molecular Biology, 2021, 2266, 187-202.	0.4	8
2360	Repurposing existing drugs: identification of SARS-CoV-2 3C-like protease inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2021, 36, 147-153.	2.5	29
2361	Automation of absolute protein-ligand binding free energy calculations for docking refinement and compound evaluation. Scientific Reports, 2021, 11, 1116.	1.6	49
2362	Coupling the high-resolution LCâ€“MS characterisation of the phenolic compounds with the antimicrobial and antibiofilm properties of helencha (Enydra fluctuans Lour.). Journal of Food Science and Technology, 2021, 58, 4755-4765.	1.4	2
2363	Insights into the structure and function of the rate-limiting enzyme of chlorophyll degradation through analysis of a bacterial Mg-dechelatase homolog. Computational and Structural Biotechnology Journal, 2021, 19, 5333-5347.	1.9	1
2364	Exploring the mechanism of Shenqisherong pill against cervical spondylotic myelopathy by network pharmacology and molecular docking. Annals of Palliative Medicine, 2021, 10, 10253-10275.	0.5	2
2365	Simulation of Ligand Transport in Receptors Using CaverDock. Methods in Molecular Biology, 2021, 2266, 105-124.	0.4	1
2366	Bionoi: A Voronoi Diagram-Based Representation of Ligand-Binding Sites in Proteins for Machine Learning Applications. Methods in Molecular Biology, 2021, 2266, 299-312.	0.4	5
2367	Molecular insights into the Patched1 drug efflux inhibitory activity of panicein A hydroquinone: a computational study. Physical Chemistry Chemical Physics, 2021, 23, 8013-8022.	1.3	2

#	Article	IF	Citations
2368	Molecular Docking Suggests the Targets of Anti-Mycobacterial Natural Products. Molecules, 2021, 26, 475.	1.7	19
2370	The Structural Properties of Odorants Modulate Their Association to Human Odorant Binding Protein. Biomolecules, 2021, 11, 145.	1.8	4
2371	Prediction of repurposed drugs for Coronaviruses using artificial intelligence and machine learning. Computational and Structural Biotechnology Journal, 2021, 19, 3133-3148.	1.9	30
2372	A Protocol to Use Comparative Binding Energy Analysis to Estimate Drug-Target Residence Time. Methods in Molecular Biology, 2021, 2266, 171-186.	0.4	1
2373	Molecular basis for the repurposing of histamine H2-receptor antagonist to treat COVID-19. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5785-5802.	2.0	8
2374	Bioactivities and in silico study of Pergularia tomentosa L. phytochemicals as potent antimicrobial agents targeting type IIA topoisomerase, TyrRS, and Sap1 virulence proteins. Environmental Science and Pollution Research, 2021, 28, 25349-25367.	2.7	18
2375	Structure-Based Identification of Potential Drugs Against FmtA of Staphylococcus aureus: Virtual Screening, Molecular Dynamics, MM-GBSA, and QM/MM. Protein Journal, 2021, 40, 148-165.	0.7	47
2376	Predicting PAMPA permeability using the 3D-RISM-KH theory: are we there yet?. Journal of Computer-Aided Molecular Design, 2021, 35, 261-269.	1.3	6
2377	Triorganotin (IV) carboxylates as potential anticancer agents: Their synthesis, physiochemical characterization, and cytotoxic activity against HeLa and MCFâ€7 cancer cells. Applied Organometallic Chemistry, 2021, 35, e6165.	1.7	8
2378	Identification of new BACE1 inhibitors for treating Alzheimerâ€™s disease. Journal of Molecular Modeling, 2021, 27, 58.	0.8	7
2379	DFT and molecular docking investigations anthocyanidin to the human epidermal receptor-2 receptor (HER-2) in breast cancer. AIP Conference Proceedings, 2021, , .	0.3	0
2380	Design, in silico Analysis, Synthesis and Evaluation of Novel Benzofused Nitrogen Containing Heterocyclic N-Substituted Mercaptobenzimidazole Derivatives as Potential Antimicrobial Agent. Asian Journal of Organic & Medicinal Chemistry, 2021, 6, 121-127.	0.1	1
2381	Drug repurposing and computational modeling for discovery of inhibitors of the main protease (M^{pro}) of SARS-CoV-2. RSC Advances, 2021, 11, 23450-23458.	1.7	15
2382	Covalent flexible peptide docking in Rosetta. Chemical Science, 2021, 12, 10836-10847.	3.7	15
2383	Ligand-based approach for predicting drug targets and for virtual screening against COVID-19. Briefings in Bioinformatics, 2021, 22, 1053-1064.	3.2	27
2384	Synthesis, Anticancer Evaluation, Computer-Aided Docking Studies, and ADMET Prediction of 1,2,3-Triazolyl-Pyridine Hybrids as Human Aurora B Kinase Inhibitors. ACS Omega, 2021, 6, 1445-1455.	1.6	29
2385	Identification of potential inhibitors for Sterol C-24 reductase of Leishmania donovani through virtual screening of natural compounds. Biocell, 2021, 45, 1601-1610.	0.4	0
2386	Drug repurposing for cancer treatment through global propagation with a greedy algorithm in a multilayer network. Cancer Biology and Medicine, 2021, 18, 0-0.	1.4	5

#	Article	IF	Citations
2387	Systematic Search for SARS-CoV-2 Main Protease Inhibitors for Drug Repurposing: Ethacrynic Acid as a Potential Drug. Viruses, 2021, 13, 106.	1.5	11
2388	Immunoinformatics-guided design of a multi-epitope vaccine based on the structural proteins of severe acute respiratory syndrome coronavirus 2. RSC Advances, 2021, 11, 18103-18121.	1.7	25
2389	Molecular docking and simulation studies of natural compounds ofVitex negundoL. against papain-like protease (PL^{pro}) of SARS CoV-2 (coronavirus) to conquer the pandemic situation in the world. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5665-5686.	2.0	24
2390	Multiple Target Drug Design Using LigBuilder 3. Methods in Molecular Biology, 2021, 2266, 279-298.	0.4	0
2391	Troubleshooting unstable molecules in chemical space. Chemical Science, 2021, 12, 5566-5573.	3.7	5
2392	Identification of potential antivirals against SARS-CoV-2 using virtual screening method. Informatics in Medicine Unlocked, 2021, 23, 100531.	1.9	17
2393	MeFSAT: a curated natural product database specific to secondary metabolites of medicinal fungi. RSC Advances, 2021, 11, 2596-2607.	1.7	16
2394	The Three Pillars of Natural Product Dereplication. Alkaloids from the Bulbs of Urceolina peruviana (C. Presl) J.F. Macbr. as a Preliminary Test Case. Molecules, 2021, 26, 637.	1.7	16
2395	Single Nucleotides Moving through Nanoslits Composed of Self-Assembled Monolayers via Equilibrium and Nonequilibrium Molecular Dynamics. Journal of Physical Chemistry B, 2021, 125, 1259-1270.	1.2	2
2396	Predictive medicinal metabolites fromMomordica dioicaagainst comorbidity related proteins of SARS-CoV-2 infections. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5175-5188.	2.0	5
2397	Mechanical Properties of Boehmite Evaluated by Atomic Force Microscopy Experiments and Molecular Dynamic Finite Element Simulations. Research Topics in Aerospace, 2021, , 91-117.	0.6	2
2398	Sparse Nonnegative Interaction Models. IEEE Access, 2021, 9, 109994-110005.	2.6	0
2399	Drug Design and Discovery: Theory, Applications, Open Issues and Challenges. Studies in Computational Intelligence, 2021, , 337-358.	0.7	0
2400	Commentary toward the 20th Anniversary of the Society ofComputer Chemistry, Japan. Journal of Computer Chemistry Japan, 2021, 20, A26-A40.	0.0	0
2401	Potential repurposing of four FDA approved compounds with antiplasmodial activity identified through proteome scale computational drug discovery and in vitro assay. Scientific Reports, 2021, 11, 1413.	1.6	14
2402	Transformer neural network for protein-specific de novo drug generation as a machine translation problem. Scientific Reports, 2021, 11, 321.	1.6	96
2403	Computer-Aided Solvent Design Integrated with a Machine Learning-based Atom Contribution Method. Computer Aided Chemical Engineering, 2021, , 69-74.	0.3	0
2404	Extracellular calcium receptor as a target for glutathione and its derivatives. SSRN Electronic Journal, 0, , .	0.4	0

#	Article	IF	Citations
2405	Application of Network Pharmacology Based on Artificial Intelligence Algorithms in Drug Development. , 2021, , 35-73.		2
2406	Accelerating high-throughput virtual screening through molecular pool-based active learning. Chemical Science, 2021, 12, 7866-7881.	3.7	115
2407	Mononuclear copper(i) complexes of triphenylphosphine and N,Nâ€²-disubstituted thioureas as potential DNA binding chemotherapeutics. New Journal of Chemistry, 2021, 45, 8925-8935.	1.4	1
2408	A systems pharmacology approach to identify the autophagy-inducing effects of Traditional Persian medicinal plants. Scientific Reports, 2021, 11, 336.	1.6	7
2409	In silico study of the inhibition of SARS-COV-2 viral cell entry by neem tree extracts. RSC Advances, 2021, 11, 26524-26533.	1.7	7
2410	Elimination of Uremic Toxins by Functionalized Graphene-Based Composite Beads for Direct Hemoperfusion. ACS Applied Materials & Interfaces, 2021, 13, 5955-5965.	4.0	19
2411	Tool recommender system in Galaxy using deep learning. GigaScience, 2021, 10, .	3.3	9
2412	In Silico Insight into the Inhibitory Effects of Active Antidiabetic Compounds from Medicinal Plants Against SARS-CoV-2 Replication and Posttranslational Modification. Coronaviruses, 2022, 3, .	0.2	2
2414	Molecular modelling as a tool for designing dipeptidylpeptidase-4 inhibitors. Journal of Analytical & Pharmaceutical Research, 2021, 10, 26-39.	0.3	0
2415	Practical and Selective sp³Câ^'H Bond Chlorination via Aminium Radicals. Angewandte Chemie, 2021, 133, 7208-7215.	1.6	1
2416	Asah2 Represses the p53â€“Hmox1 Axis to Protect Myeloid-Derived Suppressor Cells from Ferroptosis. Journal of Immunology, 2021, 206, 1395-1404.	0.4	49
2417	Imidazopyridine hydrazone derivatives exert antiproliferative effect on lung and pancreatic cancer cells and potentially inhibit receptor tyrosine kinases including c-Met. Scientific Reports, 2021, 11, 3644.	1.6	26
2418	Structureâ€“Function Relationship Study of a Secretory Amoebic Phosphatase: A Computational-Experimental Approach. International Journal of Molecular Sciences, 2021, 22, 2164.	1.8	0
2419	Cocrystal Prediction Using Machine Learning Models and Descriptors. Applied Sciences (Switzerland), 2021, 11, 1323.	1.3	22
2420	Generative chemistry: drug discovery with deep learning generative models. Journal of Molecular Modeling, 2021, 27, 71.	0.8	63
2421	Targeting allosteric pockets of SARS-CoV-2 main protease M^{pro}. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6603-6618.	2.0	11
2422	Practical and Selective sp³Câ^'H Bond Chlorination via Aminium Radicals. Angewandte Chemie - International Edition, 2021, 60, 7132-7139.	7.2	34
2423	Novel Immune Modulators Enhance Caenorhabditis elegans Resistance to Multiple Pathogens. MSphere, 2021, 6, .	1.3	17

#	Article	IF	Citations
2424	Mapping drug-target interactions and synergy in multi-molecular therapeutics for pressure-overload cardiac hypertrophy. Npj Systems Biology and Applications, 2021, 7, 11.	1.4	13
2425	Using molecular docking and molecular dynamics to investigate protein-ligand interactions. Modern Physics Letters B, 2021, 35, 2130002.	1.0	54
2426	Structure-activity relationship (SAR) and molecular dynamics study of withaferin-A fragment derivatives as potential therapeutic lead against main protease (Mpro) of SARS-CoV-2. Journal of Molecular Modeling, 2021, 27, 97.	0.8	16
2427	The B-factor index for the binding site (BFIbs) to prioritize crystal protein structures for docking. Structural Chemistry, 2021, 32, 1693-1699.	1.0	1
2428	Understanding Ring Puckering in Small Molecules and Cyclic Peptides. Journal of Chemical Information and Modeling, 2021, 61, 743-755.	2.5	20
2429	Genome-wide identification and expression profiling of glutathione S-transferase family under multiple abiotic and biotic stresses in Medicago truncatula L.. PLoS ONE, 2021, 16, e0247170.	1.1	23
2430	Synthesis and Pharmacological Evaluation of Novel Non-nucleotide Purine Derivatives as P2X7 Antagonists for the Treatment of Neuroinflammation. Journal of Medicinal Chemistry, 2021, 64, 2272-2290.	2.9	19
2431	Crystal Growth and Structure Determination of a Newly Synthesised Chalcone Derivative with Hirshfeld Surface Analysis and Energy Frame Work: (2e,4e)-5-(4-(Dimethylamino)Phenyl)-1-(Naphthalen-2-Yl)Penta-2,4-Dien-1-One. Asian Journal of Chemical Sciences, 0, , 1-13.	0.4	0
2432	Therapeutic Potentials of Colocasia affinis Leaf Extract for the Alleviation of Streptozotocin-Induced Diabetes and Diabetic Complications: In vivo and in silico-Based Studies. Journal of Inflammation Research, 2021, Volume 14, 443-459.	1.6	3
2433	Computer-assisted catalyst development via automated modelling of conformationally complex molecules: application to diphosphinoamine ligands. Scientific Reports, 2021, 11, 4534.	1.6	5
2434	Biosynthesis of glyceride glycoside (nonionic surfactant) by amylosucrase, a powerful glycosyltransferase. Food Science and Biotechnology, 2021, 30, 267-276.	1.2	3
2435	Repurposing of Omarigliptin as a Neuroprotective Agent Based on Docking with A2A Adenosine and AChE Receptors, Brain GLP-1 Response and Its Brain/Plasma Concentration Ratio after 28 Days Multiple Doses in Rats Using LC-MS/MS. Molecules, 2021, 26, 889.	1.7	10
2436	Synergistic Network Pharmacology for Traditional Chinese Medicine Liangxue Tongyu Formula in Acute Intracerebral Hemorrhagic Stroke. Neural Plasticity, 2021, 2021, 1-21.	1.0	5
2438	Artificial intelligence, machine learning, and drug repurposing in cancer. Expert Opinion on Drug Discovery, 2021, 16, 977-989.	2.5	68
2439	Crystal structure of pomalidomide Form I, C13H11N3O4. Powder Diffraction, 2021, 36, 114-119.	0.4	1
2440	In silico identification of potential inhibitor for TP53-induced glycolysis and apoptosis regulator in head and neck squamous cell carcinoma. 3 Biotech, 2021, 11, 117.	1.1	2
2441	Exploring the Impacts of Conformer Selection Methods on Ion Mobility Collision Cross Section Predictions. Analytical Chemistry, 2021, 93, 3830-3838.	3.2	8
2442	PyCHAM (v2.1.1): a Python box model for simulating aerosol chambers. Geoscientific Model Development, 2021, 14, 675-702.	1.3	9

#	Article	IF	Citations
2443	BOW-GBDT: A GBDT Classifier Combining With Artificial Neural Network for Identifying GPCRâ€“Drug Interaction Based on Wordbook Learning From Sequences. Frontiers in Cell and Developmental Biology, 2020, 8, 623858.	1.8	16
2444	Tacrine â€“ Benzothiazoles: Novel class of potential multitarget anti-AlzheimeÅ•s drugs dealing with cholinergic, amyloid and mitochondrial systems. Bioorganic Chemistry, 2021, 107, 104596.	2.0	17
2445	Synthesis and in vitro study of nitro- and methoxy-2-phenylbenzofurans as human monoamine oxidase inhibitors. Bioorganic Chemistry, 2021, 107, 104616.	2.0	12
2447	A molecular docking and dynamic approach to screen inhibitors against ZnuA1 ofCandidatusLiberibacter asiaticus. Molecular Simulation, 2021, 47, 510-525.	0.9	18
2448	QM/MM Study of the Catalytic Reaction of Myrosinase; Importance of Assigning Proper Protonation States of Active-Site Residues. Journal of Chemical Theory and Computation, 2021, 17, 1822-1841.	2.3	11
2449	In-silico strategies of some selected phytoconstituents from Melissa officinalis as SARS CoV-2 main protease and spike protein (COVID-19) inhibitors. Molecular Simulation, 2021, 47, 457-470.	0.9	19
2450	Quantum chemical benchmark databases of gold-standard dimer interaction energies. Scientific Data, 2021, 8, 55.	2.4	34
2451	Minocycline Impact on Redox Homeostasis of Normal Human Melanocytes HEMn-LP Exposed to UVA Radiation and Hydrogen Peroxide. International Journal of Molecular Sciences, 2021, 22, 1642.	1.8	8
2452	A molecular modelling approach for identifying antiviral selenium-containing heterocyclic compounds that inhibit the main protease of SARS-CoV-2: an in silico investigation. Briefings in Bioinformatics, 2021, 22, 1476-1498.	3.2	58
2453	Sensitivity of Binding Free Energy Calculations to Initial Protein Crystal Structure. Journal of Chemical Theory and Computation, 2021, 17, 1806-1821.	2.3	13
2454	Establishing an Analogue Based In Silico Pipeline in the Pursuit of Novel Inhibitory Scaffolds against the SARS Coronavirus 2 Papain-Like Protease. Molecules, 2021, 26, 1134.	1.7	11
2455	Phyto-compounds from a rather poisonous plant, Strychnos nux-vomica, show high potency against SARS-CoV-2 RNA-dependent RNA polymerase. Current Molecular Medicine, 2021, 21, .	0.6	2
2457	Exploring the active constituents of Oroxylum indicum in intervention of novel coronavirus (COVID-19) based on molecular docking method. Network Modeling Analysis in Health Informatics and Bioinformatics, 2021, 10, 8.	1.2	15
2458	A recursive molecular docking coupled with energy-based pose-rescoring and MD simulations to identify hsGC Î²H-NOX allosteric modulators for cardiovascular dysfunctions. Journal of Biomolecular Structure and Dynamics, 2021, , 1-23.	2.0	1
2459	Resveratrol Mediates the Apoptosis of Triple Negative Breast Cancer Cells by Reducing POLD1 Expression. Frontiers in Oncology, 2021, 11, 569295.	1.3	22
2460	PSC-db: A Structured and Searchable 3D-Database for Plant Secondary Compounds. Molecules, 2021, 26, 1124.	1.7	10
2461	AnnapuRNA: A scoring function for predicting RNA-small molecule binding poses. PLoS Computational Biology, 2021, 17, e1008309.	1.5	47
2462	Quantum chemical investigation of the antiradical property of avenanthramides, oat phenolics. Heliyon, 2021, 7, e06125.	1.4	9

#	Article	IF	Citations
2463	Rationalizing PROTAC-Mediated Ternary Complex Formation Using Rosetta. Journal of Chemical Information and Modeling, 2021, 61, 1368-1382.	2.5	77
2464	Fast Identification of Adverse Drug Reactions (ADRs) of Digestive and Nervous Systems of Organic Drugs by In Silico Models. Molecules, 2021, 26, 930.	1.7	1
2465	Molecular Docking Studies Reveal Rhein from rhubarb (Rheum rhabarbarum) as a Putative Inhibitor of ATP-binding Cassette Super-family G member 2. Medicinal Chemistry, 2021, 17, 273-288.	0.7	16
2467	Expanding the Coverage of Metabolic Landscape in Cultivated Rice with Integrated Computational Approaches. Genomics, Proteomics and Bioinformatics, 2022, 20, 702-714.	3.0	3
2468	Metrics for Benchmarking and Uncertainty Quantification: Quality, Applicability, and Best Practices for Machine Learning in Chemistry. Trends in Chemistry, 2021, 3, 146-156.	4.4	37
2469	Openâ€source molecular modeling software in chemical engineering focusing on the Molecular Simulation Design Framework. AICHE Journal, 2021, 67, e17206.	1.8	16
2470	Systematic Partitioning of Proteins for Quantum-Chemical Fragmentation Methods Using Graph Algorithms. Journal of Chemical Theory and Computation, 2021, 17, 1355-1367.	2.3	4
2471	Alterations in the HLA-B*57:01 Immunopeptidome by Flucloxacillin and Immunogenicity of Drug-Haptenated Peptides. Frontiers in Immunology, 2020, 11, 629399.	2.2	16
2472	QM7-X, a comprehensive dataset of quantum-mechanical properties spanning the chemical space of small organic molecules. Scientific Data, 2021, 8, 43.	2.4	46
2473	Thiazole-Based Thiosemicarbazones: Synthesis, Cytotoxicity Evaluation and Molecular Docking Study. Drug Design, Development and Therapy, 2021, Volume 15, 659-677.	2.0	55
2474	Bayesian reaction optimization as a tool for chemical synthesis. Nature, 2021, 590, 89-96.	13.7	370
2475	A New Computer Model for Evaluating the Selective Binding Affinity of Phenylalkylamines to T-Type Ca2+ Channels. Pharmaceuticals, 2021, 14, 141.	1.7	6
2476	Structure Elucidation and Cholinesterase Inhibition Activity of Two New Minor Amaryllidaceae Alkaloids. Molecules, 2021, 26, 1279.	1.7	7
2477	Identification of Inhibitors Based on Molecular Docking: Thyroid Hormone Transmembrane Transporter MCT8 as a Target. Current Drug Discovery Technologies, 2021, 18, 105-112.	0.6	1
2478	Incorporating structural similarity into a scoring function to enhance the prediction of binding affinities. Journal of Cheminformatics, 2021, 13, 11.	2.8	1
2479	Molecular docking study of fatty acids from Pliek U Oil in the inhibition of SARS-CoV-2 protein and enzymes. IOP Conference Series: Materials Science and Engineering, 2021, 1087, 012058.	0.3	6
2480	Large-Scale Analysis of Bioactive Ligand Conformational Strain Energy by Ab Initio Calculation. Journal of Chemical Information and Modeling, 2021, 61, 1180-1192.	2.5	16
2481	Evaluation of Thermochemical Machine Learning for Potential Energy Curves and Geometry Optimization. Journal of Physical Chemistry A, 2021, 125, 1987-1993.	1.1	5

#	Article	IF	Citations
2482	Molecular docking and molecular dynamic studies: screening of phytochemicals against EGFR, HER2, estrogen and NF-KB receptors for their potential use in breast cancer. Journal of Biomolecular Structure and Dynamics, 2022, 40, 6183-6192.	2.0	9
2483	Illuminating the dark conformational space of macrocycles using dominant rotors. Nature Chemistry, 2021, 13, 218-225.	6.6	31
2484	Accurate Thermochemistry of Complex Lignin Structures via Density Functional Theory, Group Additivity, and Machine Learning. ACS Sustainable Chemistry and Engineering, 2021, 9, 3043-3049.	3.2	11
2485	Metabolomics andIn SilicoDocking-Directed Discovery of Small-Molecule Enzyme Targets. Analytical Chemistry, 2021, 93, 3072-3081.	3.2	15
2486	In silico screening of therapeutic potentials from Strychnos nux-vomica against the dimeric main protease (M^{pro}) structure of SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7796-7814.	2.0	17
2487	Inhibitor Development against p7 Channel in Hepatitis C Virus. Molecules, 2021, 26, 1350.	1.7	5
2488	Phylogenic analysis of coronavirus genome and molecular studies on potential anti-COVID-19 agents from selected FDA-approved drugs. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7726-7743.	2.0	5
2489	Unraveling the potential role of bioactive molecules produced byTrichodermaspp. as inhibitors of tomatinase enzyme having an important role in wilting disease: anin-silicoapproach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7535-7544.	2.0	5
2490	Quantitative and Molecular Similarity Analyses of the Metabolites of Cold- and Hot-Natured Chinese Herbs. Evidence-based Complementary and Alternative Medicine, 2021, 2021, 1-10.	0.5	5
2491	Deciphering the multi-scale mechanisms of Tephrosia purpurea against polycystic ovarian syndrome (PCOS) and its major psychiatric comorbidities: Studies from network pharmacological perspective. Gene, 2021, 773, 145385.	1.0	12
2492	Antileishmanial Evaluation of Bark Methanolic Extract ofAcacia nilotica:In VitroandIn SilicoStudies. ACS Omega, 2021, 6, 8548-8560.	1.6	16
2493	Synthesis, Molecular Docking Studies and In Silico ADMET Screening of New Heterocycles Linked Thiazole Conjugates as Potent Anti-Hepatic Cancer Agents. Molecules, 2021, 26, 1705.	1.7	16
2494	Structure-based design of small molecule and peptide inhibitors for selective targeting of ROCK1: an integrative computational approach. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7450-7468.	2.0	3
2495	Pan-genomic analyses of 47 complete genomes of theRickettsiagenus and prediction of new vaccine targets and virulence factors of the species. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7496-7510.	2.0	2
2496	Docking and in silico toxicity assessment of Arthrospira compounds as potential antiviral agents against SARS-CoV-2. Journal of Applied Phycology, 2021, 33, 1579-1602.	1.5	29
2497	Improved Proteinâ€“Ligand Binding Affinity Prediction with Structure-Based Deep Fusion Inference. Journal of Chemical Information and Modeling, 2021, 61, 1583-1592.	2.5	140
2498	Hesperidin Targets Leishmania donovani Sterol C-24 Reductase to Fight against Leishmaniasis. ACS Omega, 2021, 6, 8112-8118.	1.6	8
2499	Structureâ€“Activity Relationship Study of Dexrazoxane Analogues Reveals ICRF-193 as the Most Potent Bisdioxopiperazine against Anthracycline Toxicity to Cardiomyocytes Due to Its Strong Topoisomerase IIÎ² Interactions. Journal of Medicinal Chemistry, 2021, 64, 3997-4019.	2.9	14

#	Article	IF	Citations
2500	Introducing DerivatizeME and its Application in the Augmentation of a Natural Product Library. Journal of Computational Biophysics and Chemistry, 2021, 20, 233-250.	1.0	1
2501	Pentagalloylglucose, a phytochemical from Terminalia chebula can efficiently prevent SARS-CoV-2 entry: In Silico study. Israel Journal of Plant Sciences, 2021, 68, 124-132.	0.3	2
2502	Identifying the Trade-off between Intramolecular Singlet Fission Requirements in Donorâ€“Acceptor Copolymers. Chemistry of Materials, 2021, 33, 2567-2575.	3.2	14
2503	The effect of nutmeg essential oil constituents on Novikoff hepatoma cell viability and communication through Cx43 gap junctions. Biomedicine and Pharmacotherapy, 2021, 135, 111229.	2.5	4
2504	Discovery of New Protein Targets of BPA Analogs and Derivatives Associated with Noncommunicable Diseases: A Virtual High-Throughput Screening. Environmental Health Perspectives, 2021, 129, 37009.	2.8	8
2505	Antiviral Essential Oil Components Against SARS-CoV-2 in Pre-procedural Mouth Rinses for Dental Settings During COVID-19: A Computational Study. Frontiers in Chemistry, 2021, 9, 642026.	1.8	29
2506	SARS-CoV-2 Main Protease Active Site Ligands in the Human Metabolome. Molecules, 2021, 26, 1409.	1.7	22
2507	Luteolin-Fabricated ZnO Nanostructures Showed PLK-1 Mediated Anti-Breast Cancer Activity. Biomolecules, 2021, 11, 385.	1.8	27
2508	In Silico Identification of Flavonoids from Corriandrum sativum Seeds against Coronavirus Covid-19 Main Protease. Journal of Drug Delivery and Therapeutics, 2021, 11, 145-152.	0.2	3
2509	Machine learning for molecular thermodynamics. Chinese Journal of Chemical Engineering, 2021, 31, 227-239.	1.7	16
2510	Pharmacoinformatics based elucidation and designing of potential inhibitors against Plasmodium falciparum to target importin Î±/Î² mediated nuclear importation. Infection, Genetics and Evolution, 2021, 88, 104699.	1.0	4
2511	Molecular dynamics analysis of phytochemicals from Ageratina adenophora against COVID-19 main protease (Mpro) and human angiotensin-converting enzyme 2 (ACE2). Biocatalysis and Agricultural Biotechnology, 2021, 32, 101924.	1.5	15
2515	In silico discovery and evaluation of phytochemicals binding mechanism against human catechol-O-methyltransferase as a putative bioenhancer of L-DOPA therapy in Parkinson disease. Genomics and Informatics, 2021, 19, e7.	0.4	3
2516	Identification of Plasmodium falciparum heat shock 90 inhibitors via molecular docking. Bioorganic and Medicinal Chemistry Letters, 2021, 35, 127818.	1.0	3
2517	Antiproliferative effect, alteration of cancer cell cycle progression and potential MET kinase inhibition induced by 3,4-dihydropyrimidin-2(1H)-one C5 amide derivatives. European Journal of Pharmacology, 2021, 894, 173850.	1.7	15
2518	Molecular and functional characterization of spotted snakehead NOD1 with an emphasis on structural insights into iE-DAP binding motifs employing advanced bioinformatic tools. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7483-7495.	2.0	5
2519	An in-silico approach to identify the potential hot spots in SARS-CoV-2 spike RBD to block the interaction with ACE2 receptor. Journal of Biomolecular Structure and Dynamics, 2021, , 1-16.	2.0	14
2520	Withanone from Withania somnifera Attenuates SARS-CoV-2 RBD and Host ACE2 Interactions to Rescue Spike Protein Induced Pathologies in Humanized Zebrafish Model. Drug Design, Development and Therapy, 2021, Volume 15, 1111-1133.	2.0	69

#	Article	IF	Citations
2521	Heteroarene-fused anthraquinone derivatives as potential modulators for human aurora kinase B. Biochimie, 2021, 182, 152-165.	1.3	9
2522	Discovery of a First-In-Class Small Molecule Antagonist against the Adrenomedullin-2 Receptor: Structureâ€“Activity Relationships and Optimization. Journal of Medicinal Chemistry, 2021, 64, 3299-3319.	2.9	6
2524	Efficacy of a Combined Antiplatelet Therapy Is Not Affected by a Simultaneous Binding of Cangrelor and PSB 0777 to Albumin. Frontiers in Pharmacology, 2021, 12, 638257.	1.6	4
2525	Gene Expression, Biochemical Characterization of a sn-1, 3 Extracellular Lipase From Aspergillus niger GZUF36 and Its Model-Structure Analysis. Frontiers in Microbiology, 2021, 12, 633489.	1.5	6
2526	Crystal structure of eltrombopag olamine Form I, (C2H8NO)2 (C25H20N4O4). Powder Diffraction, 2021, 36, 100-106.	0.4	1
2527	FRAGSITE: A Fragment-Based Approach for Virtual Ligand Screening. Journal of Chemical Information and Modeling, 2021, 61, 2074-2089.	2.5	20
2528	In silico drug designing for COVID-19: an approach of high-throughput virtual screening, molecular, and essential dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2021, , 1-15.	2.0	1
2529	Olfactory marker protein interacts with adenosine nucleotide derivatives. Biochemistry and Biophysics Reports, 2021, 25, 100887.	0.7	0
2530	EDockâ€ML: A web server for using ensemble docking with machine learning to aid drug discovery. Protein Science, 2021, 30, 1087-1097.	3.1	5
2532	Isatin-based virtual high throughput screening, molecular docking, DFT, QM/MM, MD and MM-PBSA study of novel inhibitors of SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 7852-7867.	2.0	7
2533	Soybeanâ€associated endophytic fungi as potential source for antiâ€COVIDâ€19 metabolites supported by docking analysis. Journal of Applied Microbiology, 2021, 131, 1193-1211.	1.4	29
2534	In silico prediction of GLP-1R agonists using machine learning approach. Chemical Papers, 2021, 75, 3587-3598.	1.0	0
2535	Neuroprotective and Neurorescue Mode of Action of Bacopa monnieri (L.) Wettst in 1-Methyl-4-phenyl-1,2,3,6-tetrahydropyridine-Induced Parkinsonâ€™s Disease: An In Silico and In Vivo Study. Frontiers in Pharmacology, 2021, 12, 616413.	1.6	21
2536	Rapid Identification of Inhibitors and Prediction of Ligand Selectivity for Multiple Proteins: Application to Protein Kinases. Journal of Physical Chemistry B, 2021, 125, 2288-2298.	1.2	3
2537	Screening of novel alkaloid inhibitors for vascular endothelial growth factor in cancer cells: an integrated computational approach. Genomics and Informatics, 2021, 19, e6.	0.4	2
2539	Therapeutic effects of royal jelly against sodium benzoateâ€“induced toxicity: cytotoxic, genotoxic, and biochemical assessment. Environmental Science and Pollution Research, 2021, 28, 34410-34425.	2.7	11
2541	Drug design and repurposing with DockThor-VS web server focusing on SARS-CoV-2 therapeutic targets and their non-synonym variants. Scientific Reports, 2021, 11, 5543.	1.6	63
2542	A multitarget semi-synthetic derivative of the flavonoid morin with improved in vitro vasorelaxant activity: Role of CaV1.2 and KCa1.1 channels. Biochemical Pharmacology, 2021, 185, 114429.	2.0	12

#	Article	IF	Citations
2543	In Silico Prediction of Fraction Unbound in Human Plasma from Chemical Fingerprint Using Automated Machine Learning. ACS Omega, 2021, 6, 6791-6797.	1.6	14
2544	Out-of-the-box deep learning prediction of pharmaceutical properties by broadly learned knowledge-based molecular representations. Nature Machine Intelligence, 2021, 3, 334-343.	8.3	66
2545	In Silico Investigations on the Probable Macromolecular Drug Targets Involved in the Anti-Schizophrenia Activity of Terminalia bellerica. Letters in Organic Chemistry, 2022, 19, 83-92.	0.2	1
2546	Molecular design and performance improvement in organic solar cells guided by highâ€throughput screening and machine learning. Nano Select, 2021, 2, 1629-1641.	1.9	12
2547	Developing and Implementing Cloud-Based Tutorials That Combine Bioinformatics Software, Interactive Coding, and Visualization Exercises for Distance Learning on Structural Bioinformatics. Journal of Chemical Education, 2021, 98, 1801-1807.	1.1	18
2548	JlBox v1.1: a Julia-based multi-phase atmospheric chemistry box model. Geoscientific Model Development, 2021, 14, 2187-2203.	1.3	7
2549	PyPLIF HIPPOS-Assisted Prediction of Molecular Determinants of Ligand Binding to Receptors. Molecules, 2021, 26, 2452.	1.7	1
2550	Computational and SAXS-based structure insights of pectin acetyl esterase (CtPae12B) of family 12 carbohydrate esterase from Clostridium thermocellum ATCC 27405. Journal of Biomolecular Structure and Dynamics, 2021, , 1-18.	2.0	3
2551	Structural bioinformatics survey on disease-inducing missense mutations. Journal of Bioinformatics and Computational Biology, 2021, 19, 2150008.	0.3	0
2552	Targeting sterol alphaâ€14 demethylase of Leishmania donovani to fight against leishmaniasis. Journal of Cellular Biochemistry, 2021, 122, 1037-1047.	1.2	8
2553	Inhibitory mechanism of an antifungal drug, caspofungin against amyloid Î² peptide aggregation: Repurposing via neuroinformatics and an experimental approach. Molecular and Cellular Neurosciences, 2021, 112, 103612.	1.0	3
2554	Synthesis and biological evaluation of new coumarin derivatives as cytotoxic agents. Archiv Der Pharmazie, 2021, 354, e2100029.	2.1	10
2555	STOUT: SMILES to IUPAC names using neural machine translation. Journal of Cheminformatics, 2021, 13, 34.	2.8	25
2556	Exploring the endogenous potential of Hemidesmus indicus against breast cancer using in silico studies and quantification of 2-hydroxy-4-methoxy benzaldehyde through RP-HPLC. 3 Biotech, 2021, 11, 235.	1.1	3
2557	DeepDTAF: a deep learning method to predict proteinâ€“ligand binding affinity. Briefings in Bioinformatics, 2021, 22, .	3.2	61
2558	7-phenoxytacrine is a dually acting drug with neuroprotective efficacy in vivo. Biochemical Pharmacology, 2021, 186, 114460.	2.0	12
2559	Identification of Anti-SARS-CoV-2 Compounds from Food Using QSAR-Based Virtual Screening, Molecular Docking, and Molecular Dynamics Simulation Analysis. Pharmaceuticals, 2021, 14, 357.	1.7	24
2560	A practical development of engineering simulation-assisted educational AR environments. Education for Chemical Engineers, 2021, 35, 81-93.	2.8	28

#	Article	IF	Citations
2561	Density Prediction Models for Energetic Compounds Merely Using Molecular Topology. Journal of Chemical Information and Modeling, 2021, 61, 2582-2593.	2.5	25
2562	What's Left for a Computational Chemist To Do in the Age of Machine Learning?. Israel Journal of Chemistry, 2022, 62, .	1.0	6
2564	Repurposing of <scp>FDA</scp>â€approved drugs as inhibitors of sterol Câ€24 methyltransferase of Leishmania donovani to fight against leishmaniasis. Drug Development Research, 2021, 82, 1154-1161.	1.4	13
2565	Molecular docking, SAR analysis and biophysical approaches in the study of the antibacterial activity of ceramides isolated from Cissus incisa. Bioorganic Chemistry, 2021, 109, 104745.	2.0	5
2566	Structure Elucidation and Confirmation of Phloroglucinols from the Roots of Garcinia dauphinensis by Comparison of Experimental and Calculated ECD Spectra and Specific Rotations. Journal of Natural Products, 2021, 84, 1163-1174.	1.5	2
2567	Ligand-Receptor Interactions and Machine Learning in GCGR and GLP-1R Drug Discovery. International Journal of Molecular Sciences, 2021, 22, 4060.	1.8	8
2568	The mechanism of TiaoGanYiPi formula for treating chronic hepatitis B by network pharmacology and molecular docking verification. Scientific Reports, 2021, 11, 8402.	1.6	10
2569	Computational exploration of natural peptides targeting ACE2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8018-8029.	2.0	4
2570	Development of a graph convolutional neural network model for efficient prediction of protein-ligand binding affinities. PLoS ONE, 2021, 16, e0249404.	1.1	55
2571	High-throughput screening of the ReFRAME, Pandemic Box, and COVID Box drug repurposing libraries against SARS-CoV-2 nsp15 endoribonuclease to identify small-molecule inhibitors of viral activity. PLoS ONE, 2021, 16, e0250019.	1.1	27
2572	Quinazoline Derivatives Designed as Efflux Pump Inhibitors: Molecular Modeling and Spectroscopic Studies. Molecules, 2021, 26, 2374.	1.7	20
2573	Ascidian-associated photosymbionts from Manado, Indonesia: secondary metabolites, bioactivity simulation, and biosynthetic insight. Symbiosis, 2021, 84, 71-82.	1.2	3
2574	Brassica juncea (L.) Czern. leaves alleviate adjuvant-induced rheumatoid arthritis in rats via modulating the finest disease targets - IL2RA, IL18 and VEGFA. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8155-8168.	2.0	12
2575	Enhanced validation of small-molecule ligands and carbohydrates in the Protein Data Bank. Structure, 2021, 29, 393-400.e1.	1.6	28
2576	Convolutional Neural Network-based Virtual Screening. Current Medicinal Chemistry, 2021, 28, 2033-2047.	1.2	4
2577	Identification of a novel inhibitor of SARS-CoV-2 3CL-PRO through virtual screening and molecular dynamics simulation. PeerJ, 2021, 9, e11261.	0.9	24
2578	In silico repurposing of drugs for pan-HDAC and pan-SIRT inhibitors: Consensus structure-based virtual screening and pharmacophore modeling investigations. Turkish Journal of Pharmaceutical Sciences, 2021, 18, 0-0.	0.6	2
2579	Artocarpin Targets Focal Adhesion Kinase-Dependent Epithelial to Mesenchymal Transition and Suppresses Migratory-Associated Integrins in Lung Cancer Cells. Pharmaceutics, 2021, 13, 554.	2.0	12

#	Article	IF	Citations
2580	Therapeutic development by repurposing drugs targeting SARS-CoV-2 spike protein interactions by simulation studies. Saudi Journal of Biological Sciences, 2021, 28, 4560-4568.	1.8	8
2581	Simplified Protocol for the Calculation of Multiconformer Transition State Theory Rate Constants Applied to Tropospheric OH-Initiated Oxidation Reactions. Journal of Physical Chemistry A, 2021, 125, 4499-4512.	1.1	11
2582	Aiding a Better Understanding of Molybdopterin: Syntheses, Structures, and pKa Value Determinations of Varied Pterin-Derived Organic Scaffolds Including Oxygen, Sulfur and Phosphorus Bearing Substituents. Journal of Molecular Structure, 2021, 1230, 129867.	1.8	4
2583	Inhibitors of DNA topoisomerases I and II applied to Candida dubliniensis reduce growth, viability, the generation of petite mutants and toxicity, while acting synergistically with fluconazole. FEMS Yeast Research, 2021, 21, .	1.1	4
2584	Deep Learning-Based Ligand Design Using Shared Latent Implicit Fingerprints from Collaborative Filtering. Journal of Chemical Information and Modeling, 2021, 61, 2159-2174.	2.5	5
2585	Coronavirus helicases: attractive and unique targets of antiviral drug-development and therapeutic patents. Expert Opinion on Therapeutic Patents, 2021, 31, 339-350.	2.4	31
2586	Application of Bayesian Multilevel Modeling in the Quantitative Structureâ€“Retention Relationship Studies of Heterogeneous Compounds. Analytical Chemistry, 2021, 93, 6961-6971.	3.2	8
2587	Identification of hub genes related to the progression of type 1 diabetes by computational analysis. BMC Endocrine Disorders, 2021, 21, 61.	0.9	11
2588	Alternative QSAR Study for Unsymmetrical Aromatic Disulfide Anti-SARS Inhibitors. International Journal of Quantitative Structure-Property Relationships, 2021, 6, 47-57.	1.1	0
2589	Dataset of AMBER force field parameters of drugs, natural products and steroids for simulations using GROMACS. Data in Brief, 2021, 35, 106948.	0.5	13
2590	Docking Paradigm in Drug Design. Current Topics in Medicinal Chemistry, 2021, 21, 507-546.	1.0	23
2591	Homology Modeling of Coronavirus Structural Proteins and Molecular Docking of Potential Drug Candidates for the Treatment of COVID-19. Coronaviruses, 2021, 2, 241-250.	0.2	1
2592	Structure-Based Virtual Screening to Identify Novel Potential Compound as an Alternative to Remdesivir to Overcome the RdRp Protein Mutations in SARS-CoV-2. Frontiers in Molecular Biosciences, 2021, 8, 645216.	1.6	20
2593	A COVID-19 Drug Repurposing Strategy through Quantitative Homological Similarities Using a Topological Data Analysis-Based Framework. Pharmaceutics, 2021, 13, 488.	2.0	13
2594	In silico drug repurposing for filarial infection predicts nilotinib and paritaprevir as potential inhibitors of the Wolbachia 5â€²-aminolevulinic acid synthase. Scientific Reports, 2021, 11, 8455.	1.6	4
2595	Effectiveness of Bioactive Compound as Antibacterial and Anti-Quorum Sensing Agent from Myrmecodia pendans: An In Silico Study. Molecules, 2021, 26, 2465.	1.7	7
2596	Investigation of Rosemary Active Ingredients as COVID-19 Inhibitors: Molecular Docking and DFT. Asian Journal of Applied Sciences, 2021, 9, .	0.2	0
2598	One-pot synthesis of dihydropyridine carboxylic acids via functionalization of 3-((trimethylsilyl)ethynyl)pyridines and an unusual hydration of alkynes: Molecular docking and antifungal activity. Tetrahedron, 2021, 86, 132086.	1.0	4

#	Article	IF	Citations
2599	Combined use of the hepatitis C drugs and amentoflavone could interfere with binding of the spike glycoprotein of SARS-CoV-2 to ACE2: the results of a molecular simulation study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8672-8686.	2.0	12
2600	Synthesis of New Biscoumarin Derivatives, In Vitro Cholinesterase Inhibition, Molecular Modelling and Antiproliferative Effect in A549 Human Lung Carcinoma Cells. International Journal of Molecular Sciences, 2021, 22, 3830.	1.8	3
2601	Beyond Tripeptides Two-Step Active Machine Learning for Very Large Data sets. Journal of Chemical Theory and Computation, 2021, 17, 3221-3232.	2.3	24
2602	6,7-Dihydroxycoumarin ameliorates crystal-induced necroptosis during crystal nephropathies by inhibiting MLKL phosphorylation. Life Sciences, 2021, 271, 119193.	2.0	7
2603	SMMPPI: a machine learning-based approach for prediction of modulators of proteinâ€“protein interactions and its application for identification of novel inhibitors for RBD:hACE2 interactions in SARS-CoV-2. Briefings in Bioinformatics, 2021, 22, .	3.2	22
2604	Computational Identification of Potential Anti-Inflammatory Natural Compounds Targeting the p38 Mitogen-Activated Protein Kinase (MAPK): Implications for COVID-19-Induced Cytokine Storm. Biomolecules, 2021, 11, 653.	1.8	25
2605	Fragment-Based Ab Initio Molecular Dynamics Simulation for Combustion. Molecules, 2021, 26, 3120.	1.7	1
2606	Black pepper prevents anemia of inflammation by inhibiting hepcidin over-expression through BMP6-SMAD1/ IL6-STAT3 signaling pathway. Free Radical Biology and Medicine, 2021, 168, 189-202.	1.3	9
2607	Combined in silico and in vitro approaches identified the antipsychotic drug lurasidone and the antiviral drug elbasvir as SARS-CoV2 and HCoV-OC43 inhibitors. Antiviral Research, 2021, 189, 105055.	1.9	26
2608	Separation of an aqueous mixture of 6-kestose/sucrose with zeolites: A molecular dynamics simulation. Microporous and Mesoporous Materials, 2021, 319, 111031.	2.2	3
2609	Forman persistent Ricci curvature (FPRC)-based machine learning models for proteinâ€“ligand binding affinity prediction. Briefings in Bioinformatics, 2021, 22, .	3.2	32
2610	Molecular Docking and Virtual Screening Based Prediction of Drugs for COVID-19. Combinatorial Chemistry and High Throughput Screening, 2021, 24, 716-728.	0.6	39
2611	Reverse fragment based drug discovery approach via simple estimation of fragment contributions. Mendeleev Communications, 2021, 31, 291-293.	0.6	2
2612	Multi-omics data integration and network-based analysis drives a multiplex drug repurposing approach to a shortlist of candidate drugs against COVID-19. Briefings in Bioinformatics, 2021, 22, .	3.2	18
2613	Cocrystals of Praziquantel: Discovery by Network-Based Link Prediction. Crystal Growth and Design, 2021, 21, 3428-3437.	1.4	24
2614	Toward Physics-Based Solubility Computation for Pharmaceuticals to Rival Informatics. Journal of Chemical Theory and Computation, 2021, 17, 3700-3709.	2.3	15
2615	Virtual screening FDA approved drugs against multiple targets of SARSâ€CoVâ€2. Clinical and Translational Science, 2021, 14, 1123-1132.	1.5	12
2616	Transferable Ring Corrections for Predicting Enthalpy of Formation of Cyclic Compounds. Journal of Chemical Information and Modeling, 2021, 61, 2798-2805.	2.5	5

#	Article	IF	Citations
2617	In silico identification of available drugs targeting cell surface BiP to disrupt SARS-CoV-2 binding and replication: Drug repurposing approach. European Journal of Pharmaceutical Sciences, 2021, 160, 105771.	1.9	12
2618	Drug repositioning based on similarity constrained probabilistic matrix factorization: COVID-19 as a case study. Applied Soft Computing Journal, 2021, 103, 107135.	4.1	38
2619	Proposition of a new allosteric binding site for potential SARS-CoV-2 3CL protease inhibitors by utilizing molecular dynamics simulations and ensemble docking. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9347-9360.	2.0	18
2620	Flavonoids and hERG channels: Friends or foes?. European Journal of Pharmacology, 2021, 899, 174030.	1.7	6
2621	Persistent spectralâ€“based machine learning (PerSpect ML) for protein-ligand binding affinity prediction. Science Advances, 2021, 7, .	4.7	89
2622	Acacetin and pinostrobin as a promising inhibitor of cancer-associated protein kinases. Food and Chemical Toxicology, 2021, 151, 112091.	1.8	17
2623	Bisphosphonate inhibitors of squalene synthase protect cells against cholesterolâ€dependent cytolysins. FASEB Journal, 2021, 35, e21640.	0.2	7
2625	Mutations in passive residues modulate 3D-structure of NDM (New Delhi metallo-Î²-lactamase) protein that endue in drug resistance: a MD simulation approach. Journal of Biomolecular Structure and Dynamics, 2021, , 1-17.	2.0	2
2626	New tyrosinases with putative action against contaminants of emerging concern. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1180-1192.	1.5	4
2627	Integrated bioinformatics analysis reveals novel key biomarkers and potential candidate small molecule drugs in gestational diabetes mellitus. Bioscience Reports, 2021, 41, .	1.1	7
2628	SANCDB: an update on South African natural compounds and their readily available analogs. Journal of Cheminformatics, 2021, 13, 37.	2.8	23
2629	Siteng Fang Reverses Multidrug Resistance in Gastric Cancer: A Network Pharmacology and Molecular Docking Study. Frontiers in Oncology, 2021, 11, 671382.	1.3	5
2630	Etoposide and Camptothecin Reduce Growth, Viability, the Generation of Petite Mutants, and Recognize the Active Site of DNA Topoisomerase I and II Enzymes in Candida glabrata. Indian Journal of Microbiology, 2021, 61, 306-314.	1.5	1
2631	Structural insights on the interaction potential of natural leads against major protein targets of SARS-CoV-2: Molecular modelling, docking and dynamic simulation studies. Computers in Biology and Medicine, 2021, 132, 104325.	3.9	18
2632	An Integrated Approach toward NanoBRET Tracers for Analysis of GPCR Ligand Engagement. Molecules, 2021, 26, 2857.	1.7	3
2633	Virtual Screening of FDA-Approved Drugs against Triose Phosphate Isomerase from Entamoeba histolytica and Giardia lamblia Identifies Inhibitors of Their Trophozoite Growth Phase. International Journal of Molecular Sciences, 2021, 22, 5943.	1.8	11
2634	Genotoxic effects and molecular docking of 1,4-dioxane: combined protective effects of trans-resveratrol. Environmental Science and Pollution Research, 2021, 28, 54922-54935.	2.7	14
2635	Reverse fragment based drug discovery approach via simple estimation of fragment contributions. Mendeleev Communications, 2021, 31, 291-293.	0.6	1

#	Article	IF	Citations
2636	Phytochemical Moieties From Indian Traditional Medicine for Targeting Dual Hotspots on SARS-CoV-2 Spike Protein: An Integrative in-silico Approach. Frontiers in Medicine, 2021, 8, 672629.	1.2	34
2637	Effect of Positional Isomerism on Some Alcohol Based Drug towards Anti-Viral Activity against SARS-Cov-2: A Molecular Modeling Based Investigation. Journal of Biomedical Research & Environmental Sciences, 2021, 2, 383-391.	0.1	0
2638	Partial Agonist Activity of Neonicotinoids on Rat Nicotinic Receptors: Consequences over Epinephrine Secretion and In Vivo Blood Pressure. International Journal of Molecular Sciences, 2021, 22, 5106.	1.8	5
2639	VirtualFlow Antsâ€"Ultra-Large Virtual Screenings with Artificial Intelligence Driven Docking Algorithm Based on Ant Colony Optimization. International Journal of Molecular Sciences, 2021, 22, 5807.	1.8	16
2640	Integrated support vector machine and pharmacophore based virtual screening driven identification of thiophene carboxamide scaffold containing compound as potential PARP1 inhibitor. Journal of Biomolecular Structure and Dynamics, 2021, , 1-14.	2.0	5
2641	Seeking the exclusive binding region of phenylalkylamine derivatives on human Tâ€type calcium channels via homology modeling and molecular dynamics simulation approach. Pharmacology Research and Perspectives, 2021, 9, e00783.	1.1	1
2642	In-silico screening and identification of potential inhibitors against 2Cys peroxiredoxin ofCandidatusLiberibacter asiaticus. Journal of Biomolecular Structure and Dynamics, 2022, 40, 8725-8739.	2.0	10
2643	RiPPMiner-Genome: A Web Resource for Automated Prediction of Crosslinked Chemical Structures of RiPPs by Genome Mining. Journal of Molecular Biology, 2021, 433, 166887.	2.0	19
2644	Revving up 13C NMR shielding predictions across chemical space: benchmarks for atoms-in-molecules kernel machine learning with new data for 134 kilo molecules. Machine Learning: Science and Technology, 2021, 2, 035010.	2.4	13
2645	Investigation of Antifungal Properties of Synthetic Dimethyl-4-Bromo-1-(Substituted Benzoyl) Pyrrolo[1,2-a] Quinoline-2,3-Dicarboxylates Analogues: Molecular Docking Studies and Conceptual DFT-Based Chemical Reactivity Descriptors and Pharmacokinetics Evaluation. Molecules, 2021, 26, 2722.	1.7	18
2646	Exploring weak intermolecular interactions in two bis-1,3,4-oxadiazoles derivatives: A combined X-ray diffraction, Hirshfeld surface analysis and theoretical studies. Journal of Molecular Structure, 2021, 1232, 130030.	1.8	7
2647	A study of deregulated MMR pathways and anticancer potential of curcuma derivatives using computational approach. Scientific Reports, 2021, 11, 10110.	1.6	1
2648	Rifampicin and Letermovir as potential repurposed drug candidate for COVID-19 treatment: insights from an in-silico study. Pharmacological Reports, 2021, 73, 926-938.	1.5	16
2649	Discovery of Natural Products Targeting NQO1 via an Approach Combining Network-Based Inference and Identification of Privileged Substructures. Journal of Chemical Information and Modeling, 2021, 61, 2486-2498.	2.5	7
2650	A large-scale computational screen identifies strong potential inhibitors for disrupting SARS-CoV-2â€‰S-protein and human ACE2 interaction. Journal of Biomolecular Structure and Dynamics, 2021, , 1-14.	2.0	4
2651	A Computational Approach to Investigate the HDAC6 and HDAC10 Binding Propensity of Psidium guajava-derived Compounds as Potential Anticancer Agents. Current Drug Discovery Technologies, 2021, 18, 423-436.	0.6	3
2652	Virtual screening of natural compounds for potential inhibitors of Sterol Câ€24 methyltransferase of Leishmania donovani to overcome leishmaniasis. Journal of Cellular Biochemistry, 2021, 122, 1216-1228.	1.2	9
2653	A deep neural network inverse solution to recover pre-crash impact data of car collisions. Transportation Research Part C: Emerging Technologies, 2021, 126, 103009.	3.9	27

#	Article	IF	Citations
2655	Can molecular dynamics simulations improve the structural accuracy and virtual screening performance of GPCR models?. PLoS Computational Biology, 2021, 17, e1008936.	1.5	16
2656	Characterization of ribonucleotide reductases of emerging pathogensElizabethkingia anophelisandElizabethkingia meningosepticaand streptonigrin as their inhibitor: a computational study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9509-9521.	2.0	4
2657	Discovery of a Potent and Selective Chikungunya Virus Envelope Protein Inhibitor through Computer-Aided Drug Design. ACS Infectious Diseases, 2021, 7, 1503-1518.	1.8	9
2658	Molecular dynamics simulation of bioactive compounds of Withania somnifera leaf extract as DNA gyrase inhibitor. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9279-9286.	2.0	5
2660	Additive CHARMM36 Force Field for Nonstandard Amino Acids. Journal of Chemical Theory and Computation, 2021, 17, 3554-3570.	2.3	39
2661	Binding free energy predictions in host-guest systems using Autodock4. A retrospective analysis on SAMPL6, SAMPL7 and SAMPL8 challenges. Journal of Computer-Aided Molecular Design, 2021, 35, 721-729.	1.3	9
2662	Artificial Intelligence-Guided De Novo Molecular Design Targeting COVID-19. ACS Omega, 2021, 6, 12557-12566.	1.6	22
2663	Discovery of Potent Coumarin-Based Kinetic Stabilizers of Amyloidogenic Immunoglobulin Light Chains Using Structure-Based Design. Journal of Medicinal Chemistry, 2021, 64, 6273-6299.	2.9	16
2664	Synthesis, in vitro bioassays, and computational study of heteroaryl nitazoxanide analogs. Pharmacology Research and Perspectives, 2021, 9, e00800.	1.1	8
2665	Discovery of anti-MERS-CoV small covalent inhibitors through pharmacophore modeling, covalent docking and molecular dynamics simulation. Journal of Molecular Liquids, 2021, 330, 115699.	2.3	35
2666	The accelerated weight histogram method for alchemical free energy calculations. Journal of Chemical Physics, 2021, 154, 204103.	1.2	15
2667	Improving virtual screening results with MM/GBSA and MM/PBSA rescoring. Journal of Computer-Aided Molecular Design, 2021, 35, 731-736.	1.3	36
2668	Natural plant products as potential inhibitors of RNA dependent RNA polymerase of Severe Acute Respiratory Syndrome Coronavirus-2. PLoS ONE, 2021, 16, e0251801.	1.1	25
2669	Repurposing potential of posaconazole and grazoprevir as inhibitors of SARS-CoV-2 helicase. Scientific Reports, 2021, 11, 10290.	1.6	16
2670	Trimethoxymethylsilane as a solid-electrolyte interphases improver for graphite anode. Current Applied Physics, 2021, 26, 72-77.	1.1	5
2671	Efficient Quantum-Chemical Calculations of Acid Dissociation Constants from Free-Energy Relationships. Journal of Physical Chemistry A, 2021, 125, 5681-5692.	1.1	18
2672	GNINA 1.0: molecular docking with deep learning. Journal of Cheminformatics, 2021, 13, 43.	2.8	185
2673	Molecular screening of glycyrrhizin-based inhibitors against ACE2 host receptor of SARS-CoV-2. Journal of Molecular Modeling, 2021, 27, 206.	0.8	28

#	Article	IF	Citations
2674	3D-QSAR and Molecular Docking Approaches for the Identification of Novel Phyto-inhibitors of the Cyclin-dependent Kinase 4. Science Letters, 2021, 9, 42-48.	0.7	2
2675	Phycobilins as Potent Food Bioactive Broad-Spectrum Inhibitors Against Proteases of SARS-CoV-2 and Other Coronaviruses: A Preliminary Study. Frontiers in Microbiology, 2021, 12, 645713.	1.5	23
2676	Identification of average molecular weight (AMW) as a useful chemical descriptor to discriminate liver injury-inducing drugs. PLoS ONE, 2021, 16, e0253855.	1.1	2
2677	Synthesis, Characterization, Molecular Docking and Antimicrobial Activity of Novel Spiropyrrolidine Derivatives. Polycyclic Aromatic Compounds, 2022, 42, 5385-5397.	1.4	8
2678	Structure-Based Virtual Screening Reveals Ibrutinib and Zanubrutinib as Potential Repurposed Drugs against COVID-19. International Journal of Molecular Sciences, 2021, 22, 7071.	1.8	22
2679	Docking-based virtual screening studies aiming at the covalent inhibition of SARS-CoV-2 MPro by targeting the cysteine 145. Computational Biology and Chemistry, 2021, 92, 107463.	1.1	10
2680	Elucidating an Atmospheric Brown Carbon Speciesâ€"Toward Supplanting Chemical Intuition with Exhaustive Enumeration and Machine Learning. Environmental Science & Technology, 2021, 55, 8447-8457.	4.6	6
2681	Evaluation of logÂP, pKa, and logÂD predictions from the SAMPL7 blind challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 771-802.	1.3	42
2682	Molecular docking-aided identification of small molecule inhibitors targeting Î²-catenin-TCF4 interaction. IScience, 2021, 24, 102544.	1.9	6
2683	Docking and antibacterial activity of novel nontoxic 5-arylidenepyrimidine-triones as inhibitors of NDM-1 and MetAP-1. Future Medicinal Chemistry, 2021, 13, 1041-1055.	1.1	1
2684	From Genome to Drugs: New Approaches in Antimicrobial Discovery. Frontiers in Pharmacology, 2021, 12, 647060.	1.6	16
2685	Homology modelling and analysis of structure predictions of human tumour necrosis factor ligand superfamily member 8. Future Journal of Pharmaceutical Sciences, 2021, 7, .	1.1	4
2686	Data-Driven Ensemble Docking to Map Molecular Interactions of Steroid Analogs with Hepatic Organic Anion Transporting Polypeptides. Journal of Chemical Information and Modeling, 2021, 61, 3109-3127.	2.5	7
2687	Design, Synthesis, and Bioactivity Evaluation of Dual-Target Inhibitors of Tubulin and Src Kinase Guided by Crystal Structure. Journal of Medicinal Chemistry, 2021, 64, 8127-8141.	2.9	19
2688	A Computational Protocol Combining DFT and Cheminformatics for Prediction of pH-Dependent Redox Potentials. Molecules, 2021, 26, 3978.	1.7	13
2689	Hierarchical Harmonization of Atom-Resolved Metabolic Reactions across Metabolic Databases. Metabolites, 2021, 11, 431.	1.3	4
2690	Druggability of cavity pockets within SARS-CoV-2 spike glycoprotein and pharmacophore-based drug discovery. Future Virology, 2021, 16, 389-397.	0.9	10
2691	Alkali metal ion-induced conformation changes of methionine- and leucine enkephalin investigated by gas-phase hydrogen/deuterium exchange combined with theoretical calculations. Journal of Molecular Structure, 2021, 1233, 130113.	1.8	0

#	Article	IF	Citations
2692	Discovery of a â€œCocktailâ€•of Potential SARS-COV-2 Main Protease Inhibitors through Virtual Screening of Known Chemical Components of Vitex negundo L. (â€œLagundiâ€). Medicinal Chemistry, 2022, 18, 364-381.	0.7	3
2693	Encoding the atomic structure for machine learning in materials science. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, e1558.	6.2	29
2694	Discovery and Engineering of Bacterial (â˜)â€‘Isopiperitenol Dehydrogenases to Enhance (â˜)â€‘Menthol Precursor Biosynthesis. Advanced Synthesis and Catalysis, 2021, 363, 3973-3982.	2.1	3
2695	Subtractive proteomics approach to Unravel the druggable proteins of the emerging pathogen Waddlia chondrophila and drug repositioning on its MurB protein. Heliyon, 2021, 7, e07320.	1.4	2
2697	Design, synthesis, and anticancer activities of 8,9-substituted Luotonin A analogs as novel topoisomerase I inhibitors. Medicinal Chemistry Research, 2021, 30, 1512-1522.	1.1	1
2698	Eco-Friendly Synthesis, Biological Evaluation, and In Silico Molecular Docking Approach of Some New Quinoline Derivatives as Potential Antioxidant and Antibacterial Agents. Frontiers in Chemistry, 2021, 9, 679967.	1.8	13
2699	Data on the docking of phytoconstituents of betel plant and matcha green tea on SARS-CoV-2. Data in Brief, 2021, 36, 107049.	0.5	4
2700	Identification of non-covalent SARS-CoV-2 main protease inhibitors by a virtual screen of commercially available drug-like compounds. Bioorganic and Medicinal Chemistry Letters, 2021, 41, 127990.	1.0	2
2702	Effect of thymoquinone on high fat diet and STZâ€‘induced experimental type 2 diabetes: A mechanistic insight by in vivo and in silico studies. Journal of Food Biochemistry, 2021, 45, e13807.	1.2	10
2703	Cardiovascular effects of farnesol and its Î²-cyclodextrin complex in normotensive and hypertensive rats. European Journal of Pharmacology, 2021, 901, 174060.	1.7	8
2704	Molecular docking and toxicity assessment of spirodiclofen: protective role of lycopene. Environmental Science and Pollution Research, 2021, 28, 57372-57385.	2.7	18
2705	Bioinformatics Accelerates the Major Tetrad: A Real Boost for the Pharmaceutical Industry. International Journal of Molecular Sciences, 2021, 22, 6184.	1.8	16
2706	A computational toolbox for molecular property prediction based on quantum mechanics and quantitative structure-property relationship. Frontiers of Chemical Science and Engineering, 0, , 1.	2.3	7
2707	Molecular docking and dynamics studies of curcumin with COVID-19 proteins. Network Modeling Analysis in Health Informatics and Bioinformatics, 2021, 10, 44.	1.2	19
2708	Potential Biological Targets Prediction, ADME Profiling, & Molecular Docking studies of Novel Steroidal Products from Cunninghamella Blakesleana. Medicinal Chemistry, 2021, 17, .	0.7	0
2709	Small-Molecule Inhibitors Targeting Proteasome-Associated Deubiquitinases. International Journal of Molecular Sciences, 2021, 22, 6213.	1.8	12
2710	Synthesis, biological evaluation and molecular docking studies of heterocycle encompassed benzoxazole derivatives as antimicrobial agents. Materials Today: Proceedings, 2022, 49, 849-853.	0.9	3
2711	Predicting partition coefficients for the SAMPL7 physical property challenge using the ClassicalGSG method. Journal of Computer-Aided Molecular Design, 2021, 35, 819-830.	1.3	5

#	Article	IF	Citations
2713	Targeting the NS2B-NS3 protease of tick-borne encephalitis virus with pan-flaviviral protease inhibitors. Antiviral Research, 2021, 190, 105074.	1.9	12
2714	Corilagin inhibits SARS-CoV-2 replication by targeting viral RNA-dependent RNA polymerase. Acta Pharmaceutica Sinica B, 2021, 11, 1555-1567.	5.7	42
2715	Potential phytochemical inhibitors of SARS-CoV-2 helicase Nsp13: a molecular docking and dynamic simulation study. Molecular Diversity, 2022, 26, 429-442.	2.1	27
2716	Identification of FDA approved drugs against SARS-CoV-2 RNA dependent RNA polymerase (RdRp) and 3-chymotrypsin-like protease (3CLpro), drug repurposing approach. Biomedicine and Pharmacotherapy, 2021, 138, 111544.	2.5	44
2717	Studies on Histamine H2-Receptor Antagonists by Using Density Functional Theory. , 0, , .		0
2718	Structural variants ofRM734in the design of splay nematic materials. Liquid Crystals, 2021, 48, 1780-1790.	0.9	39
2719	Combination of consensus and ensemble docking strategies for the discovery of human dihydroorotate dehydrogenase inhibitors. Scientific Reports, 2021, 11, 11417.	1.6	9
2720	Molecular Design of Dispersed Nickel Phthalocyanine@Nanocarbon Hybrid Catalyst for Active and Stable Electroreduction of CO₂. Journal of Physical Chemistry C, 2021, 125, 13836-13849.	1.5	16
2721	Identification of potential inhibitors for LLM ofStaphylococcus aureus: structure-based pharmacophore modeling, molecular dynamics, and binding free energy studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 9833-9847.	2.0	28
2722	Molecular modeling of organic corrosion inhibitors: Calculations, pitfalls, and conceptualization of moleculeâ€“surface bonding. Corrosion Science, 2021, 193, 109650.	3.0	70
2723	Catechin isolated from faba beans (Vicia faba L.): insights from oxidative stress and hypoglycemic effect in yeast cells through confocal microscopy, flow cytometry, and in silico strategy. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10470-10480.	2.0	2
2724	Identification of 13 Guanidinobenzoyl- or Aminidinobenzoyl-Containing Drugs to Potentially Inhibit TMPRSS2 for COVID-19 Treatment. International Journal of Molecular Sciences, 2021, 22, 7060.	1.8	10
2725	pâ€cymene impairs SARSâ€CoVâ€2 and Influenza A (H1N1) viral replication: In silico predicted interaction with SARSâ€CoVâ€2 nucleocapsid protein and H1N1 nucleoprotein. Pharmacology Research and Perspectives, 2021, 9, e00798.	1.1	15
2726	Low Carbon Footprint Recycling of Postâ€Consumer PET Plastic with a Metagenomic Polyester Hydrolase. ChemSusChem, 2022, 15, .	3.6	70
2727	Structure and lipid dynamics in the maintenance of lipid asymmetry inner membrane complex of A. baumannii. Communications Biology, 2021, 4, 817.	2.0	31
2728	Sub-structure-based screening and molecular docking studies of potential enteroviruses inhibitors. Computational Biology and Chemistry, 2021, 92, 107499.	1.1	0
2729	Evolving scenario of big data and Artificial Intelligence (AI) in drug discovery. Molecular Diversity, 2021, 25, 1439-1460.	2.1	38
2730	Learning the Exciton Properties of Azo-dyes. Journal of Physical Chemistry Letters, 2021, 12, 5957-5962.	2.1	4

#	Article	IF	Citations
2731	The Detosylation of Chiral 1,2-Bis(tosylamides). Journal of Organic Chemistry, 2021, 86, 9163-9180.	1.7	5
2732	Relating molecular descriptors to frontier orbital energy levels, singlet and triplet excited states of fused tricyclics using machine learning. Journal of Molecular Graphics and Modelling, 2021, 105, 107891.	1.3	5
2734	Synthesis and Antiviral Evaluation of Nucleoside Analogues Bearing One Pyrimidine Moiety and Two D-Ribofuranosyl Residues. Molecules, 2021, 26, 3678.	1.7	7
2735	Antiviral Activity of Two Marine Carotenoids against SARS-CoV-2 Virus Entry In Silico and In Vitro. International Journal of Molecular Sciences, 2021, 22, 6481.	1.8	20
2736	Dehalogenation of Dichlorobenzoates by Acidovorax sp. KKS102â€™s beta class Glutathione S-transferase and its Mutants. UMYU Journal of Microbiology Research, 2021, 6, 70-76.	0.1	0
2737	EXPRORER: Rational Cosolvent Set Construction Method for Cosolvent Molecular Dynamics Using Large-Scale Computation. Journal of Chemical Information and Modeling, 2021, 61, 2744-2753.	2.5	6
2738	â€œIdentification of Nafamostat and VR23 as COVID-19 drug candidates by targeting 3CLpro and PLpro". Journal of Molecular Structure, 2021, 1233, 130094.	1.8	17
2739	A metabolic modeling approach reveals promising therapeutic targets and antiviral drugs to combat COVID-19. Scientific Reports, 2021, 11, 11982.	1.6	27
2740	A comprehensive comparative assessment of 3D molecular similarity tools in ligand-based virtual screening. Briefings in Bioinformatics, 2021, 22, .	3.2	11
2741	In Silico Repositioning of Dopamine Modulators with Possible Application to Schizophrenia: Pharmacophore Mapping, Molecular Docking and Molecular Dynamics Analysis. ACS Omega, 2021, 6, 14748-14764.	1.6	2
2742	WormPaths: Caenorhabditis elegans metabolic pathway annotation and visualization. Genetics, 2021, 219, .	1.2	17
2743	Unveiling Potential Active Constituents and Pharmacological Mechanisms of Pudilanxiaoyan Oral Liquid for Anti-Coronavirus Pneumonia Using Network Pharmacology. Pharmaceutical Fronts, 2021, 03, e65-e76.	0.4	0
2745	In silicoscreening of small molecule modulators and their binding studies against human sirtuin-6 protein. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10033-10044.	2.0	1
2747	Improving Docking Power for Short Peptides Using Random Forest. Journal of Chemical Information and Modeling, 2021, 61, 3074-3090.	2.5	11
2748	Finding Druggable Sites in Proteins Using TACTICS. Journal of Chemical Information and Modeling, 2021, 61, 2897-2910.	2.5	13
2749	Inhibition of the 3CL Protease and SARS-CoV-2 Replication by Dalcetrapib. ACS Omega, 2021, 6, 16584-16591.	1.6	17
2750	Molecular fingerprint and machine learning to accelerate design of <scp>highâ€performance</scp> homochiral metalâ€“organic frameworks. AICHE Journal, 2021, 67, e17352.	1.8	15
2751	Inhibitors of bacterial H ₂ S biogenesis targeting antibiotic resistance and tolerance. Science, 2021, 372, 1169-1175.	6.0	112

#	Article	IF	Citations
2752	Ensemble-based screening of natural products and FDA-approved drugs identified potent inhibitors of SARS-CoV-2 that work with two distinct mechanisms. Journal of Molecular Graphics and Modelling, 2021, 105, 107871.	1.3	7
2753	Molecular insights on ABL kinase activation using tree-based machine learning models and molecular docking. Molecular Diversity, 2021, 25, 1301-1314.	2.1	10
2754	Exploring the octanolâ€“water partition coefficient dataset using deep learning techniques and data augmentation. Communications Chemistry, 2021, 4, .	2.0	22
2755	Simultaneously improving reaction coverage and computational cost in automated reaction prediction tasks. Nature Computational Science, 2021, 1, 479-490.	3.8	28
2756	PyRMD: A New Fully Automated AI-Powered Ligand-Based Virtual Screening Tool. Journal of Chemical Information and Modeling, 2021, 61, 3835-3845.	2.5	21
2757	Identification of novel inhibitors of <scp>SARSâ€CoV</scp>â€2 main protease (M^{pro}) from Withania sp. by molecular docking and molecular dynamics simulation. Journal of Computational Chemistry, 2021, 42, 1861-1872.	1.5	21
2758	Reappraisal of trifluperidol against Nsp3 as a potential therapeutic for novel COVID-19: aÂmolecular docking and dynamics study. Future Virology, 2021, 16, 491-506.	0.9	4
2759	2-Hydroxy-5-(3,5,7-trihydroxy-4-oxo-4H-chromen-2-yl)phenyl (E)-3-(4-hydroxy-3-methoxyphenyl)acrylate: Synthesis, In Silico Analysis and In Vitro Pharmacological Evaluation. MolBank, 2021, 2021, M1258.	0.2	1
2761	Grand canonical Monte Carlo simulations of methane adsorption in fullerene pillared graphene nanocomposites. Journal of Molecular Graphics and Modelling, 2021, 106, 107909.	1.3	5
2762	Identification of Vitamin K3 and its analogues as covalent inhibitors of SARS-CoV-2 3CLpro. International Journal of Biological Macromolecules, 2021, 183, 182-192.	3.6	22
2763	DihydroazuleneâEAzobenzeneâEDihydroazulene Triad Photoswitches. Chemistry - A European Journal, 2021, 27, 12437-12446.	1.7	8
2764	Atom Equivalent Energies for the Rapid Estimation of the Heat of Formation of Explosive Molecules from Density Functional Tight Binding Theory. Journal of Chemical Information and Modeling, 2021, 61, 3337-3347.	2.5	10
2765	A Machine Learning Model to Predict Drug Transfer Across the Human Placenta Barrier. Frontiers in Chemistry, 2021, 9, 714678.	1.8	9
2767	An annotation database for chemicals of emerging concern in exposome research. Environment International, 2021, 152, 106511.	4.8	29
2768	Repurposing of <scp>FDA</scp>â€approved drugs against active site and potential allosteric drugâ€binding sites of <scp>COVID</scp>â€19 main protease. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1425-1441.	1.5	30
2770	Computational studies on phylogeny and drug designing using molecular simulations for COVID-19. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10753-10762.	2.0	16
2771	The impact of curcumin derived polyphenols on the structure and flexibility COVID-19 main protease binding pocket: a molecular dynamics simulation study. PeerJ, 2021, 9, e11590.	0.9	9
2772	Dual targeting of cytokine storm and viral replication in COVID-19 by plant-derived steroidal pregnanes: An in silico perspective. Computers in Biology and Medicine, 2021, 134, 104406.	3.9	14

#	Article	IF	Citations
2773	Structure and mechanism of secondary sulfonamide binding to carbonic anhydrases. European Biophysics Journal, 2021, 50, 993-1011.	1.2	5
2774	Supercomputing, Docking and Quantum Mechanics in Quest for Inhibitors of Papain-like Protease of SARS-CoV-2. Lobachevskii Journal of Mathematics, 2021, 42, 1571-1579.	0.1	4
2775	Comprehensive in silico Characterization of Universal Stress Proteins in Rice (Oryza sativa L.) With Insight Into Their Stress-Specific Transcriptional Modulation. Frontiers in Plant Science, 2021, 12, 712607.	1.7	11
2776	Identification of Natural Compounds with Analgesic and Antiinflammatory Properties Using Machine Learning and Molecular Docking Studies. Letters in Drug Design and Discovery, 2022, 19, 256-262.	0.4	0
2777	Leveraging high-throughput screening data, deep neural networks, and conditional generative adversarial networks to advance predictive toxicology. PLoS Computational Biology, 2021, 17, e1009135.	1.5	23
2778	The Effect of Hartree-Fock Exchange on Scaling Relations and Reaction Energetics for Câ€“H Activation Catalysts. Topics in Catalysis, 2022, 65, 296-311.	1.3	11
2779	Simulations of Promising Indolizidineâ€”Î±-Î²2 Nicotinic Acetylcholine Receptor Complexes. International Journal of Molecular Sciences, 2021, 22, 7934.	1.8	1
2780	In Silico Structural Modeling and Analysis of Interactions of Tremellomycetes Cytochrome P450 Monooxygenases CYP51s with Substrates and Azoles. International Journal of Molecular Sciences, 2021, 22, 7811.	1.8	4
2782	A biphenyl inhibitor of eIF4E targeting an internal binding site enables the design of cell-permeable PROTAC-degraders. European Journal of Medicinal Chemistry, 2021, 219, 113435.	2.6	15
2783	Elucidation of Teicoplanin Interactions with Drug Targets Related to COVID-19. Antibiotics, 2021, 10, 856.	1.5	22
2784	Comprehensive virtual screening of 4.8Âk flavonoids reveals novel insights into allosteric inhibition of SARS-CoV-2 MPRO. Scientific Reports, 2021, 11, 15452.	1.6	36
2785	High-temperature decomposition of amorphous and crystalline cellulose: reactive molecular simulations. Cellulose, 2021, 28, 8987-9005.	2.4	15
2786	Kinetic Modeling of API Oxidation: (1) The AIBN/H₂O/CH₃OH Radical â€œSoupâ€• Molecular Pharmaceutics, 2021, 18, 3037-3049.	2.3	12
2787	Tetrazoles as PPARÎ³ ligands: A structural and computational investigation. Journal of Molecular Graphics and Modelling, 2021, 106, 107932.	1.3	1
2788	Prediction of n-octanol/water partition coefficients and acidity constants (pKa) in the SAMPL7 blind challenge with the IEFPCM-MST model. Journal of Computer-Aided Molecular Design, 2021, 35, 803-811.	1.3	10
2789	Identification, ADMET evaluation and molecular docking analysis of Phytosterols from Banaba (Lagerstroemia speciosa (L.)Pers) seed extract against breast cancer. In Silico Pharmacology, 2021, 9, 43.	1.8	5
2790	Effect of dapagliflozin on diabetic patients with cardiovascular disease via MAPK signalling pathway. Journal of Cellular and Molecular Medicine, 2021, 25, 7500-7512.	1.6	7
2791	In silicoidentification of antidiabetic target for phytochemicals ofA. marmelosand mechanistic insights by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2022, 40, 10543-10560.	2.0	8

#	Article	IF	Citations
2792	Target-Based In Silico Screening for Phytoactive Compounds Targeting SARS-CoV-2. Interdisciplinary Sciences, Computational Life Sciences, 2021, , 1.	2.2	5
2793	Identification of non-classical hCA XII inhibitors using combination of computational approaches for drug design and discovery. Scientific Reports, 2021, 11, 15516.	1.6	5
2794	A Comparison of Nine Machine Learning Mutagenicity Models and Their Application for Predicting Pyrrolizidine Alkaloids. Frontiers in Pharmacology, 2021, 12, 708050.	1.6	6
2795	Identification of candidate biomarkers and therapeutic agents for heart failure by bioinformatics analysis. BMC Cardiovascular Disorders, 2021, 21, 329.	0.7	28
2796	Evaluation of the Antidepressant-like Effect of Total Sterols Fraction and Stigmasterol Isolated from Leaves of Aegle marmelos and Possible Mechanism(s) of Action Involved. Current Drug Discovery Technologies, 2022, 19, .	0.6	9
2797	Impact of the Characteristics of Quantum Chemical Databases on Machine Learning Prediction of Tautomerization Energies. Journal of Chemical Theory and Computation, 2021, 17, 4769-4785.	2.3	12
2798	QSAR modeling and pharmacoinformatics of SARS coronavirus 3C-like protease inhibitors. Computers in Biology and Medicine, 2021, 134, 104483.	3.9	12
2799	Facilitating SARS CoV-2 RNA-Dependent RNA polymerase (RdRp) drug discovery by the aid of HCV NS5B palm subdomain binders: In silico approaches and benchmarking. Computers in Biology and Medicine, 2021, 134, 104468.	3.9	15
2800	Virtual screening of potential anticancer drugs based on microbial products. Seminars in Cancer Biology, 2022, 86, 1207-1217.	4.3	6
2801	Prediction of the Drugâ€“Target Binding Kinetics for Flexible Proteins by Comparative Binding Energy Analysis. Journal of Chemical Information and Modeling, 2021, 61, 3708-3721.	2.5	12
2802	Learning Chemistry of Complex Reaction Systems via a Python First-Principles Reaction Rule Stencil (pReSt) Generator. Journal of Chemical Information and Modeling, 2021, 61, 3431-3441.	2.5	12
2803	Development of QSAR models for prediction of fish bioconcentration factors using physicochemical properties and molecular descriptors with machine learning algorithms. Ecological Informatics, 2021, 63, 101285.	2.3	14
2804	Luteolin: a blocker of SARS-CoV-2 cell entry based on relaxed complex scheme, molecular dynamics simulation, and metadynamics. Journal of Molecular Modeling, 2021, 27, 221.	0.8	17
2805	Sequence similarity in 3D for comparison of protein families. Journal of Molecular Graphics and Modelling, 2021, 106, 107906.	1.3	3
2806	Phytocompounds of Rheum emodi, Thymus serpyllum, and Artemisia annua Inhibit Spike Protein of SARS-CoV-2 Binding to ACE2 Receptor: In Silico Approach. Current Pharmacology Reports, 2021, 7, 135-149.	1.5	50
2807	Determination of Ligand Binding Modes in Hydrated Viral Ion Channels to Foster Drug Design and Repositioning. Journal of Chemical Information and Modeling, 2021, 61, 4011-4022.	2.5	10
2808	Strengths and Weaknesses of Docking Simulations in the SARS-CoV-2 Era: the Main Protease (Mpro) Case Study. Journal of Chemical Information and Modeling, 2021, 61, 3758-3770.	2.5	32
2809	Combining SARS-CoV-2 Proofreading Exonuclease and RNA-Dependent RNA Polymerase Inhibitors as a Strategy to Combat COVID-19: A High-Throughput in silico Screening. Frontiers in Microbiology, 2021, 12, 647693.	1.5	43

#	Article	IF	Citations
2811	Discovery of new vascular disrupting agents based on evolutionarily conserved drug action, pesticide resistance mutations, and humanized yeast. Genetics, 2021, 219, .	1.2	6
2812	Chromosome-level genome of Himalayan yew provides insights into the origin and evolution of the paclitaxel biosynthetic pathway. Molecular Plant, 2021, 14, 1199-1209.	3.9	46
2813	Fisetin Prevents Oxidized Low-density Lipoproteinâ€“Induced Macrophage Foam Cell Formation. Journal of Cardiovascular Pharmacology, 2021, 78, e729-e737.	0.8	7
2814	In Vitro and In Silico Evaluation for the Inhibitory Action of O. basilicum Methanol Extract on Î±-Glucosidase and Î±-Amylase. Evidence-based Complementary and Alternative Medicine, 2021, 2021, 1-9.	0.5	9
2815	Computational Discovery of Transition-metal Complexes: From High-throughput Screening to Machine Learning. Chemical Reviews, 2021, 121, 9927-10000.	23.0	110
2816	The structure of CO2 and CH4 at the interface of a poly(urethane urea) oligomer model from the microscopic point of view. Journal of Chemical Physics, 2021, 155, 044704.	1.2	3
2817	Investigation into Small Molecule Isomeric Glucuronide Metabolite Differentiation Using In Silico and Experimental Collision Cross-Section Values. Journal of the American Society for Mass Spectrometry, 2021, 32, 1976-1986.	1.2	11
2818	DFT Study of Structure and Radical Scavenging Activity of Natural Pigment Delphinidin and Derivatives. , 0, , .		0
2819	Solubilized ubiquinol for preserving corneal function. Biomaterials, 2021, 275, 120842.	5.7	13
2820	Learning protein-ligand binding affinity with atomic environment vectors. Journal of Cheminformatics, 2021, 13, 59.	2.8	29
2821	Machine Learning-Enabled Pipeline for Large-Scale Virtual Drug Screening. Journal of Chemical Information and Modeling, 2021, 61, 4236-4244.	2.5	19
2822	In silico discovery of SARS-CoV-2 main protease inhibitors from the carboline and quinoline database. Future Virology, 2021, 16, 507-518.	0.9	1
2823	Assessing the binding properties of <scp>CASP14</scp> targets and models. Proteins: Structure, Function and Bioinformatics, 2021, 89, 1922-1939.	1.5	11
2824	NICEdrug.ch, a workflow for rational drug design and systems-level analysis of drug metabolism. ELife, 2021, 10, .	2.8	8
2825	Chemometric analysis of bio-inspired micellar electrokinetic chromatographic systems â€“ modelling of retention mechanism and prediction of biological properties using bile salts surfactants. Microchemical Journal, 2021, 167, 106340.	2.3	7
2826	Quantum chemical calculations of lithium-ion battery electrolyte and interphase species. Scientific Data, 2021, 8, 203.	2.4	19
2827	Cordycepin as a Promising Inhibitor of SARS-CoV-2 RNA Dependent RNA Polymerase (RdRp). Current Medicinal Chemistry, 2022, 29, 152-162.	1.2	31
2828	Drug Repurposing Against SARS-CoV-2: Targeting NSP16-NSP10 Interaction. Journal of the Turkish Chemical Society, Section A: Chemistry, 0, , 933-940.	0.4	1

#	Article	IF	Citations
2829	Molecular modelling on SARS-CoV-2 papain-like protease: an integrated study with homology modelling, molecular docking, and molecular dynamics simulations. SAR and QSAR in Environmental Research, 2021, 32, 699-718.	1.0	7
2830	Machine learning to accelerate screening for Marcus reorganization energies. Journal of Chemical Physics, 2021, 155, 054106.	1.2	14
2831	Borneol dehydrogenase from Pseudomonas sp. TCU-HL1 possesses novel quinuclidinone reductase activities. Biocatalysis and Biotransformation, 0, , 1-8.	1.1	0
2832	Mechanistic and Predictive QSAR Analysis of Diverse Molecules to Capture Salient and Hidden Pharmacophores for Anti-Thrombotic Activity. International Journal of Molecular Sciences, 2021, 22, 8352.	1.8	4
2833	A computational approach for rational discovery of inhibitors for non-structural protein 1 of SARS-CoV-2. Computers in Biology and Medicine, 2021, 135, 104555.	3.9	60
2834	Discovering potential inhibitors against SARS-CoV-2 by targeting Nsp13 Helicase. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12062-12074.	2.0	8
2835	Computational investigation of phytoalexins as potential antiviral RAP-1 and RAP-2 (Replication) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 5 modeling,in silicodocking and MM-GBSA study. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12165-12183.	2.0	2
2836	Fluorescent Phthalocyanine-Encapsulated Bovine Serum Albumin Nanoparticles: Their Deployment as Therapeutic Agents in the NIR Region. Molecules, 2021, 26, 4679.	1.7	9
2837	Finding inhibitors for PCSK9 using computational methods. PLoS ONE, 2021, 16, e0255523.	1.1	13
2838	2D-QSAR modeling and two-fold classification of 1,2,4-triazole derivatives for antitubercular potency against the dormant stage of Mycobacterium tuberculosis. Molecular Diversity, 2022, 26, 1227-1242.	2.1	5
2839	Molecular solvation theory studies of liquid oleyl alcohol and molecular partitioning in water-oleyl alcohol mixture. Chemical Physics Letters, 2021, 777, 138726.	1.2	0
2840	Effective Use of Empirical Data for Virtual Screening against APJR GPCR Receptor. Molecules, 2021, 26, 4894.	1.7	0
2841	A multiscale approach for bridging the gap between potency, efficacy, and safety of small molecules directed at membrane proteins. Scientific Reports, 2021, 11, 16580.	1.6	10
2842	Inhibition of multiple SARS-CoV-2 proteins by an antiviral biomolecule, seselin fromAegle marmelosdeciphered using molecular docking analysis. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11070-11081.	2.0	9
2843	Shape-Restrained Modeling of Proteinâ€“Small-Molecule Complexes with High Ambiguity Driven DOCKing. Journal of Chemical Information and Modeling, 2021, 61, 4807-4818.	2.5	11
2844	Potansiyel SARS CoV-2 Ana proteaz inhibitÃ¶rleri olarak Corylus avellana L.'nin fenolik asitlerinin deÄŸerlendirilmesi. Erzincan Ãœniversitesi Fen Bilimleri EnstitÃ¼sÃ¼ Dergisi, 2021, 14, 492-509.	0.1	1
2845	Drugs repurposing against SARS-CoV2 and the new variant B.1.1.7 (alpha strain) targeting the spike protein: molecular docking and simulation studies. Heliyon, 2021, 7, e07803.	1.4	13
2846	Structural investigation of tetrahydropteridin analogues as selective PLK1 inhibitors for treating cancer through combined QSAR techniques, molecular docking, and molecular dynamics simulations. Journal of Molecular Liquids, 2021, 335, 116235.	2.3	17

#	Article	IF	Citations
2847	A synthetic small molecule stalls pre-mRNA splicing by promoting an early-stage U2AF2-RNA complex. Cell Chemical Biology, 2021, 28, 1145-1157.e6.	2.5	24
2848	Dietary bioactive diindolylmethane enhances the therapeutic efficacy of centchroman in breast cancer cells by regulating ABCB1/P-gp efflux transporter. Journal of Nutritional Biochemistry, 2021, 94, 108749.	1.9	21
2849	Incorporation of 4J-HMBC and NOE Data into Computer-Assisted Structure Elucidation with WebCocon. Molecules, 2021, 26, 4846.	1.7	5
2850	Phenolics-Rich Extracts of Dietary Plants as Regulators of Fructose Uptake in Caco-2 Cells via GLUT5 Involvement. Molecules, 2021, 26, 4745.	1.7	6
2851	In silico analysis of marine natural product from sponge (Clathria Sp.) for their activity as inhibitor of SARS-CoV-2 Main Protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11526-11532.	2.0	8
2852	Genomics-guided identification of potential modulators of SARS-CoV-2 entry proteases, TMPRSS2 and Cathepsins B/L. PLoS ONE, 2021, 16, e0256141.	1.1	12
2853	Molecular modeling and dynamics simulation of alcohol dehydrogenase enzyme from high efficacy cellulosic ethanol-producing yeast mutant strainPichia kudriavzeviiBGY1-Î³m. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12022-12036.	2.0	4
2854	Therapeutic effect of certain Indian medicinal compounds against the Corona Virus: An in-silico study. Asian Journal of Pharmaceutical Research, 2021, , 167-172.	0.2	1
2855	Identification and Structureâ€“Activity Relationships of Dietary Flavonoids as Human Macrophage Migration Inhibitory Factor (MIF) Inhibitors. Journal of Agricultural and Food Chemistry, 2021, 69, 10138-10150.	2.4	3
2856	An in-silico analysis reveals 7,7â€²-bializarin as a promising DNA gyrase B inhibitor on Gram-positive and Gram-negative bacteria. Computers in Biology and Medicine, 2021, 135, 104626.	3.9	8
2857	Molecular Conditional Generation and Property Analysis of Non-Fullerene Acceptors with Deep Learning. International Journal of Molecular Sciences, 2021, 22, 9099.	1.8	0
2858	SARS-CoV-2 host cell entry: an in silico investigation of potential inhibitory roles of terpenoids. Journal of Genetic Engineering and Biotechnology, 2021, 19, 113.	1.5	10
2859	A combinatorial approach to screen structurally diverse acetylcholinesterase inhibitory plant secondary metabolites targeting Alzheimerâ€™s disease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11705-11718.	2.0	5
2860	A fragment-based approach identifies an allosteric pocket that impacts malate dehydrogenase activity. Communications Biology, 2021, 4, 949.	2.0	2
2861	Reaction Data Curation I: Chemical Structures and Transformations Standardization. Molecular Informatics, 2021, 40, e2100119.	1.4	15
2862	Network pharmacology study on the mechanism of Qiangzhifang in the treatment of panic disorder. Annals of Translational Medicine, 2021, 9, 1350-1350.	0.7	5
2863	Ugonin J Acts as a SARS-CoV-2 3C-like Protease Inhibitor and Exhibits Anti-inflammatory Properties. Frontiers in Pharmacology, 2021, 12, 720018.	1.6	11
2864	In silico molecular docking of SARS-CoV-2 surface proteins with microbial non-ribosomal peptides: identification of potential drugs. Journal of Proteins and Proteomics, 2021, 12, 177-184.	1.0	12

#	Article	IF	Citations
2865	Cyclodextrin Complex Formation with Water-Soluble Drugs: Conclusions from Isothermal Titration Calorimetry and Molecular Modeling. AAPS PharmSciTech, 2021, 22, 232.	1.5	4
2866	Recent Advances in In Silico Target Fishing. Molecules, 2021, 26, 5124.	1.7	29
2867	Entry-inhibitory role of catechins against SARS-CoV-2 and its UK variant. Computers in Biology and Medicine, 2021, 135, 104560.	3.9	21
2868	Evaluation of COVID-19 protease and HIV inhibitors interactions. Acta Pharmaceutica, 2022, 72, 1-8.	0.9	3
2869	Persicaria strigosa (R.Br.) Nakai: a natural anthelmintic?. Parasitology Research, 2021, 120, 3215-3227.	0.6	0
2870	Polypharmacology of some medicinal plant metabolites against SARS-CoV-2 and host targets: Molecular dynamics evaluation of NSP9 RNA binding protein. Journal of Biomolecular Structure and Dynamics, 2022, 40, 11467-11483.	2.0	7
2872	Computational Drug Repurposing for Antituberculosis Therapy: Discovery of Multi-Strain Inhibitors. Antibiotics, 2021, 10, 1005.	1.5	16
2873	Structural insights into ligand recognition and activation of the melanocortin-4 receptor. Cell Research, 2021, 31, 1163-1175.	5.7	26
2874	Identification of Natural Inhibitors Against SARS-CoV-2 Drugable Targets Using Molecular Docking, Molecular Dynamics Simulation, and MM-PBSA Approach. Frontiers in Cellular and Infection Microbiology, 2021, 11, 730288.	1.8	46
2875	Machine Learning of Interstellar Chemical Inventories. Astrophysical Journal Letters, 2021, 917, L6.	3.0	11
2876	Phytochemicals present in Indian ginseng possess potential to inhibit SARS-CoV-2 virulence: A molecular docking and MD simulation study. Microbial Pathogenesis, 2021, 157, 104954.	1.3	33
2877	A distinct <scp>ssDNA</scp>/<scp>RNA</scp> binding interface in the Nsp9 protein from <scp>SARSâ€CoV</scp>â€2. Proteins: Structure, Function and Bioinformatics, 2022, 90, 176-185.	1.5	20
2878	Synthesis, Biological Evaluation, and In Silico Studies of New Acetylcholinesterase Inhibitors Based on Quinoxaline Scaffold. Molecules, 2021, 26, 4895.	1.7	21
2879	Anti-Ebola: an initiative to predict Ebola virus inhibitors through machine learning. Molecular Diversity, 2022, 26, 1635-1644.	2.1	6
2880	Nutraceutical potential of Pennisetum typhoides microgreens: In vitro evaluation of antioxidant and antibacterial activities and in silico Staphylococcus aureus FtsZ inhibition. Food Bioscience, 2021, 42, 101151.	2.0	5
2881	Evaluating the performance of drug-repurposing technologies. Drug Discovery Today, 2022, 27, 49-64.	3.2	18
2882	GraphDTI: A robust deep learning predictor of drug-target interactions from multiple heterogeneous data. Journal of Cheminformatics, 2021, 13, 58.	2.8	12
2883	Molecular Dynamics-Derived Pharmacophore Model Explaining the Nonselective Aspect of KV10.1 Pore Blockers. International Journal of Molecular Sciences, 2021, 22, 8999.	1.8	3

#	Article	IF	Citations
2884	Suppression of LPS-Induced Inflammation and Cell Migration by Azelastine through Inhibition of JNK/NF-ÎºB Pathway in BV2 Microglial Cells. International Journal of Molecular Sciences, 2021, 22, 9061.	1.8	18
2885	Non-competitive interactions between hydroxychloroquine and azithromycin: Systematic density functional, molecular dynamics, and docking calculations. Chemical Physics Letters, 2021, 777, 138745.	1.2	5
2886	Adamantane-derived scaffolds targeting the sigma-2 receptor; an in vitro and in silico study. Saudi Pharmaceutical Journal, 2021, 29, 1166-1172.	1.2	2
2887	Amaryllidaceae Alkaloids of Norbelladine-Type as Inspiration for Development of Highly Selective Butyrylcholinesterase Inhibitors: Synthesis, Biological Activity Evaluation, and Docking Studies. International Journal of Molecular Sciences, 2021, 22, 8308.	1.8	5
2888	Determination of the interaction between the receptor binding domain of 2019-nCoV spike protein, TMPRSS2, cathepsin B and cathepsin L, and glycosidic and aglycon forms of some flavonols. Turkish Journal of Biology, 2021, 45, 484-502.	2.1	5
2889	Effects of carbamate pesticides intermediates on Escherichia coli membrane architecture: An in vitro and in silico approach. Environmental Analysis, Health and Toxicology, 2021, 36, e2021020.	0.7	1
2890	Synthesis, Characterization, Antimicrobial Activity Screening, and Molecular Docking Study of Pyrimidine Carbonitrile Derivatives. Russian Journal of Organic Chemistry, 2021, 57, 1352-1360.	0.3	2
2891	Learning from Docked Ligands: Ligand-Based Features Rescue Structure-Based Scoring Functions When Trained on Docked Poses. Journal of Chemical Information and Modeling, 2022, 62, 5329-5341.	2.5	10
2892	Compound Prioritization through Meta-Analysis Enhances the Discovery of Antimicrobial Hits against Bacterial Pathogens. Antibiotics, 2021, 10, 1065.	1.5	2
2893	An LC-MS/MS assay and complementary web-based tool to quantify and predict compound accumulation in E. coli. Nature Protocols, 2021, 16, 4833-4854.	5.5	26
2894	Gamma-decanolactone: Preliminary evaluation as potential antiparkinsonian drug. European Journal of Pharmacology, 2021, 906, 174276.	1.7	2
2895	Identification of SARS-CoV-2 inhibitors from extracts of Houttuynia cordata Thunb.. Saudi Journal of Biological Sciences, 2021, 28, 7517-7527.	1.8	13
2896	Syzygium aromaticum Extracts as a Potential Antibacterial Inhibitors against Clinical Isolates of Acinetobacter baumannii: An In-Silico-Supported In-Vitro Study. Antibiotics, 2021, 10, 1062.	1.5	5
2897	Predicting 1,9-Decadieneâ"Water Partition Coefficients Using the 3D-RISM-KH Molecular Solvation Theory. Physchem, 2021, 1, 215-224.	0.5	0
2898	Molecular docking, modeling, semiempirical calculations studies and in vitro evaluation of new synthesized pyrimidin-imide derivatives. Journal of Molecular Structure, 2022, 1249, 131548.	1.8	9
2899	Barks of Three Wild Pyrus Taxa: Phenolic Constituents, Antioxidant Activity, and in Vitro and in Silico Investigations of Î± â€Amylase and Î± â€Glucosidase Inhibition. Chemistry and Biodiversity, 2021, 18, e2100446.	1.0	2
2900	In silico and in vitro assays reveal potential inhibitors against 3CL^{pro} main protease of SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12800-12811.	2.0	2
2901	A Novel Glutathione S-Transferase Gtt2 Class (VpGSTT2) Is Found in the Genome of the AHPND/EMS Vibrio parahaemolyticus Shrimp Pathogen. Toxins, 2021, 13, 664.	1.5	1

#	Article	IF	Citations
2903	A natural derivative from ethnomedicinal mushroom potentiates apoptosis, autophagy and attenuates cell migration, via fine tuning the <scp>Akt</scp> signaling in human lung adenocarcinoma cells (<scp>A549</scp>). Environmental Toxicology, 2022, 37, 52-68.	2.1	3
2904	The anti-cancer potential of 2,4,6 tris-methyphenylamino1,3,5-triazine compound against mammary glands cancer: Via down-regulating the hormonal, inflammatory mediators, and oxidative stress. Life Sciences, 2021, 285, 119994.	2.0	5
2905	Systematic analysis of the mechanism of Xiaochaihu decoction in hepatitis B treatment via network pharmacology and molecular docking. Computers in Biology and Medicine, 2021, 138, 104894.	3.9	10
2906	Predicting octanol/water partition coefficients using molecular simulation for the SAMPL7 challenge: comparing the use of neat and water saturated 1-octanol. Journal of Computer-Aided Molecular Design, 2021, 35, 1009-1024.	1.3	5
2907	Anthraquinolone and quinolizine derivatives as an alley of future treatment for COVID-19: an in silico machine learning hypothesis. Scientific Reports, 2021, 11, 17915.	1.6	1
2908	Predicting gasâ€“particle partitioning coefficients of atmospheric molecules with machine learning. Atmospheric Chemistry and Physics, 2021, 21, 13227-13246.	1.9	15
2909	Ligand-based virtual screening, molecular docking, and molecular dynamics of eugenol analogs as potential acetylcholinesterase inhibitors with biological activity against Spodoptera frugiperda. Molecular Diversity, 2021, , 1.	2.1	6
2910	Inhibition of Aminoglycoside 6â€²-N-acetyltransferase Type Ib (AAC(6â€²)-Ib): Structureâ€“Activity Relationship of Substituted Pyrrolidine Pentamine Derivatives as Inhibitors. Biomedicines, 2021, 9, 1218.	1.4	1
2911	Functional variation (Q63R) in the cannabinoid CB2 receptor may affect the severity of COVID-19: a human study and molecular docking. Archives of Virology, 2021, 166, 3117-3126.	0.9	6
2913	Potential natural products that target the SARS-CoV-2 spike protein identified by structure-based virtual screening, isothermal titration calorimetry and lentivirus particles pseudotyped (Vpp) infection assay. Journal of Traditional and Complementary Medicine, 2022, 12, 73-89.	1.5	16
2914	Cell-free chemoenzymatic starch synthesis from carbon dioxide. Science, 2021, 373, 1523-1527.	6.0	274
2915	In Silico Identification and Evaluation of Natural Products as Potential Tumor Necrosis Factor Function Inhibitors Using Advanced Enalos Asclepios KNIME Nodes. International Journal of Molecular Sciences, 2021, 22, 10220.	1.8	10
2916	Biochemical Characterization of 13-Lipoxygenases of Arabidopsis thaliana. International Journal of Molecular Sciences, 2021, 22, 10237.	1.8	9
2917	Selection of the Optimal L-asparaginase II Against Acute Lymphoblastic Leukemia: An In Silico Approach. Jmirx Med, 2021, 2, e29844.	0.2	11
2918	buildH: Build hydrogen atoms from united-atom molecular dynamics of lipids and calculate the order parameters. Journal of Open Source Software, 2021, 6, 3521.	2.0	0
2919	Inhibitory potential of plant-derived metabolites against Zika virus: a computational-aided approach. Phytomedicine Plus, 2021, 1, 100129.	0.9	7
2920	Functional annotation and sequence-structure characterization of a hypothetical protein putatively involved in carotenoid biosynthesis in microalgae. South African Journal of Botany, 2021, 141, 219-226.	1.2	31
2921	3-(5-(1H-imidazol-1-yl) pent-1-en-1-yl)-9-ethyl-9H-carbazole: synthesis, characterization (IR, NMR), DFT, antimicrobial-antioxidant activities and docking study. Journal of Biomolecular Structure and Dynamics, 2021, , 1-11.	2.0	3

#	Article	IF	Citations
2922	Exploring the Regulatory Function of the Nâ€terminal Domain of SARSâ€CoVâ€2 Spike Protein through Molecular Dynamics Simulation. Advanced Theory and Simulations, 2021, 4, 2100152.	1.3	17
2923	Bioisosteric Modification of To042: Synthesis and Evaluation of Promising Useâ€Dependent Inhibitors of Voltageâ€Gated Sodium Channels. ChemMedChem, 2021, 16, 3588-3599.	1.6	3
2924	Identifying potential inhibitors of biofilm-antagonistic proteins to promote biofilm formation: a virtual screening and molecular dynamics simulations approach. Molecular Diversity, 2022, 26, 2135-2147.	2.1	4
2925	Synthesis, in vivo and in silico analgesic and anti-inflammatory studies of Î±-D-ribofuranose derivatives. Saudi Pharmaceutical Journal, 2021, 29, 981-991.	1.2	3
2926	Structural, CSD, and computational studies of 6b, 11b-Dihydroxy-6b, 11-b-dihydro-7H-indeno[1,2-b]naptho[2,1-d]furan-7-one, a therapeutic potential small molecule. Journal of Molecular Structure, 2021, 1240, 130600.	1.8	1
2927	Exploring EZH2-Proteasome Dual-Targeting Drug Discovery through a Computational Strategy to Fight Multiple Myeloma. Molecules, 2021, 26, 5574.	1.7	2
2928	Identification of SARS-CoV-2 RNA-dependent RNA polymerase inhibitors from the major phytochemicals of Nigella sativa: An in silico approach. Saudi Journal of Biological Sciences, 2022, 29, 394-401.	1.8	17
2929	Identification of a small molecule splicing inhibitor targeting UHM domains. FEBS Journal, 2022, 289, 682-698.	2.2	8
2932	Phytochemical Characterization, Antioxidant, Anti-inflammatory, Anti-diabetic properties, Molecular Docking, Pharmacokinetic Profiling, and Network Pharmacology Analysis of the Major Phytoconstituents of Raw and Differently Dried Mangifera indica (Himsagar cultivar): an In Vitro and In Silico Investigations. Applied Biochemistry and Biotechnology, 2022, 194, 950-987.	1.4	32
2933	Transferable Gaussian Attractive Potentials for Organic/Oxide Interfaces. Journal of Physical Chemistry B, 2021, 125, 10843-10853.	1.2	8
2934	Integrated Multi-omics, Virtual Screening and Molecular Docking Analysis of Methicillin-Resistant Staphylococcus aureus USA300 for the Identification of Potential Therapeutic Targets: An In-Silico Approach. International Journal of Peptide Research and Therapeutics, 2021, 27, 2735-2755.	0.9	7
2935	Abrogating the nsp10â€“nsp16 switching mechanisms in SARS-CoV-2 by phytochemicals from Withania somnifera: a molecular dynamics study. Molecular Simulation, 0, , 1-9.	0.9	1
2936	Molecular modelling studies unveil potential binding sites on human serum albumin for selected experimental and in silico COVID-19 drug candidate molecules. Saudi Journal of Biological Sciences, 2022, 29, 53-64.	1.8	10
2937	Fenugreek steroidal saponins hinder osteoclastogenic bone resorption by targeting CSF-1R which diminishes the RANKL/OPG ratio. International Journal of Biological Macromolecules, 2021, 186, 351-364.	3.6	17
2938	New Amino Acid Schiff Bases as Anticancer Agents via Potential Mitochondrial Complex I-Associated Hexokinase Inhibition and Targeting AMP-Protein Kinases/mTOR Signaling Pathway. Molecules, 2021, 26, 5332.	1.7	27
2939	Lin_F9: A Linear Empirical Scoring Function for Proteinâ€“Ligand Docking. Journal of Chemical Information and Modeling, 2021, 61, 4630-4644.	2.5	13
2940	Benchmark study on the optical and thermochemical properties of the norbornadiene-quadricyclane photoswitch. Chemical Physics Letters, 2021, 779, 138665.	1.2	8
2941	Tyrp1 Mutant Variants Associated with OCA3: Computational Characterization of Protein Stability and Ligand Binding. International Journal of Molecular Sciences, 2021, 22, 10203.	1.8	7

#	Article	IF	Citations
2942	Drug repositioning based on gene expression data for human HER2-positive breast cancer. Archives of Biochemistry and Biophysics, 2021, 712, 109043.	1.4	4
2945	NLDock: a Fast Nucleic Acidâ€“Ligand Docking Algorithm for Modeling RNA/DNAâ€“Ligand Complexes. Journal of Chemical Information and Modeling, 2021, 61, 4771-4782.	2.5	25
2946	Automated Construction and Optimization Combined with Machine Learning to Generate Pt(II) Methane Câ€“H Activation Transition States. Topics in Catalysis, 2022, 65, 312-324.	1.3	11
2947	Reliable Prediction of the Octanolâ€“Air Partition Ratio. Environmental Toxicology and Chemistry, 2021, 40, 3166-3180.	2.2	22
2948	Genome Scale Modeling to Study the Metabolic Competition between Cells in the Tumor Microenvironment. Cancers, 2021, 13, 4609.	1.7	15
2949	Structures of a Phosphoryl Derivative of 4-Allyl-2,4-dihydro-3H-1,2,4-triazole-3-thione: An Illustrative Example of Conformational Polymorphism. Crystals, 2021, 11, 1126.	1.0	3
2950	Evaluation of flavonoids from banana pseudostem and flower (quercetin and catechin) as potent inhibitors of Î±-glucosidase: An in silico perspective. Journal of Biomolecular Structure and Dynamics, 2022, 40, 12491-12505.	2.0	29
2951	PUResNet: prediction of protein-ligand binding sites using deep residual neural network. Journal of Cheminformatics, 2021, 13, 65.	2.8	59
2952	Structure-based virtual screening suggests inhibitors of 3-Chymotrypsin-Like Protease of SARS-CoV-2 from Vernonia amygdalina and Occinum gratissimum. Computers in Biology and Medicine, 2021, 136, 104671.	3.9	22
2953	Naturally Occurring Mutations to Muscle-Type Creatine Kinase Impact Its Canonical and Pharmacological Activities in a Substrate-Dependent Manner In Vitro. Molecular Pharmacology, 2021, 100, 588-596.	1.0	5
2954	A structural, DFT and experimental investigation of the ring stability and ring-opening polymerization behaviour of cyclic thionylphosphazenes in the presence of Lewis acid catalysts. Polymer, 2021, 233, 124196.	1.8	4
2955	The machine-learned radii of atoms. Computational and Theoretical Chemistry, 2021, 1204, 113389.	1.1	1
2956	Multistep rational molecular design and combined docking for discovery of novel classes of inhibitors of SARS-CoV-2 main protease 3CLpro. Chemical Physics Letters, 2021, 780, 138894.	1.2	22
2957	Non-target analysis of organic waste amended agricultural soils: Characterization of added organic pollution. Chemosphere, 2021, 280, 130582.	4.2	21
2958	Amyloid Î² fibrils disruption by kolaviron: Molecular docking and extended molecular dynamics simulation studies. Computational Biology and Chemistry, 2021, 94, 107557.	1.1	14
2959	Calculation of diffusion coefficients of pesticides by employing molecular dynamics simulations. Journal of Molecular Liquids, 2021, 340, 117106.	2.3	10
2960	In silico and in vitro study of epiisopiloturine/ hydroxypropyl-Î²-cyclodextrin inclusion complexes obtained by different methods. Journal of Drug Delivery Science and Technology, 2021, 65, 102658.	1.4	6
2961	Integrated molecular dynamics and experimental approach to characterize low-free-energy perfluoro-decyl-acrylate (PFDA) coated silicon. Materials and Design, 2021, 208, 109902.	3.3	6

#	Article	IF	Citations
2962	Structural deformability induced in proteins of potential interest associated with COVID-19 by binding of homologues present in ivermectin: Comparative study based in elastic networks models. Journal of Molecular Liquids, 2021, 340, 117284.	2.3	5
2963	CAT-COSMO-CAMPD: Integrated in silico design of catalysts and processes based on quantum chemistry. Computers and Chemical Engineering, 2021, 153, 107438.	2.0	6
2964	Identification of Plasmodium falciparum Falcilysin Inhibitors by a Virtual Screen. Bioorganic and Medicinal Chemistry Letters, 2021, 52, 128394.	1.0	1
2965	Chemical profiling and in-vitro anti-inflammatory activity of bioactive fraction(s) from Trichodesma indicum (L.) R.Br. against LPS induced inflammation in RAW 264.7 murine macrophage cells. Journal of Ethnopharmacology, 2021, 279, 114235.	2.0	5
2966	Predicting zebrafish (Danio rerio) embryo developmental toxicity through a non-conformational QSAR approach. Science of the Total Environment, 2021, 796, 148820.	3.9	11
2967	Exploration of brominated Plastoquinone analogs: Discovery and structure-activity relationships of small antimicrobial lead molecules. Bioorganic Chemistry, 2021, 116, 105316.	2.0	7
2968	Genomics-guided targeting of stress granule proteins G3BP1/2 to inhibit SARS-CoV-2 propagation. International Journal of Biological Macromolecules, 2021, 190, 636-648.	3.6	13
2969	Identification of bioactive natural compounds as efficient inhibitors against Mycobacterium tuberculosis protein-targets: A molecular docking and molecular dynamics simulation study. Journal of Molecular Liquids, 2021, 341, 117340.	2.3	27
2970	Cytotoxic effects of butyric acid derivatives through GPR109A receptor in Colorectal Carcinoma cells by in silico and in vitro methods. Journal of Molecular Structure, 2021, 1243, 130832.	1.8	4
2971	Exploring the conformational space of a receptor for drug design: An ERÎ± case study. Journal of Molecular Graphics and Modelling, 2021, 108, 107974.	1.3	2
2972	An in silico pipeline for the discovery of multitarget ligands: A case study for epi-polypharmacology based on DNMT1/HDAC2 inhibition. Artificial Intelligence in the Life Sciences, 2021, 1, 100008.	1.6	1
2973	Targeting SARS-CoV-2 main protease by teicoplanin: A mechanistic insight by docking, MM/GBSA and molecular dynamics simulation. Journal of Molecular Structure, 2021, 1246, 131124.	1.8	22
2974	Development of prediction models for adsorption properties of chitin and chitosan for micropollutants. Chemical Engineering Journal, 2021, 426, 131341.	6.6	25
2975	3CLpro and PLpro affinity, a docking study to fight COVID19 based on 900 compounds from PubChem and literature. Are there new drugs to be found?. Journal of Molecular Structure, 2021, 1245, 130968.	1.8	15
2976	In search of SARS CoV-2 replication inhibitors: Virtual screening, molecular dynamics simulations and ADMET analysis. Journal of Molecular Structure, 2021, 1246, 131190.	1.8	46
2977	Synthesis of 7-azaindole based carbohydrazides and 1,3,4-oxadiazoles; Antioxidant activity, Î±-glucosidase inhibition properties and docking study. Journal of Molecular Structure, 2022, 1247, 131343.	1.8	13
2978	Screening and verification of CYP3A4 inhibitors from Bushen-Yizhi formula to enhance the bioavailability of osthole in rat plasma. Journal of Ethnopharmacology, 2022, 282, 114643.	2.0	11
2979	A facile synthesis and structural elucidation for furfural based chromophores: Prediction of linear and nonlinear optical properties. Journal of Molecular Structure, 2022, 1249, 131543.	1.8	5

#	Article	IF	Citations
2980	Schiff Bases of Isatin and Adamantane-1-Carbohydrazide: Synthesis, Characterization and Anticonvulsant Activity. Journal of Chemistry, 2021, 2021, 1-11.	0.9	9
2981	Synthesis of new chrysin derivatives with substantial antibiofilm activity. Molecular Diversity, 2022, 26, 137-156.	2.1	3
2982	Elucidation of the Effects of Bisphenol A and Structural Analogs on Germ and Steroidogenic Cells Using Single Cell High-Content Imaging. Toxicological Sciences, 2021, 180, 224-238.	1.4	13
2983	Molecular modelling and de novo fragment-based design of potential inhibitors of beta-tubulin gene of Necator americanus from natural products. Informatics in Medicine Unlocked, 2021, 26, 100734.	1.9	4
2984	Anti-Tuberculosis Activity in Punica granatum: In silico Validation and Identification of Lead Molecules. , 0, , .		2
2985	Rational engineering of the lccÎ² T. versicolor laccase for the mediator-less oxidation of large polycyclic aromatic hydrocarbons. Computational and Structural Biotechnology Journal, 2021, 19, 2213-2222.	1.9	16
2986	WADDAICA: A webserver for aiding protein drug design by artificial intelligence and classical algorithm. Computational and Structural Biotechnology Journal, 2021, 19, 3573-3579.	1.9	17
2987	Cheminformatics-Based Identification of Potential Novel Anti-SARS-CoV-2 Natural Compounds of African Origin. Molecules, 2021, 26, 406.	1.7	35
2988	Emacs as a Tool for Modern Science. Johnson Matthey Technology Review, 2022, 66, 122-129.	0.5	1
2989	Linarin Protects the Kidney against Ischemia/Reperfusion Injury <i>via</i> the Inhibition of Bioactive ETS2/IL-12. Biological and Pharmaceutical Bulletin, 2021, 44, 25-31.	0.6	8
2990	In silico investigation of phytoconstituents of medicinal herb â€˜Piper Longumâ€™ against SARS-CoV-2 by molecular docking and molecular dynamics analysis. Results in Chemistry, 2021, 3, 100199.	0.9	32
2991	A data-driven perspective on the colours of metalâ€“organic frameworks. Chemical Science, 2021, 12, 3587-3598.	3.7	16
2992	Biomolecular Talksâ€”Part 2: Applications and Challenges of Molecular Docking Approaches. , 2021, , 245-269.		1
2993	Biased Docking for Proteinâ€“Ligand Pose Prediction. Methods in Molecular Biology, 2021, 2266, 39-72.	0.4	9
2994	Screening and Validation of Vitamin D₃ Hydroxylase Substrate Profile Based on Molecular Docking Technique. Journal of Advances in Physical Chemistry, 2021, 10, 9-19.	0.1	0
2995	Structural Modeling in Systems Biology. , 2021, , 446-468.		0
2996	Application of grouping and read-across for the evaluation of parabens of different chain lengths with a particular focus on endocrine properties. Archives of Toxicology, 2021, 95, 853-881.	1.9	3
2998	Synthesis and evaluation of benzenesulfonic acid derivatives as human neutrophil elastase (hNE) inhibitors. Medicinal Chemistry Research, 2021, 30, 387-398.	1.1	2

#	Article	IF	Citations
2999	Multifaceted activity of polyciclic MDR revertant agents in drug-resistant leukemic cells: Role of the spacer. Bioorganic Chemistry, 2021, 106, 104460.	2.0	5
3000	Known Drugs Identified by Structure-Based Virtual Screening Are Able to Bind Sigma-1 Receptor and Increase Growth of Huntington Disease Patient-Derived Cells. International Journal of Molecular Sciences, 2021, 22, 1293.	1.8	5
3001	Chebulinic Acid for Alternative Treatment of Vulvovaginal Candidiasis by Targeting Agglutinin-Like Sequence Protein 3 in Candida albicans: In silico Approach. , 2021, 83, .		1
3002	Potential of MurA Enzyme and GBAP in Fsr Quorum Sensing System as Antibacterial Drugs Target: In vitro and In silico Study of Antibacterial Compounds from Myrmecodia pendans. Combinatorial Chemistry and High Throughput Screening, 2021, 24, 109-118.	0.6	7
3003	Virtual screening and repurposing of FDA-approved drugs from ZINC database to identify potential autophagy inhibitors exploiting autophagy related 4A cysteine peptidase as a target: potential as novel anti-cancer molecule.. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5266-5282.	2.0	3
3004	High-throughput virtual screening for organic electronics: a comparative study of alternative strategies. Journal of Materials Chemistry C, 2021, 9, 13557-13583.	2.7	20
3005	Botanical drugs: a new strategy for structure-based target prediction. Briefings in Bioinformatics, 2022, 23, .	3.2	7
3006	In silico analysis of novel dipeptidyl peptidase-IV inhibitory peptides released from Macadamia integrifolia antimicrobial protein 2 (MiAMP2) and the possible pathways involved in diabetes protection. Current Research in Food Science, 2021, 4, 603-611.	2.7	20
3007	GPR55 Receptor Activation by the N-Acyl Dopamine Family Lipids Induces Apoptosis in Cancer Cells via the Nitric Oxide Synthase (nNOS) Over-Stimulation. International Journal of Molecular Sciences, 2021, 22, 622.	1.8	13
3008	Exploring structure-property relationships in magnesium dissolution modulators. Npj Materials Degradation, 2021, 5, .	2.6	17
3009	Anin silicoanalysis of Ibuprofen enantiomers in high concentrations of sodium chloride with SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5653-5664.	2.0	6
3010	Application and assessment of deep learning for the generation of potential NMDA receptor antagonists. Physical Chemistry Chemical Physics, 2021, 23, 1197-1214.	1.3	9
3011	Evaluating Deep Learning models for predicting ALK-5 inhibition. PLoS ONE, 2021, 16, e0246126.	1.1	10
3012	Assessment of the Antileishmanial Potential of Cassia fistula Leaf Extract. ACS Omega, 2021, 6, 2318-2327.	1.6	9
3014	QSAR/QSPR Revisited. , 0, , 465-495.		6
3015	Ursolic acid ameliorates hypobaric hypoxiaâ€induced skeletal muscle protein loss via upregulating Akt pathway: An experimental study using rat model. IUBMB Life, 2021, 73, 375-389.	1.5	9
3016	<scp>IOData</scp>: A python library for reading, writing, and converting computational chemistry file formats and generating input files. Journal of Computational Chemistry, 2021, 42, 458-464.	1.5	17
3017	Computational Methods and Tools for Repurposing of Drugs Against Coronaviruses. Methods in Pharmacology and Toxicology, 2021, , 163-177.	0.1	1

#	Article	IF	Citations
3018	Ligand Biological Activity Predictions Using Fingerprint-Based Artificial Neural Networks (FANN-QSAR). Methods in Molecular Biology, 2015, 1260, 149-164.	0.4	12
3019	Small-Molecule Library Screening by Docking with PyRx. Methods in Molecular Biology, 2015, 1263, 243-250.	0.4	1,807
3020	Computational Approaches to Developing Short Cyclic Peptide Modulators of Proteinâ€“Protein Interactions. Methods in Molecular Biology, 2015, 1268, 241-271.	0.4	27
3021	A Computational Fragment-Based De Novo Design Protocol Guided by Ligand Efficiency Indices (LEI). Methods in Molecular Biology, 2015, 1289, 89-100.	0.4	5
3022	Structure-Based Virtual Screening. Methods in Molecular Biology, 2017, 1558, 111-124.	0.4	44
3023	Computational Methods to Assess the Production Potential of Bio-Based Chemicals. Methods in Molecular Biology, 2018, 1671, 97-116.	0.4	4
3024	Open-Access Activity Prediction Tools for Natural Products. Case Study: hERG Blockers. Progress in the Chemistry of Organic Natural Products, 2019, 110, 177-238.	0.8	3
3025	A Density-Functional Perspective on the Chorismate Mutase Enzyme. Springer Theses, 2015, , 111-141.	0.0	1
3026	Topic Models with Relational Features for Drug Design. Lecture Notes in Computer Science, 2013, , 45-57.	1.0	7
3027	The Graph Grammar Library - A Generic Framework for Chemical Graph Rewrite Systems. Lecture Notes in Computer Science, 2013, , 52-53.	1.0	8
3028	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
3029	Artificial Intelligence in Drug Discovery: A Comprehensive Review of Data-driven and Machine Learning Approaches. Biotechnology and Bioprocess Engineering, 2020, 25, 895-930.	1.4	43
3030	Design, synthesis, DNA binding studies and evaluation of anticancer potential of novel substituted biscarbazole derivatives against human glioma U87 MG cell line. Bioorganic Chemistry, 2020, 100, 103911.	2.0	14
3031	1,2,4 triazolo[1,5-a] pyrimidin-7-ones as novel SARS-CoV-2 Main protease inhibitors: In silico screening and molecular dynamics simulation of potential COVID-19 drug candidates. Biophysical Chemistry, 2020, 267, 106478.	1.5	18
3032	Isoform-Selective Enzyme Inhibitors by Exploring Pocket Size According to the Lock-and-Key Principle. Biophysical Journal, 2020, 119, 1513-1524.	0.2	6
3033	Identification of Potential Flavonoid Inhibitors of the SARS-CoV-2 Main Protease 6YNQ: A Molecular Docking Study. Digital Chinese Medicine, 2020, 3, 239-248.	0.5	25
3034	Evaluation of consensus scoring methods for AutoDock Vina, smina and idock. Journal of Molecular Graphics and Modelling, 2020, 96, 107532.	1.3	48
3035	Identification of potential natural neuroprotective molecules for Parkinsonâ€™s disease by using chemoinformatics and molecular docking. Journal of Molecular Graphics and Modelling, 2020, 97, 107547.	1.3	6

#	Article	IF	Citations
3036	TrypInDB: A searchable online resource of small molecule inhibitors against Trypanosoma sp.. Parasitology International, 2020, 78, 102131.	0.6	1
3037	Expression of recombinant SnRK1 in E. coli. Characterization of adenine nucleotide binding to the SnRK1.1/AKINÎ²Î³-Î²3 complex. Plant Science, 2017, 263, 116-125.	1.7	11
3038	Predicting Partition Coefficients of Short-Chain Chlorinated Paraffin Congeners by COSMO-RS-Trained Fragment Contribution Models. Environmental Science & Technology, 2020, 54, 15162-15169.	4.6	12
3040	Diphenylalanine-Derivative Peptide Assemblies with Increased Aromaticity Exhibit Metal-like Rigidity and High Piezoelectricity. ACS Nano, 2020, 14, 7025-7037.	7.3	59
3041	Autonomous molecule generation using reinforcement learning and docking to develop potential novel inhibitors. Scientific Reports, 2020, 10, 22104.	1.6	43
3042	Improving the prediction of organism-level toxicity through integration of chemical, protein target and cytotoxicity qHTS data. Toxicology Research, 2016, 5, 883-894.	0.9	10
3043	Generating transition states of isomerization reactions with deep learning. Physical Chemistry Chemical Physics, 2020, 22, 23618-23626.	1.3	35
3044	Quantifying soft degrees of freedom in volatile organic compounds: insight from quantum chemistry and focused single molecule experiments. Physical Chemistry Chemical Physics, 2020, 22, 27850-27860.	1.3	2
3045	Accelerating the repurposing of FDA-approved drugs against coronavirus disease-19 (COVID-19). RSC Advances, 2020, 10, 40867-40875.	1.7	17
3046	Lattice energies of molecular solids from the random phase approximation with singles corrections. Journal of Chemical Physics, 2016, 145, 094506.	1.2	26
3047	Identification of compounds that bind the centriolar protein SAS-6 and inhibit its oligomerization. Journal of Biological Chemistry, 2020, 295, 17922-17934.	1.6	2
3048	In-silico identification of new inhibitors for Low-density lipoprotein receptor-related protein6 (LRP6). Journal of Biomolecular Structure and Dynamics, 2022, 40, 4440-4450.	2.0	51
3049	Thousands of reactants and transition states for competing E2 and S N 2 reactions. Machine Learning: Science and Technology, 2020, 1, 045026.	2.4	33
3050	The proto-Nucleic Acid Builder: a software tool for constructing nucleic acid analogs. Nucleic Acids Research, 2021, 49, 79-89.	6.5	10
3051	Potential RNA-dependent RNA polymerase inhibitors as prospective therapeutics against SARS-CoV-2. Journal of Medical Microbiology, 2020, 69, 864-873.	0.7	49
3083	CrystalCMP: automatic comparison of molecular structures. Journal of Applied Crystallography, 2020, 53, 841-847.	1.9	16
3084	Virtual Screening for the Identification of Potential Candidate Molecules Against Envelope (E) and Membrane (M) Proteins of SARS-CoV-2. Journal of Computational Biophysics and Chemistry, 2021, 20, 209-224.	1.0	5
3085	GPU-Accelerated Drug Discovery with Docking on the Summit Supercomputer. , 2020, , .		36

#	Article	IF	Citations
3086	Alkaloids and flavonoids from African phytochemicals as potential inhibitors of SARS-Cov-2 RNA-dependent RNA polymerase: anin silicoperspective. Antiviral Chemistry and Chemotherapy, 2020, 28, 204020662098407.	0.3	26
3087	A European proposal for quality control and quality assurance of tandem mass spectral libraries. Environmental Sciences Europe, 2020, 32, .	2.6	53
3088	AutoGrow4: an open-source genetic algorithm for de novo drug design and lead optimization. Journal of Cheminformatics, 2020, 12, 25.	2.8	68
3089	Molecular docking and molecular dynamics simulation study of inositol phosphorylceramide synthase â€“ inhibitor complex in leishmaniasis: Insight into the structure based drug design. F1000Research, 2016, 5, 1610.	0.8	11
3090	Computational Discovery of Putative Leads for Drug Repositioning through Drug-Target Interaction Prediction. PLoS Computational Biology, 2016, 12, e1005219.	1.5	32
3091	The Chemical Information Ontology: Provenance and Disambiguation for Chemical Data on the Biological Semantic Web. PLoS ONE, 2011, 6, e25513.	1.1	86
3092	Homology Modeling of Dopamine D2 and D3 Receptors: Molecular Dynamics Refinement and Docking Evaluation. PLoS ONE, 2012, 7, e44316.	1.1	62
3093	Binding Pocket Optimization by Computational Protein Design. PLoS ONE, 2012, 7, e52505.	1.1	39
3094	Predicting Binding within Disordered Protein Regions to Structurally Characterised Peptide-Binding Domains. PLoS ONE, 2013, 8, e72838.	1.1	33
3095	In Silico Prediction of Mutant HIV-1 Proteases Cleaving a Target Sequence. PLoS ONE, 2014, 9, e95833.	1.1	12
3096	Integrated Analysis of Residue Coevolution and Protein Structures Capture Key Protein Sectors in HIV-1 Proteins. PLoS ONE, 2015, 10, e0117506.	1.1	11
3097	tRNAGlu Increases the Affinity of Glutamyl-tRNA Synthetase for Its Inhibitor Glutamyl-Sulfamoyl-Adenosine, an Analogue of the Aminoacylation Reaction Intermediate Glutamyl-AMP: Mechanistic and Evolutionary Implications. PLoS ONE, 2015, 10, e0121043.	1.1	4
3098	Structural Models of Zebrafish (Danio rerio) NOD1 and NOD2 NACHT Domains Suggest Differential ATP Binding Orientations: Insights from Computational Modeling, Docking and Molecular Dynamics Simulations. PLoS ONE, 2015, 10, e0121415.	1.1	31
3099	The Use of Chemical-Chemical Interaction and Chemical Structure to Identify New Candidate Chemicals Related to Lung Cancer. PLoS ONE, 2015, 10, e0128696.	1.1	9
3100	JMS: An Open Source Workflow Management System and Web-Based Cluster Front-End for High Performance Computing. PLoS ONE, 2015, 10, e0134273.	1.1	12
3101	A Teach-Discover-Treat Application of ZincPharmer: An Online Interactive Pharmacophore Modeling and Virtual Screening Tool. PLoS ONE, 2015, 10, e0134697.	1.1	15
3102	Adaptive Neuro-Fuzzy Inference System Applied QSAR with Quantum Chemical Descriptors for Predicting Radical Scavenging Activities of Carotenoids. PLoS ONE, 2015, 10, e0140154.	1.1	5
3103	Mining Chemical Activity Status from High-Throughput Screening Assays. PLoS ONE, 2015, 10, e0144426.	1.1	15

#	Article	IF	Citations
3104	Characterising Complex Enzyme Reaction Data. PLoS ONE, 2016, 11, e0147952.	1.1	13
3105	Drug Repositioning for Cancer Therapy Based on Large-Scale Drug-Induced Transcriptional Signatures. PLoS ONE, 2016, 11, e0150460.	1.1	71
3106	Vinardo: A Scoring Function Based on Autodock Vina Improves Scoring, Docking, and Virtual Screening. PLoS ONE, 2016, 11, e0155183.	1.1	222
3107	Integrated Computational Solution for Predicting Skin Sensitization Potential of Molecules. PLoS ONE, 2016, 11, e0155419.	1.1	7
3108	A Novel Phenanthridionone Based Scaffold As a Potential Inhibitor of the BRD2 Bromodomain: Crystal Structure of the Complex. PLoS ONE, 2016, 11, e0156344.	1.1	11
3109	A Large and Phylogenetically Diverse Class of Type 1 Opsins Lacking a Canonical Retinal Binding Site. PLoS ONE, 2016, 11, e0156543.	1.1	11
3110	A Novel Class of Small Molecule Agonists with Preference for Human over Mouse TLR4 Activation. PLoS ONE, 2016, 11, e0164632.	1.1	16
3111	Predicting the Metabolic Sites by Flavin-Containing Monooxygenase on Drug Molecules Using SVM Classification on Computed Quantum Mechanics and Circular Fingerprints Molecular Descriptors. PLoS ONE, 2017, 12, e0169910.	1.1	8
3112	A single amino acid mutation affects elicitor and expansins-like activities of cerato-platanin, a non-catalytic fungal protein. PLoS ONE, 2017, 12, e0178337.	1.1	14
3113	TopicalPdb: A database of topically delivered peptides. PLoS ONE, 2018, 13, e0190134.	1.1	10
3114	CONSTRUCTION AND RETROSPECTIVE VALIDATION OF STRUCTURE-BASED VIRTUAL SCREENING PROTOCOLS TO IDENTIFY POTENT LIGANDS FOR HUMAN ADRENERGIC BETA-2 RECEPTOR. Indonesian Journal of Pharmacy, 2015, 26, 20.	0.3	2
3115	Supercomputer Simulations of Dopamine-Derived Ligands Complexed with Cyclooxygenases. Supercomputing Frontiers and Innovations, 2018, 5, .	0.5	3
3116	Accounting of Receptor Flexibility in Ultra-Large Virtual Screens with VirtualFlow Using a Grey Wolf Optimization Method. Supercomputing Frontiers and Innovations, 2020, 7, 4-12.	0.5	7
3117	In Search of Non-covalent Inhibitors of SARS-CoV-2 Main Protease: Computer Aided Drug Design Using Docking and Quantum Chemistry. Supercomputing Frontiers and Innovations, 2020, 7, .	0.5	7
3118	Computational approaches to chemical hazard assessment. ALTEX: Alternatives To Animal Experimentation, 2017, 34, 459-478.	0.9	41
3119	Bioinformatics Approach for COVID-19 (Coronavirus) Disease Prevention Treatment and Drug Validation. Eurasian Journal of Medicine and Oncology, 0, , .	1.0	2
3120	Targeting prolyl tripeptidyl peptidase from Porphyromonas gingivalis with the bioactive compounds from Rosmarinus officinalis. Asian Biomedicine, 2019, 13, 197-203.	0.2	3
3121	Identification of new superwarfarin-type rodenticides by structural similarity. The docking of ligands on the vitamin K epoxide reductase enzymeâ€™s active site. Acta Universitatis Sapientiae: Agriculture and Environment, 2015, 7, 108-122.	0.1	2

#	Article	IF	Citations
3122	Computer-based techniques for lead identification and optimization II: Advanced search methods. Physical Sciences Reviews, 2020, 5, .	0.8	8
3123	Neonicotinoids in vector control: In silico approach. , 2014, 4, 25-29.		5
3124	In silico-Based Virtual Drug Screening and Molecular Docking Analysis of Phyto Chemical Derived Compounds and FDA Approved Drugs against BRCA1 Receptor. Journal of Cancer Prevention & Current Research, 2017, 8, .	0.1	7
3125	Synthesis, Docking and Anti-inflammatory Activity of Some Newer Triazole Derivatives as Potential PDE7 Inhibitors. Journal of Medicinal Chemistry and Toxicology, 2017, 2, 55-61.	0.2	5
3127	Systematic approach identifies RHOA as a potential biomarker therapeutic target for Asian gastric cancer. Oncotarget, 2016, 7, 81435-81451.	0.8	17
3128	Novel galeterone analogs act independently of AR and AR-V7 for the activation of the unfolded protein response and induction of apoptosis in the CWR22Rv1 prostate cancer cell model. Oncotarget, 2017, 8, 88501-88516.	0.8	10
3129	Salinomycin exerts anti-angiogenic and anti-tumorigenic activities by inhibiting vascular endothelial growth factor receptor 2-mediated angiogenesis. Oncotarget, 2016, 7, 26580-26592.	0.8	35
3134	SMACT: Semiconducting Materials by Analogy and Chemical Theory. Journal of Open Source Software, 2019, 4, 1361.	2.0	21
3135	LiSIs: An Online Scientific Workflow System for Virtual Screening. Combinatorial Chemistry and High Throughput Screening, 2015, 18, 281-295.	0.6	2
3136	Predicting the types of metabolic pathway of compounds using molecular fragments and sequential minimal optimization. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 136-143.	0.6	38
3137	Prediction of bioactive compound pathways using chemical interaction and structural information. Combinatorial Chemistry and High Throughput Screening, 2016, 19, 161-169.	0.6	2
3138	Survey of Machine Learning Techniques for Prediction of the Isoform Specificity of Cytochrome P450 Substrates. Current Drug Metabolism, 2019, 20, 229-235.	0.7	26
3139	Enabling Virtual Screening of Potent and Safer Antimicrobial Agents Against Noma: mtk-QSBER Model for Simultaneous Prediction of Antibacterial Activities and ADMET Properties. Mini-Reviews in Medicinal Chemistry, 2015, 15, 194-202.	1.1	19
3140	Design, Synthesis, Molecular Docking Study and Anti-Hepatocellular Carcinoma Evaluation of New Bis-Triazolothiadiazines. Mini-Reviews in Medicinal Chemistry, 2020, 20, 788-800.	1.1	13
3141	Evolution of Graph Theory-Based QSAR Methods and their Applications to the Search for New Antibacterial Agents. Current Topics in Medicinal Chemistry, 2013, 13, 3101-3117.	1.0	4
3142	A Survey of Molecular Descriptors Used in Mass Spectrometry Based Proteomics. Current Topics in Medicinal Chemistry, 2014, 14, 388-397.	1.0	5
3143	Virtual Screening Strategies in Medicinal Chemistry: The State of the Art and Current Challenges. Current Topics in Medicinal Chemistry, 2014, 14, 1899-1912.	1.0	57
3144	Screening of Anti-mycobacterial Phytochemical Compounds for Potential Inhibitors against Mycobacterium Tuberculosis Isocitrate Lyase. Current Topics in Medicinal Chemistry, 2019, 19, 600-608.	1.0	8

#	Article	IF	Citations
3145	Forging New Scaffolds from Old: Combining Scaffold Hopping and Hierarchical Virtual Screening for Identifying Novel Bcl-2 Inhibitors. Current Topics in Medicinal Chemistry, 2019, 19, 1162-1172.	1.0	5
3146	Pharmacophore Modeling, Synthesis, Scaffold Hopping and Biological Î²- Hematin Inhibition Interaction Studies for Anti-malaria Compounds. Current Topics in Medicinal Chemistry, 2020, 19, 2743-2765.	1.0	9
3147	Molecular Modeling of an Orphan GPR18 Receptor. Letters in Drug Design and Discovery, 2019, 16, 1167-1174.	0.4	6
3148	Monoamine Oxidase Inhibition and Molecular Modeling Studies of Piperidyl-thienyl and 2-Pyrazoline Derivatives of Chalcones. Medicinal Chemistry, 2015, 11, 497-505.	0.7	19
3149	Graph-Based Processing of Macromolecular Information. Current Bioinformatics, 2015, 10, 606-631.	0.7	4
3150	Investigating the Conformation of S100Î² Protein Under Physiological Parameters Using Computational Modeling: A Clue for Rational Drug Design. Open Biomedical Engineering Journal, 2018, 12, 36-50.	0.7	3
3151	Successes and Pitfalls in Automated Dereplication Strategy Using Mass Spectrometry Data: a CASMI Experience. Current Metabolomics, 2017, 5, 25-34.	0.5	2
3152	Binary Quantitative Structure-Activity Relationship Analysis to Increase the Predictive Ability of Structure-Based Virtual Screening Campaigns Targeting Cyclooxygenase-2. Indonesian Journal of Chemistry, 2017, 17, 322.	0.3	4
3153	In silico Molecular Docking Analysis Targeting SARS-CoV-2 Spike Protein and Selected Herbal Constituents. Journal of Pure and Applied Microbiology, 2020, 14, 989-998.	0.3	49
3164	Cembranoid Diterpenes as Antitumor: Molecular Docking Study to Several Protein Receptor Targets. , 0, , .		1
3165	Search for Human Lactate Dehydrogenase A Inhibitors Using Structure-Based Modeling. Acta Naturae, 2015, 7, 57-63.	1.7	11
3166	Virtual Screening, Oriented-synthesis and Evaluation of Lipase Inhibitory Activity of Benzyl Amino Chalcone Derivatives. Y Hoc Thanh Pho Ho Chi Minh, 2017, 1, 26-36.	0.1	5
3167	Best Practices for Alchemical Free Energy Calculations [Article v1.0]. Living Journal of Computational Molecular Science, 2020, 2, .	2.2	125
3168	Hybrid MM/CG Webserver: Automatic Set Up of Molecular Mechanics/Coarse-Grained Simulations for Human G Protein-Coupled Receptor/Ligand Complexes. Frontiers in Molecular Biosciences, 2020, 7, 576689.	1.6	7
3169	RASPD+: Fast Protein-Ligand Binding Free Energy Prediction Using Simplified Physicochemical Features. Frontiers in Molecular Biosciences, 2020, 7, 601065.	1.6	15
3170	Potential Inhibitors for Novel Coronavirus Protease Identified by Virtual Screening of 606 Million Compounds. International Journal of Molecular Sciences, 2020, 21, 3626.	1.8	131
3171	In Silico Analysis of Ethanol Binding Activity in Neuronal Nicotinic Acetylcholine Receptors. Malaysian Journal of Applied Sciences, 2020, 5, 54-61.	0.2	1
3172	Machine-learning Prediction of Infrared Spectra of Interstellar Polycyclic Aromatic Hydrocarbons. Astrophysical Journal, 2020, 902, 100.	1.6	16

#	Article	IF	Citations
3173	Molecular Docking of Biologically Active Substances to Double Helical Nucleic Acids. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 127-157.	0.3	1
3174	Binding mode of triazole derivatives as aromatase inhibitors based on docking, protein ligand interaction fingerprinting, and molecular dynamics simulation studies. Research in Pharmaceutical Sciences, 2017, 12, 21.	0.6	45
3175	In vitro H⁺/K⁺-ATPase Inhibition, Antiradical effects of a flavonoid-rich fraction of Dissotis rotundifolia, and In silico PASS Prediction of its isolated compounds. Journal of Natural Science, Biology and Medicine, 2018, 9, 47.	1.0	8
3176	A bioinformatics-based investigation to screen and analyze the bioactivity of Piper longum Linn. compounds as a ground-breaking hostile to antidiabetic activity. Pharmacognosy Magazine, 2020, 16, 199.	0.3	3
3178	Database for the kinetics of the gas-phase atmospheric reactions of organic compounds. Earth System Science Data, 2020, 12, 1203-1216.	3.7	50
3179	ConfBuster: Open-Source Tools for Macrocycle Conformational Search and Analysis. Journal of Open Research Software, 2018, 6, 1.	2.7	7
3180	Regulation by Phloroglucinol of Nrf2/Maf-Mediated Expression of Antioxidant Enzymes and Inhibition of Osteoclastogenesis via the RANKL/RANK Signaling Pathway: In Silico study. Acta Informatica Medica, 2015, 23, 228.	0.5	7
3181	Selective Inhibition on RAGE-binding AGEs Required by Bioactive Peptide Alpha-S2 Case in Protein from Goat Ethawah Breed Milk: Study of Biological Modeling. Acta Informatica Medica, 2015, 23, 90.	0.5	21
3182	In Silico Interaction of the Active Compounds of Scurrula Atropurpurea with the RANK/RANKL/OPG System in Diabetoporosis. Acta Informatica Medica, 2019, 27, 8.	0.5	4
3183	In Silico Analysis of the Potential of the Active Compounds Fucoidan and Alginate Derived from Sargassum Sp. as Inhibitors of COX-1 and COX-2. Medicinski Arhiv = Medical Archives = Archives De MÃ©decine, 2016, 70, 172.	0.4	5
3184	Glycosyl flavones from Humulus japonicus suppress MMP-1 production via decreasing oxidative stress in UVB irradiated human dermal fibroblasts. BMB Reports, 2020, 53, 379-384.	1.1	12
3185	Structure-Based Virtual Screening: Identification of Novel Quorum-Sensing Inhibitors to Interfere with the Formation of Pseudomonas aeruginosa Biofilm. Journal of Archives in Military Medicine, 2017, 5, .	0.0	2
3186	Bactenecin and Its Three Improved Derivatives for Enhancement of Antibacterial Activity Against Escherichia coli. Jundishapur Journal of Microbiology, 2019, 12, .	0.2	2
3187	Comparative modeling and molecular docking of orphan human CYP4V2 protein with fatty acid substrates: Insights into substrate specificity. Bioinformation, 2011, 7, 360-365.	0.2	14
3188	Homology modelling of CB1 receptor and selection of potential inhibitor against Obesity. Bioinformation, 2012, 8, 523-528.	0.2	14
3189	Molecular Docking Study of Beta-Glucosidase with Cellobiose, Cellotetraose and Cellotetriose. Bioinformation, 2013, 9, 813-817.	0.2	18
3190	A Script for Automated 3-Dimentional Structure Generation and Conformer Search from 2-Dimentional Chemical Drawing. Bioinformation, 2013, 9, 988-992.	0.2	10
3191	Virtual Screening of Indonesian Herbal Database as HIV-1 Protease Inhibitor. Bioinformation, 2014, 10, 52-55.	0.2	12

#	Article	IF	Citations
3192	Evaluation of novel Saquinavir analogs for resistance mutation compatibility and potential as an HIV-Protease inhibitor drug. Bioinformation, 2014, 10, 227-232.	0.2	3
3193	A QSAR model of benzoxazole derivatives as potential inhibitors for inosine 5`-monophosphate dehydrogenase from Cryptosporidium parvum. Bioinformation, 2016, 12, 119-123.	0.2	2
3194	Simian Virus 40 Large T Antigen as a Model to Test the Efficacy of Flouroquinolones against Viral Helicases. Bioinformation, 2018, 14, 75-79.	0.2	2
3195	Repurposing of known anti-virals as potential inhibitors for SARS-CoV-2 main protease using molecular docking analysis. Bioinformation, 2020, 16, 301.	0.2	32
3196	OrCanome: a Comprehensive Resource for Oral Cancer. Asian Pacific Journal of Cancer Prevention, 2016, 17, 1333-1336.	0.5	4
3197	Interaction of Ketoconazole with Bovine Serum Albumin: Electrochemical, Spectroscopic and Molecular Modeling Studies. Journal of Applied Pharmaceutical Science, 0, , 37-44.	0.7	8
3198	Site-specific effects of neurosteroids on GABAA receptor activation and desensitization. ELife, 2020, 9, .	2.8	32
3199	Exploring the chemical space of influenza neuraminidase inhibitors. PeerJ, 2016, 4, e1958.	0.9	27
3200	Prediction of pKa values using the PM6 semiempirical method. PeerJ, 2016, 4, e2335.	0.9	29
3201	FragBuilder: an efficient Python library to setup quantum chemistry calculations on peptides models. PeerJ, 2014, 2, e277.	0.9	6
3202	Data-mining of potential antitubercular activities from molecular ingredients of traditional Chinese medicines. PeerJ, 2014, 2, e476.	0.9	4
3203	Impacts of Analogy and Dimerization of Bioactive Compounds on Molecular Biological Functions. Journal of Advances in Medical and Pharmaceutical Sciences, 2018, 19, 1-14.	0.2	3
3204	Identification of the acetaldehyde oxide Criegee intermediate reaction network in the ozone-assisted low-temperature oxidation of trans-2-butene. Physical Chemistry Chemical Physics, 2021, 23, 23554-23566.	1.3	10
3205	G4LDB 2.2: a database for discovering and studying G-quadruplex and i-Motif ligands. Nucleic Acids Research, 2022, 50, D150-D160.	6.5	43
3206	Dietary stigmastane-type saponins as promising dual-target directed inhibitors of SARS-CoV-2 proteases: a structure-based screening. RSC Advances, 2021, 11, 33380-33398.	1.7	16
3207	Precipitation-induced transport and phase partitioning of organophosphate esters (OPEs) in urban and rural watersheds. Environmental Science: Water Research and Technology, 2021, 7, 2106-2115.	1.2	6
3208	N-stearoylethanolamine - a new inhibitor of the hepatitis C virus reproduction. Biopolymers and Cell, 2021, 37, 167-176.	0.1	0
3209	Screening and functional evaluation of the glucose-lowering active compounds of total saponins of Baibiandou (Lablab Semen Album). Digital Chinese Medicine, 2021, 4, 229-240.	0.5	1

#	Article	IF	Citations
3210	Do Lipids Influence Gastrointestinal Processing: A Case Study of Major Soybean Allergen Gly m 4. Membranes, 2021, 11, 754.	1.4	2
3211	Structure and inhibition of Cryptococcus neoformans sterylglucosidase to develop antifungal agents. Nature Communications, 2021, 12, 5885.	5.8	13
3212	Biological Profile of Two Gentiana lutea L. Metabolites Using Computational Approaches and In Vitro Tests. Biomolecules, 2021, 11, 1490.	1.8	3
3213	Development of Range-Corrected Deep Learning Potentials for Fast, Accurate Quantum Mechanical/Molecular Mechanical Simulations of Chemical Reactions in Solution. Journal of Chemical Theory and Computation, 2021, 17, 6993-7009.	2.3	47
3214	Type 2 Diabetes Mellitus Mediation by the Disruptive Activity of Environmental Toxicants on Sex Hormone Receptors: In Silico Evaluation. Toxics, 2021, 9, 255.	1.6	3
3215	Inhibition Potencies of Phytochemicals Derived from Sesame Against SARS-CoV-2 Main Protease: A Molecular Docking and Simulation Study. Frontiers in Chemistry, 2021, 9, 744376.	1.8	24
3216	Evaluating Molecular Docking Software for Small Molecule Binding to G-Quadruplex DNA. International Journal of Molecular Sciences, 2021, 22, 10801.	1.8	11
3217	Potential efficacy of existing drug molecules against severe fever with thrombocytopenia syndrome virus: an in silico study. Scientific Reports, 2021, 11, 20857.	1.6	3
3218	Phosphoinositide-binding activity of Smad2 is essential for its function in TGF-Î² signaling. Journal of Biological Chemistry, 2021, 297, 101303.	1.6	5
3219	Benchmarking Free Energy Calculations in Liquid Aliphatic Ketone Solvents Using the 3D-RISM-KH Molecular Solvation Theory. J, 2021, 4, 604-613.	0.6	1
3220	A Comparative Analysis of Punicalagin Interaction with PDIA1 and PDIA3 by Biochemical and Computational Approaches. Biomedicines, 2021, 9, 1533.	1.4	3
3221	Bio-Mechanism of Catechin as Pheromone Signal Inhibitor: Prediction of Antibacterial Agent Action Mode by In Vitro and In Silico Study. Molecules, 2021, 26, 6381.	1.7	8
3222	In silico screening and molecular docking study of compounds from Pedalium murex L. with Vasopressin2 receptor target for Autosomal Dominant Polycystic Kidney Disease. Beni-Suef University Journal of Basic and Applied Sciences, 2021, 10, .	0.8	1
3223	FBXL2 counteracts Grp94 to destabilize EGFR and inhibit EGFR-driven NSCLC growth. Nature Communications, 2021, 12, 5919.	5.8	29
3224	Identification of novel small molecule inhibitors for endoplasmic reticulum oxidoreductase 1Î± (ERO1Î±) enzyme: structure-based molecular docking and molecular dynamic simulation studies. Journal of Biomolecular Structure and Dynamics, 2021, , 1-15.	2.0	1
3225	Development of homology model, docking protocol and Machine-Learning based scoring functions for identification of Equus caballusâ€™s butyrylcholinesterase inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13693-13710.	2.0	3
3226	Novel Benzotriazole Acetamide Derivatives as Benzo-Fused Five- Membered Nitrogen-Containing Heterocycles - In silico Screening, Molecular Docking, and Synthesis. Letters in Drug Design and Discovery, 2022, 19, 337-349.	0.4	2
3227	The impact of cross-docked poses on performance of machine learning classifier for proteinâ€“ligand binding pose prediction. Journal of Cheminformatics, 2021, 13, 81.	2.8	18

#	Article	IF	Citations
3228	Screening of Î²1- and Î²2-Adrenergic Receptor Modulators through Advanced Pharmacoinformatics and Machine Learning Approaches. International Journal of Molecular Sciences, 2021, 22, 11191.	1.8	3
3229	Computer-Aided Design and Synthesis of a New Class of PEX14 Inhibitors: Substituted 2,3,4,5-Tetrahydrobenzo[F][1,4]oxazepines as Potential New Trypanocidal Agents. Journal of Chemical Information and Modeling, 2021, 61, 5256-5268.	2.5	1
3230	Human Estrogen Receptor Î± Antagonists. Part 1: 3-D QSAR-Driven Rational Design of Innovative Coumarin-Related Antiestrogens as Breast Cancer Suppressants through Structure-Based and Ligand-Based Studies. Journal of Chemical Information and Modeling, 2021, 61, 5028-5053.	2.5	5
3231	New Pyridone-Based Derivatives as Cannabinoid Receptor Type 2 Agonists. International Journal of Molecular Sciences, 2021, 22, 11212.	1.8	10
3232	Crystal structure of osimertinib mesylate Form B (Tagrisso), (C₂₈H₃₄N₇O₂)(CH₃O₃S). Powder Diffraction, 2021, 36, 282-290.	0.4	0
3233	Improving Structure-Based Virtual Screening with Ensemble Docking and Machine Learning. Journal of Chemical Information and Modeling, 2021, 61, 5362-5376.	2.5	27
3234	Structure-guided steric hindrance engineering of Bacillus badius phenylalanine dehydrogenase for efficient l-homophenylalanine synthesis. Biotechnology for Biofuels, 2021, 14, 207.	6.2	17
3235	Transport Dynamics of MtrD: An RND Multidrug Efflux Pump from Neisseria gonorrhoeae. Biochemistry, 2021, 60, 3098-3113.	1.2	2
3236	Protein Data Bank Japan: Celebrating our 20th anniversary during a global pandemic as the Asian hub of three dimensional macromolecular structural data. Protein Science, 2022, 31, 173-186.	3.1	28
3237	A Novel Method for Predicting the Human Inherent Clearance and Its Application in the Study of the Pharmacokinetics and Drugâ€“Drug Interaction between Azidothymidine and Fluconazole Mediated by UGT Enzyme. Pharmaceutics, 2021, 13, 1734.	2.0	1
3238	Potential Inhibitors of Fascin From A Database of Marine Natural Products: A Virtual Screening and Molecular Dynamics Study. Frontiers in Chemistry, 2021, 9, 719949.	1.8	5
3239	Navigating Chemical Space by Interfacing Generative Artificial Intelligence and Molecular Docking. Journal of Chemical Information and Modeling, 2021, 61, 5589-5600.	2.5	12
3240	An automatized workflow from molecular dynamic simulation to quantum chemical methods to identify elementary reactions and compute reaction constants. Journal of Computational Chemistry, 2021, 42, 2264-2282.	1.5	6
3241	Point mutations in Candida glabrata 3-hydroxy-3-methylglutaryl-coenzyme A reductase (CgHMGR) decrease enzymatic activity and substrate/inhibitor affinity. Scientific Reports, 2021, 11, 20842.	1.6	0
3242	Swertia purpurascens Wall ethanolic extract mitigates hepatic fibrosis and restores hepatic hepcidin levels via inhibition of TGFÎ²/SMAD/NFÎºB signaling in rats. Journal of Ethnopharmacology, 2022, 284, 114741.	2.0	4
3243	Identification of key structural features of phosphate and thiophosphate tricyclic coumarin analogs as STS inhibitors. Medicine in Drug Discovery, 2021, 12, 100108.	2.3	1
3244	Phytocompounds from Himalayan Medicinal Plants as Potential Drugs to Treat Multidrug-Resistant SalmonellaÂtyphimurium: An In Silico Approach. Biomedicines, 2021, 9, 1402.	1.4	18
3245	Translating the InChI: adapting neural machine translation to predict IUPAC names from a chemical identifier. Journal of Cheminformatics, 2021, 13, 79.	2.8	7

#	Article	IF	Citations
3246	In silicoidentification of novel benzophenoneâ€“coumarin derivatives as SARS-CoV-2 RNA-dependent RNA polymerase (RdRp) inhibitors. Journal of Biomolecular Structure and Dynamics, 2022, 40, 13032-13048.	2.0	24
3247	A Novel Sesquiterpene Lactone Xanthatin-13-(pyrrolidine-2-carboxylic acid) Isolated from Burdock Leaf Up-Regulates Cellsâ€™ Oxidative Stress Defense Pathway. Antioxidants, 2021, 10, 1617.	2.2	5
3249	Mechanistic Insights on the Anionic Polymerization of Aliphatic Aldehydes. Macromolecules, 2021, 54, 9165-9173.	2.2	2
3250	A fluorescent sensor recognized by the FA1 site for highly sensitive detection of HSA. Analytica Chimica Acta, 2021, 1188, 339201.	2.6	11
3251	Virtual screening using docking and molecular dynamics of cannabinoid analogs against CB1 and CB2 receptors. Computational Biology and Chemistry, 2021, 95, 107590.	1.1	14
3252	A deep learning ensemble approach to prioritize antiviral drugs against novel coronavirus SARS-CoV-2 for COVID-19 drug repurposing. Applied Soft Computing Journal, 2021, 113, 107945.	4.1	14
3253	Beware of proper validation of models for ionic Liquids!. Journal of Molecular Liquids, 2021, 344, 117722.	2.3	19
3254	Identification of Berbamine, Oxyacanthine and Rutin from Berberis asiatica as anti-SARS-CoV-2 compounds: An in silico study. Journal of Molecular Graphics and Modelling, 2021, 109, 108028.	1.3	10
3255	A Database of Experimentally Derived and Estimated Octanolâ€“Air Partition Ratios (KOA). Journal of Physical and Chemical Reference Data, 2021, 50, .	1.9	34
3256	Reactive liquid-liquid test system ZnSO4/D2EHPA: Equilibrium, thermochemical, structural, and spectroscopic insights from experiments and density functional theory. Hydrometallurgy, 2021, 206, 105760.	1.8	4
3257	Personalization of structural PDB files.. Acta Biochimica Polonica, 2013, 60, .	0.3	0
3258	Compound Design Using Predictive In Silico Chemistry and Chem(o)informatics. , 2014, , .		0
3260	In-Silico Identification of Potential Inhibitors Against AChE Using Cheminformatics Approach. MOJ Proteomics & Bioinformatics, 2014, 1, .	0.1	2
3262	Successes and Pitfalls in Scoring Molecular Interactions. Lecture Notes in Computer Science, 2015, , 231-237.	1.0	0
3263	Computerized Models of Carbohydrates. , 2015, , 1397-1440.		0
3265	Homology Modeling of DNA polymerases of Herpesviridae family and structure-based virtual screening for inhibitor identification.. Journal of Applied Pharmaceutical Science, 0, , 048-055.	0.7	0
3266	HOODS: finding context-specific neighborhoods of proteins, chemicals and diseases. PeerJ, 2015, 3, e1057.	0.9	1
3269	Iran Virtual Screening (IranVScreen): An Integrated Virtual Screening Interface. Journal of Archives in Military Medicine, 2015, 3, .	0.0	1

#	Article	IF	Citations
3270	Homology Modeling and Docking Studies of a Cell Division Protein, FtsZ: Taxanes and Flavonoids as Anti-FtsZ Agents. International Journal of Scientific Research in Environmental Sciences, 2015, 3, 322-333.	0.1	0
3273	Sequence Retriever for Known, Discovered, and User-Specified Molecular Fragments. Advances in Intelligent Systems and Computing, 2016, , 51-58.	0.5	0
3274	Open Source Chemoinformatics Software including KNIME Analytics Platform. , 2016, , 1-30.		0
3275	Open-Source Chemoinformatics Software. , 2016, , 1-30.		0
3276	Online Molecular Docking Resources. Advances in Medical Technologies and Clinical Practice Book Series, 2016, , 360-379.	0.3	0
3279	Constrained Group Testing to Predict Binding Response of Candidate Compounds. , 2016, , .		0
3281	VIRTUAL SCREENING OF GINKGO BILOBA FOR THERAPEUTIC POTENTIALS AGAINST PARKINSONâ€™S DISEASE. Kongunadu Research Journal, 2016, 3, 6-11.	0.1	0
3288	Online Molecular Docking Resources. , 2017, , 941-959.		0
3289	Examples of SAR-Centric Patent Mining Using Open Resources. , 2017, , 464-487.		1
3290	Design, Synthesis and Cytotoxicity Evaluation of Structural Analogues of Imatinib. Journal of Drug Design and Medicinal Chemistry, 2017, 3, 27.	0.1	0
3291	Akar Kuning (Arcangelisia Flava) As Neuraminidase Inhibitor: Molecular Docking And Pharmacophore Optimization Approach. , 2017, , .		1
3292	Influence of the Method of Hydrogen Atoms Incorporation Into the Target Protein on the Protein-Ligand Binding Energy. Bulletin of the South Ural State University, Series: Mathematical Modelling, Programming and Computer Software, 2017, 10, 94-107.	0.1	9
3296	Synthesis, Docking and Evaluation of Novel Pyrazole Carboxamide Derivatives as Multifunctional Anti-Alzheimer's Agents. Journal of Medicinal Chemistry and Toxicology, 2017, 2, 47-54.	0.2	2
3298	EXPLORING ANTI-HYPERGLYCEMIC POTENTIAL OF ALKALOID COMPOUNDS FROM CATHARANTHUS ROSEUS G. DON (L) AGAINST VARIOUS TYPE II DIABETES TARGETS BY IN SILICO VIRTUAL SCREENING. World Journal of Pharmacy and Pharmaceutical Sciences, 2017, , 82-110.	0.0	0
3299	Marine sponge derived natural products as inhibitors of mycothiol-S-conjugate amidase. Bioinformation, 2017, 13, 256-260.	0.2	1
3301	Modeling the photoreduction of amines by the triplet nitromethane. , 0, , .		1
3303	Continuous Evaluation of Ligand Protein Predictions: A Weekly Community Challenge for Drug Docking. SSRN Electronic Journal, 0, , .	0.4	0
3305	Computational Pharmacogenetics of P-Glycoprotein Mediated Antiepileptic Drug Resistance. Open Bioinformatics Journal, 2018, 11, 197-207.	1.0	2

#	Article	IF	Citations
3315	CBSF: A New Empirical Scoring Function for Docking Parameterized by Weights of Neural Network. Computational and Mathematical Biophysics, 2019, 7, 121-134.	0.6	0
3316	Target Identification Among Known Drugs by Deep Learning from Heterogeneous Networks. SSRN Electronic Journal, 0, , .	0.4	3
3317	Structure-Activity Relationship of Anthocyanidins as an Inhibitory Effect on Osteoclast Differentiation. BPB Reports, 2019, 2, 1-6.	0.1	1
3318	Consice Synthesis of TAN1251C. Heterocycles, 2019, 99, 1095.	0.4	0
3326	Docking-based virtual screening of pyrrole containing imatinib structure analogs. , 2019, 63, 37-43.	0.0	0
3332	The Synthesis and Theoretical Anti-Tumor Studies of Some New Monoaza-10H-Phenothiazine and 10H-Phenoxazine Heterocycles. Chemistry and Chemical Technology, 2019, 13, 288-295.	0.2	1
3335	Crystal structure, DFT study and Hirshfeld surface analysis of 1-nonyl-2,3-dihydro-1H-indole-2,3-dione. Acta Crystallographica Section E: Crystallographic Communications, 2019, 75, 1140-1144.	0.2	2
3337	Computational investigation of marine bioactive compounds reveals frigocyclinone as a potent inhibitor of Kaposiâ€™s Sarcoma Associated Herpesvirus (KSHV) targets. Biomedical and Pharmacology Journal, 2019, 12, 1289-1302.	0.2	1
3339	Molecular docking analysis of flavonoid compounds with HIV-1 Reverse transcriptase for the identification of potential effective inhibitors. Bioinformation, 2019, 15, 646-656.	0.2	1
3341	In silico Identification of High-Affinity Ligands of the Hiv-1 Gp120 Protein, Potential Peptidomimetics of Neutralizing Antibody N6. Mathematical Biology and Bioinformatics, 2019, 14, 430-449.	0.1	2
3342	In Silico Laboratory: Tools for Similarity-Based Drug Discovery. Methods in Molecular Biology, 2020, 2089, 1-28.	0.4	2
3343	Molecular Hybrids of N-Phthaloylglycyl Hydrazide and Hydrazinecarbothioamide with Anti-inflammatory and Anti-oxidant Activities. Current Organic Synthesis, 2019, 16, 1055-1066.	0.7	1
3344	Molecular Docking Study of Akar Kuning (Arcangelisia flava) Secondary Metabolites as Src Inhibitor. Indonesian Journal of Cancer Chemoprevention, 2019, 10, 122.	0.3	0
3348	An integrated approach of network based system pharmacology approach and molecular docking to explore multiscale role of Pinus roxburghii and investigation into its mechanism. Pharmacognosy Magazine, 2020, 16, 586.	0.3	1
3349	In SilicoStudy of 1, 4 Alpha Glucan Branching Enzyme and Substrate Docking Studies. Current Proteomics, 2020, 17, 40-50.	0.1	0
3350	Multi-scale QSAR Approach for Simultaneous Modeling of Ecotoxic Effects of Pesticides. Methods in Pharmacology and Toxicology, 2020, , 639-660.	0.1	8
3360	Identification of Novel Human Serum Albumin (SA) Inhibitors from Scoparia Dulsis for Urolithiasis. Current Computer-Aided Drug Design, 2020, 16, 308-317.	0.8	1
3362	IN SILICO STUDIES OF SOPHORAFLAVANONE G: QUANTUM CHARACTERIZATION AND ADMET. International Journal of Research -GRANTHAALAYAH, 2019, 7, 160-179.	0.1	2

#	Article	IF	Citations
3364	Machine Learning Strategies to Distinguish Oral Cancer from Periodontitis Using Salivary Metabolites. Advances in Intelligent Systems and Computing, 2021, , 511-526.	0.5	3
3366	Evaluation of Phytochemicals of Cassia occidentalis L. for their Binding Affinities to SARS-CoV-2 3C-Like Protease: An in Silico Approach. Asian Journal of Research in Infectious Diseases, 0, , 8-14.	0.0	1
3368	Reverse Docking for the Identification of Molecular Targets of Anticancer Compounds. Methods in Molecular Biology, 2021, 2174, 31-43.	0.4	3
3369	Drug screening with the Autodock Vina on a set of kinases without experimentally established structures. , 2020, , .		0
3370	Influence of Membrane Phase on the Optical Properties of DPH. Molecules, 2020, 25, 4264.	1.7	4
3371	Compound Segmentation via Clustering on Mol2Vec-based Embeddings. , 2021, , .		0
3372	Siâ‹¯O proximity in imidosilanesÂâ€“ absence of orbital interactions. Zeitschrift Fur Naturforschung - Section B Journal of Chemical Sciences, 2022, 77, 55-67.	0.3	2
3373	Analysis of the uncharted, druglike property space by self-organizing maps. Molecular Diversity, 2021, , 1.	2.1	3
3374	Hydroquinone 5-O-Cinnamoyl Ester of Renieramycin M Suppresses Lung Cancer Stem Cells by Targeting Akt and Destabilizes c-Myc. Pharmaceuticals, 2021, 14, 1112.	1.7	8
3375	Flexible CDOCKER: Hybrid Searching Algorithm and Scoring Function with Side Chain Conformational Entropy. Journal of Chemical Information and Modeling, 2021, 61, 5535-5549.	2.5	13
3376	OrbNet Denali: A machine learning potential for biological and organic chemistry with semi-empirical cost and DFT accuracy. Journal of Chemical Physics, 2021, 155, 204103.	1.2	40
3377	SSIPTools: Software and Methodology for Surface Site Interaction Point (SSIP) Approach and Applications. Journal of Chemical Information and Modeling, 2021, 61, 5331-5335.	2.5	6
3378	Integrative Modeling of PROTAC-Mediated Ternary Complexes. Journal of Medicinal Chemistry, 2021, 64, 16271-16281.	2.9	51
3379	Automated Exploration of Prebiotic Chemical Reaction Space: Progress and Perspectives. Life, 2021, 11, 1140.	1.1	6
3380	New Antagonists of the Membrane Androgen Receptor OXER1 from the ZINC Natural Product Database. ACS Omega, 2021, 6, 29664-29674.	1.6	8
3381	Three-Component Synthesis of 2-Amino-3-cyano-4H-chromenes, In Silico Analysis of Their Pharmacological Profile, and In Vitro Anticancer and Antifungal Testing. Pharmaceuticals, 2021, 14, 1110.	1.7	6
3382	Synthesis and molecular docking studies of 5-acetyl-2-(arylidenehydrazin-1-yl)-4-methyl-1,3-thiazoles as Î±-amylase inhibitors. Journal of Molecular Structure, 2021, 1250, 131807.	1.8	7
3383	A Search for Antiâ€inflammatory Therapies: Synthesis, In silico Investigation of the Mode of Action and In vitro Analyses of New Quinazolinâ€2,4â€dione Derivatives Targeting Phosphodiesteraseâ€4 Enzyme. Journal of Heterocyclic Chemistry, 0, , .	1.4	8

#	Article	IF	Citations
3384	Amino Alcohols from Eugenol as Potential Semisynthetic Insecticides: Chemical, Biological, and Computational Insights. Molecules, 2021, 26, 6616.	1.7	12
3385	V-Dock: Fast Generation of Novel Drug-like Molecules Using Machine-Learning-Based Docking Score and Molecular Optimization. International Journal of Molecular Sciences, 2021, 22, 11635.	1.8	15
3386	Computational-Designed Enzyme for Î²-Tyrosine Production in Lignin Valorization. Catalysts, 2021, 11, 1310.	1.6	2
3387	ScaffComb: A Phenotypeâ€Based Framework for Drug Combination Virtual Screening in Largeâ€Scale Chemical Datasets. Advanced Science, 2021, 8, e2102092.	5.6	7
3388	Extracting Predictive Representations from Hundreds of Millions of Molecules. Journal of Physical Chemistry Letters, 2021, 12, 10793-10801.	2.1	28
3389	Effective Search of Triterpenes with Anti-HSV-1 Activity Using a Classification Model by Logistic Regression. Frontiers in Chemistry, 2021, 9, 763794.	1.8	3
3390	A Comprehensive Computational Platform to Guide Drug Development Using Graph-Based Signature Methods. Methods in Molecular Biology, 2020, 2112, 91-106.	0.4	5
3391	Fine tuning by protein kinases of CaV1.2 channel current in rat tail artery myocytes. Biochemical Pharmacology, 2020, 182, 114263.	2.0	3
3392	Predictive Quantitative Structureâ€“Activity Relationship Modeling of the Antifungal and Antibiotic Properties of Triazolothiadiazine Compounds. Methods and Protocols, 2021, 4, 2.	0.9	2
3395	Exploring the structural basis of conformational alterations of myoglobin in the presence of spermine through computational modeling, molecular dynamics simulations, and spectroscopy methods. Journal of Biomolecular Structure and Dynamics, 2022, 40, 3581-3594.	2.0	11
3396	Oxygenated PAH Formation Chemistry Investigation in Anisole Jet Stirred Reactor Oxidation by a Thermodynamic Approach. Energy & Fuels, 2021, 35, 1535-1545.	2.5	8
3398	Convolutional neural networks for the design and analysis of nonfullerene acceptors. , 2022, , 231-256.		25
3399	On the transport and dynamics of disaccharides: H-bonding effect in sucrose and sucralose. Journal of Molecular Liquids, 2022, 345, 117855.	2.3	8
3400	Introductory chapter. , 2022, , 1-37.		0
3401	Predicting novel drug candidates against Covid-19 using generative deep neural networks. Journal of Molecular Graphics and Modelling, 2022, 110, 108045.	1.3	12
3402	Comparison results of eight oxygenated organic molecules: Unexpected contribution to new particle formation in the atmosphere. Atmospheric Environment, 2022, 268, 118817.	1.9	5
3403	Ferrocene-functionalized anilines as potent anticancer and antidiabetic agents: Synthesis, spectroscopic elucidation, and DFT calculations. Journal of Molecular Structure, 2022, 1249, 131632.	1.8	7
3404	Cluster-Based Regression Model for Predicting Aqueous Solubility of the Molecules. Communications in Computer and Information Science, 2020, , 14-24.	0.4	0

#	Article	IF	Citations
3405	New 2-(4-(4-bromophenylsulfonyl)phenyl)-4-arylidene-oxazol-5(4H)-ones: analgesic activity and histopathological assessment. Romanian Journal of Morphology and Embryology, 2020, 61, 493-502.	0.4	1
3406	Propolis Components and Biological Activities from Stingless Bees Collected on South Sulawesi, Indonesia. HAYATI Journal of Biosciences, 2020, 27, 82.	0.1	10
3407	Action mode of ursolic acid as a natural antioxidant and inhibitor of superoxide dismutase: In vitro and in silico study. Journal of Advanced Pharmaceutical Technology and Research, 2021, 12, 389.	0.4	4
3408	From Groove Binding to Intercalation: Unravelling the Weak Interactions and Other Factors Modulating the Modes of Interaction between Methylated Phenanthroline Based Drugs and Duplex DNA. Physical Chemistry Chemical Physics, 2021, 23, 26680-26695.	1.3	4
3410	BESTox: A Convolutional Neural Network Regression Model Based on Binary-Encoded SMILES for Acute Oral Toxicity Prediction of Chemical Compounds. Lecture Notes in Computer Science, 2020, , 155-166.	1.0	7
3411	Benchmarking Small-Dataset Structure-Activity-Relationship Models for Prediction of Wnt Signaling Inhibition. IEEE Access, 2020, 8, 228831-228840.	2.6	9
3412	Design, synthesis, and in vitro evaluation of novel dipeptidyl peptidase IV inhibitors. Biomedical Research and Clinical Practice, 2020, 5, .	0.3	0
3413	Pascal Programming in Neural Data Server for Indonesian Elementary Schools. , 0, , .		0
3414	In silicoEvaluation of Substrate Binding Site and Rare Codons in the Structure of CYP152A1. Current Proteomics, 2020, 17, 10-22.	0.1	0
3415	Natural Products as Potential Inhibitors for SARS-CoV-2 Papain-Like Protease: An in Silico Study. Lecture Notes in Computer Science, 2020, , 265-270.	1.0	0
3416	Concomitant prediction of environmental fate and toxicity of chemical compounds. Biology Methods and Protocols, 2020, 5, bpaa025.	1.0	3
3419	Virtual Screening of Anticancer Drugs Using Deep Learning. , 2020, , 1293-1298.		1
3420	Identification of phenolic acids of Pandan anggur (Sararanga sinuosa Hemsley) fruits and their potential antiglycation through molecular docking study. Journal of Applied Pharmaceutical Science, 0, , .	0.7	1
3421	Computational Studies of Drug Repurposing Targeting P-Glycoprotein-Mediated Multidrug Resistance Phenotypes in Priority Infectious Agents. , 0, , .		2
3422	Exploring public health benefits of Dolichos lablab as a dietary supplement during the COVID-19 outbreak: A computational study. Journal of Applied Pharmaceutical Science, 0, , .	0.7	3
3423	SwissBioisostere 2021: updated structural, bioactivity and physicochemical data delivered by a reshaped web interface. Nucleic Acids Research, 2022, 50, D1382-D1390.	6.5	17
3427	DeepBindPoc: a deep learning method to rank ligand binding pockets using molecular vector representation. PeerJ, 2020, 8, e8864.	0.9	11
3430	DeepStack-DTIs: Predicting Drugâ€“Target Interactions Using LightGBM Feature Selection and Deep-Stacked Ensemble Classifier. Interdisciplinary Sciences, Computational Life Sciences, 2022, 14, 311-330.	2.2	14

#	Article	IF	Citations
3431	Identification of potential inhibitory analogs of metastasis tumor antigens (MTAs) using bioactive compounds: revealing therapeutic option to prevent malignancy. Molecular Diversity, 2022, 26, 2473-2502.	2.1	1
3432	Hydrophobic Cargo Encapsulation into Virus Protein Cages by Self-Assembly in an Aprotic Organic Solvent. Bioconjugate Chemistry, 2021, 32, 2366-2376.	1.8	1
3433	In Silico End-to-End Proteinâ€“Ligand Interaction Characterization Pipeline: The Case of SARS-CoV-2. ACS Synthetic Biology, 2021, 10, 3209-3235.	1.9	9
3434	Relaxed complex scheme and molecular dynamics simulation suggests small molecule inhibitor of human TMPRSS2 for combating COVID-19. Journal of Biomolecular Structure and Dynamics, 2021, , 1-11.	2.0	1
3435	A target fishing study to spot possible biological targets of fusaric acid: Inhibition of protein kinase-A and insights on the underpinning mechanisms. Food and Chemical Toxicology, 2022, 159, 112663.	1.8	6
3436	Quantum computational, spectroscopic and molecular docking studies of potent tuberculosis drug 2,6-dihydroxypyridine-4-carboxylic acid and 2â€hydroxy -6-methylpyridine-4-carboxylic acid. Journal of Molecular Structure, 2022, 1250, 131895.	1.8	4
3437	Ultrahigh Throughput Proteinâ€“Ligand Docking with Deep Learning. Methods in Molecular Biology, 2022, 2390, 301-319.	0.4	3
3438	AroCageDB: A Web-Based Resource for Aromatic Cage Binding Sites and Their Intrinsic Ligands. Journal of Chemical Information and Modeling, 2021, 61, 5327-5330.	2.5	3
3439	Molecular Docking and Virtual Screening of an Influenza Virus Inhibitor That Disrupts Proteinâ€“Protein Interactions. Viruses, 2021, 13, 2229.	1.5	10
3440	Binding affinity prediction for proteinâ€“ligand complex using deep attention mechanism based on intermolecular interactions. BMC Bioinformatics, 2021, 22, 542.	1.2	32
3441	Tyrosine kinase inhibitor prodrug-loaded liposomes for controlled release at tumor microenvironment. Journal of Controlled Release, 2021, 340, 318-330.	4.8	8
3442	Synthesis, In-vitro Antioxidant, Anti-diabetic Evaluation and Docking Studies of Newly Synthesized Benzoxazole Derivatives. Trends in Sciences, 2021, 18, 35.	0.2	4
3443	Cosolvent and Dynamic Effects in Binding Pocket Search by Docking Simulations. Journal of Chemical Information and Modeling, 2021, 61, 5508-5523.	2.5	3
3445	From atoms to bonds, angles and torsions: molecular metrics from crystal space, and two Excel implementations. Journal of Applied Crystallography, 2020, 53, 1101-1107.	1.9	0
3450	The inhibitory effect of KN-93 and KN-62 as a result of CaM-directed blocking animal CaMK2 and plant CDPK activation. Faktori Eksperimental Noi Evolucii Organizmiv, 0, 26, 298-304.	0.0	0
3451	Simulation of Proteins Modified with a Fluorescent Label. Methods in Molecular Biology, 2021, 2199, 289-313.	0.4	1
3452	Characterization of sulfated polysaccharide activity against virulent Plasmodium falciparum PHISTb/RLP1 protein. F1000Research, 0, 9, 1268.	0.8	1
3458	Antiproliferative potential, quantitative structure-activity relationship, cheminformatic and molecular docking analysis of quinoline and benzofuran derivatives. European Journal of Chemistry, 2020, 11, 223-234.	0.3	3

#	Article	IF	Citations
3459	Crystal structure of hyoscyamine sulfate monohydrate, (C₁₇H₂₄NO₃)₂(SO₄)(H₂O). Powder Diffraction, 2020, 35, 286-292.	0.4	0
3461	Identification of bioactive compounds by GC-MS and Î±-amylase and Î±-glucosidase inhibitory activity of Rauvolfia tetraphylla L. and Oroxylum indicum (L.) Kurz: an in vitro and in silico approach. Clinical Phytoscience, 2020, 6, .	0.8	5
3462	Molecular docking and simulation investigation: effect of beta-sesquiphellandrene with ionic integration on SARS-CoV2 and SFTS viruses. Journal of Genetic Engineering and Biotechnology, 2020, 18, 78.	1.5	22
3463	Mechanistic insight into the interactions between thiazolidinedione derivatives and PTP-1B combining 3D QSAR and molecular docking in the treatment of type 2 diabetes. ChemistrySelect, 2022, 7, 645-664.	0.7	0
3464	Identification of Novel Phyto-chemicals from Ocimum basilicum for the Treatment of Parkinsonâ€™s Disease using In Silico Approach. Current Computer-Aided Drug Design, 2020, 16, 420-434.	0.8	8
3465	Molecular Docking of Novel 5-O-benzoylpinostrobin Derivatives as SARS-CoV-2 Main Protease Inhibitors. Pharmaceutical Sciences, 2020, 26, S63-S77.	0.1	2
3466	GABAergic and Serotonergic System Mediated Psychoneuropharmacological Activities of Essential Oil from the Leaves of Aegle marmelos: An in vivo and in silico Approach. Journal of Essential Oil-bearing Plants: JEOP, 2020, 23, 1265-1282.	0.7	2
3467	Molecular Insights into the Interaction of Ursolic Acid and Cucurbitacin from Colocynth with Therapeutic Targets of Mycobacterium tuberculosis. Letters in Drug Design and Discovery, 2020, 17, 1309-1318.	0.4	1
3468	Gossypetin Derivatives are also Putative Inhibitors of SARS-COV 2: Results of a Computational Study. , 2020, 1, 201-212.		2
3469	In Silico Docking, ADMET and QSAR Study of few Antimalarial Phytoconstituents as Inhibitors of Plasmepsin II of P. falciparum Against Malaria. Current Drug Therapy, 2020, 15, 264-273.	0.2	1
3470	Activation of Caspase-3 by Terpenoids and Flavonoids in Different Types of Cancer Cells. Current Topics in Medicinal Chemistry, 2020, 20, 1876-1887.	1.0	5
3473	Search for Human Lactate Dehydrogenase A Inhibitors Using Structure-Based Modeling. Acta Naturae, 2015, 7, 57-63.	1.7	6
3474	Coumarin derivatives bearing benzoheterocycle moiety: synthesis, cholinesterase inhibitory, and docking simulation study. Iranian Journal of Basic Medical Sciences, 2017, 20, 631-638.	1.0	7
3475	Oleanolic Acids Inhibit Vascular Endothelial Growth Factor Receptor 2 Signaling in Endothelial Cells: Implication for Anti-Angiogenic Therapy. Molecules and Cells, 2018, 41, 771-780.	1.0	7
3476	Computational Investigation of Ginsenoside F1 from Meyer as p38 MAP Kinase Inhibitor: Molecular Docking and Dynamics Simulations, ADMET Analysis, and Drug Likeness Prediction. Iranian Journal of Pharmaceutical Research, 2018, 17, 1318-1327.	0.3	4
3477	Study of lipase producing gene in wheat - an in silico approach. Journal of Genetic Engineering and Biotechnology, 2021, 19, 73.	1.5	0
3478	estrogen receptor alpha antagonist studies and toxicity prediction of leaves bioactive ethyl acetate fraction. Journal of Advanced Pharmaceutical Technology and Research, 2021, 12, 236-241.	0.4	0
3479	Computer modeling and numerical studies of peptide nanotubes based on diphenylalanine. Keldysh Institute Preprints, 2021, , 1-54.	0.1	1

#	Article	IF	Citations
3480	Molecular persistent spectral image (Mol-PSI) representation for machine learning models in drug design. Briefings in Bioinformatics, 2022, 23, .	3.2	12
3481	Unraveling the differential impact of PAHs and dioxin-like compounds on AKR1C3 reveals the EGFR extracellular domain as a critical determinant of the AHR response. Environment International, 2022, 158, 106989.	4.8	15
3482	Novel O-acylated (E)-3-aryl-6,7-dihydrobenzisoxazol-4(5H)-one oximes targeting HSP90-HER2 axis in breast cancer cells. Bioorganic and Medicinal Chemistry, 2022, 53, 116521.	1.4	4
3483	Integrative analysis of the molecular mechanisms, immunological features and immunotherapy response of ferroptosis regulators across 33 cancer types. International Journal of Biological Sciences, 2022, 18, 180-198.	2.6	28
3484	A computer-aided drug design approach to discover tumour suppressor p53 protein activators for colorectal cancer therapy. Bioorganic and Medicinal Chemistry, 2022, 53, 116530.	1.4	8
3485	Monoterpene indole alkaloids from Vinca minor L. (Apocynaceae): Identification of new structural scaffold for treatment of Alzheimer's disease. Phytochemistry, 2022, 194, 113017.	1.4	7
3486	De-Novo Design of Hits Against New Delhi Metallo-Î²-Lactamase Enzyme. International Journal of Quantitative Structure-Property Relationships, 2022, 7, 1-13.	1.1	1
3487	2D-QSAR Modeling of Quinazolinone Derivatives as Angiotensin II Type 1a Receptor Blockers. International Journal of Quantitative Structure-Property Relationships, 2022, 7, 1-20.	1.1	1
3488	In Silico Molecular Dynamics Docking of Drugs to the Inhibitory Active Site of SARS-CoV-2 Protease and Their Predicted Toxicology and ADME. , 2021, 1, 16.		2
3489	Investigation of anticancer phytomolecule, chlorophyll catabolite of Capsicum annuum, targeting MECOM protein: molecular docking insight. , 2021, , .		0
3490	Virtual screening of new targets and inhibitors for Candida albicans infection control. , 2021, , .		0
3493	Structural Diversity and Role of Phytochemicals against P38-Î± Mitogen-activated Protein Kinase and Epidermal Growth Factor Receptor Kinase Domain: A Privileged Computational Approach. Journal of Pure and Applied Microbiology, 2021, 15, 2263-2269.	0.3	4
3494	Identification of diverse lipidâ€binding modes in the groove of zinc Î±₂ glycoprotein reveals its functional versatility. FEBS Journal, 2022, 289, 1876-1896.	2.2	3
3495	Synthesis, Identification, Computer-Aided Docking Studies, and ADMET Prediction of Novel Benzimidazo-1,2,3-triazole Based Molecules as Potential Antimicrobial Agents. Molecules, 2021, 26, 7119.	1.7	15
3496	Identification of Novel Antistaphylococcal Hit Compounds Targeting Sortase A. Molecules, 2021, 26, 7095.	1.7	7
3497	CHARMM-GUI Ligand Designer for Template-Based Virtual Ligand Design in a Binding Site. Journal of Chemical Information and Modeling, 2021, 61, 5336-5342.	2.5	8
3498	Evaluation of the inhibitory potentials of selected compounds from Costus spicatus (Jacq.) rhizome towards enzymes associated with insulin resistance in polycystic ovarian syndrome: an in silico study. Journal of Genetic Engineering and Biotechnology, 2021, 19, 176.	1.5	2
3499	Molecular Docking Simulation Studies Identifies Potential Natural Product Derived-Antiwolbachial Compounds as Filaricides against Onchocerciasis. Biomedicines, 2021, 9, 1682.	1.4	17

#	Article	IF	Citations
3500	LCP: Simple Representation of Docking Poses for Machine Learning: A Case Study on Xanthine Oxidase Inhibitors. Molecular Informatics, 2022, 41, e2100245.	1.4	0
3501	Use of Poly(vinyl alcohol)-Malic Acid (CLHPMA) Hydrogels and Chitosan Coated Calcium Alginate (CCCA) Microparticles as Potential Sorbent Phases for the Extraction and Quantitative Determination of Pesticides from Aqueous Solutions. Polymers, 2021, 13, 3993.	2.0	8
3502	Which of the (Mixed) Halogenated n-Alkanes Are Likely To Be Persistent Organic Pollutants?. Environmental Science & Technology, 2021, 55, 15912-15920.	4.6	16
3503	Identifying organic chemicals not subject to bioaccumulation in airâ€breathing organisms using predicted partitioning and biotransformation properties. Integrated Environmental Assessment and Management, 2022, 18, 1297-1312.	1.6	7
3504	Chemical properties of key metabolites determine the global distribution of lichens. Ecology Letters, 2022, 25, 416-426.	3.0	6
3505	MRlogP: Transfer Learning Enables Accurate logP Prediction Using Small Experimental Training Datasets. Processes, 2021, 9, 2029.	1.3	4
3506	Computational resources in healthcare. Wiley Interdisciplinary Reviews: Data Mining and Knowledge Discovery, 2022, 12, e1437.	4.6	1
3507	Building Unit Extractor for Metalâ€“Organic Frameworks. Journal of Chemical Information and Modeling, 2021, 61, 5827-5840.	2.5	7
3508	A System Pharmacology Model for Decoding the Synergistic Mechanisms of Compound Kushen Injection in Treating Breast Cancer. Frontiers in Pharmacology, 2021, 12, 723147.	1.6	0
3509	Iminoâ€2Hâ€Chromene Based Derivatives as Potential Antiâ€Alzheimer's Agents: Design, Synthesis, Biological Evaluation and in Silico Study. Chemistry and Biodiversity, 2022, 19, e2100599.	1.0	4
3511	De novo protein fold families expand the designable ligand binding site space. PLoS Computational Biology, 2021, 17, e1009620.	1.5	3
3512	Repurposing the Trypanosomatidic GSK Kinetobox for the Inhibition of Parasitic Pteridine and Dihydrofolate Reductases. Pharmaceuticals, 2021, 14, 1246.	1.7	2
3514	Genome-Guided Discovery of Natural Products through Multiplexed Low-Coverage Whole-Genome Sequencing of Soil Actinomycetes on Oxford Nanopore Flongle. MSystems, 2021, 6, e0102021.	1.7	6
3515	Accelerated dinuclear palladium catalyst identification through unsupervised machine learning. Science, 2021, 374, 1134-1140.	6.0	63
3516	Identification of megacerotonic acid and a quinazoline derivative from Universal Natural Product Database as potential inhibitors ofTrypanosoma brucei bruceialternative oxidase: molecular docking, molecular dynamic simulation and MM/PBSA analysis. Journal of Biomolecular Structure and Dynamics, 2023, 41, 45-54.	2.0	3
3517	A 3D structural SARS-CoV-2â€“human interactome to explore genetic and drug perturbations. Nature Methods, 2021, 18, 1477-1488.	9.0	17
3518	DockStream: a docking wrapper to enhance de novo molecular design. Journal of Cheminformatics, 2021, 13, 89.	2.8	24
3519	A novel synthetic protocol for the synthesis of pulvinones, and naturally occurring Aspulvinone E, molecules of medicinal interest. Synthetic Communications, 2022, 52, 117-128.	1.1	2

#	Article	IF	Citations
3520	Computational Network Pharmacologyâ€“Based Strategy to Capture Key Functional Components and Decode the Mechanism of Chai-Hu-Shu-Gan-San in Treating Depression. Frontiers in Pharmacology, 2021, 12, 782060.	1.6	6
3521	Designing of a Multi-epitope Vaccine against the Structural Proteins of Marburg Virus Exploiting the Immunoinformatics Approach. ACS Omega, 2021, 6, 32043-32071.	1.6	43
3522	Interactions of chlorophyll-derived photosensitizers with human serum albumin are determined by the central metal ion. Journal of Biomolecular Structure and Dynamics, 2023, 41, 479-492.	2.0	5
3523	Evaluation of Substitution of Small Branches with Roots of Desmodium gangeticum (Physicochemical) Tj ETQq1 1 0.784314 rgBT /Ov Applied Biochemistry and Biotechnology, 2021, , 1.	1.4	2
3524	VRChem: A Virtual Reality Molecular Builder. Applied Sciences (Switzerland), 2021, 11, 10767.	1.3	7
3526	Protein domain-based prediction of drug/compoundâ€“target interactions and experimental validation on LIM kinases. PLoS Computational Biology, 2021, 17, e1009171.	1.5	13
3527	Computational and In Vitro Experimental Investigations Reveal Anti-Viral Activity of Licorice and Glycyrrhizin against Severe Acute Respiratory Syndrome Coronavirus 2. Pharmaceuticals, 2021, 14, 1216.	1.7	13
3528	Screening of Severe Acute Respiratory Syndrome Coronavirus 2 RNA-Dependent RNA Polymerase Inhibitors Using Computational Approach. Journal of Computational Biology, 2021, 28, 1228-1247.	0.8	13
3530	A New Paradigm for KIM-PTP Drug Discovery: Identification of Allosteric Sites with Potential for Selective Inhibition Using Virtual Screening and LEI Analysis. International Journal of Molecular Sciences, 2021, 22, 12206.	1.8	4
3531	Antimalarial Drug Predictions Using Molecular Descriptors and Machine Learning against Plasmodium Falciparum. Biomolecules, 2021, 11, 1750.	1.8	8
3532	Investigation of Thiocarbamates as Potential Inhibitors of the SARS-CoV-2 Mpro. Pharmaceuticals, 2021, 14, 1153.	1.7	1
3533	DD-GUI: a graphical user interface for deep learning-accelerated virtual screening of large chemical libraries (Deep Docking). Bioinformatics, 2022, 38, 1146-1148.	1.8	4
3534	Anti-neoplastic phramacophore benzophenone-1 coumarin (BP-1C) targets JAK2 to induce apoptosis in lung cancer. Apoptosis: an International Journal on Programmed Cell Death, 2021, , 1.	2.2	3
3536	High-Throughput Screening Reveals New Glutaminase Inhibitor Molecules. ACS Pharmacology and Translational Science, 2021, 4, 1849-1866.	2.5	3
3537	Hibiscus sabdariffa anthocyanins are potential modulators of estrogen receptor alpha activity with favourable toxicology: a computational analysis using molecular docking, ADME/Tox prediction, 2D/3D QSAR and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 611-633.	2.0	16
3538	In silicoscreening of natural compounds to inhibit interaction of human ACE2 receptor and spike protein of SARS-CoV-2 for the prevention of COVID-19. Journal of Biomolecular Structure and Dynamics, 2023, 41, 646-658.	2.0	6
3539	Automated discovery of noncovalent inhibitors of SARS-CoV-2 main protease by consensus Deep Docking of 40 billion small molecules. Chemical Science, 2021, 12, 15960-15974.	3.7	36
3540	Trustworthy Deep Neural Network for Inferring Anticancer Synergistic Combinations. IEEE Journal of Biomedical and Health Informatics, 2023, 27, 1691-1700.	3.9	1

#	Article	IF	Citations
3541	Effective synthesis of novel dihydrobenzisoxazoles bearing the 2-aminothiazole moiety and evaluation of the antiproliferative activity of their acylated derivatives. Organic and Biomolecular Chemistry, 2021, 19, 10432-10443.	1.5	4
3542	Implementing in vitro bioactivity data to modernize priority setting of chemical inventories. ALTEX: Alternatives To Animal Experimentation, 2021, , .	0.9	6
3543	In vitro antioxidant and anti-inflammatory activities of green cardamom essential oil and in silico molecular docking of its major bioactives. Journal of Taibah University for Science, 2021, 15, 757-768.	1.1	29
3544	ADENet: a novel network-based inference method for prediction of drug adverse events. Briefings in Bioinformatics, 2022, 23, .	3.2	4
3545	Identification of SARS-CoV-2 main protease inhibitors from FDA-approved drugs by artificial intelligence-supported activity prediction system. Journal of Biomolecular Structure and Dynamics, 2023, 41, 1767-1775.	2.0	2
3546	Multi-scale mechanism of antiviral drug-alike phytoligands from Ayurveda in managing COVID-19 and associated metabolic comorbidities: insights from network pharmacology. Molecular Diversity, 2022, 26, 2575-2594.	2.1	6
3547	Antiproliferative pharmacophore azo-hydrazone analogue BT-1F exerts death signalling pathway targeting STAT3 in solid tumour. Pharmacological Reports, 2022, , 1.	1.5	3
3548	Quantum Chemical Prediction of Electron Ionization Mass Spectra of Trimethylsilylated Metabolites. Analytical Chemistry, 2022, , .	3.2	5
3549	From Platform to Knowledge Graph: Evolution of Laboratory Automation. Jacs Au, 2022, 2, 292-309.	3.6	42
3550	wSDTNBI: a novel network-based inference method for virtual screening. Chemical Science, 2022, 13, 1060-1079.	3.7	11
3552	A 5-FU Precursor Designed to Evade Anabolic and Catabolic Drug Pathways and Activated by Pd Chemistry In Vitro and In Vivo. Journal of Medicinal Chemistry, 2022, 65, 552-561.	2.9	20
3553	A benchmark study of machine learning methods for molecular electronic transition: Treeâ€based ensemble learning versus graph neural network. Bulletin of the Korean Chemical Society, 2022, 43, 328-335.	1.0	9
3554	In Silico Screening of Potential Phytocompounds from Several Herbs against SARS-CoV-2 Indian Delta Variant B.1.617.2 to Inhibit the Spike Glycoprotein Trimer. Applied Sciences (Switzerland), 2022, 12, 665.	1.3	8
3555	Indoles and 1-(3-(benzyloxy)benzyl)piperazines: Reversible and selective monoamine oxidase B inhibitors identified by screening an in-house compound library. Bioorganic Chemistry, 2022, 119, 105581.	2.0	2
3556	Picolylamine-functionalized benz[e]indole squaraine dyes: Synthetic approach, characterization and inÂvitro efficacy as potential anticancer phototherapeutic agents. European Journal of Medicinal Chemistry, 2022, 229, 114071.	2.6	11
3557	Evolution of Pharmacological activity with Molecular Docking of active constituents present in roots and small branches of Aegle Marmelos: A comparative study using HPLC, GCâ€“MS, LC-MS. Phytomedicine Plus, 2022, 2, 100210.	0.9	1
3558	Molecular insights of oxadiazole benzene sulfonamides as human carbonic anhydrase IX inhibitors: Combined molecular docking, molecular dynamics, and 3D QSAR studies. Journal of the Indian Chemical Society, 2022, 99, 100339.	1.3	4
3559	Virtual screening and in vitro validation of natural compound inhibitors against SARS-CoV-2 spike protein. Bioorganic Chemistry, 2022, 119, 105574.	2.0	10

#	Article	IF	Citations
3560	Studies on physicochemical, phytochemicals, chromatographic profiling & estimation and in-silico study of Negundoside in roots & small branches of Vitex Negundo plant. Phytomedicine Plus, 2022, 2, 100205.	0.9	6
3561	Molecular basis for stereoselective transport of fenoterol by the organic cation transporters 1 and 2. Biochemical Pharmacology, 2022, 197, 114871.	2.0	7
3562	Anti-diabetic potential, crystal structure, molecular docking, DFT, and optical-electrochemical studies of new dimethyl and diethyl carbamoyl-N, Nâ€²-disubstituted based thioureas. Journal of Molecular Structure, 2022, 1253, 132207.	1.8	11
3563	Alpha-lipoic acid analogues in the regulation of redox balance in epilepsy: A molecular docking and simulation study. Journal of Molecular Graphics and Modelling, 2022, 112, 108116.	1.3	5
3564	Molecular dynamics simulations of the flexibility and inhibition of SARS-CoV-2 NSP 13 helicase. Journal of Molecular Graphics and Modelling, 2022, 112, 108122.	1.3	3
3565	Deep learning-assisted pipeline for Virtual Screening of ligand compound databases: Application on inhibiting the entry of SARS-CoV-2 into human cells. , 2020, , .		1
3566	In Silico Identification of Protein Targets Associated to the Insecticide Activity of Eugenol Derivatives. Chemistry Proceedings, 2020, 3, .	0.1	0
3567	Virtual Screening of the Active Components of Garcinia mangostana Linn. Potentially Inhibiting the Interaction of Advanced Glycation End-products and their Receptor. Open Access Macedonian Journal of Medical Sciences, 2020, 8, 921-927.	0.1	1
3568	Limonin inhibits angiogenesis and metastasis of human breast cancer cells by suppressing the VEGFR2/IGFR1-mediated STAT3 signaling pathway. Translational Cancer Research, 2020, 9, 6820-6832.	0.4	5
3569	Ligand Docking Methods to Recognize Allosteric Inhibitors for G-Protein-Coupled Receptors. Bioinformatics and Biology Insights, 2021, 15, 117793222110377.	1.0	3
3570	Application of Indian Pennywort Centella asiatica in Carp Aquaculture against Flavobacterium columnare Infection. , 2021, , 535-572.		0
3571	Modeling the Interaction of the UxuRâ€“ExuR Heterodimer with the Components of the Metabolic Pathway of Escherichia coli for Hexuronate Utilization. Biophysics (Russian Federation), 2021, 66, 753-763.	0.2	0
3572	In vitro and in silico studies of fluorinated 2,3â€disubstituted thiazolidinoneâ€pyrazoles as potential Î±â€amylase inhibitors and antioxidant agents. Archiv Der Pharmazie, 2022, 355, e2100342.	2.1	30
3573	Mechanism of biotin carboxylase inhibition by ethyl 4-[[2-chloro-5-(phenylcarbamoyl)phenyl]sulphonylamino]benzoate. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 100-108.	2.5	2
3574	Lignin Nanoparticles Deliver Novel Thymine Biomimetic Photo-Adducts with Antimelanoma Activity. International Journal of Molecular Sciences, 2022, 23, 915.	1.8	9
3575	Transport mechanisms and desalination performance of the PSF/UiO-66 thin-film composite membrane: a molecular dynamics study. Molecular Simulation, 2022, 48, 427-437.	0.9	0
3576	Synthesis of New 3-Arylcoumarins Bearing N-Benzyl Triazole Moiety: Dual Lipoxygenase and Butyrylcholinesterase Inhibitors With Anti-Amyloid Aggregation and Neuroprotective Properties Against Alzheimerâ€™s Disease. Frontiers in Chemistry, 2021, 9, 810233.	1.8	5
3577	Search for long-lasting electronic coherence using on-the-fly ab initio semiclassical dynamics. Journal of Chemical Physics, 2022, 156, 034104.	1.2	10

#	Article	IF	Citations
3578	Investigation of SARS-CoV-2 Main Protease Potential Inhibitory Activities of Some Natural Antiviral Compounds Via Molecular Docking and Dynamics Approaches. Phyton, 2022, 91, 1089-1104.	0.4	3
3579	Antenna-Biased Odorant Receptor HvarOR25 in Hippodamia variegata Tuned to Allelochemicals from Hosts and Habitat Involved in Perceiving Preys. Journal of Agricultural and Food Chemistry, 2022, 70, 1090-1100.	2.4	13
3580	Synthesis and biological evaluation of novel thiazolo[4,5-d]pyrimidin-7(6H)-ones as topoisomerase I inhibitors. Chemistry of Heterocyclic Compounds, 2021, 57, 1220-1229.	0.6	1
3581	Accurate Prediction of Inhibitor Binding to HIV-1 Protease Using CANDOCK. Frontiers in Chemistry, 2021, 9, 775513.	1.8	3
3582	Effect of Chain Length on the Dipole Moment of Polyisobutylene Succinate Anhydride. Industrial & Engineering Chemistry Research, 2022, 61, 2359-2365.	1.8	3
3583	EnzyHTP: A High-Throughput Computational Platform for Enzyme Modeling. Journal of Chemical Information and Modeling, 2022, 62, 647-655.	2.5	16
3584	Negative Modulation of the Angiogenic Cascade Induced by Allosteric Kinesin Eg5 Inhibitors in a Gastric Adenocarcinoma In Vitro Model. Molecules, 2022, 27, 957.	1.7	10
3585	Machine Learning for Melting Temperature Predictions and Design in Polyhydroxyalkanoate-Based Biopolymers. Journal of Physical Chemistry B, 2022, 126, 934-945.	1.2	15
3586	Functional, electrophysiology, and molecular dynamics analysis of quercetin-induced contraction of rat vascular musculature. European Journal of Pharmacology, 2022, 918, 174778.	1.7	9
3587	ChemSpaX: exploration of chemical space by automated functionalization of molecular scaffold. , 2022, 1, 8-25.		5
3588	New Hypercoordinating Organostannanes for the Modular Functionalization of Monoâ€•and Polystannanes: Synthetic and Computational Studies**. European Journal of Inorganic Chemistry, 2022, 2022, .	1.0	0
3589	Molecular determinants of GPCR pharmacogenetics: Deconstructing the population variants in Î²2-adrenergic receptor. Advances in Protein Chemistry and Structural Biology, 2022, 128, 361-396.	1.0	1
3591	Evaluating the Accuracy of the QCEIMS Approach for Computational Prediction of Electron Ionization Mass Spectra of Purines and Pyrimidines. Metabolites, 2022, 12, 68.	1.3	4
3592	In silico profiling of histone deacetylase inhibitory activity of compounds isolated from Cajanus cajan. Beni-Suef University Journal of Basic and Applied Sciences, 2022, 11, .	0.8	2
3593	New Secondary Metabolites from the Marine-Derived Fungus Talaromyces mangshanicus BTBU20211089. Marine Drugs, 2022, 20, 79.	2.2	10
3594	ER/AR Multi-Conformational Docking Server: A Tool for Discovering and Studying Estrogen and Androgen Receptor Modulators. Frontiers in Pharmacology, 2022, 13, 800885.	1.6	1
3595	Identification of selective mtbDHFR inhibitors by virtual screening and experimental approaches. Chemical Biology and Drug Design, 2022, 100, 1005-1016.	1.5	7
3596	Target-Based Virtual Screening and LC/MS-Guided Isolation Procedure for Identifying Phloroglucinol-Terpenoid Inhibitors of SARS-CoV-2. Journal of Natural Products, 2022, 85, 327-336.	1.5	13

#	Article	IF	Citations
3597	Cancer Chemopreventive Potential and Chemical Profiling of Euphorbia abyssinica Endowed with Docking Studies. ACS Omega, 2022, 7, 3596-3604.	1.6	4
3598	Valence-, Dipole- and Quadropole-Bound Electronically Excited States of Closed-Shell Anions Formed by Deprotonation of Cyano- and Ethynyl-Disubstituted Polycyclic Aromatic Hydrocarbons. Chemistry, 2022, 4, 42-56.	0.9	4
3599	Machineâ€Learning Prediction of Metalâ€“Organic Framework Guest Accessibility from Linker and Metal Chemistry. Angewandte Chemie - International Edition, 2022, 61, .	7.2	24
3600	Inhibition of Collagenase Q1 of Bacillus cereus as a Novel Antivirulence Strategy for the Treatment of Skinâ€Wound Infections. Advanced Therapeutics, 2022, 5, 2100222.	1.6	4
3601	In silico prediction and structure-based multitargeted molecular docking analysis of selected bioactive compounds against mucormycosis. Bulletin of the National Research Centre, 2022, 46, 24.	0.7	12
3602	A New Series of Aryloxyacetic Acids Endowed with Multi-Target Activity towards Peroxisome Proliferator-Activated Receptors (PPARs), Fatty Acid Amide Hydrolase (FAAH), and Acetylcholinesterase (AChE). Molecules, 2022, 27, 958.	1.7	7
3603	Insect RDL Receptor Models for Virtual Screening: Impact of the Template Conformational State in Pentameric Ligand-Gated Ion Channels. ACS Omega, 2022, 7, 1988-2001.	1.6	2
3604	Targeting mucormycosis polyprotein (RVT_1 region) through antifungal phytochemicals: An in-silico perspective. Informatics in Medicine Unlocked, 2022, 29, 100851.	1.9	1
3605	DeepSide: A Deep Learning Approach for Drug Side Effect Prediction. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2022, PP, 1-1.	1.9	6
3606	Computational investigations on the potential role of hygrophorones as quorum sensing inhibitors against LasR protein ofPseudomonas aeruginosa. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2249-2259.	2.0	3
3607	DOTA: Deep Learning Optimal Transport Approach to Advance Drug Repositioning for Alzheimerâ€™s Disease. Biomolecules, 2022, 12, 196.	1.8	8
3608	Representations and strategies for transferable machine learning improve model performance in chemical discovery. Journal of Chemical Physics, 2022, 156, 074101.	1.2	11
3609	Phytochemicals and in silico investigations of Sudanese roselle. South African Journal of Science, 2022, 118, .	0.3	2
3610	Supramolecular gating of guest release from cucurbit[7]uril using de novo design. Npj Computational Materials, 2022, 8, .	3.5	9
3611	Computational Scaling Relationships Predict Experimental Activity and Rate-Limiting Behavior in Homogeneous Water Oxidation. Inorganic Chemistry, 2022, 61, 2186-2197.	1.9	3
3612	Phytochemical Screening, In Vitro and In Silico Studies of Volatile Compounds from Petroselinum crispum (Mill) Leaves Grown in Saudi Arabia. Molecules, 2022, 27, 934.	1.7	14
3613	Drug Repurposing Targeting Pseudomonas aeruginosa MvfR Using Docking, Virtual Screening, Molecular Dynamics, and Free-Energy Calculations. Antibiotics, 2022, 11, 185.	1.5	14
3614	DeepDrug: Applying AI for the Advancement of Drug Discovery. , 2022, , .		2

#	Article	IF	Citations
3615	Extracellular Calcium Receptor as a Target for Glutathione and Its Derivatives. International Journal of Molecular Sciences, 2022, 23, 717.	1.8	6
3616	Diosgenin From Dioscorea Nipponica Rhizoma Against Gravesâ€™ Diseaseâ€”On Network Pharmacology and Experimental Evaluation. Frontiers in Pharmacology, 2021, 12, 806829.	1.6	4
3617	Synthesis, Molecular Docking Analysis and in Vitro Biological Evaluation of Some New Heterocyclic Scaffolds-Based Indole Moiety as Possible Antimicrobial Agents. Frontiers in Molecular Biosciences, 2021, 8, 775013.	1.6	3
3618	The SwissSimilarity 2021 Web Tool: Novel Chemical Libraries and Additional Methods for an Enhanced Ligand-Based Virtual Screening Experience. International Journal of Molecular Sciences, 2022, 23, 811.	1.8	53
3619	In silicoscreening-based discovery of inhibitors against glycosylation proteins dysregulated in cancer. Journal of Biomolecular Structure and Dynamics, 2023, 41, 1540-1552.	2.0	6
3620	NNAIMQ: A neural network model for predicting QTAIM charges. Journal of Chemical Physics, 2022, 156, 014112.	1.2	5
3621	Trehaloseâ€6â€phosphate phosphatases are involved in the trehalose synthesis and metamorphosis in Bactrocera minax. Insect Science, 2022, , .	1.5	2
3622	Screening toward the Development of Fingerprints of Atomic Environments Using Bond-Orientational Order Parameters. ACS Omega, 2022, 7, 4606-4613.	1.6	2
3623	Improving proteinâ€“ligand docking and screening accuracies by incorporating a scoring function correction term. Briefings in Bioinformatics, 2022, 23, .	3.2	41
3624	Theoretical insights into the radical scavenging activity of glipizide: DFT and molecular docking studies. Free Radical Research, 2022, 56, 53-62.	1.5	5
3625	Machineâ€Learning Prediction of Metalâ€“Organic Framework Guest Accessibility from Linker and Metal Chemistry. Angewandte Chemie, 2022, 134, .	1.6	2
3626	Zeolite Phase Selectivity Using the Same Organic Structure-Directing Agent in Fluoride and Hydroxide Media. Journal of Physical Chemistry C, 2022, 126, 2078-2087.	1.5	8
3627	In-silico interactions of eugenol and temephos with metabolic detoxifying enzymes of Aedes aegypti (Diptera: Culicidae). International Journal of Tropical Insect Science, 2022, 42, 1987.	0.4	0
3628	The potential role of U2AF1L4 cDNA 3â€™ stretch mutations in oral carcinogenesis. Advances in Cancer Biology Metastasis, 2022, 4, 100030.	1.1	1
3629	Interplay Between Applied Force and Radical Attack in the Mechanochemical Chain Scission of Poly(acrylic acid). Journal of Physical Chemistry A, 2022, 126, 521-528.	1.1	2
3630	Elucidating the inhibitory mechanism of yeast Î±-glucosidase by phytocompounds from Scoparia dulcis through inÂvitro and in silico approach. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2574-2586.	2.0	1
3631	Emergence of Meropenem Resistance Among Cefotaxime Non-susceptible Streptococcus pneumoniae: Evidence and Challenges. Frontiers in Microbiology, 2021, 12, 810414.	1.5	17
3632	Intermolecular interactions between imidazolium- and cholinium-based ionic liquids and lysozyme: Regularities and peculiarities. Journal of Molecular Liquids, 2022, 348, 118426.	2.3	11

#	Article	IF	Citations
3633	Structural, Electronic, Elastic and Dynamical Properties of MCO₃ (M: Mn, Co, Ni) Precursor Materials for Li-Ion Batteries: A First-Principles Study. Journal of the Electrochemical Society, 2022, 169, 020540.	1.3	3
3634	Design, synthesis and molecular docking studies of new azomethine derivatives as promising anti-inflammatory agents. Bioorganic Chemistry, 2022, 120, 105595.	2.0	1
3635	Identification of novel bioactive compounds from Olea europaea by evaluation of chemical compounds in the OliveNetâ„¢ library: in silico bioactivity and molecular modelling, and in vitro validation of hERG activity. Computers in Biology and Medicine, 2022, 142, 105247.	3.9	5
3636	Structural-based virtual screening and identification of novel potent antimicrobial compounds against YsxC of Staphylococcus aureus. Journal of Molecular Structure, 2022, 1255, 132476.	1.8	29
3637	Ecdysterone prevents negative effect of acute immobilization stress on energy metabolism of rat liver mitochondria. Journal of Steroid Biochemistry and Molecular Biology, 2022, 219, 106066.	1.2	4
3638	Synthesis, characterization, crystal structure determination, computational modelling and biological studies of a new tetrakis-(2-hydroxy-5-methylphenyl)(1H-pyrazol-4-yl)methanonezinc(II) complex. Journal of Molecular Structure, 2022, 1255, 132377.	1.8	5
3639	Generating 3D molecules conditional on receptor binding sites with deep generative models. Chemical Science, 2022, 13, 2701-2713.	3.7	60
3641	Identification of novel SARS-CoV-2 RNA dependent RNA polymerase (RdRp) inhibitors: From in silico screening to experimentally validated inhibitory activity. Computational and Structural Biotechnology Journal, 2022, 20, 882-890.	1.9	10
3642	Accelerating the discovery of the beyond rule of five compounds that have high affinities toward SARS-CoV-2 spike RBD. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2518-2527.	2.0	1
3643	Artificial intelligenceâ€“enabled virtual screening of ultra-large chemical libraries with deep docking. Nature Protocols, 2022, 17, 672-697.	5.5	107
3644	Potential Fluorinated Antiâ€MRSA Thiazolidinone Derivatives with Antibacterial, Antitubercular Activity and Molecular Docking Studies. Chemistry and Biodiversity, 2022, 19, .	1.0	22
3645	Synthesis of Dihydrobenzofuro[3,2â€b]chromenes as Potential 3CLpro Inhibitors of SARSâ€CoVâ€2: A Molecular Docking and Molecular Dynamics Study. ChemMedChem, 2022, 17, .	1.6	20
3646	Molecular docking analysis of FDA approved drugs with the glycoprotein from Junin and Machupo viruses. Bioinformation, 2022, 18, 119-126.	0.2	2
3647	BINANA 2: Characterizing Receptor/Ligand Interactions in Python and JavaScript. Journal of Chemical Information and Modeling, 2022, 62, 753-760.	2.5	12
3648	PyPAn: An Automated Graphical User Interface for Protein Sequence and Structure Analyses. Protein and Peptide Letters, 2022, 29, 306-312.	0.4	2
3649	Structure-Based Discovery of N-Sulfonylpiperidine-3-Carboxamides as Novel Capsid Assembly Modulators for Potent Inhibition of HBV Replication. Viruses, 2022, 14, 348.	1.5	5
3650	Screening of antibacterial compounds with novel structure from the FDA approved drugs using machine learning methods. Aging, 2022, 14, 1448-1472.	1.4	4
3651	Phytochemicals of Euphorbia hirta L. and Their Inhibitory Potential Against SARS-CoV-2 Main Protease. Frontiers in Molecular Biosciences, 2021, 8, 801401.	1.6	7

#	Article	IF	Citations
3652	Chemical Distance Measurement and System Pharmacology Approach Uncover the Novel Protective Effects of Biotransformed Ginsenoside C-Mc against UVB-Irradiated Photoaging. Oxidative Medicine and Cellular Longevity, 2022, 2022, 1-23.	1.9	2
3653	Repurposing Ayush-64 for COVID-19: A Computational Study Based on Network Pharmacology and Molecular Docking. Combinatorial Chemistry and High Throughput Screening, 2022, 25, 2089-2102.	0.6	1
3655	Efficient Reaction Space Exploration with ChemTraYzer-TAD. Journal of Chemical Information and Modeling, 2022, 62, 890-902.	2.5	11
3656	In silicoevaluation of binding of phytochemicals from bayati (Anamirta cocculusLinn) to the glutathione-s-transferase of Asian Corn Borer (Ostrinia furnacalisGuenÃ©e). Journal of Biomolecular Structure and Dynamics, 2023, 41, 2660-2666.	2.0	6
3657	Evidence that nuclear receptors are related to terpene synthases. Journal of Molecular Endocrinology, 2022, 68, 153-166.	1.1	0
3658	Possibilities and Challenges of Using Educational Cheminformatics for STEM Education: A SWOT Analysis of a Molecular Visualization Engineering Project. Journal of Chemical Education, 2022, 99, 1190-1200.	1.1	9
3659	Assessment of the ameliorative effect of curcumin on pendimethalin-induced genetic and biochemical toxicity. Scientific Reports, 2022, 12, 2195.	1.6	7
3660	Computational studies on the cholinesterase, beta-secretase 1 (BACE1) and monoamine oxidase (MAO) inhibitory activities of endophytes-derived compounds: towards discovery of novel neurotherapeutics. Journal of Biomolecular Structure and Dynamics, 2022, , 1-15.	2.0	3
3661	Revealing 2-dimethylhydrazino-2-alkyl alkynyl sphingosine derivatives as sphingosine kinase 2 inhibitors: Some hints on the structural basis for selective inhibition. Bioorganic Chemistry, 2022, 121, 105668.	2.0	2
3662	Plasma Bead Entrapped Liposomes as a Potential Drug Delivery System to Combat Fungal Infections. Molecules, 2022, 27, 1105.	1.7	1
3663	A Lead-Based Fragment Library Screening of the Glycosyltransferase WaaG from Escherichia coli. Pharmaceuticals, 2022, 15, 209.	1.7	3
3664	Exploring the Natural Compounds in Flavonoids for Their Potential Inhibition of Cancer Therapeutic Target MEK1 Using Computational Methods. Pharmaceuticals, 2022, 15, 195.	1.7	5
3665	Predicting Antifouling Activity and Acetylcholinesterase Inhibition of Marine-Derived Compounds Using a Computer-Aided Drug Design Approach. Marine Drugs, 2022, 20, 129.	2.2	8
3666	Exploration of potential inhibitors for autophagyâ€related protein 8 as antileishmanial agents. Chemical Biology and Drug Design, 2022, 99, 816-827.	1.5	3
3667	Discover, Sample, and Refine: Exploring Chemistry with Enhanced Sampling Techniques. Journal of Physical Chemistry Letters, 2022, 13, 1424-1430.	2.1	12
3668	Unusual substrate specificity in GH family 12: structureâ€“function analysis of glucanases Bgh12A and Xgh12B from Aspergillus cervinus, and Egh12 from Thielavia terrestris. Applied Microbiology and Biotechnology, 2022, 106, 1493-1509.	1.7	4
3669	NMR study of the inclusion complexes of Î²-cyclodextrin with diphenhydramine, clonidine and tolperisone. SN Applied Sciences, 2022, 4, 1.	1.5	0
3670	Detailed Analyses of Molecular Interactions between Favipiravir and RNA Viruses In Silico. Viruses, 2022, 14, 338.	1.5	0

#	Article	IF	Citations
3672	Structureâ€“Activity Relationships of Novel Tau Ligands: Passive Fibril Binders and Active Aggregation Inhibitors. ACS Chemical Biology, 2022, 17, 701-708.	1.6	4
3673	Chemical synthesis, biological activities and action on nuclear receptors of 20S(OH)D3, 20S,25(OH)2D3, 20S,23S(OH)2D3 and 20S,23R(OH)2D3. Bioorganic Chemistry, 2022, 121, 105660.	2.0	10
3674	Investigation of the Mechanism of Zishen Yutai Pills on Polycystic Ovary Syndrome: A Network Pharmacology and Molecular Docking Approach. Evidence-based Complementary and Alternative Medicine, 2021, 2021, 1-14.	0.5	5
3675	Targeting Epigenetic Regulators Using Machine Learning: Potential Sirtuin 2 Inhibitors. Journal of Computational Biophysics and Chemistry, 2021, 20, 841-851.	1.0	1
3676	Molecular Docking and Dynamics Investigations for Identifying Potential Inhibitors of the 3-Chymotrypsin-like Protease of SARS-CoV-2: Repurposing of Approved Pyrimidonic Pharmaceuticals for COVID-19 Treatment. Molecules, 2021, 26, 7458.	1.7	11
3677	Catechin Derivatives as Inhibitor of COVID-19 Main Protease (Mpro): Molecular Docking Studies Unveil an Opportunity Against CORONA. Combinatorial Chemistry and High Throughput Screening, 2021, 25, 197-203.	0.6	6
3678	In Silico Prediction and Bioactivity Evaluation of Chemical Ingredients Against Influenza A Virus From Isatis tinctoria L. Frontiers in Pharmacology, 2021, 12, 755396.	1.6	6
3679	Identification of Major Compounds and Î±-Amylase and Î±-Glucosidase Inhibitory Activity of Rhizome of Musa balbisiana Colla: An in-vitro and in-silico Study. Combinatorial Chemistry and High Throughput Screening, 2021, 25, 139-148.	0.6	0
3680	The Effect of Energy Minimization on The Molecular Docking of Acetone-Based Oxindole Derivatives. JKPK (Jurnal Kimia Dan Pendidikan Kimia), 2021, 6, 69.	0.1	4
3681	Identification of novel candidates for inhibition ofLasR, a quorum-sensing receptor of multidrug resistantPseudomonas aeruginosa, through a specialized multi-levelin silicoapproach. Molecular Systems Design and Engineering, 2022, 7, 434-446.	1.7	12
3682	2D QSAR of 3-(Piperidin-1-yl)-5,6,7,8-Tetrahydropyrido[3,4-b] Pyrazine Derivatives With GPCR-6 Inhibitory Activity. International Journal of Quantitative Structure-Property Relationships, 2022, 7, 1-27.	1.1	1
3683	Network pharmacology combined with metabolomics and lipidomics to reveal the hypolipidemic mechanism ofAlismatis rhizomain hyperlipidemic mice. Food and Function, 2022, 13, 4714-4733.	2.1	16
3684	Unlocking the computational design of metalâ€“organic cages. Chemical Communications, 2022, 58, 3717-3730.	2.2	24
3685	Implementation of predictive models: Practical aspects. Theoretical and Computational Chemistry, 2022, , 405-433.	0.2	0
3686	<i>In Silico</i> Evaluation for the Inhibitory Action of Curcumin Derivatives on the SARS-CoV-2 Proteins. Journal of Biosciences and Medicines, 2022, 10, 63-76.	0.1	0
3687	Machine Learning Models for Predicting Liver Toxicity. Methods in Molecular Biology, 2022, 2425, 393-415.	0.4	7
3688	Virtual screening of phytochemicals from Indian medicinal plants against the endonuclease domain of SFTS virus L polymerase. RSC Advances, 2022, 12, 6234-6247.	1.7	10
3690	Discovery of lead low-potential radical candidates for organic radical polymer batteries with machine-learning-assisted virtual screening. Journal of Materials Chemistry A, 2022, 10, 8273-8282.	5.2	15

#	Article	IF	Citations
3691	Auto-QChem: an automated workflow for the generation and storage of DFT calculations for organic molecules. Reaction Chemistry and Engineering, 2022, 7, 1276-1284.	1.9	16
3692	An automated framework for high-throughput predictions of NMR chemical shifts within liquid solutions. Nature Computational Science, 2022, 2, 112-122.	3.8	4
3693	Anti-Adhesion and Antibiofilm Activity of Eruca sativa Miller Extract Targeting Cell Adhesion Proteins of Food-Borne Bacteria as a Potential Mechanism: Combined In Vitro-In Silico Approach. Plants, 2022, 11, 610.	1.6	15
3694	An Integrative Pharmacology Model for Decoding the Underlying Therapeutic Mechanisms of Ermiao Powder for Rheumatoid Arthritis. Frontiers in Pharmacology, 2022, 13, 801350.	1.6	3
3695	An Enhanced Hybrid Screening Approach to Identify Potent Inhibitors for the SARS-CoV-2 Main Protease From the NCI Compound Library. Frontiers in Chemistry, 2022, 10, 816576.	1.8	6
3696	Inverse design of 3d molecular structures with conditional generative neural networks. Nature Communications, 2022, 13, 973.	5.8	70
3697	Enhancing the Antipsychotic Effect of Risperidone by Increasing Its Binding Affinity to Serotonin Receptor via Picric Acid: A Molecular Dynamics Simulation. Pharmaceuticals, 2022, 15, 285.	1.7	21
3698	Virtual Screening, Synthesis and Biological Evaluation of Streptococcus mutans Mediated Biofilm Inhibitors. Molecules, 2022, 27, 1455.	1.7	3
3699	Investigation of Unprecedented Sites and Proposition of New Ligands for Programmed Cell Death Protein I through Molecular Dynamics with Probes and Virtual Screening. Journal of Chemical Information and Modeling, 2022, 62, 1236-1248.	2.5	2
3700	Elucidating Antiangiogenic Potential of Rauwolfia serpentina: VEGFR-2 Targeting-Based Molecular Docking Study. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-10.	0.5	14
3701	A Molecular Investigation of the Solvent Influence on Inter- and Intra-Molecular Hydrogen Bond Interaction of Linamarin. Processes, 2022, 10, 352.	1.3	2
3702	Nontarget mass spectrometry and in silico molecular characterization of air pollution from the Indian subcontinent. Communications Earth & Environment, 2022, 3, .	2.6	14
3703	In Search of HIV Entry Inhibitors Using Molecular Docking, ADME, and Toxicity Studies of Some Thiazolidinone-Pyrazine Derivatives Against CXCR4 Co-receptor. Current HIV Research, 2022, 20, 152-162.	0.2	1
3704	In silicoandinÂvitroevaluation of imatinib as an inhibitor for SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3052-3061.	2.0	5
3705	Dynamics of natural product Lupenone as a potential fusion inhibitor against the spike complex of novel Semliki Forest Virus. PLoS ONE, 2022, 17, e0263853.	1.1	25
3706	PSnpBind: a database of mutated binding site proteinâ€“ligand complexes constructed using a multithreaded virtual screening workflow. Journal of Cheminformatics, 2022, 14, 8.	2.8	5
3707	Virtual screening of small natural compounds against NS1 protein of DENV, YFV and ZIKV. Journal of Biomolecular Structure and Dynamics, 2022, , 1-11.	2.0	5
3708	Network-Based Pharmacology Study Reveals Protein Targets for Medical Benefits and Harms of Cannabinoids in Humans. Applied Sciences (Switzerland), 2022, 12, 2205.	1.3	1

#	Article	IF	Citations
3709	Molecular modelling studies and identification of novel phytochemical inhibitor of DLL3. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3089-3109.	2.0	0
3710	Synthesis and in silico anti-metastatic evaluation of carvacrol derivative, 2-hydroxy-6-isopropyl-3-methylbenzalehyde. Materials Today: Proceedings, 2022, 57, 739-747.	0.9	1
3711	In Silico Screening of Bioactive Compounds of Representative Seaweeds to Inhibit SARS-CoV-2 ACE2-Bound Omicron B.1.1.529 Spike Protein Trimer. Marine Drugs, 2022, 20, 148.	2.2	19
3712	Z16b, a natural compound from Ganoderma cochlear is a novel RyR2 stabilizer preventing catecholaminergic polymorphic ventricular tachycardia. Acta Pharmacologica Sinica, 2022, 43, 2340-2350.	2.8	3
3713	Synthesis of N-Methylspiropyrrolidine Hybrids for Their Structural Characterization, Biological and Molecular Docking Studies. Polycyclic Aromatic Compounds, 2023, 43, 2430-2443.	1.4	3
3714	A new bio-active asymmetric-Schiff base: synthesis and evaluation of calf thymus DNA interaction, topoisomerase IÎ± inhibition,inÂvitroantiproliferative activity, SEM analysis and molecular docking studies. Journal of Biomolecular Structure and Dynamics, 2023, 41, 2804-2822.	2.0	0
3715	Identification of promising multi-targeting inhibitors of obesity from Vernonia amygdalina through computational analysis. Molecular Diversity, 2023, 27, 1-25.	2.1	17
3716	In silico analyses of the human spermâ€specific antigen 2 and its role in oral squamous cell carcinoma. , 0, , .		1
3717	PTML Modeling for Pancreatic Cancer Research: In Silico Design of Simultaneous Multi-Protein and Multi-Cell Inhibitors. Biomedicines, 2022, 10, 491.	1.4	10
3718	iCn3D: From Web-Based 3D Viewer to Structural Analysis Tool in Batch Mode. Frontiers in Molecular Biosciences, 2022, 9, 831740.	1.6	26
3719	DEPACT and PACMatch: A Workflow of Designing De Novo Protein Pockets to Bind Small Molecules. Journal of Chemical Information and Modeling, 2022, 62, 971-985.	2.5	4
3720	FitDock: proteinâ€“ligand docking by template fitting. Briefings in Bioinformatics, 2022, 23, .	3.2	38
3722	In silicoÂdiscovery of potential azole-containing mPGES-1 inhibitors by virtual screening, pharmacophore modeling and molecular dynamics simulations. Structural Chemistry, 0, , 1.	1.0	1
3723	Prediction of Water Distributions and Displacement at Proteinâ€“Ligand Interfaces. Journal of Chemical Information and Modeling, 2022, 62, 1489-1497.	2.5	5
3724	Characterizations of botanical attractant of Halyomorpha halys and selection of relevant deorphanization candidates via computational approach. Scientific Reports, 2022, 12, 4170.	1.6	3
3725	Phytoconstituents of traditional Himalayan Herbs as potential inhibitors of Human Papillomavirus (HPV-18) for cervical cancer treatment: An In silico Approach. PLoS ONE, 2022, 17, e0265420.	1.1	15
3726	Neem and Turmeric in the management of Covid Associated Mucormycosis (CAM) derived through network pharmacology. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3281-3294.	2.0	4
3727	Decomposing compounds enables reconstruction of interaction fingerprints for structure-based drug screening. Journal of Cheminformatics, 2022, 14, 17.	2.8	3

#	Article	IF	Citations
3728	Adding hydrogen atoms to molecular models via fragment superimposition. Algorithms for Molecular Biology, 2022, 17, 7.	0.3	1
3729	Paraquat toxicity in different cell types of Swiss albino mice. Scientific Reports, 2022, 12, 4818.	1.6	8
3730	Design, Synthesis, Biological Evaluation, and Computational Studies of Novel Ureidopropanamides as Formyl Peptide Receptor 2 (FPR2) Agonists to Target the Resolution of Inflammation in Central Nervous System Disorders. Journal of Medicinal Chemistry, 2022, 65, 5004-5028.	2.9	7
3731	Molecular modelling and computational studies of peptide diphenylalanine nanotubes, containing waters: structural and interactions analysis. Journal of Molecular Modeling, 2022, 28, 81.	0.8	7
3732	Design, Synthesis and 5-HT1A Binding Affinity of N-(3-(4-(2-Methoxyphenyl)piperazin-1-yl)propyl)tricyclo[3.3.1.13,7]decan-1-amine and N-(3-(4-(2-Methoxyphenyl)piperazin-1-yl)propyl)-3,5-dimethyl-tricylo[3.3.1.13,7]decan-1-amine. MolBank, 2022, 2022, M1353.	0.2	0
3733	Molecular docking studies of natural immunomodulators indicate their interactions with the CD40L of CD40/CD40L pathway and CSF1R kinase domain of microglia. Journal of Molecular Modeling, 2022, 28, 101.	0.8	3
3734	ELECTRA-DTA: a new compound-protein binding affinity prediction model based on the contextualized sequence encoding. Journal of Cheminformatics, 2022, 14, 14.	2.8	11
3735	Automated Virtual Design of Organic Semiconductors Based on Metal-Organic Frameworks. Frontiers in Materials, 2022, 9, .	1.2	8
3736	Benchmarking Semiempirical QM Methods for Calculating the Dipole Moment of Organic Molecules. Journal of Physical Chemistry A, 2022, 126, 1905-1921.	1.1	8
3737	Discovery of Cinnamylidene Derivative of Rhodanine with High Anthelmintic Activity against Rhabditis sp.. Molecules, 2022, 27, 2155.	1.7	5
3738	Computational profiling of natural compounds as promising inhibitors against the spike proteins of SARSâ€CoVâ€2 wildâ€type and the variants of concern, viral cellâ€entry process, and cytokine storm in COVIDâ€19. Journal of Cellular Biochemistry, 2022, 123, 964-986.	1.2	8
3739	In silico prediction and analysis of dielectric constant of ionic liquids. Korean Journal of Chemical Engineering, 2022, 39, 1651-1657.	1.2	1
3740	A novel antibacterial tyroscherin derivative with a natural unprecedented morpholine-2, 3-dione structural unit from the fungus Pseudallescheria boydii. Natural Product Research, 2022, 36, 5977-5983.	1.0	3
3741	Design, synthesis and screening of pyridothieno[3,2-b]indole and pyridothieno[3,2-c]cinnoline derivatives as potential biological active molecules. Synthesis, 0, 0, .	1.2	0
3742	Synthesis, molecular docking and dynamics study of novel epoxide derivatives of 1,2,4-trioxanes as antimalarial agents. Structural Chemistry, 2022, 33, 907-919.	1.0	5
3743	AtomNet PoseRanker: Enriching Ligand Pose Quality for Dynamic Proteins in Virtual High-Throughput Screens. Journal of Chemical Information and Modeling, 2022, 62, 1178-1189.	2.5	13
3744	Cov_DOX: A Method for Structure Prediction of Covalent Proteinâ€“Ligand Bindings. Journal of Medicinal Chemistry, 2022, 65, 5528-5538.	2.9	16
3745	Exploring the Prominent and Concealed Inhibitory Features for Cytoplasmic Isoforms of Hsp90 Using QSAR Analysis. Pharmaceuticals, 2022, 15, 303.	1.7	2

#	Article	IF	Citations
3746	Nonlinear molecular dynamics of quercetin in Gynocardia odorata and Diospyros malabarica fruits: Its mechanistic role in hepatoprotection. PLoS ONE, 2022, 17, e0263917.	1.1	12
3747	Resveratrol-Based MTDLs to Stimulate Defensive and Regenerative Pathways and Block Early Events in Neurodegenerative Cascades. Journal of Medicinal Chemistry, 2022, 65, 4727-4751.	2.9	10
3748	Bioprospecting for Microorganisms in Peloidsâ€"Extreme Environment Known for Its Healing Properties. Frontiers in Marine Science, 2022, 9, .	1.2	6
3749	pyscreener: A Python Wrapper for Computational Docking Software. Journal of Open Source Software, 2022, 7, 3950.	2.0	2
3750	DeLA-Drug: A Deep Learning Algorithm for Automated Design of Druglike Analogues. Journal of Chemical Information and Modeling, 2022, 62, 1411-1424.	2.5	18
3751	Discovery and Structure-Based Optimization of Novel Atg4B Inhibitors for the Treatment of Castration-Resistant Prostate Cancer. Journal of Medicinal Chemistry, 2022, 65, 4878-4892.	2.9	4
3753	An integrated computational approach to screening of alkaloids inhibitors of TBX3 in breast cancer cell lines. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3025-3041.	2.0	5
3755	Free and open source software for computational chemistry education. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2022, 12, .	6.2	19
3756	Expanding biochemical knowledge and illuminating metabolic dark matter with ATLASx. Nature Communications, 2022, 13, 1560.	5.8	19
3757	A female-biased odorant receptor tuned to the lepidopteran sex pheromone in parasitoid Microplitis mediator guiding habitat of host insects. Journal of Advanced Research, 2023, 43, 1-12.	4.4	9
3758	Molecular docking assisted biological functions and phytochemical screening of Amaranthus lividus L. extract. Scientific Reports, 2022, 12, 4308.	1.6	17
3759	Integrated Machine Learning and Chemoinformatics-Based Screening of Mycotic Compounds against Kinesin Spindle ProteinEg5 for Lung Cancer Therapy. Molecules, 2022, 27, 1639.	1.7	7
3760	In SilicoDrug Discovery Strategies Identified ADMET Properties of Decoquinate RMB041 and Its Potential Drug Targets against Mycobacterium tuberculosis. Microbiology Spectrum, 2022, 10, e0231521.	1.2	8
3761	Molecular charge transfer: annealed, pendant, and analyte cases. European Physical Journal B, 2022, 95, 1.	0.6	0
3762	Mechanistic basis of choline import involved in teichoic acids and lipopolysaccharide modification. Science Advances, 2022, 8, eabm1122.	4.7	11
3763	Interaction Analysis of MRP1 with Anticancer Drugs Used in Ovarian Cancer: In Silico Approach. Life, 2022, 12, 383.	1.1	9
3764	Structure determination from unindexed powder data from scratch by a global optimization approach using pattern comparison based on cross-correlation functions. Acta Crystallographica Section B: Structural Science, Crystal Engineering and Materials, 2022, 78, 195-213.	0.5	6
3765	In Silico Investigation of Some Compounds from the N-Butanol Extract of Centaurea tougourensis Boiss. & Reut.. Crystals, 2022, 12, 355.	1.0	1

#	Article	IF	Citations
3766	In Silico Multi-Target Approach Revealed Potential Lead Compounds as Scaffold for the Synthesis of Chemical Analogues Targeting SARS-CoV-2. Biology, 2022, 11, 465.	1.3	2
3767	Identification of Potential Poly (ADP-Ribose) Polymerase-1 Inhibitors Derived from Rauwolfia serpentina: Possible Implication in Cancer Therapy. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-9.	0.5	12
3768	Hybrid Classification/Regression Approach to QSAR Modeling of Stoichiometric Antiradical Capacity Assaysâ€™ Endpoints. Molecules, 2022, 27, 2084.	1.7	0
3769	Eucommia ulmoides Oliver-Tribulus terrestris L. Drug Pair Regulates Ferroptosis by Mediating the Neurovascular-Related Ligand-Receptor Interaction Pathway- A Potential Drug Pair for Treatment Hypertension and Prevention Ischemic Stroke. Frontiers in Neurology, 2022, 13, 833922.	1.1	16
3770	Screening of Phytoconstituents from Traditional Plants against SARSCoV- 2 using Molecular Docking Approach. Letters in Drug Design and Discovery, 2022, 19, 1022-1038.	0.4	2
3771	Density Functional Theory Study of Carbamoyl-Substituted Dihydroazulene/Vinylheptafulvene Derivatives and Solvent Effects. Journal of Physical Chemistry C, 2022, 126, 4815-4825.	1.5	1
3772	Methylxanthines as Potential Inhibitor of SARS-CoV-2: an In Silico Approach. Current Pharmacology Reports, 2022, 8, 149-170.	1.5	15
3773	Optimizing Multisite Î»-Dynamics Throughput with Charge Renormalization. Journal of Chemical Information and Modeling, 2022, 62, 1479-1488.	2.5	8
3774	Evolution of the Automatic Rhodopsin Modeling (ARM) Protocol. Topics in Current Chemistry, 2022, 380, 21.	3.0	7
3775	Fragment-based virtual screening discovers potential new Plasmodium PI4KIIIÎ² ligands. BMC Chemistry, 2022, 16, 19.	1.6	3
3776	NMS-873 Leads to Dysfunctional Glycometabolism in A p97-Independent Manner in HCT116 Colon Cancer Cells. Pharmaceutics, 2022, 14, 764.	2.0	5
3777	Modeling the Conformational Preference of the Lignocellulose Interface and Its Interaction with Weak Acids. Journal of Physical Chemistry A, 2022, 126, 2119-2126.	1.1	8
3778	Identification of Zinc-Binding Inhibitors of Matrix Metalloproteinase-9 to Prevent Cancer Through Deep Learning and Molecular Dynamics Simulation Approach. Frontiers in Molecular Biosciences, 2022, 9, 857430.	1.6	5
3779	Polymer Structure Predictor (PSP): A Python Toolkit for Predicting Atomic-Level Structural Models for a Range of Polymer Geometries. Journal of Chemical Theory and Computation, 2022, 18, 2737-2748.	2.3	7
3780	A Comprehensive Analysis of Calmodulin-Like Proteins of Glycine max Indicates Their Role in Calcium Signaling and Plant Defense Against Insect Attack. Frontiers in Plant Science, 2022, 13, 817950.	1.7	16
3781	Collaborative Approach between Explainable Artificial Intelligence and Simplified Chemical Interactions to Explore Active Ligands for Cyclin-Dependent Kinase 2. ACS Omega, 2022, 7, 10372-10381.	1.6	9
3782	AutoSolvate: A toolkit for automating quantum chemistry design and discovery of solvated molecules. Journal of Chemical Physics, 2022, 156, 124801.	1.2	12
3783	Identifying HSV-1 Inhibitors from Natural Compounds via Virtual Screening Targeting Surface Glycoprotein D. Pharmaceuticals, 2022, 15, 361.	1.7	3

#	Article	IF	Citations
3784	MOFSimplify, machine learning models with extracted stability data of three thousand metalâ€“organic frameworks. Scientific Data, 2022, 9, 74.	2.4	34
3785	Molecular docking prediction and in vitro studies elucidate anti-inflammatory effect of Garcinia extract against inducible nitric oxide synthase and cyclooxygenase-2 targets. Beni-Suef University Journal of Basic and Applied Sciences, 2022, 11, .	0.8	6
3786	In Silico Structure-Based Approach for Group Efficiency Estimation in Fragment-Based Drug Design Using Evaluation of Fragment Contributions. Molecules, 2022, 27, 1985.	1.7	2
3789	In Silico and In Vitro Evaluations of Fluorophoric Thiazolo-[2,3-b]quinazolinones as Anti-cancer Agents Targeting EGFR-TKD. Applied Biochemistry and Biotechnology, 2022, 194, 4292-4318.	1.4	13
3790	Triamcinolone as a Potential Inhibitor of SARS-CoV-2 Main Protease and Cytokine Storm: An In silico Study. Letters in Drug Design and Discovery, 2023, 20, 1230-1242.	0.4	1
3791	Repurposing dyphylline as a pan-coronavirus antiviral therapy. Future Medicinal Chemistry, 2022, 14, 685-699.	1.1	3
3792	Accurate evaluation of combustion enthalpy by ab-initio computations. Scientific Reports, 2022, 12, 5834.	1.6	3
3793	Novel drug-target interactions via link prediction and network embedding. BMC Bioinformatics, 2022, 23, 121.	1.2	6
3794	[^{99m}Tc]Tc-DTPA-Bis(cholineethylamine) as an Oncologic Tracer for the Detection of Choline Transporter (ChT) and Choline Kinase (ChK) Expression in Cancer. ACS Omega, 2022, 7, 12509-12523.	1.6	3
3795	Defining the Role of Isoeugenol from Ocimum tenuiflorum against Diabetes Mellitus-Linked Alzheimerâ€™s Disease through Network Pharmacology and Computational Methods. Molecules, 2022, 27, 2398.	1.7	41
3796	ELIXIR-A: An Interactive Visualization Tool for Multi-Target Pharmacophore Refinement. ACS Omega, 2022, 7, 12707-12715.	1.6	6
3797	Identification of potent aldose reductase inhibitors as antidiabetic (Anti-hyperglycemic) agents using QSAR based virtual Screening, molecular Docking, MD simulation and MMGBSA approaches. Saudi Pharmaceutical Journal, 2022, 30, 693-710.	1.2	16
3798	3Î²-Acetoxy-21Î±-H-hop-22(29)ene, a novel multitargeted phytocompound against SARS-CoV-2: in silico screening. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3884-3891.	2.0	1
3799	Activation of retinoic acid-related orphan receptor Î³(t) by parabens and benzophenone UV-filters. Toxicology, 2022, 471, 153159.	2.0	5
3800	Identification of a novel anticancer mechanism of Paeoniae Radix extracts based on systematic transcriptome analysis. Biomedicine and Pharmacotherapy, 2022, 148, 112748.	2.5	9
3801	Enhancement of Methane Catalysis Rates in Methylosinus trichosporium OB3b. Biomolecules, 2022, 12, 560.	1.8	6
3802	AB-DB: Force-Field parameters, MD trajectories, QM-based data, and Descriptors of Antimicrobials. Scientific Data, 2022, 9, 148.	2.4	6
3803	In Silico Identification and Mechanism Exploration of Active Ingredients against Stroke from An-Gong-Niu-Huang-Wan (AGNHW) Formula. Oxidative Medicine and Cellular Longevity, 2022, 2022, 1-16.	1.9	3

#	Article	IF	Citations
3804	Identification of Entry Inhibitors against Delta and Omicron Variants of SARS-CoV-2. International Journal of Molecular Sciences, 2022, 23, 4050.	1.8	17
3805	Machine learned calibrations to high-throughput molecular excited state calculations. Journal of Chemical Physics, 2022, 156, 134116.	1.2	5
3806	Synthesis of (S)- and (R)-Î²-Tyrosine by Redesigned Phenylalanine Aminomutase. Catalysts, 2022, 12, 397.	1.6	0
3807	Genome-wide expression reveals potential biomarkers in breast cancer bone metastasis. Journal of Integrative Bioinformatics, 2022, .	1.0	0
3808	Phenolic compounds as Î±-glucosidase inhibitors: a docking and molecular dynamics simulation study. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3862-3871.	2.0	10
3809	Dowker complex based machine learning (DCML) models for protein-ligand binding affinity prediction. PLoS Computational Biology, 2022, 18, e1009943.	1.5	14
3810	In search of novel inhibitors of anti-cancer drug target fibroblast growth factor receptors: Insights from virtual screening, molecular docking, and molecular dynamics. Arabian Journal of Chemistry, 2022, 15, 103882.	2.3	15
3811	Systemic evolutionary chemical space exploration for drug discovery. Journal of Cheminformatics, 2022, 14, 19.	2.8	6
3812	In silico and in vitro evaluation of silibinin: a promising anti-Chikungunya agent. In Vitro Cellular and Developmental Biology - Animal, 2022, 58, 255-267.	0.7	1
3813	The physiological role of complex V in ATP synthesis: Murzyme functioning is viable whereas rotary conformation change model is untenable. Journal of Biomolecular Structure and Dynamics, 2022, , 1-20.	2.0	9
3814	Implementation and Optimization of the Embedded Cluster Reference Interaction Site Model with Atomic Charges. Journal of Physical Chemistry A, 2022, 126, 2417-2429.	1.1	1
3815	Structure-Based Discovery of Potent Staphylococcus aureus Thymidylate Kinase Inhibitors by Virtual Screening. Medicinal Chemistry, 2023, 19, 75-90.	0.7	0
3816	Elucidating novel antibacterial compounds from the NPASS database against the FimH lectin domain for the treatment of urinary tract infections: an in-silico study. Journal of Biomolecular Structure and Dynamics, 2023, 41, 3914-3925.	2.0	1
3817	A highly sensitive cell-based luciferase assay for high-throughput automated screening of SARS-CoV-2 nsp5/3CLpro inhibitors. Antiviral Research, 2022, 201, 105272.	1.9	9
3818	Natural alkaloids targeting EGFR in non-small cell lung cancer: Molecular docking and ADMET predictions. Chemico-Biological Interactions, 2022, 358, 109901.	1.7	11
3819	Combining multi-dimensional molecular fingerprints to predict the hERG cardiotoxicity of compounds. Computers in Biology and Medicine, 2022, 144, 105390.	3.9	3
3820	Network pharmacology prediction and molecular docking-based strategy to explore the potential mechanism of Huanglian Jiedu Decoction against sepsis. Computers in Biology and Medicine, 2022, 144, 105389.	3.9	137
3821	New N-aryl-Nâ€²-aryl-/(thio)ureido-/sulfamoylamino-derivatives of alkyl/alkylcarbamoyl piperazines: Effect of structural modifications on selectivity over 5-HT1A receptor. European Journal of Medicinal Chemistry, 2022, 235, 114319.	2.6	5

#	Article	IF	Citations
3822	The behaviour of aluminium ions in artificial saliva and the impact of the chlorhexidine digluconate on its removal â€“ A diffusion model. Journal of Molecular Liquids, 2022, 353, 118749.	2.3	1
3823	Iloneoside, an antimalarial pregnane glycoside isolated from Gongronema latifolium leaf, potentiates the activity of chloroquine against multidrug resistant Plasmodium falciparum. Molecular and Biochemical Parasitology, 2022, 249, 111474.	0.5	1
3824	Physical properties of N-Cbz-protected amino acids in methanol as predicted through molecular dynamics calculations at different temperatures and constant pressure. Journal of Molecular Liquids, 2022, 355, 118935.	2.3	0
3825	Adjusted degradation of BRD4 S and BRD4 L based on fine structural modifications of the pyrrolopyridone scaffold. European Journal of Medicinal Chemistry, 2022, 236, 114259.	2.6	8
3826	Machine learning prediction of 3CL SARS-CoV-2 docking scores. Computational Biology and Chemistry, 2022, 98, 107656.	1.1	9
3827	Anti-influenza mechanism of phenolic phytochemicals from Canarium album (Lour.) DC. leaf extract. Journal of Ethnopharmacology, 2022, 292, 115175.	2.0	7
3828	Identification of bio-active food compounds as potential SARS-CoV-2 PLpro inhibitors-modulators via negative image-based screening and computational simulations. Computers in Biology and Medicine, 2022, 145, 105474.	3.9	4
3829	The data on molecular docking of cinnamic acid amide on dengue viral target NS2B/NS3. Data in Brief, 2022, 42, 108036.	0.5	0
3830	Robust and predictive QSAR models for predicting the D2, 5-HT1A, and 5-HT2A inhibition activities of fused tricyclic heterocycle piperazine (piperidine) derivatives as atypical antipsychotic drugs. Journal of Molecular Structure, 2022, 1259, 132753.	1.8	2
3831	Molecular-fingerprint machine-learning-assisted design and prediction for high-performance MOFs for capture of NMHCs from air. , 2022, 1, 100026.		18
3832	An overview on applications of SwissADME web tool in the design and development of anticancer, antitubercular and antimicrobial agents: A medicinal chemist's perspective. Journal of Molecular Structure, 2022, 1259, 132712.	1.8	52
3833	Virtual screening of molecular databases for potential inhibitors of the NSP16/NSP10 methyltransferase from SARS-CoV-2. Journal of Molecular Structure, 2022, 1261, 132951.	1.8	4
3834	Understanding the I/O Impact on the Performance of High-Throughput Molecular Docking. , 2021, , .		7
3835	Comparison of performance of two virtual screening software on acetylcholinesterase protein molecular docking. , 2021, , .		0
3836	Predictions of drug metabolism pathways through CYP 3A4 enzyme by analysing drug-target interactions network graph. , 2021, , .		0
3837	Molecular Informatics of Trypanothione Reductase of Leishmania major Reveals Novel Chromen-2-One Analogues as Potential Leishmanicides. , 0, , .		0
3838	Epitope-Based Vaccine of a Brucella abortus Putative Small RNA Target Induces Protection and Less Tissue Damage in Mice. Frontiers in Immunology, 2021, 12, 778475.	2.2	3
3839	Identifying Molecular Fragments That Drive 7-Dehydrocholesterol Elevation. ACS Pharmacology and Translational Science, 2022, 5, 3-7.	2.5	1

#	Article	IF	Citations
3840	Wet-dry-wet drug screen leads to the synthesis of TS1, a novel compound reversing lung fibrosis through inhibition of myofibroblast differentiation. Cell Death and Disease, 2022, 13, 2.	2.7	3
3841	Benzophenone Glucosides and B-Type Proanthocyanidin Dimers from Zambian Cassia abbreviata and Their Trypanocidal Activities. Journal of Natural Products, 2022, 85, 91-104.	1.5	2
3842	Selection of Promising Novel Fragment Sized S. aureus SrtA Noncovalent Inhibitors Based on QSAR and Docking Modeling Studies. Molecules, 2021, 26, 7677.	1.7	6
3843	Identifying FAAH Inhibitors as New Therapeutic Options for the Treatment of Chronic Pain through Drug Repurposing. Pharmaceuticals, 2022, 15, 38.	1.7	12
3844	Computational Study of the Therapeutic Potential of Novel Heterocyclic Derivatives against SARS-CoV-2. Covid, 2021, 1, 757-774.	0.7	7
3845	Enantiomeric Separation and Molecular Modelling of Bioactive 4-Aryl-3,4-dihydropyrimidin-2(1H)-one Ester Derivatives on Teicoplanin-Based Chiral Stationary Phase. Separations, 2022, 9, 7.	1.1	3
3846	Eugenol carbonate activity against Plasmodium falciparum , Leishmania braziliensis , and Trypanosoma cruzi. Archiv Der Pharmazie, 2022, 355, 2100432.	2.1	7
3847	Computational Discovery of TTF Molecules with Deep Generative Models. Frontiers in Chemistry, 2021, 9, 800133.	1.8	4
3848	Inhibition of MurA Enzyme from Escherichia coli and Staphylococcus aureus by Diterpenes from Lepechinia meyenii and Their Synthetic Analogs. Antibiotics, 2021, 10, 1535.	1.5	8
3849	Computational investigation of potent inhibitors against YsxC: structure-based pharmacophore modeling, molecular docking, molecular dynamics, and binding free energy. Journal of Biomolecular Structure and Dynamics, 2023, 41, 930-941.	2.0	15
3850	Dietary Intake of Flavonoids and Carotenoids Is Associated with Anti-Depressive Symptoms: Epidemiological Study and In Silicoâ€”Mechanism Analysis. Antioxidants, 2022, 11, 53.	2.2	19
3851	A computational biology approach for the identification of potential SARS-CoV-2 main protease inhibitors from natural essential oil compounds.. F1000Research, 0, 10, 1313.	0.8	1
3852	Development of Computational Approaches with a Fragment-Based Drug Design Strategy: In Silico Hsp90 Inhibitors Discovery. International Journal of Molecular Sciences, 2021, 22, 13226.	1.8	2
3853	Not Drug-like, but Like Drugs: Cnidaria Natural Products. Marine Drugs, 2022, 20, 42.	2.2	5
3854	Targeting Neuraminidase A of Multidrug-Resistant Streptococcus pneumoniae: Molecular Docking and Redesign of Traditional Chinese Medicine Compounds. , 2021, , .		0
3855	Virtual Screening with Gnina 1.0. Molecules, 2021, 26, 7369.	1.7	20
3856	A Benchmark Study of Quantum Mechanics and Quantum Mechanics-Molecular Mechanics Methods for Carbocation Chemistry. Journal of Chemical Theory and Computation, 2022, 18, 167-178.	2.3	11
3857	Discovery of Novel BRD4 Ligand Scaffolds by Automated Navigation of the Fragment Chemical Space. Journal of Medicinal Chemistry, 2021, 64, 17887-17900.	2.9	6

#	Article	IF	Citations
3859	Screening of phytochemicals as potential anti-breast cancer agents targeting HER2: an in-silico approach. Journal of Biomolecular Structure and Dynamics, 2021, , 1-15.	2.0	3
3860	Entrectinibâ€"A SARS-CoV-2 Inhibitor in Human Lung Tissue (HLT) Cells. International Journal of Molecular Sciences, 2021, 22, 13592.	1.8	7
3861	Sdfconf: A Novel, Flexible, and Robust Molecular Data Management Tool. Journal of Chemical Information and Modeling, 2022, 62, 9-15.	2.5	3
3862	Data-driven modeling of S â†' S1 excitation energy in the BODIPY chemical space: High-throughput computation, quantum machine learning, and inverse design. Journal of Chemical Physics, 2021, 155, 244102.	1.2	11
3863	Appraisal of Bioactive Compounds of Betel Fruit as Antimalarial Agents by Targeting Plasmepsin 1 and 2: A Computational Approach. Pharmaceuticals, 2021, 14, 1285.	1.7	3
3864	Hydroxychloroquine (HCQ) Exhibits Better Binding to the Main Protease (Mpro) Compared to Spike Protein (S protein) of SARS-CoV-2: An In-silico Analysis. Clinical Cancer Drugs, 2021, 8, 106-115.	0.3	0
3865	Synthesis, structure determination, Hirshfeld surfaces analysis and anticancer activity study of a new biomolecule: (2E)-2-{[4-(benzyloxy)phenyl]methylidene}-3,4-dihydronaphthalen-1(2H)-one. Phosphorus, Sulfur and Silicon and the Related Elements, 2022, 197, 269-275.	0.8	0
3866	Using NCBI Entrez Direct (EDirect) for Small Molecule Chemical Information Searching in a Unix Terminal. Journal of Chemical Education, 2021, 98, 3904-3914.	1.1	2
3867	PreBINDS: An Interactive Web Tool to Create Appropriate Datasets for Predicting Compoundâ€"Protein Interactions. Frontiers in Molecular Biosciences, 2021, 8, 758480.	1.6	1
3869	Protein pK_a Prediction with Machine Learning. ACS Omega, 2021, 6, 34823-34831.	1.6	14
3870	Candidates for Repurposing as Anti-Virulence Agents Based on the Structural Profile Analysis of Microbial Collagenase Inhibitors. Pharmaceutics, 2022, 14, 62.	2.0	9
3871	Modular characteristics and the mechanism of Chinese medicineâ€™s treatment of gastric cancer: a data mining and pharmacology-based identification. Annals of Translational Medicine, 2021, 9, 1777-1777.	0.7	6
3873	MODOMICS: a database of RNA modification pathways. 2021 update. Nucleic Acids Research, 2022, 50, D231-D235.	6.5	374
3875	Discovery of Novel Small Molecule HDAC1, 2, 3 Inhibitors -- Combined Receptor-Based and Ligand-Based Virtual Screening Strategy. Letters in Drug Design and Discovery, 2022, 19, 627-636.	0.4	0
3876	Bioconjugation of Active Ingredients to Plant Viral Nanoparticles Is Enhanced by Preincubation with a Pluronic F127 Polymer Scaffold. ACS Applied Materials & Interfaces, 2021, 13, 59618-59632.	4.0	10
3877	Dielectric Polymer Genome: Integrating Valence-Aware Polarizable Reactive Force Fields and Machine Learning. Transactions on Computational Science and Computational Intelligence, 2021, , 51-64.	0.3	2
3878	Visualising Metabolic Pathways and Networks: Past, Present, Future. , 2022, , 237-267.		2
3879	D3AI-CoV: a deep learning platform for predicting drug targets and for virtual screening against COVID-19. Briefings in Bioinformatics, 2022, 23, .	3.2	13

#	Article	IF	Citations
3880	TeachOpenCADD 2022: open source and FAIR Python pipelines to assist in structural bioinformatics and cheminformatics research. Nucleic Acids Research, 2022, 50, W753-W760.	6.5	6
3881	Uncovering a Hub Signaling Pathway of Antimicrobial-Antifungal-Anticancer Peptidesâ€™ Axis on Short Cationic Peptides via Network Pharmacology Study. International Journal of Molecular Sciences, 2022, 23, 2055.	1.8	1
3882	Computational Study on SARS-CoV-2 Viral Protein Interaction with Natural Compounds of Coriandrum sativum L. , 2022, , .		0
3883	Molecular docking studies of Amidoxime-containing heterocyclic compounds from Zinc database against homology modelled PfADSL. IOP Conference Series: Earth and Environmental Science, 2022, 993, 012026.	0.2	0
3884	In Silico Prediction of Metabolite in Petroselinum Crispum in Inhibiting Androgen Receptor as Treatment for Alopecia. Research Journal of Pharmacy and Technology, 2022, , 1211-1218.	0.2	3
3885	Ab initio development of generalized Lennard-Jones (Mie) force fields for predictions of thermodynamic properties in advanced molecular-based SAFT equations of state. Journal of Chemical Physics, 2022, 156, 154106.	1.2	6
3886	Proteochemometrics modeling for prediction of the interactions between caspase isoforms and their inhibitors. Molecular Diversity, 2022, , 1.	2.1	0
3887	Network Pharmacology and Molecular Docking to Elucidate the Potential Mechanism of Ligusticum Chuanxiong Against Osteoarthritis. Frontiers in Pharmacology, 2022, 13, 854215.	1.6	23
3888	Preparation, physicochemical characterization, docking and antiarrhythmic effect of d-limonene and d-limonene hydroxypropyl-Î²-cyclodextrin complex. Journal of Drug Delivery Science and Technology, 2022, , 103350.	1.4	3
3889	ï»¿Inhibitory effects of Moringa oleifera leaves extract on xanthine oxidase activity from bovine milk. Pharmacia, 2022, 69, 363-375.	0.4	4
3890	TLR8 is activated by 5Ê¹-methylthioinosine, a Plasmodium falciparum-derived intermediate of the purine salvage pathway. Cell Reports, 2022, 39, 110691.	2.9	6
3891	Identification of potent inhibitors of NEK7 protein using a comprehensive computational approach. Scientific Reports, 2022, 12, 6404.	1.6	48
3892	SAMPL7 protein-ligand challenge: A community-wide evaluation of computational methods against fragment screening and pose-prediction. Journal of Computer-Aided Molecular Design, 2022, 36, 291-311.	1.3	10
3893	Galaxy workflows for fragment-based virtual screening: a case study on the SARS-CoV-2 main protease. Journal of Cheminformatics, 2022, 14, 22.	2.8	2
3895	Current Trends in Computational Quantum Chemistry Studies on Antioxidant Radical Scavenging Activity. Journal of Chemical Information and Modeling, 2022, 62, 2639-2658.	2.5	33
3897	Comprehensive interpretation of in vitro micronucleus test results for 292 chemicals: from hazard identification to risk assessment application. Archives of Toxicology, 2022, 96, 2067-2085.	1.9	15
3898	Machine Learning-Based Retention Time Prediction of Trimethylsilyl Derivatives of Metabolites. Biomedicines, 2022, 10, 879.	1.4	5
3899	Lipophilic Constituents in Salvia miltiorrhiza Inhibit Activation of the Hepatic Stellate Cells by Suppressing the JAK1/STAT3 Signaling Pathway: A Network Pharmacology Study and Experimental Validation. Frontiers in Pharmacology, 2022, 13, 770344.	1.6	1

#	Article	IF	Citations
3900	A new ChEMBL dataset for the similarity-based target fishing engine FastTargetPred: Annotation of an exhaustive list of linear tetrapeptides. Data in Brief, 2022, 42, 108159.	0.5	2
3901	Conformational Sampling for Transition State Searches on a Computational Budget. Journal of Chemical Theory and Computation, 2022, 18, 3006-3016.	2.3	15
3902	Structure-based design of novel donepezil-like hybrids for a multi-target approach to the therapy of Alzheimer's disease. European Journal of Medicinal Chemistry, 2022, 237, 114358.	2.6	14
3903	Computational evolution of high-performing unfused non-fullerene acceptors for organic solar cells. Journal of Chemical Physics, 2022, 156, 174107.	1.2	9
3904	A single-molecule with multiple investigations: Synthesis, characterization, computational methods, inhibitory activity against Alzheimer's disease, toxicity, and ADME studies. Computers in Biology and Medicine, 2022, 146, 105514.	3.9	8
3905	African derived phytocompounds may interfere with SARS-CoV-2 RNA capping machinery via inhibition of 2â€²-O-ribose methyltransferase: An in silico perspective. Journal of Molecular Structure, 2022, 1262, 133019.	1.8	3
3906	New aldo-keto reductase 1C3 (AKR1C3) inhibitors based on the hydroxytriazole scaffold. European Journal of Medicinal Chemistry, 2022, 237, 114366.	2.6	7
3907	Characterization of an alcohol acetyltransferase GcAAT responsible for the production of antifungal volatile esters in endophytic Geotrichum candidum PF005. Microbiological Research, 2022, 260, 127021.	2.5	3
3954	Identification of potential andrographolide-based drug candidate against Keap1-Nrf2 pathway through rigorous cheminformatics screening. Molecular Diversity, 2022, , 1.	2.1	0
3955	Genotoxic and cytotoxic effects of pethoxamid herbicide on Allium cepa cells and its molecular docking studies to unravel genotoxicity mechanism. Environmental Science and Pollution Research, 2022, 29, 63127-63140.	2.7	13
3956	AA-Score: a New Scoring Function Based on Amino Acid-Specific Interaction for Molecular Docking. Journal of Chemical Information and Modeling, 2022, 62, 2499-2509.	2.5	11
3957	Î”-Quantum machine-learning for medicinal chemistry. Physical Chemistry Chemical Physics, 2022, 24, 10775-10783.	1.3	21
3958	Identification of potential bioactive natural compounds from Indonesian medicinal plants against 3-chymotrypsin-like protease (3CL^{pro}) of SARS-CoV-2: molecular docking, ADME/T, molecular dynamic simulations, and DFT analysis. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4467-4484.	2.0	10
3959	Structural insights into inhibition of PRRSV Nsp4 revealed by structure-based virtual screening, molecular dynamics, and MM-PBSA studies. Journal of Biological Engineering, 2022, 16, 4.	2.0	14
3960	Study of lipase producing gene in wheat â€“ an in silico approach. Journal of Genetic Engineering and Biotechnology, 2021, 19, 73.	1.5	1
3962	Application of PolyPRep tools on HIV protease polyproteins using molecular docking. Brazilian Journal of Biology, 2021, 84, e245592.	0.4	0
3963	In-silico Optimization of Frizzled-8 Receptor Inhibition Activity of Carbamazepine: Design New Anti-Cancer Agent. Combinatorial Chemistry and High Throughput Screening, 2022, 25, .	0.6	1
3965	Target Specific Inhibition of Protein Tyrosine Kinase in Conjunction With Cancer and SARS-COV-2 by Olive Nutraceuticals. Frontiers in Pharmacology, 2021, 12, 812565.	1.6	17

#	Article	IF	Citations
3966	A Set of Experimentally Validated Decoys for the Human CC Chemokine Receptor 7 (CCR7) Obtained by Virtual Screening. Frontiers in Pharmacology, 2022, 13, 855653.	1.6	2
3968	Synthesis, characterization,in silicomolecular docking, and antibacterial activities of some new nitrogen-heterocyclic analogues based on ap-phenolic unit. RSC Advances, 2022, 12, 12607-12621.	1.7	8
3969	Computer-aided identification of potential inhibitors against Necator americanus glutathione S-transferase 3. Informatics in Medicine Unlocked, 2022, 30, 100957.	1.9	1
3970	CB-Dock2: improved proteinâ€“ligand blind docking by integrating cavity detection, docking and homologous template fitting. Nucleic Acids Research, 2022, 50, W159-W164.	6.5	219
3971	Antimicrobial Activity of Some Celastroloids and Their Derivatives. SSRN Electronic Journal, 0, , .	0.4	0
3972	fastDRH: a webserver to predict and analyze proteinâ€“ligand complexes based on molecular docking and MM/PB(GB)SA computation. Briefings in Bioinformatics, 2022, 23, .	3.2	34
3973	Prediction of Multi Class Drugs: A Perspective for Designing Drug with Many Uses. , 2022, , .		1
3974	Interaction of Pelargonium sidoides Compounds with Lactoferrin and SARS-CoV-2: Insights from Molecular Simulations. International Journal of Environmental Research and Public Health, 2022, 19, 5254.	1.2	5
3975	Drugsniffer: An Open Source Workflow for Virtually Screening Billions of Molecules for Binding Affinity to Protein Targets. Frontiers in Pharmacology, 2022, 13, 874746.	1.6	7
3976	Anti-breast cancer potential of MnO2 nanoparticles using Terminalia chebula fruit extract against MCF-7 cell line through in vitro cell cycle and apoptotic studies. Materials Today: Proceedings, 2022, , .	0.9	3
3977	Structure-based virtual screening, ADMET profiling, and molecular dynamics simulation studies on HIV-1 protease for identification of active phytocompounds as potential anti-HIV agents. Molecular Simulation, 2022, 48, 1031-1049.	0.9	7
3978	Optimizing the Thermodynamics and Kinetics of the Triplet-Pair Dissociation in Donorâ€“Acceptor Copolymers for Intramolecular Singlet Fission. Chemistry of Materials, 2022, 34, 4115-4121.	3.2	6
3979	Synthesis, Biological Activity, and Molecular Modelling Studies of Naphthoquinone Derivatives as Promising Anticancer Candidates Targeting COX-2. Pharmaceuticals, 2022, 15, 541.	1.7	11
3980	Advances in Activity/Property Prediction from Chemical Structures. Critical Reviews in Analytical Chemistry, 2024, 54, 135-147.	1.8	0
3981	Identification of Bioactive Components of Stephania epigaea Lo and Their Potential Therapeutic Targets by UPLC-MS/MS and Network Pharmacology. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-11.	0.5	1
3982	Quantum Mechanics/Molecular Mechanics Studies on the Catalytic Mechanism of a Novel Esterase (FmtA) of Staphylococcus aureus. Journal of Chemical Information and Modeling, 2022, 62, 2409-2420.	2.5	23
3983	Are Vanadium Intermediates Suitable Mimics in Non-Heme Iron Enzymes? An Electronic Structure Analysis. ACS Catalysis, 2022, 12, 5489-5501.	5.5	5
3984	Targeting Omicron (B.1.1.529) SARS CoV-2 spike protein with selected phytochemicals: an in-silico approach for identification of potential drug. Journal of Experimental Biology and Agricultural Sciences, 2022, 10, 396-404.	0.1	5

#	Article	IF	Citations
3985	Classification-based QSARs for predicting dietary biomagnification in fish. SAR and QSAR in Environmental Research, 2022, 33, 259-271.	1.0	5
3986	Jiedu Huoxue Decoction for Cytokine Storm and Thrombosis in Severe COVID-19: A Combined Bioinformatics and Computational Chemistry Approach. Natural Product Communications, 2022, 17, 1934578X2210969.	0.2	0
3987	Development of an Automatic Pipeline for Participation in the CELPP Challenge. International Journal of Molecular Sciences, 2022, 23, 4756.	1.8	1
3988	Characterization of sulfated polysaccharide activity against virulent Plasmodium falciparum PHISTb/RLP1 protein. F1000Research, 0, 9, 1268.	0.8	1
3989	New Strategies for Direct Methane-to-Methanol Conversion from Active Learning Exploration of 16 Million Catalysts. Jacs Au, 2022, 2, 1200-1213.	3.6	23
3990	Extending NMR Quantum Computation Systems by Employing Compounds with Several Heavy Metals as Qubits. Magnetochemistry, 2022, 8, 47.	1.0	5
3991	CELLOPT: improved unit-cell parameters for electron diffraction data of small-molecule crystals. Journal of Applied Crystallography, 2022, 55, 647-655.	1.9	1
3992	Virtual Screening and Molecular Docking Analysis of Degradation Products of Curcumin as Inhibitors of EGFR. Journal of Computational Biophysics and Chemistry, 2022, 21, 629-646.	1.0	2
3993	Rules of Chinese Herbal Intervention of Radiation Pneumonia Based on Network Pharmacology and Data Mining. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-13.	0.5	7
3994	Synthesis, structure determination, molecular interaction analysis, molecular docking studies, and anticancer activity investigation of a chalcone derivative: (2E)-2-[(2,4-dimethoxyphenyl)methylidene]-3,4 dihydronaphthalen-1(2H)-one. Materials Today: Proceedings, 2022, 65, 2506-2514.	0.9	2
3995	Anticancer Agents Derived from Cyclic Thiosulfonates: Structureâ€Reactivity and Structureâ€Activity Relationships. ChemMedChem, 2022, 17, .	1.6	1
3996	Soyasapogenol-B as a Potential Multitarget Therapeutic Agent for Neurodegenerative Disorders: Molecular Docking and Dynamics Study. Entropy, 2022, 24, 593.	1.1	10
3997	Design, synthesis and docking study of Vortioxetine derivatives as a SARS-CoV-2 main protease inhibitor. DARU, Journal of Pharmaceutical Sciences, 2022, 30, 139-152.	0.9	9
3998	Automated generation of molecular derivatives â€“ DerGen software package. Materials Today: Proceedings, 2022, , .	0.9	1
3999	Bioinformatic Screening of Compounds from Iranian Lamiaceae Family Members against SARS-CoV-2 Spike Protein. Letters in Drug Design and Discovery, 2023, 20, 684-698.	0.4	1
4000	Advances and Challenges in De Novo Drug Design Using Three-Dimensional Deep Generative Models. Journal of Chemical Information and Modeling, 2022, 62, 2269-2279.	2.5	25
4001	Molecular Dynamics Study of the Photodegradation of Polymeric Chains. Journal of Physical Chemistry Letters, 2022, 13, 4374-4380.	2.1	2
4002	Phenyl Bis-Sulfonamide Keap1-Nrf2 Proteinâ€“Protein Interaction Inhibitors with an Alternative Binding Mode. Journal of Medicinal Chemistry, 2022, 65, 7380-7398.	2.9	14

#	Article	IF	Citations
4003	Novel peptides with xanthine oxidase inhibitory activity identified from macadamia nuts: integrated in silico and in vitro analysis. European Food Research and Technology, 2022, 248, 2031-2042.	1.6	6
4004	Identification of the target and mode of action for the prokaryotic nucleotide excision repair inhibitor ATBC. Bioscience Reports, 2022, 42, .	1.1	4
4005	Indexing Ultrafast Shape-Based Descriptors in MongoDB to Identify TLR4 Pathway Agonists. Journal of Chemical Information and Modeling, 2022, 62, 2446-2455.	2.5	1
4006	Tuaimenal A, a Meroterpene from the Irish Deep-Sea Soft Coral Duva florida, Displays Inhibition of the SARS-CoV-2 3CLpro Enzyme. Journal of Natural Products, 2022, 85, 1315-1323.	1.5	6
4007	Data mining and structural analysis for multi-tissue regeneration potential of BMP-4 and activator drugs. Journal of Biomolecular Structure and Dynamics, 2022, , 1-16.	2.0	0
4008	Promising antivirals for PLpro of SARS-CoV-2 using virtual screening, molecular docking, dynamics, and MMPBSA. Journal of Biomolecular Structure and Dynamics, 2023, 41, 4650-4666.	2.0	18
4009	Indole alkaloids as potential candidates against COVID-19: an in silico study. Journal of Molecular Modeling, 2022, 28, 144.	0.8	7
4010	EVALUATION OF ANTAGONIST ACTIVITY OF IFENPRODIL AND THEIR ANALOGOUS AGAINST GLUN1/GLUN2B USING IN SILICO MOLECULAR DOCKING AND ABSORPTION-DISTRIBUTIONMETABOLISM- EXCRETION TOXICITY. Asian Journal of Pharmaceutical and Clinical Research, 0, , 34-40.	0.3	0
4011	Lactiplantibacillus plantarum-Derived Biosurfactant Attenuates Quorum Sensing-Mediated Virulence and Biofilm Formation in Pseudomonas aeruginosa and Chromobacterium violaceum. Microorganisms, 2022, 10, 1026.	1.6	13
4012	Allelic Variation in Zmfatb Gene Defines Variability for Fatty Acids Composition Among Diverse Maize Genotypes. Frontiers in Nutrition, 2022, 9, .	1.6	8
4013	Computational Modeling of Supramolecular Metallo-organic Cagesâ€“Challenges and Opportunities. ACS Catalysis, 2022, 12, 5806-5826.	5.5	24
4014	Choline chloride attenuates the allergic airway disease by inhibiting the lysophosphatidylcholine induced response in mouse model. Current Research in Pharmacology and Drug Discovery, 2022, , 100109.	1.7	0
4015	Toward the Discovery of a Novel Class of Leads for High Altitude Disorders by Virtual Screening and Molecular Dynamics Approaches Targeting Carbonic Anhydrase. International Journal of Molecular Sciences, 2022, 23, 5054.	1.8	13
4016	Investigation of the tight binding mechanism of a new anticoagulant DD217 to factor Xa by means of molecular docking and molecular dynamics. Journal of Biomolecular Structure and Dynamics, 2022, , 1-11.	2.0	0
4017	PLATO: A Predictive Drug Discovery Web Platform for Efficient Target Fishing and Bioactivity Profiling of Small Molecules. International Journal of Molecular Sciences, 2022, 23, 5245.	1.8	15
4018	Potential of Natural Alkaloids From Jadwar (Delphinium denudatum) as Inhibitors Against Main Protease of COVID-19: A Molecular Modeling Approach. Frontiers in Molecular Biosciences, 2022, 9, .	1.6	3
4019	Anti-COVID-19 and antidiabetic activities of new oleanane and ursane-type triterpenoids from Salvia grossheimii: an in-silico approach. Journal of Receptor and Signal Transduction Research, 2022, 42, 540-548.	1.3	2
4020	High-Throughput Measurement and Machine Learning-Based Prediction of Collision Cross Sections for Drugs and Drug Metabolites. Journal of the American Society for Mass Spectrometry, 2022, 33, 1061-1072.	1.2	13

#	Article	IF	Citations
4021	Targeting non-structural proteins and 3CLpro in SARS-CoV-2 virus using phytochemicals from medicinal plants - In-silico approach. Journal of the Indian Chemical Society, 2022, 99, 100488.	1.3	2
4022	ï»¿Dynamics insights into aggregation of phospholipid species with cholesterol and vitamin C. Pharmacia, 2022, 69, 385-391.	0.4	1
4023	Atomevo: a web server combining protein modelling, docking, molecular dynamic simulation and MMPBSA analysis of Candida antarctica lipase B (CalB) fusion protein. Bioresources and Bioprocessing, 2022, 9, .	2.0	2
4024	Understanding the Driving Forces That Trigger Mutations in SARS-CoV-2: Mutational Energetics and the Role of Arginine Blockers in COVID-19 Therapy. Viruses, 2022, 14, 1029.	1.5	17
4025	An in silico approach unveils the potential of antiviral compounds in preclinical and clinical trials as SARS-CoV-2 omicron inhibitors. Saudi Journal of Biological Sciences, 2022, 29, 103297.	1.8	11
4026	Protective effects of E Se tea extracts against alcoholic fatty liver disease induced by high fat/alcohol diet: In vivo biological evaluation and molecular docking study. Phytomedicine, 2022, 101, 154113.	2.3	11
4027	Direct space approach in action: Challenging structure solution of microcrystalline materials using the EXPO software. Computational Materials Science, 2022, 210, 111465.	1.4	0
4028	Interpretable machine learning for accelerating the discovery of metal-organic frameworks for ethane/ethylene separation. Chemical Engineering Journal, 2022, 444, 136651.	6.6	27
4029	Preparation, Physicochemical Characterization, Docking and Antiarrhythmic Effect of D-Limonene and D-Limonene Hydroxypropyl-Î²-Cyclodextrin Complex. SSRN Electronic Journal, 0, , .	0.4	0
4030	Extension of the approximate 3D-RISM-KH molecular solvation theory to liquid aniline and pyridines. Results in Chemistry, 2022, 4, 100365.	0.9	1
4031	Applied Machine Learning Toward Drug Discovery Enhancement: Leishmaniases as a Case Study. Bioinformatics and Biology Insights, 2022, 16, 117793222210903.	1.0	1
4032	Molecular docking reveals Chitosan nanoparticle protection mechanism for dentin against Collagen-binding bacteria. Journal of Materials Science: Materials in Medicine, 2022, 33, 43.	1.7	1
4033	Interaction of the New Inhibitor Paxlovid (PF-07321332) and Ivermectin With the Monomer of the Main Protease SARS-CoV-2: A Volumetric Study Based on Molecular Dynamics, Elastic Networks, Classical Thermodynamics and SPT. Computational Biology and Chemistry, 2022, , 107692.	1.1	1
4034	Data considerations for predictive modeling applied to the discovery of bioactive natural products. Drug Discovery Today, 2022, 27, 2235-2243.	3.2	7
4035	Anti-viral herbal phytoconstituents of tulsi (Ocimum sanctum) against Covid-19. IP International Journal of Comprehensive and Advanced Pharmacology, 2022, 7, 77-80.	0.1	1
4036	Automated In silico EGFR Peptide Inhibitor Elongation Using Self-Evolving Peptide Algorithm. Current Computer-Aided Drug Design, 2022, 18, .	0.8	1
4037	Delta Machine Learning to Improve Scoring-Ranking-Screening Performances of Proteinâ€“Ligand Scoring Functions. Journal of Chemical Information and Modeling, 2022, 62, 2696-2712.	2.5	26
4038	First QSPR models to predict the thermal stability of potential self-reactive substances. Chemical Engineering Research and Design, 2022, 163, 191-199.	2.7	4

#	Article	IF	Citations
4039	Crystal structure of merimepodib, C₂₃H₂₄N₄O₆. Powder Diffraction, 0, , 1-7.	0.4	0
4040	A Combination of Pharmacophore-Based Virtual Screening, Structure-Based Lead Optimization, and DFT Study for the Identification of S. epidermidis TcaR Inhibitors. Pharmaceuticals, 2022, 15, 635.	1.7	4
4041	In Silico Screening and Testing of FDA-Approved Small Molecules to Block SARS-CoV-2 Entry to the Host Cell by Inhibiting Spike Protein Cleavage. Viruses, 2022, 14, 1129.	1.5	3
4042	Computational attributes of protein kinase-C gamma C2-domain & virtual screening for small molecules: elucidation from meta-dynamics simulations & free-energy calculations. Journal of Biomolecular Structure and Dynamics, 0, , 1-12.	2.0	2
4043	Repurposing of berbamine hydrochloride to inhibit Ebola virus by targeting viral glycoprotein. Acta Pharmaceutica Sinica B, 2022, 12, 4378-4389.	5.7	5
4044	Enhancement of Haloperidol Binding Affinity to Dopamine Receptor via Forming a Charge-Transfer Complex with Picric Acid and 7,7,8,8-Tetracyanoquinodimethane for Improvement of the Antipsychotic Efficacy. Molecules, 2022, 27, 3295.	1.7	11
4045	A survey on computational taste predictors. European Food Research and Technology, 2022, 248, 2215-2235.	1.6	9
4046	Synthesis of alkoxy-isoflavones as potential Î±-glucosidase inhibitors. Medicinal Chemistry Research, 2022, 31, 1298-1312.	1.1	3
4047	A Comprehensive Database for DNA Adductomics. Frontiers in Chemistry, 2022, 10, .	1.8	8
4048	Novel ¹⁸F-Labeled PET Tracers Specific to Aromatase: Design, Synthesis, and Biological Evaluation. Molecular Pharmaceutics, 2022, 19, 2456-2470.	2.3	2
4049	Identification of potential inhibitors against FemX of Staphylococcus aureus: A hierarchial in-silico drug repurposing approach. Journal of Molecular Graphics and Modelling, 2022, 115, 108215.	1.3	5
4050	Modelling Approaches for Studies of Drug-Polymer Interactions in Drug Delivery Systems. , 2022, , 561-591.		1
4051	MolE8: finding DFT potential energy surface minima values from force-field optimised organic molecules with new machine learning representations. Chemical Science, 2022, 13, 7204-7214.	3.7	1
4052	CORAL: Development of a hybrid descriptor based QSTR model to predict the toxicity of dioxins and dioxin-like compounds with correlation intensity index and consensus modelling. Environmental Toxicology and Pharmacology, 2022, 93, 103893.	2.0	18
4053	PDAUG: a Galaxy based toolset for peptide library analysis, visualization, and machine learning modeling. BMC Bioinformatics, 2022, 23, .	1.2	5
4054	Antimalarial phytochemicals as potential inhibitors of SARS-CoV-2 guanine N7-methyltransferase (nsp) Tj ETQq1 1 0.784314 rgBT /Ov	2.0	1
4055	Unveiling the Possible Oryzalin-Binding Site in the Î±-Tubulin of Toxoplasma gondii. ACS Omega, 2022, 7, 18434-18442.	1.6	5
4056	Based on network pharmacology and molecular docking to predict the mechanism of Huangqi in the treatment of castration-resistant prostate cancer. PLoS ONE, 2022, 17, e0263291.	1.1	4

#	Article	IF	Citations
4057	Dual transcriptome based reconstruction of Salmonella-human integrated metabolic network to screen potential drug targets. PLoS ONE, 2022, 17, e0268889.	1.1	7
4058	Computer-Aided Identification of Cholinergic and Monoaminergic Inhibitory Flavonoids from Hibiscus sabdariffa L.. Current Drug Discovery Technologies, 2022, 19, .	0.6	1
4059	QSPRs for Predicting Equilibrium Partitioning in Solventâ€“Air Systems from the Chemical Structures of Solutes and Solvents. Journal of Solution Chemistry, 2022, 51, 1101-1132.	0.6	20
4060	The Antidiabetic Effect and Mechanism of JinXiaoXiaoKe Decoction in type 2 diabetic Gotoâ€“Kakizaki rats. Clinical Complementary Medicine and Pharmacology, 2022, , 100049.	0.9	1
4061	Integrated metalâ€organic framework (<scp>MOF</scp>) and pressure/vacuum swing adsorption process design:<scp>MOF</scp>matching. AICHE Journal, 2022, 68, .	1.8	7
4062	Increasing the Efficacy of Seproxetine as an Antidepressant Using Chargeâ€“Transfer Complexes. Molecules, 2022, 27, 3290.	1.7	11
4064	Molecular Modelling and Docking Analysis of Filarial Targets by using New Lead Compounds identified from Psoralea corylifolia and Mimusops elengi. Current Biotechnology, 2022, 11, 123-130.	0.2	0
4065	Design and Synthesis of Novel Bis-Imidazolyl Phenyl Butadiyne Derivatives as HCV NS5A Inhibitors. Pharmaceuticals, 2022, 15, 632.	1.7	2
4066	In silico and in vitro study of Mycobacterium tuberculosisÂH37Rv uncharacterized protein (RipD): an insight on tuberculosis therapeutics. Journal of Molecular Modeling, 2022, 28, .	0.8	0
4068	Effect of starch-catechin interaction on regulation of starch digestibility during hot-extrusion 3D printing: Structural analysis and simulation study. Food Chemistry, 2022, 393, 133394.	4.2	31
4069	fingeRNAtâ€”A novel tool for high-throughput analysis of nucleic acid-ligand interactions. PLoS Computational Biology, 2022, 18, e1009783.	1.5	9
4070	Protein-Ligand Identification andIn VitroInhibitory Effects of Cathine on 11 Major Human Drug Metabolizing Cytochrome P450s. International Journal of Toxicology, 2022, 41, 355-366.	0.6	4
4071	Deciphering the role of Trichoderma sp. bioactives in combating the wilt causing cell wall degrading enzyme polygalacturonase produced by Fusarium oxysporum: An in-silico approach. Microbial Pathogenesis, 2022, 168, 105610.	1.3	8
4072	Tilianin Reduces Apoptosis via the ERK/EGR1/BCL2L1 Pathway in Ischemia/Reperfusion-Induced Acute Kidney Injury Mice. Frontiers in Pharmacology, 0, 13, .	1.6	6
4073	ADME PROPERTIES PREDICTION OF 5-PHENYL-5,6-DIHYDROTETRAZOLO[1,5-c] QUINAZOLINES. Grail of Science, 2022, , 684-692.	0.0	2
4075	Towards the discovery of potential RdRp inhibitors for the treatment of COVID-19: structure guided virtual screening, computational ADME and molecular dynamics study. Structural Chemistry, 2022, 33, 1569-1583.	1.0	5
4076	In silico prediction of chemical aquatic toxicity by multiple machine learning and deep learning approaches. Journal of Applied Toxicology, 2022, 42, 1766-1776.	1.4	3
4077	Anti-Proliferative and Cytoprotective Activity of Aryl Carbamate and Aryl Urea Derivatives with Alkyl Groups and Chlorine as Substituents. Molecules, 2022, 27, 3616.	1.7	2

#	Article	IF	Citations
4078	idse-HE: Hybrid embedding graph neural network for drug side effects prediction. Journal of Biomedical Informatics, 2022, 131, 104098.	2.5	13
4079	Mapping of Protein Binding Sites using clustering algorithms - Development of a pharmacophore based drug discovery tool. Journal of Molecular Graphics and Modelling, 2022, 115, 108228.	1.3	3
4080	Molecular docking of ethanol extracts of katuk leaf (Sauropus androgynus) on functional proteins of severe acute respiratory syndrome coronavirus 2. South African Journal of Botany, 2022, 149, 1-5.	1.2	3
4081	Construction of New Medicines via Game Proof Search. Proceedings of the AAAI Conference on Artificial Intelligence, 2012, 26, 1564-1570.	3.6	8
4082	Synthesis and In Silico Evaluation of Potential Insecticide Activity of Benzamides. , 0, , .		0
4083	Metal Chelation Ability of Protocatechuic Acid Anion with Radioactive 210po84; a Theoretical Insight. SSRN Electronic Journal, 0, , .	0.4	0
4084	Benzo[d]Thiazole-2-Carboxamides/Carbanilides as New Anti-TB Chemotypes Inhibiting the Mycobacterial ATP-Phosphoribosyl Transferase (HisG). SSRN Electronic Journal, 0, , .	0.4	0
4085	Synthesis, computational and nanoencapsulation studies on eugenol-derived insecticides. New Journal of Chemistry, 2022, 46, 14375-14387.	1.4	3
4086	Inorganic Polyphosphate and F0F1-ATP Synthase of Mammalian Mitochondria. Progress in Molecular and Subcellular Biology, 2022, , 1-13.	0.9	4
4087	The effect of non-specific binding of Pd(II) complexes with N-heteroaromatic hydrazone ligands on the protein structure. Journal of the Serbian Chemical Society, 2022, 87, 1143-1156.	0.4	0
4088	Synthesis of new 3-substituted quinolone derivatives with benzene sulfonamide group using hydrazine linker with their docking and antibacterial studies in vitro. Results in Chemistry, 2022, 4, 100397.	0.9	1
4089	Metal Chelation Ability of Protocatechuic Acid Anion with Radioactive 210po84; a Theoretical Insight. SSRN Electronic Journal, 0, , .	0.4	0
4090	AnÃ¡lise da interaÃ§Ã£o do contaminante metilmercÃºrio com hemoglobina do peixe matrinxÃ£ Brycon cephalus (GÃ¼nther, 1869). Journal of Education, Science and Health, 2022, 2, 1-6.	0.1	0
4091	IMPDB: Indian Medicinal Phytochemical Database Curated for Drug Designing. Journal of Computational Biophysics and Chemistry, 0, , .	1.0	1
4092	Synthesis and characterization of singleâ€walled carbon nanotube: Cytoâ€genotoxicity in Allium cepa root tips and molecular docking studies. Microscopy Research and Technique, 2022, 85, 3193-3206.	1.2	7
4093	Combined QM/MM, Machine Learning Path Integral Approach to Compute Free Energy Profiles and Kinetic Isotope Effects in RNA Cleavage Reactions. Journal of Chemical Theory and Computation, 2022, 18, 4304-4317.	2.3	17
4094	In silico screening of c-Met tyrosine kinase inhibitors targeting nucleotide and drug-substrate binding sites of ABCB1 as potential MDR reversal agents. Journal of Receptor and Signal Transduction Research, 2022, 42, 549-561.	1.3	4
4095	Efficient Enumeration of Branched Novel Biochemical Pathways Using a Probabilistic Technique. Industrial & Engineering Chemistry Research, 0, , .	1.8	1

#	Article	IF	Citations
4096	In Silico ADME Profiling of Salubrinal and Its Analogues. Future Pharmacology, 2022, 2, 160-197.	0.6	11
4097	Learning About Allosteric Drugs and Ways to Design Them. Journal of Molecular Biology, 2022, 434, 167692.	2.0	13
4098	Commentary: the first twelve years of the Journal of Cheminformatics. Journal of Cheminformatics, 2022, 14, .	2.8	0
4099	Structure-Based Virtual Screening Identifies Novobiocin, Montelukast, and Cinnarizine as TRPV1 Modulators with Anticonvulsant Activity In Vivo. Journal of Chemical Information and Modeling, 2022, 62, 3008-3022.	2.5	7
4100	Modeling of Anticancer Sulfonamide Derivatives Lipophilicity by Chemometric and Quantitative Structure-Retention Relationships Approaches. Molecules, 2022, 27, 3965.	1.7	4
4101	Withania somnifera phytochemicals possess SARS-CoV-2 RdRp and human TMPRSS2 protein binding potential. Vegetos, 2023, 36, 701-720.	0.8	5
4102	Inverse molecular design of alkoxides and phenoxides for aqueous direct air capture of CO ₂. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	3.3	8
4103	Evaluation of the inhibitory potential of Valproic acid against histone deacetylase ofLeishmania donovaniand computational studies of Valproic acid derivatives. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5447-5464.	2.0	0
4104	In silico study to identify novel potential thiadiazole-based molecules as anti-Covid-19 candidates by hierarchical virtual screening and molecular dynamics simulations. Structural Chemistry, 2022, 33, 1727-1739.	1.0	9
4105	Design of SARS-CoV-2 Main Protease Inhibitors Using Artificial Intelligence and Molecular Dynamic Simulations. Molecules, 2022, 27, 4020.	1.7	14
4106	Computational Study of Asian Propolis Compounds as Potential Anti-Type 2 Diabetes Mellitus Agents by Using Inverse Virtual Screening with the DIA-DB Web Server, Tanimoto Similarity Analysis, and Molecular Dynamic Simulation. Molecules, 2022, 27, 3972.	1.7	4
4107	Menthol carbonates as potent antiparasitic agents: synthesis and in vitro studies along with computer-aided approaches. BMC Complementary Medicine and Therapies, 2022, 22, .	1.2	3
4108	Gaining deeper insights into 2,5-disubstituted furan derivatives as potent Î±-glucosidase inhibitors and discovery of putative targets associated with diabetes diseases using an integrative computational approach. Structural Chemistry, 2023, 34, 519-538.	1.0	4
4109	Computational Identification of Potential Multitarget Inhibitors of Nipah Virus by Molecular Docking and Molecular Dynamics. Microorganisms, 2022, 10, 1181.	1.6	14
4110	In Silico Models on Algal Cultivation and Processing. Impact of Meat Consumption on Health and Environmental Sustainability, 2022, , 228-255.	0.4	0
4111	Octanolâ€“Water Partition Coefficients of Fluorinated Drug Molecules with Continuum Solvation Models. Journal of Physical Chemistry A, 0, , .	1.1	3
4112	The functional mechanisms of synchronizing royal jelly consumption and physical activity on rat with multiple sclerosis-like behaviors hallmarks based on bioinformatics analysis, and experimental survey. BMC Neuroscience, 2022, 23, .	0.8	3
4113	The Optimal Permeation of Cyclic Boronates to Cross the Outer Membrane via the Porin Pathway. Antibiotics, 2022, 11, 840.	1.5	3

#	Article	IF	Citations
4114	Discovery of potential mTOR inhibitors from Cichorium intybus to find new candidate drugs targeting the pathological protein related to the breast cancer: an integrated computational approach. Molecular Diversity, 2023, 27, 1141-1162.	2.1	9
4115	Synthesis, In Silico and Pharmacological Evaluation of New Thiazolidine-4-Carboxylic Acid Derivatives Against Ethanol-Induced Neurodegeneration and Memory Impairment. Journal of Inflammation Research, 0, Volume 15, 3643-3660.	1.6	1
4116	Mechanistic Analysis of Chemically Diverse Bromodomain-4 Inhibitors Using Balanced QSAR Analysis and Supported by X-ray Resolved Crystal Structures. Pharmaceuticals, 2022, 15, 745.	1.7	1
4117	Rational Design, Synthesis, in Vitro, and in Silico Studies of Chlorophenylquinazolinâ€4(3H)â€One Containing Different Aryl Acetohydrazides as Tyrosinase Inhibitors. Chemistry and Biodiversity, 2022, 19, .	1.0	8
4118	Exploring a Computational Method for Evaluating the Epinecidin-1 and Its Variants Binding Efficacy with Breast Cancer Receptor (HER-2). International Journal of Peptide Research and Therapeutics, 2022, 28, .	0.9	4
4121	Data-Driven Mapping of Inorganic Chemical Space for the Design of Transition Metal Complexes and Metal-Organic Frameworks. ACS Symposium Series, 0, , 127-179.	0.5	0
4122	Attacking the SARS-CoV-2 replication machinery with the Pathogen Boxâ€™s molecules. Letters in Drug Design and Discovery, 2022, 19, .	0.4	0
4124	An Integrated Mass Spectrometry-Based Glycomics-Driven Glycoproteomics Analytical Platform to Functionally Characterize Glycosylation Inhibitors. Molecules, 2022, 27, 3834.	1.7	6
4125	A computational biology approach for the identification of potential SARS-CoV-2 main protease inhibitors from natural essential oil compounds.. F1000Research, 0, 10, 1313.	0.8	2
4126	In Silico Screening of Some Anti-Cancer Drugs Against the Main Protease of COVID-19 Using Molecular Docking. Letters in Organic Chemistry, 2023, 20, 77-90.	0.2	2
4128	Machine Learning Models Predict Calculation Outcomes with the Transferability Necessary for Computational Catalysis. Journal of Chemical Theory and Computation, 2022, 18, 4282-4292.	2.3	9
4129	Acute behavioral and Neurochemical Effects of NovelN-Benzyl-2-Phenylethylamine Derivatives in Adult Zebrafish. ACS Chemical Neuroscience, 2022, 13, 1902-1922.	1.7	4
4130	Allosteric regulation of the inactive to active state conformational transition in CDPK1 protein of Plasmodium falciparum. International Journal of Biological Macromolecules, 2022, 215, 489-500.	3.6	1
4131	Computational approach to decode the mechanism of curcuminoids against neuropathic pain. Computers in Biology and Medicine, 2022, 147, 105739.	3.9	5
4132	In-Silico targeting of SARS-CoV-2 NSP6 for drug and natural products repurposing. Virology, 2022, 573, 96-110.	1.1	7
4134	Covid-19 and Flavonoids: In silico Molecular Dynamics Docking to the Active Catalytic Site of SARS-CoV and SARS-CoV-2 Main Protease. , 2022, 2, 23-42.		0
4135	Targeting non-structural proteins of Hepatitis C virus for predicting repurposed drugs using QSAR and machine learning approaches. Computational and Structural Biotechnology Journal, 2022, 20, 3422-3438.	1.9	5
4136	Characterization of Structure Isomers of Ethylbenzalkyl Dimethyl Ammonium Chloride and Quantification in Commercial Household Disinfectant Products. SSRN Electronic Journal, 0, , .	0.4	0

#	Article	IF	Citations
4137	In Silico Prediction Model of STAT3 Inhibition and in Vivo Antitumor Activity of Cucurbitacin IIb and Kinoin a from Ibervillea Sonorae. SSRN Electronic Journal, 0, , .	0.4	1
4138	Molecular dynamic simulation, free binding energy calculation of Thiazolo-[2,3-b]quinazolinone derivatives against EGFR-TKD and their anticancer activity. Results in Chemistry, 2022, 4, 100418.	0.9	10
4139	Coupling of acceptor-substituted diazo compounds and tertiary thioamides: synthesis of enamino carbonyl compounds and their pharmacological evaluation. RSC Advances, 2022, 12, 19431-19444.	1.7	1
4140	Targetâ€based virtual screening, computational multiscoring docking and molecular dynamics simulation of small molecules as promising drug candidate affecting kinesinâ€like protein KIFC1. Cell Biochemistry and Function, 2022, 40, 451-472.	1.4	3
4141	Sfcnn: a novel scoring function based on 3D convolutional neural network for accurate and stable proteinâ€“ligand affinity prediction. BMC Bioinformatics, 2022, 23, .	1.2	16
4142	Structureâ€based study to identify alkaloids as promising cytochrome P450 (CYP1A1) inhibitors: An in silico approach using virtual screening, molecular dynamic simulations, and binding free energy calculation. Journal of Cellular Biochemistry, 2022, 123, 1422-1439.	1.2	3
4143	Crescent-shaped meta-substituted benzene derivatives as a new class of non-nucleoside ribonuclease A inhibitors. Bioorganic and Medicinal Chemistry, 2022, 71, 116888.	1.4	4
4144	Effect of Key Phytochemicals from Andrographis paniculata, Tinospora cordifolia, and Ocimum sanctum on PLpro-ISG15 De-Conjugation Machineryâ€”A Computational Approach. Computation, 2022, 10, 109.	1.0	2
4145	Investigation of the Fluorescence Turn-off Mechanism, Genome, Molecular Docking In Silico and In Vitro Studies of 2-Acetyl-3H-benzo[f]chromen-3-one. ACS Omega, 2022, 7, 23759-23770.	1.6	4
4146	In Silico Study of Alkaloids: Neferine and Berbamine Potentially Inhibit the SARS-CoV-2 RNA-Dependent RNA Polymerase. Journal of Chemistry, 2022, 2022, 1-9.	0.9	9
4147	Investigation of the Captoprilâ€“Insulin Interaction by Mass Spectrometry and Computational Approaches Reveals that Captopril Induces Structural Changes in Insulin. ACS Omega, 2022, 7, 23115-23126.	1.6	0
4148	Design, synthesis and evaluation of novel tetrahydropyridothienopyrimidin-ureas as cytotoxic and anti-angiogenic agents. Scientific Reports, 2022, 12, .	1.6	0
4149	Curcumin improves D-galactose and normal-aging associated memory impairment in mice: In vivo and in silico-based studies. PLoS ONE, 2022, 17, e0270123.	1.1	10
4150	Newly Synthesized Pyrazolinone Chalcones as Anticancer Agents via Inhibiting the PI3K/Akt/ERK1/2 Signaling Pathway. ACS Omega, 2022, 7, 25265-25277.	1.6	23
4151	Accelerating Discovery of High Fractional Free Volume Polymers from a Data-Driven Approach. ACS Applied Materials & Interfaces, 2022, 14, 31203-31215.	4.0	8
4152	Metabolic activation of tachysterol ₃ to biologically active hydroxyderivatives that act on <scp>VDR</scp> , <scp>AhR</scp> , <scp>LXRs,</scp> and <scp>PPARÎ³</scp> receptors. FASEB Journal, 2022, 36, .	0.2	29
4153	Prediction of CIAPIN1 (Cytokine-Induced Apoptosis Inhibitor 1) Signaling Pathway and Its Role in Cholangiocarcinoma Metastasis. Journal of Clinical Medicine, 2022, 11, 3826.	1.0	0
4154	Synthesis of Novel Benzoxazole Derivatives: Exploration of Their Possible Pharmacological Profiles with Computational Studies. Polycyclic Aromatic Compounds, 2023, 43, 3853-3886.	1.4	0

#	Article	IF	Citations
4155	Spectroscopic and Molecular Docking Studies of Cu(II), Ni(II), Co(II), and Mn(II) Complexes with Anticonvulsant Therapeutic Agent Gabapentin. Molecules, 2022, 27, 4311.	1.7	5
4156	Variations of SARS-CoV-2 in the Iranian population and candidate putative drug-like compounds to inhibit the mutated proteins. Heliyon, 2022, 8, e09910.	1.4	1
4157	DockingPie: a consensus docking plugin for PyMOL. Bioinformatics, 2022, 38, 4233-4234.	1.8	8
4158	Biochemical characterization and structure-basedin silicoscreening of potent inhibitor molecules against the 1 cys peroxiredoxin of bacterioferritin comigratory protein family fromCandidatus Liberibacter asiaticus. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5776-5788.	2.0	4
4159	DOCKSTRING: Easy Molecular Docking Yields Better Benchmarks for Ligand Design. Journal of Chemical Information and Modeling, 2022, 62, 3486-3502.	2.5	25
4160	Structure Prediction, Evaluation, and Validation of GPR18 Lipid Receptor Using Free Programs. International Journal of Molecular Sciences, 2022, 23, 7917.	1.8	0
4161	Does an Ionomer Penetrate a Carbon Mesopore? Free-Energy Analysis Using Molecular Dynamics Simulations. Journal of Physical Chemistry C, 2022, 126, 11518-11528.	1.5	5
4162	Machine Learning and Artificial Intelligence: A Paradigm Shift in Big Data-Driven Drug Design and Discovery. Current Topics in Medicinal Chemistry, 2022, 22, 1692-1727.	1.0	8
4163	In Silico Drug Repurposing of FDA-Approved Drugs Highlighting Promacta as a Potential Inhibitor of H7N9 Influenza Virus. Molecules, 2022, 27, 4515.	1.7	4
4164	Proteinâ€“Ligand Docking in the Machine-Learning Era. Molecules, 2022, 27, 4568.	1.7	37
4165	The heterogeneous pharmacological medical biochemical network PharMeBINet. Scientific Data, 2022, 9, .	2.4	2
4166	Toxicological Evaluation and In Silico Identification of Acetylcholinesterase Inhibitors in a Commercial Polyherbal Formulation (KWAPF01). Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-9.	0.5	0
4167	Biomarker Profiling Revealed Carcinoembryonic Antigen as a Target of Artesunate in a Ductal Breast Cancer Patient. Anticancer Research, 2022, 42, 3483-3494.	0.5	1
4168	Investigation of potential inhibitor properties of violacein against HIV-1 RT and CoV-2 Spike RBD:ACE-2. World Journal of Microbiology and Biotechnology, 2022, 38, .	1.7	11
4170	Bis-1,2,4-triazol derivatives: Synthesis, characterization, DFT, antileishmanial activity and molecular docking study. Journal of Biomolecular Structure and Dynamics, 2023, 41, 5970-5980.	2.0	1
4171	Automation of chemical kinetics: Status and challenges. Proceedings of the Combustion Institute, 2023, 39, 11-28.	2.4	8
4173	A computational chemistry-driven hypothesis on the mode of action of Hipposudoric Acid and related analogs. Future Medicinal Chemistry, 0, , .	1.1	1
4174	Perceiving the Concealed and Unreported Pharmacophoric Features of the 5-Hydroxytryptamine Receptor Using Balanced QSAR Analysis. Pharmaceuticals, 2022, 15, 834.	1.7	4

#	Article	IF	Citations
4175	The therapeutic effect of Fufang Zhenshu Tiaozhi (FTZ) on osteoclastogenesis and ovariectomized-induced bone loss: evidence from network pharmacology, molecular docking and experimental validation. Aging, 2022, 14, 5727-5748.	1.4	3
4176	Antimicrobial activity of some celastroloids and their derivatives. Medicinal Chemistry Research, 0, , .	1.1	0
4177	The Use of AlphaFold for In Silico Exploration of Drug Targets in the Parasite Trypanosoma cruzi. Frontiers in Cellular and Infection Microbiology, 0, 12, .	1.8	7
4178	In Silico Insights on the Pro-Inflammatory Potential of Polycyclic Aromatic Hydrocarbons and the Prospective Anti-Inflammatory Capacity of Andrographis paniculata Phytocompounds. International Journal of Environmental Research and Public Health, 2022, 19, 8588.	1.2	6
4179	Fundamentals of Molecular Docking and Comparative Analysis of Proteinâ€“Small-Molecule Docking Approaches. , 0, , .		1
4180	Modeling Gd³⁺ Complexes for Molecular Dynamics Simulations: Toward a Rational Optimization of MRI Contrast Agents. Inorganic Chemistry, 2022, 61, 11837-11858.	1.9	3
4181	A Path-Based Analysis of Infected Cell Line and COVID-19 Patient Transcriptome Reveals Novel Potential Targets and Drugs Against SARS-CoV-2. Frontiers in Immunology, 0, 13, .	2.2	6
4183	In-silico screening and in-vitro assay show the antiviral effect of Indomethacin against SARS-CoV-2. Computers in Biology and Medicine, 2022, 147, 105788.	3.9	10
4184	Comparative molecular dynamics analyses on PIK3CA hotspot mutations with PI3KÎ± specific inhibitors and ATP. Computational Biology and Chemistry, 2022, 99, 107726.	1.1	2
4185	Crystal structure and molecular characterization of NADP+-farnesol dehydrogenase from cotton bollworm, Helicoverpa armigera. Insect Biochemistry and Molecular Biology, 2022, 147, 103812.	1.2	8
4186	Repurposing of FDA approved drugs against uropathogenic Escherichia coli: In silico, in vitro, and in vivo analysis. Microbial Pathogenesis, 2022, 169, 105665.	1.3	5
4187	Intermolecular charge-transfer complexes between chlorothiazide antihypertensive drug against iodine sigma and picric acid pi acceptors: DFT and molecular docking interaction study with Covid-19 protease. Journal of the Indian Chemical Society, 2022, 99, 100605.	1.3	1
4188	An integrated understanding of the evolutionary and structural features of the SARS-CoV-2 spike receptor binding domain (RBD). International Journal of Biological Macromolecules, 2022, 217, 492-505.	3.6	9
4189	Pharmacoinformatics based screening discovers swertianolin from Lavandula angustifolia as a novel neuromodulator targeting epilepsy, depression, and anxiety. South African Journal of Botany, 2022, 149, 712-730.	1.2	21
4190	Gas-phase OH-oxidation of 2-butanethiol: Multiconformer transition state theory rate constant with constrained transition state randomization. Chemical Physics Letters, 2022, 803, 139829.	1.2	7
4191	Discovery of benzyloxyphenyl- and phenethylphenyl-imidazole derivatives as a new class of anteâ€“drug type boosters. Bioorganic and Medicinal Chemistry Letters, 2022, 72, 128868.	1.0	1
4192	Hyjapones Aâ^'D, trimethylated acyphloroglucinol meroterpenoids from Hypericum japonicum thunb. With anti-inflammatory activity. Phytochemistry, 2022, 202, 113308.	1.4	6
4193	7-Azaindole, 2,7-diazaindole, and 1H-pyrazole as core structures for novel anticancer agents with potential chemosensitizing properties. European Journal of Medicinal Chemistry, 2022, 240, 114580.	2.6	3

#	Article	IF	Citations
4194	The nucleoside adenosine inhibits intracellular microvascular Î±2C-adrenoceptor surface trafficking. Journal of Molecular Structure, 2022, 1267, 133637.	1.8	2
4195	An efficient pâ€TSA catalyzed synthesis of some new substitutedâ€(5â€hydroxyâ€3â€phenylisoxazolâ€4â€yl)â€1,3â€dimethylâ€1Hâ€chromeno[2,3â€d]pyrimidineâ€2,4(3H,5H)â€dione/ scaffolds and evaluation of their pharmacological and computational investigations. Journal of Molecular Structure, 2022, 1267, 133587.	1.8	7
4196	In-silico functional and structural annotation of hypothetical protein from Klebsiella pneumonia: A potential drug target. Journal of Molecular Graphics and Modelling, 2022, 116, 108262.	1.3	23
4197	Calculation of Gas-phase Standard Formation Enthalpy via Ring-Preserved Connectivity-Based Hierarchy and Automatic Bond Separation Reaction Platform. Fuel, 2022, 327, 125203.	3.4	7
4198	Syzygium aromaticum (L.) Merr. & L.M.Perry mitigates iron-mediated oxidative brain injury via in vitro, ex vivo, and in silico approaches. Journal of Molecular Structure, 2022, 1268, 133675.	1.8	8
4199	Towards Covid-19 TMPRSS2 enzyme inhibitors and antimicrobial agents: Synthesis, antimicrobial potency, molecular docking, and drug-likeness prediction of thiadiazole-triazole hybrids. Journal of Molecular Structure, 2022, 1268, 133659.	1.8	8
4200	Eugenol Ester Derivatives: Synthesis, Insecticidal Activity and Computational Studies. , 0, , .		0
4201	Electron Transfer of Functionalised Quinones in Acetonitrile. Journal of Chemical Physics, 0, , .	1.2	0
4202	SCORCH: Improving structure-based virtual screening with machine learning classifiers, data augmentation, and uncertainty estimation. Journal of Advanced Research, 2023, 46, 135-147.	4.4	7
4203	Target-based in-silico screening of basil polysaccharides against different epigenetic targets responsible for breast cancer. Journal of Receptor and Signal Transduction Research, 0, , 1-10.	1.3	0
4204	Diminazene Aceturate Reduces Angiotensin II Constriction and Interacts with the Spike Protein of Severe Acute Respiratory Syndrome Coronavirus 2. Biomedicines, 2022, 10, 1731.	1.4	8
4205	Machine intelligence-driven framework for optimized hit selection in virtual screening. Journal of Cheminformatics, 2022, 14, .	2.8	9
4206	QSAR Evaluations to Unravel the Structural Features in Lysine-Specific Histone Demethylase 1A Inhibitors for Novel Anticancer Lead Development Supported by Molecular Docking, MD Simulation and MMGBSA. Molecules, 2022, 27, 4758.	1.7	4
4207	Machine Learning for Electrocatalyst and Photocatalyst Design and Discovery. Chemical Reviews, 2022, 122, 13478-13515.	23.0	120
4208	Mebendazoleâ€™s Conformational Space and Its Predicted Binding to Human Heat-Shock Protein 90. Journal of Chemical Information and Modeling, 2022, 62, 3604-3617.	2.5	1
4209	De Novo Molecule Design Using Molecular Generative Models Constrained by Ligandâ€“Protein Interactions. Journal of Chemical Information and Modeling, 2022, 62, 3291-3306.	2.5	17
4210	Deep Learning for Additive Screening in Perovskite Lightâ€Emitting Diodes. Angewandte Chemie, 0, , .	1.6	0
4211	Deep Learning for Additive Screening in Perovskite Lightâ€Emitting Diodes. Angewandte Chemie - International Edition, 2022, 61, .	7.2	14

#	Article	IF	Citations
4212	Exploration of Diazaspiro Cores as Piperazine Bioisosteres in the Development of Ïƒ2 Receptor Ligands. International Journal of Molecular Sciences, 2022, 23, 8259.	1.8	6
4213	Development of Fenofibrate/Randomly Methylated Î²-Cyclodextrin-Loaded EudragitÂ® RL 100 Nanoparticles for Ocular Delivery. Molecules, 2022, 27, 4755.	1.7	9
4214	In silico disrupting quorum sensing of porphyromonas gingivalis via essential oils and coumarin derivatives. Annals of Proteomics and Bioinformatics, 2022, 6, 001-005.	1.0	0
4215	Preliminary Discovery of Small Molecule Inhibitors of Epidermal Growth Factor Receptor (EGFR) That Bind to the Extracellular Domain. Cancers, 2022, 14, 3647.	1.7	2
4216	Pharmacophore-based virtual screening, molecular docking and molecular dynamics simulations study for the identification of LIM kinase-1 inhibitors. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6089-6103.	2.0	5
4217	Combining empirical knowledge, in silico molecular docking and ADMET profiling to identify therapeutic phytochemicals from Brucea antidysentrica for acute myeloid leukemia. PLoS ONE, 2022, 17, e0270050.	1.1	5
4219	TRPC6 N338S is a gain-of-function mutant identified in patient with doxorubicin-induced cardiotoxicity. Biochimica Et Biophysica Acta - Molecular Basis of Disease, 2022, 1868, 166505.	1.8	1
4220	Molecular Docking of Gallic Acid and Its Derivatives as the Potential nNOS Inhibitors. Jurnal Kimia Sains Dan Aplikasi, 2022, 25, 197-204.	0.1	1
4221	Molecular Docking Study of IPBCC.08.610 Glucose Oxidase Mutant for Increasing Gluconic Acid Production. Jurnal Kimia Sains Dan Aplikasi, 2022, 25, 169-178.	0.1	0
4222	Network Pharmacology and Molecular Docking Analysis on Mechanisms of Isobavachalcone in Parkinsonâ€™s Disease. , 2022, 2, 1-9.		0
4223	In-silico and in-vivo evaluation of comparative enhanced neurogenic performance by energy drinks. International Journal of Health Sciences, 0, , 5439-5454.	0.0	0
4224	Human TMPRSS2 non-catalytic ectodomain and SARS-CoV-2 S2' subunit interaction mediated SARS-CoV-2 endocytosis: a model proposal with virtual screening for potential drug molecules to inhibit this interaction. Journal of Biomolecular Structure and Dynamics, 0, , 1-12.	2.0	0
4225	Synthesis of Two Novel Copper (II) Complexes as Potential Inhibitors of HIV-1 Protease Enzyme: Experimental and Theoretical Investigations. Crystals, 2022, 12, 1066.	1.0	3
4226	Biofilm-i: A Platform for Predicting Biofilm Inhibitors Using Quantitative Structureâ€"Relationship (QSAR) Based Regression Models to Curb Antibiotic Resistance. Molecules, 2022, 27, 4861.	1.7	4
4227	Docking and Molecular Dynamics Study to Identify Novel Phytobiologics from Dracaena trifasciata against Metabolic Reprogramming in Rheumatoid Arthritis. Life, 2022, 12, 1148.	1.1	2
4228	Spectroscopic and Molecular Docking Studies of a Novel Biologically Active Heterocyclic Compound 2-Chloro-6-Methoxypyridine-4-Carboxylic Acid by Quantum Computational Method. Polycyclic Aromatic Compounds, 2023, 43, 5404-5436.	1.4	1
4229	Imidazole and nitroimidazole derivatives as <scp>NADH</scp>â€fumarate reductase inhibitors: <scp>Density functional theory</scp> studies, homology modeling, and molecular docking. Journal of Computational Chemistry, 2022, 43, 1573-1595.	1.5	3
4231	Molecular dynamics simulations reveal the inhibitory mechanism of Withanolide A against Î±-glucosidase and Î±-amylase. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6203-6218.	2.0	7

#	Article	IF	Citations
4232	Toward the General Mechanistic Model of Liquid Chromatographic Retention. Analytical Chemistry, 2022, 94, 11070-11080.	3.2	5
4233	Targeting SARS-CoV-2 endoribonuclease: a structure-based virtual screening supported by in vitro analysis. Scientific Reports, 2022, 12, .	1.6	7
4234	Assessing the Persistence and Mobility of Organic Substances to Protect Freshwater Resources. ACS Environmental Au, 2022, 2, 482-509.	3.3	17
4235	Structural and Biochemical Analysis Reveals Catalytic Mechanism of Fucoidan Lyase from Flavobacterium sp. SA-0082. Marine Drugs, 2022, 20, 533.	2.2	2
4236	Repurposing food molecules as a potential BACE1 inhibitor for Alzheimerâ€™s disease. Frontiers in Aging Neuroscience, 0, 14, .	1.7	16
4237	Molecular modelling of antiproliferative inhibitors based on SMILES descriptors using Monte-Carlo method, docking, MD simulations and ADME/Tox studies. Molecular Simulation, 2022, 48, 1575-1591.	0.9	12
4238	Inhibition mechanism of alpha-amylase, a diabetes target, by a steroidal pregnane and pregnane glycosides derived from Gongronema latifolium Benth. Frontiers in Molecular Biosciences, 0, 9, .	1.6	17
4239	Identification of small molecules targeting homoserine acetyl transferase from Mycobacterium tuberculosis and Staphylococcus aureus. Scientific Reports, 2022, 12, .	1.6	1
4240	Novel psoralen derivatives as anti-breast cancer agents and their light-activated cytotoxicity against HER2 positive breast cancer cells. Scientific Reports, 2022, 12, .	1.6	5
4241	Profiling prediction of nuclear receptor modulators with multi-task deep learning methods: toward the virtual screening. Briefings in Bioinformatics, 2022, 23, .	3.2	7
4242	FPocketWeb: protein pocket hunting in a web browser. Journal of Cheminformatics, 2022, 14, .	2.8	6
4243	Oxygen heterocyclic Diels-Alder-Type sesquiterpenoid dimers from Vernonia anthelmintica. Phytochemistry, 2022, 203, 113386.	1.4	2
4244	DRPADC: A novel drug repositioning algorithm predicting adaptive drugs for COVID-19. Computers and Chemical Engineering, 2022, 166, 107947.	2.0	3
4245	Density Functional Theory with Implicit Solvents for Accurate Estimation of Aqueous and Organic Solvation Free Energies of Lignin Fragments. ACS Sustainable Chemistry and Engineering, 2022, 10, 10870-10878.	3.2	5
4246	Preserving the Integrity of Empirical Force Fields. Journal of Chemical Information and Modeling, 2022, 62, 3825-3831.	2.5	5
4247	Antibacterial Potential of Bacopa monnieri (L.) Wettst. and Its Bioactive Molecules against Uropathogensâ€”An In Silico Study to Identify Potential Lead Molecule(s) for the Development of New Drugs to Treat Urinary Tract Infections. Molecules, 2022, 27, 4971.	1.7	17
4248	Dose-dependent toxicity profile and genotoxicity mechanism of lithium carbonate. Scientific Reports, 2022, 12, .	1.6	16
4249	Glutathione degradation activity of <scp>Î³â€glutamyl</scp> peptidase 1 manifests its dual roles in primary and secondary sulfur metabolism in Arabidopsis. Plant Journal, 2022, 111, 1626-1642.	2.8	10

#	Article	IF	Citations
4250	Evaluation of the toxicological effects of atrazine-metolachlor in male rats: in vivo and in silico studies. Environmental Analysis, Health and Toxicology, 2022, 37, e2022021.	0.7	2
4251	Effective Proteinâ€“Ligand Docking Strategy via Fragment Reuse and a Proof-of-Concept Implementation. ACS Omega, 2022, 7, 30265-30274.	1.6	1
4252	In Silico Repurposed Drugs against Monkeypox Virus. Molecules, 2022, 27, 5277.	1.7	39
4253	Interaction of the Emerging Mycotoxins Beauvericin, Cyclopiazonic Acid, and Sterigmatocystin with Human Serum Albumin. Biomolecules, 2022, 12, 1106.	1.8	9
4254	Phytochemical drug discovery for COVID-19 using high-resolution computational docking and machine learning assisted binder prediction. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6643-6663.	2.0	2
4256	In silico analysis of the C-terminal domain of big defensin from the Pacific oyster. Journal of Biomolecular Structure and Dynamics, 0, , 1-13.	2.0	0
4257	Chemical Composition of Various Nepeta cataria Plant Organsâ€™ Methanol Extracts Associated with In Vivo Hepatoprotective and Antigenotoxic Features as well as Molecular Modeling Investigations. Plants, 2022, 11, 2114.	1.6	3
4258	Evaluating the therapeutic role of selected active compounds in Plumula Nelumbinis on pulmonary hypertension via network pharmacology and experimental analysis. Frontiers in Pharmacology, 0, 13, .	1.6	6
4259	A computational study to target necroptosis via RIPK1 inhibition. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6502-6517.	2.0	1
4260	Virtual screening and molecular dynamics study of natural products against Rab10 for the treatment of Alzheimerâ€™s disease. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6728-6748.	2.0	1
4261	Probing interactions of aminoacyl-adenylate with Mycobacterium tuberculosis methionyl-tRNA synthetase through in silico site-directed mutagenesis and free energy calculation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6450-6458.	2.0	1
4262	Nonâ€physical Species in Chemical Kinetic Models: A Case Study of Diazenyl Hydroxy and Diazenyl Peroxide. ChemPhysChem, 0, , .	1.0	2
4264	Virtual Screening for FDA-Approved Drugs That Selectively Inhibit Arginase Type 1 and 2. Molecules, 2022, 27, 5134.	1.7	7
4265	Graph-based Automated Macro-Molecule Assembly. Journal of Chemical Information and Modeling, 2022, 62, 3714-3723.	2.5	0
4266	Towards systematic exploration of chemical space: building the fragment library module in molecular property diagnostic suite. Molecular Diversity, 2023, 27, 1459-1468.	2.1	8
4267	Critical Assessment of Stateâ€ofâ€theâ€Art Ligandâ€Based Virtual Screening Methods. Molecular Informatics, 2022, 41, .	1.4	3
4268	Identification of Potential Cytochrome P450 3A5 Inhibitors: An Extensive Virtual Screening through Molecular Docking, Negative Image-Based Screening, Machine Learning and Molecular Dynamics Simulation Studies. International Journal of Molecular Sciences, 2022, 23, 9374.	1.8	1
4269	Atmospheric Degradation of Two Hydrofluoroketones: Theoretical Rate Constants for the Gas-Phase OH-Oxidation of HFK-447mcc and HFK-465mc. Atmosphere, 2022, 13, 1256.	1.0	3

#	Article	IF	Citations
4270	Antioxidant Capacities and Enzymatic Inhibitory Effects of Different Solvent Fractions and Major Flavones from Celery Seeds Produced in Different Geographic Areas in China. Antioxidants, 2022, 11, 1542.	2.2	5
4272	Using network pharmacology to explore the mechanism of Danggui-Shaoyao-San in the treatment of diabetic kidney disease. Frontiers in Pharmacology, 0, 13, .	1.6	2
4273	<scp>Conformerâ€RL</scp>: A deep reinforcement learning library for conformer generation. Journal of Computational Chemistry, 2022, 43, 1880-1886.	1.5	2
4274	Artificial intelligence uncovers carcinogenic human metabolites. Nature Chemical Biology, 2022, 18, 1204-1213.	3.9	9
4275	Combined docking and machine learning identify key molecular determinants of ligand pharmacological activity on Î²2 adrenoceptor. Pharmacology Research and Perspectives, 2022, 10, .	1.1	5
4277	Novel Phenothiazine/Donepezil-like Hybrids Endowed with Antioxidant Activity for a Multi-Target Approach to the Therapy of Alzheimerâ€™s Disease. Antioxidants, 2022, 11, 1631.	2.2	6
4279	Digging for the discovery of SARS-CoV-2 nsp12 inhibitors: a pharmacophore-based and molecular dynamics simulation study. Future Virology, 0, , .	0.9	1
4280	Bovine Serum Amine Oxidase and Polyamine Analogues: Chemical Synthesis and Biological Evaluation Integrated with Molecular Docking and 3-D QSAR Studies. Journal of Chemical Information and Modeling, 2022, 62, 3910-3927.	2.5	0
4281	Phytochemical Discrimination, Biological Activity and Molecular Docking of Water-Soluble Inhibitors from Saussurea costus Herb against Main Protease of SARS-CoV-2. Molecules, 2022, 27, 4908.	1.7	9
4282	Pharmacological and In Silico Analysis of Oat Avenanthramides as EGFR Inhibitors: Effects on EGF-Induced Lung Cancer Cell Growth and Migration. International Journal of Molecular Sciences, 2022, 23, 8534.	1.8	8
4283	Novel drug design framework as a response to neglected and emerging diseases. Journal of Biomolecular Structure and Dynamics, 2023, 41, 6664-6675.	2.0	0
4284	Essential oil from Oliveria decumbens accelerates in vivo wound healing: a possible mechanism by the involvement of glycogen synthase kinase-3. Zanco Journal of Medical Sciences, 2022, 26, 118-126.	0.0	1
4285	Computational and Experimental Design of Quinones for Electrochemical CO₂ Capture and Concentration. ACS Sustainable Chemistry and Engineering, 2022, 10, 11387-11395.	3.2	5
4286	Pharmacokinetics and molecular docking of novel antineoplastic sesquiterpene lactone from Tarchonanthus camphoratus L: an in silico approaches. Structural Chemistry, 2023, 34, 703-712.	1.0	1
4288	Non-steroidal anti-inflammatory drugs ketorolac and etodolac can augment the treatment against pneumococcal meningitis by targeting penicillin-binding proteins. Microbial Pathogenesis, 2022, 170, 105694.	1.3	10
4289	Synthesis of 4-substituted benzyl-2-triazole-linked-tryptamine-paeonol derivatives and evaluation of their selective inhibitions against butyrylcholinesterase and monoamine oxidase-B. International Journal of Biological Macromolecules, 2022, 217, 910-921.	3.6	16
4290	The drp-1-mediated mitochondrial fission inhibitor mdivi-1 impacts the function of ion channels and pathways underpinning vascular smooth muscle tone. Biochemical Pharmacology, 2022, 203, 115205.	2.0	1
4291	â€œVirtual patch clamp analysisâ€•for predicting the functional significance of pathogenic variants in sodium channels. Epilepsy Research, 2022, 186, 107002.	0.8	2

#	Article	IF	Citations
4292	Predicting 2H NMR acyl chain order parameters with graph neural networks. Computational Biology and Chemistry, 2022, 100, 107750.	1.1	2
4293	Prediction of ligand binding sites using improved blind docking method with a Machine Learning-Based scoring function. Chemical Engineering Science, 2022, 261, 117962.	1.9	4
4294	Integrated strategy of network pharmacology, molecular docking, HPLC-DAD and mice model for exploring active ingredients and pharmacological mechanisms of Penthorum chinense Pursh against alcoholic liver injury. Journal of Ethnopharmacology, 2022, 298, 115589.	2.0	9
4295	Targeting the gp130_D5 domain through pharmacophore modelling and structure-based virtual screening using natural plant products: A detailed molecular dynamics study for development of novel anti-cancer therapeutics. Journal of Molecular Graphics and Modelling, 2022, 117, 108290.	1.3	0
4299	Crystal structure of aminopentamide hydrogen sulfate, (C₁₉H₂₅N₂O)(HSO₄). Powder Diffraction, 0, , 1-6.	0.4	0
4300	In silico studies disclose the underlying link between binding affinity and redox potential in laccase isoforms. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7265-7276.	2.0	1
4301	Structural and functional implications of leucine-rich repeats in toll-like receptor1 subfamily. Journal of Biosciences, 2022, 47, .	0.5	0
4302	High-Throughput Screening and Molecular Dynamics Simulation of Natural Products for the Identification of Anticancer Agents against MCM7 Protein. Applied Bionics and Biomechanics, 2022, 2022, 1-12.	0.5	3
4303	Abetting host immune response by inhibiting rhipicephalus sanguineus Evasin-1: An in silico approach. PLoS ONE, 2022, 17, e0271401.	1.1	3
4304	Diffusion of small molecule drugs is affected by surface interactions and crowder proteins. IScience, 2022, 25, 105088.	1.9	5
4305	Computational exploration of the dual role of the phytochemical fortunellin: Antiviral activities against SARS-CoV-2 and immunomodulatory abilities against the host. Computers in Biology and Medicine, 2022, 149, 106049.	3.9	3
4306	New carbazol derivatives containing 1,2,4-triazole: Synthesis, characterization, DFT study, acetylcholinesterase activity and docking study. Journal of the Indian Chemical Society, 2022, 99, 100690.	1.3	0
4307	Bacterial FtsZ inhibition by benzo[d]imidazole-2-carboxamide derivative with anti-TB activity. Future Medicinal Chemistry, 2022, 14, 1361-1373.	1.1	6
4308	Molecular interactions of hesperidin with DMPC/cholesterol bilayers. Chemico-Biological Interactions, 2022, 366, 110131.	1.7	3
4309	Potential inhibitory activity of phytoconstituents against black fungus: In silico ADMET, molecular docking and MD simulation studies. Computational Toxicology, 2022, 24, 100247.	1.8	20
4310	Machine learning models for phase transition and decomposition temperature of ionic liquids. Journal of Molecular Liquids, 2022, 366, 120247.	2.3	7
4311	Structural insights of a putative Î²-1,4-xylosidase (PsGH43F) of glycoside hydrolase family 43 from Pseudopedobacter saltans. International Journal of Biological Macromolecules, 2022, 221, 751-762.	3.6	1
4312	Mahanimbine isolated from Murraya koenigii inhibits P-glycoprotein involved in lung cancer chemoresistance. Bioorganic Chemistry, 2022, 129, 106170.	2.0	7

#	Article	IF	Citations
4313	Antibacterial activity and molecular studies of non-symmetric POCOP-Pd(II) pincer complexes derived from 2,4-dihydroxybenzaldehyde (2,4-DHBA). Polyhedron, 2022, 227, 116115.	1.0	0
4314	A comprehensive analysis on the relationship between BDE-209 exposure and erectile dysfunction. Chemosphere, 2022, 308, 136486.	4.2	3
4315	Targeting neuronal calcium channels and GSK3Î² for Alzheimerâ€™s disease with naturally-inspired Diels-Alder adducts. Bioorganic Chemistry, 2022, 129, 106152.	2.0	1
4316	Non-covalent acetylcholinesterase inhibitors: In vitro screening and molecular modeling for novel selective insecticides. Toxicology in Vitro, 2022, 85, 105463.	1.1	2
4317	Design of organic materials with tailored optical properties: Predicting quantum-chemical polarizabilities and derived quantities. , 2023, , 653-674.		0
4318	Learning excited-state properties. , 2023, , 467-488.		1
4319	Immunomodulatory efficacy of Cousinia thomsonii C.B. Clarke in ameliorating inflammatory cascade expressions. Journal of Ethnopharmacology, 2023, 300, 115727.	2.0	0
4320	Identification of upregulated genes in glioblastoma and glioblastoma cancer stem cells using bioinformatics analysis. Gene, 2023, 848, 146895.	1.0	4
4321	Computational Docking Study of Calanolides as Potential Inhibitors of SARS-CoV-2 Main Protease. French-Ukrainian Journal of Chemistry, 2022, 10, 48-59.	0.1	0
4322	A structure-guided computational screening approach for predicting plant enzymeâ€“metabolite interactions. Methods in Enzymology, 2022, , .	0.4	0
4323	Virus-host interaction analysis in colorectal cancer identifies core virus network signature and small molecules. Computational and Structural Biotechnology Journal, 2022, 20, 4025-4039.	1.9	2
4324	Whole proteome mapping of compound-protein interactions. Current Research in Chemical Biology, 2022, 2, 100035.	1.4	1
4325	Evaluating fast methods for static polarizabilities on extended conjugated oligomers. Physical Chemistry Chemical Physics, 2022, 24, 23173-23181.	1.3	1
4326	Identification of Potential Ligands of the Main Protease of Coronavirus SARS-CoV-2 (2019-nCoV) Using Multimodal Generative Neural-Networks. French-Ukrainian Journal of Chemistry, 2022, 10, 30-47.	0.1	0
4327	Design, synthesis, and cytotoxicity evaluation of novel indole-acylhydrazone derivatives of 4-pyridinone as potential histone deacetylase-2 inhibitors. Research in Pharmaceutical Sciences, 2022, 17, 572.	0.6	1
4328	Dayak Onions (Eleutherine americana L Merr) Reduced Mesothelial Cell Detachment After Laparoscopy in Rats. Open Access Macedonian Journal of Medical Sciences, 2022, 10, 1321-1329.	0.1	0
4329	Discovery of compounds with viscosity-reducing effects on biopharmaceutical formulations with monoclonal antibodies. Computational and Structural Biotechnology Journal, 2022, 20, 5420-5429.	1.9	3
4330	DenovoProfiling: A webserver for de novo generated molecule library profiling. Computational and Structural Biotechnology Journal, 2022, 20, 4082-4097.	1.9	1

#	Article	IF	Citations
4331	Impact of solvent interactions on¹H and¹³C chemical shifts investigated using DFT and a reference dataset recorded in CDCl₃and CCl₄. Physical Chemistry Chemical Physics, 2022, 24, 23551-23560.	1.3	4
4332	Molecular Docking Studies and in silico ADMET Screening of Indazole Scaffolds as VEGFR and Enoyl-ACP (CoA) Reductase Inhibitors. Asian Journal of Chemistry, 2022, 34, 2311-2317.	0.1	0
4333	New inhibitors of cathepsin V impair tumor cell proliferation and elastin degradation and increase immune cell cytotoxicity. Computational and Structural Biotechnology Journal, 2022, 20, 4667-4687.	1.9	5
4334	Unsupervised Prediction Method for Drug-Target Interactions Based on Structural Similarity. Lecture Notes in Computer Science, 2022, , 517-532.	1.0	1
4335	Protein-Ligand Binding Affinity Prediction Based on Deep Learning. Lecture Notes in Computer Science, 2022, , 310-316.	1.0	0
4336	Synthesis, antitumor activity, 3D-QSAR and molecular docking studies of new iodinated 4-(3H)-quinazolinones 3N-substituted. RSC Advances, 2022, 12, 21340-21352.	1.7	1
4337	Prediction and validation of host-pathogen interactions by a versatile inference approach using Aspergillus fumigatus as a case study. Computational and Structural Biotechnology Journal, 2022, 20, 4225-4237.	1.9	1
4338	Molecular docking analysis of fluoroquinolones and other natural and synthetic compounds with the HCV NS3 helicase. Bioinformation, 2022, 18, 147-154.	0.2	2
4339	Molecular docking analysis of estrogen receptor binding phytocomponents identified from the ethyl acetate extract of Salicornia herbacea (L). Bioinformation, 2022, 18, 273-283.	0.2	2
4340	The COVID-19 Oral Drug Molnupiravir Is a CES2 Substrate: Potential Drug-Drug Interactions and Impact of CES2 Genetic Polymorphism In Vitro. Drug Metabolism and Disposition, 2022, 50, 1151-1160.	1.7	12
4341	Mechanism of Astragali Radix for the treatment of osteoarthritis: A study based on network pharmacology and molecular docking. Medicine (United States), 2022, 101, e29885.	0.4	3
4342	Novel Approaches for Inhibiting the Indoor Allergen Der f 2 Excreted from House Dust Mites by Todomatsu Oil Produced from Woodland Residues. International Journal of Environmental Research and Public Health, 2022, 19, 10881.	1.2	3
4343	Mechanisms and network pharmacological analysis of Yangyin Fuzheng Jiedu prescription in the treatment of hepatocellular carcinoma. Cancer Medicine, 2023, 12, 3237-3259.	1.3	3
4344	A Computational approach in identifying the herbal compounds as Lactation inducer. Research Journal of Pharmacy and Technology, 2022, , 3345-3350.	0.2	0
4345	Homology modeling of human BAP1 and analysis of its binding properties through molecular docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7158-7173.	2.0	1
4346	Computational Assessment of Xanthones from African Medicinal Plants as Aldose Reductase Inhibitors. Computation, 2022, 10, 146.	1.0	5
4347	SMICLR: Contrastive Learning on Multiple Molecular Representations for Semisupervised and Unsupervised Representation Learning. Journal of Chemical Information and Modeling, 2022, 62, 3948-3960.	2.5	10
4348	Molecular Docking, Molecular Dynamics Simulations, and Free Energy Calculation Insights into the Binding Mechanism between VS-4718 and Focal Adhesion Kinase. ACS Omega, 2022, 7, 32442-32456.	1.6	10

#	Article	IF	Citations
4349	De Novo Prediction of Drug Targets and Candidates by Chemical Similarity-Guided Network-Based Inference. International Journal of Molecular Sciences, 2022, 23, 9666.	1.8	2
4350	Deciphering the Potential of Pre and Pro-Vitamin D of Mushrooms against Mpro and PLpro Proteases of COVID-19: An In Silico Approach. Molecules, 2022, 27, 5620.	1.7	2
4351	Mechanistic study of the antibacterial potential of the prenylated flavonoid auriculasin against Escherichia coli. Archiv Der Pharmazie, 2022, 355, .	2.1	5
4352	Virtual Screening of Native Variants of Focal Adhesion Kinase - A QSAR, Molecular Docking, and Dynamic Simulation Study. Letters in Drug Design and Discovery, 2024, 21, 254-269.	0.4	0
4353	Modulation of mitochondrial permeability transition pore opening by Myricetin and prediction of its-drug-like potential usingin silicoapproach. Drug and Chemical Toxicology, 2023, 46, 1004-1014.	1.2	0
4354	Some New 1,2,4-triazole Derivatives Bearing the Pyrimidine Moiety as Potential Antimycobacterial Agents: Synthesis and Docking Analysis. Letters in Drug Design and Discovery, 2023, 20, 1664-1674.	0.4	0
4355	Targeting Protein Pockets with Halogen Bonds: The Role of the Halogen Environment. Journal of Chemical Information and Modeling, 0, , .	2.5	7
4356	TAIGET: A small-molecule target identification and annotation web server. Frontiers in Pharmacology, 0, 13, .	1.6	2
4357	Anti-asthmatic fraction screening and mechanisms prediction of Schisandrae Sphenantherae Fructus based on a combined approach. Frontiers in Pharmacology, 0, 13, .	1.6	1
4358	Consensus docking and MM-PBSA computations identify putative furin protease inhibitors for developing potential therapeutics against COVID-19. Structural Chemistry, 2022, 33, 2221-2241.	1.0	7
4359	Structure-based discovery of small molecules that disaggregate Alzheimerâ€™s disease tissue derived tau fibrils in vitro. Nature Communications, 2022, 13, .	5.8	68
4360	Pharmacoinformatic study of inhibitory potentials of selected flavonoids against papain-like protease and 3-chymotrypsin-like protease of SARS-CoV-2. Clinical Phytoscience, 2022, 8, .	0.8	1
4361	Ilimaquinone (Marine Sponge Metabolite) Induces Apoptosis in HCT-116 Human Colorectal Carcinoma Cells via Mitochondrial-Mediated Apoptosis Pathway. Marine Drugs, 2022, 20, 582.	2.2	6
4362	Assessing Molecular Docking Tools to Guide the Design of Polymeric Materials Formulations: A Case Study of Canola and Soybean Protein. Polymers, 2022, 14, 3690.	2.0	2
4363	A Combined Bayesian and Similarity-Based Approach for Predicting E. coli Biofilm Inhibition by Phenolic Natural Compounds. Journal of Natural Products, 2022, 85, 2255-2265.	1.5	3
4364	In-Silico Molecular Modeling Studies to Identify Novel Potential Inhibitors of HPV E6 Protein. Vaccines, 2022, 10, 1452.	2.1	3
4365	Structural modeling of the hERG potassium channel and associated drug interactions. Frontiers in Pharmacology, 0, 13, .	1.6	7
4366	Epicatechin analogues may hinder human parainfluenza virus infection by inhibition of hemagglutinin neuraminidase protein and prevention of cellular entry. Journal of Molecular Modeling, 2022, 28, .	0.8	1

#	Article	IF	Citations
4367	Predicting octanol/water partition coefficients and pKa for the SAMPL7 challenge using the SM12, SM8 and SMD solvation models. Journal of Computer-Aided Molecular Design, 2022, 36, 687-705.	1.3	4
4368	Skin permeability prediction with MD simulation sampling spatial and alchemical reaction coordinates. Biophysical Journal, 2022, 121, 3837-3849.	0.2	6
4369	Multi-Level High-Throughput Screening for Discovery of Ligands That Inhibit Insulin Aggregation. Molecular Pharmaceutics, 2022, 19, 3770-3783.	2.3	0
4370	Identification of Monobenzone as a Novel Potential Anti-Acute Myeloid Leukaemia Agent That Inhibits RNR and Suppresses Tumour Growth in Mouse Xenograft Model. Cancers, 2022, 14, 4710.	1.7	0
4371	How do we further enhance 2D fingerprint similarity searching for novel drug discovery?. Expert Opinion on Drug Discovery, 2022, 17, 1173-1176.	2.5	2
4372	Identification of Novel Ribonucleotide Reductase Inhibitors for Therapeutic Application in Bile Tract Cancer: An Advanced Pharmacoinformatics Study. Biomolecules, 2022, 12, 1279.	1.8	1
4373	A pocket-based 3D molecule generative model fueled by experimental electron density. Scientific Reports, 2022, 12, .	1.6	8
4374	Computational discovery of novel inhibitory candidates targeting versatile transcriptional repressor MBD2. Journal of Molecular Modeling, 2022, 28, .	0.8	1
4376	Attempting to Increase the Effectiveness of the Antidepressant Trazodone Hydrochloride Drug Using Ï€-Acceptors. International Journal of Environmental Research and Public Health, 2022, 19, 11281.	1.2	0
4377	Inhibitory potentials of phytocompounds from Ocimum gratissimum against anti-apoptotic BCL-2 proteins associated with cancer: an integrated computational study. Egyptian Journal of Basic and Applied Sciences, 2022, 9, 588-608.	0.2	0
4378	Fe₃O₄â€supported sulfonated graphene oxide as a green and magnetically separable nanocatalyst for synthesis of 2-amino-3-cyano-4H-chromene derivatives and their in-silico studies. Synthetic Communications, 2022, 52, 1926-1955.	1.1	8
4379	Virtual Screening and Quantum Chemistry Analysis for SARS-CoV-2 RNA-Dependent RNA Polymerase Using the ChEMBL Database: Reproduction of the Remdesivir-RTP and Favipiravir-RTP Binding Modes Obtained from Cryo-EM Experiments with High Binding Affinity. International Journal of Molecular Sciences, 2022, 23, 11009.	1.8	1
4380	Docking Study on Caspase 3 Inhibitors As Potential Drugs For Traumatic Brain Cell Apoptosis. Letters in Drug Design and Discovery, 2024, 21, 542-551.	0.4	0
4381	Auto3D: Automatic Generation of the Low-Energy 3D Structures with ANI Neural Network Potentials. Journal of Chemical Information and Modeling, 2022, 62, 5373-5382.	2.5	16
4382	The First 5â€²-Phosphorylated 1,2,3-Triazolyl Nucleoside Analogues with Uracil and Quinazoline-2,4-Dione Moieties: A Synthesis and Antiviral Evaluation. Molecules, 2022, 27, 6214.	1.7	9
4383	Anti-angiogenic potential of bioactive phytochemicals fromHelicteres isoratargeting VEGFR-2 to fight cancer through molecular docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7447-7462.	2.0	7
4384	Natural Xylooligosaccharides Exert Antitumor Activity via Modulation of Cellular Antioxidant State and TLR4. International Journal of Molecular Sciences, 2022, 23, 10430.	1.8	10
4385	GCMM: graph convolution network based on multimodal attention mechanism for drug repurposing. BMC Bioinformatics, 2022, 23, .	1.2	5

#	Article	IF	Citations
4386	Molecular Docking and Drug-likeness Prediction of New Potent Tubulin Colchicine Binding Site Inhibitors for Potential Antitumor Drug. Cumhuriyet Science Journal, 2022, 43, 398-403.	0.1	0
4387	Crystal structure and reaction mechanism of a bacterial Mgâ€dechelatase homolog from the Chloroflexi Anaerolineae. Protein Science, 2022, 31, .	3.1	0
4388	Chemoinformatic Design and Profiling of Derivatives of Dasabuvir, Efavirenz, and Tipranavir as Potential Inhibitors of Zika Virus RNA-Dependent RNA Polymerase and Methyltransferase. ACS Omega, 2022, 7, 33330-33348.	1.6	4
4389	A novel phenolic derivative inhibits AHL-dependent quorum sensing signaling in Pseudomonas aeruginosa. Frontiers in Pharmacology, 0, 13, .	1.6	6
4391	Multispectral and Molecular Docking Studies Reveal Potential Effectiveness of Antidepressant Fluoxetine by Forming Ï€-Acceptor Complexes. Molecules, 2022, 27, 5883.	1.7	0
4392	The latest guidance on the simultaneous design of virtually active and non-hemolytic peptides. Expert Opinion on Drug Discovery, 0, , 1-3.	2.5	0
4393	Cheminformatics-Based Discovery of Potential Chemical Probe Inhibitors of Omicron Spike Protein. International Journal of Molecular Sciences, 2022, 23, 10315.	1.8	7
4394	MGPLI: exploring multigranular representations for proteinâ€“ligand interaction prediction. Bioinformatics, 2022, 38, 4859-4867.	1.8	7
4395	Promising antibacterials for LLM ofStaphylococcus aureususing virtual screening, molecular docking, dynamics, and MMPBSA. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7277-7289.	2.0	2
4396	Development of a Deep Learning Generative Neural Network for Computer-Aided Design of Potential SARS-Cov-2 Inhibitors. Mathematical Biology and Bioinformatics, 2022, 17, 188-207.	0.1	2
4397	Is an Inductive Effect Explicit Account Required for Atomic Charges Aimed at Use within the Force Fields?. Journal of Physical Chemistry A, 2022, 126, 6278-6294.	1.1	3
4398	Aptasensors Based on Graphene Field-Effect Transistors for Arsenite Detection. ACS Applied Nano Materials, 2022, 5, 12848-12854.	2.4	6
4399	Glycosylated Flavonoid Compounds as Potent CYP121 Inhibitors of Mycobacterium tuberculosis. Biomolecules, 2022, 12, 1356.	1.8	8
4400	Individual and Synergistic Potential of Bioactive Compounds from Chrysopogon Zizanioides Against Main-Protease of SARSCov-2 using Computational Approach. Biosciences, Biotechnology Research Asia, 2022, 19, 657-670.	0.2	0
4401	Identification of novel pyrrolopyrimidine and pyrrolopyridine derivatives as potent ENPP1 inhibitors. Journal of Enzyme Inhibition and Medicinal Chemistry, 2022, 37, 2434-2451.	2.5	8
4402	MISPR: an open-source package for high-throughput multiscale molecular simulations. Scientific Reports, 2022, 12, .	1.6	5
4403	Expression and estrogen regulation of G proteinâ€coupled estrogen receptor in human glioblastoma cells. Oncology Letters, 2022, 24, .	0.8	6
4404	Lignin Nanoparticle Morphology Depends on Polymer Properties and Solvent Composition: an Experimental and Computational Study. ACS Applied Polymer Materials, 2022, 4, 6925-6935.	2.0	6

#	Article	IF	Citations
4405	In silico studies of natural product-like caffeine derivatives as potential MAO-B inhibitors/AA_{2A}R antagonists for the treatment of Parkinson's disease. Journal of Integrative Bioinformatics, 2022, 19, .	1.0	7
4407	Antiviral activity of Cenostigma pluviosum var. peltophoroides extract and fractions against SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7297-7308.	2.0	5
4408	New Chemicals Suppressing SARS-CoV-2 Replication in Cell Culture. Molecules, 2022, 27, 5732.	1.7	2
4409	Rosavin Ameliorates Hepatic Inflammation and Fibrosis in the NASH Rat Model via Targeting Hepatic Cell Death. International Journal of Molecular Sciences, 2022, 23, 10148.	1.8	7
4410	In-Silico Drug Toxicity and Interaction Prediction for Plant Complexes Based on Virtual Screening and Text Mining. International Journal of Molecular Sciences, 2022, 23, 10056.	1.8	0
4411	Discovery of novel IDH1-R132C inhibitors through structure-based virtual screening. Frontiers in Pharmacology, 0, 13, .	1.6	1
4412	Exploring Anti-osteoporosis Medicinal Herbs using Cheminformatics and Deep Learning Approaches. Combinatorial Chemistry and High Throughput Screening, 2022, 25, .	0.6	0
4413	In Silico Pharmacokinetic Profiling of the Identified Bioactive Metabolites of Pergularia tomentosa L. Latex Extract and In Vitro Cytotoxic Activity via the Induction of Caspase-Dependent Apoptosis with S-Phase Arrest. Pharmaceuticals, 2022, 15, 1132.	1.7	3
4414	In-silico Approach to Investigate the Phytochemicals of Terminalia arjuna as Multitarget Inhibitors of Proteins Involved with Lung Cancer. Letters in Drug Design and Discovery, 2024, 21, 329-338.	0.4	0
4415	DFT and In-silico Investigations along with In-vitro Antitumor and Antimicrobial Assessments of Pharmacological Molecules. Current Organic Synthesis, 2022, 19, .	0.7	0
4416	StackPR is a new computational approach for large-scale identification of progesterone receptor antagonists using the stacking strategy. Scientific Reports, 2022, 12, .	1.6	7
4417	Clustering Analysis, Structure Fingerprint Analysis, and Quantum Chemical Calculations of Compounds from Essential Oils of Sunflower (Helianthus annuus L.) Receptacles. International Journal of Molecular Sciences, 2022, 23, 10169.	1.8	2
4418	Quantum chemistry calculation and experimental research on the component proportion of black disperse dye. Textile Reseach Journal, 2023, 93, 750-761.	1.1	1
4419	Shionone-Targeted Pneumolysin to Ameliorate Acute Lung Injury Induced by Streptococcus pneumoniae In Vivo and In Vitro. Molecules, 2022, 27, 6258.	1.7	3
4420	Prioritizing Virtual Screening with Interpretable Interaction Fingerprints. Journal of Chemical Information and Modeling, 2022, 62, 4300-4318.	2.5	13
4421	Novel machine learning models to predict endocrine disruption activity for high-throughput chemical screening. Frontiers in Toxicology, 0, 4, .	1.6	6
4422	In silicoapproach identified benzoylguanidines as SARS-CoV-2 main protease (M^{pro}) potential inhibitors. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7686-7699.	2.0	2
4423	Screening of the Role of the Chemical Structure in the Electrochemical Stability Window of Ionic Liquids: DFT Calculations Combined with Data Mining. Journal of Chemical Information and Modeling, 2022, 62, 4702-4712.	2.5	4

#	Article	IF	Citations
4424	Nanomaterialsâ€Mediated Coâ€Stimulation of Tollâ€Like Receptors and CD40 for Antitumor Immunity. Advanced Materials, 2022, 34, .	11.1	19
4425	Odorant-Binding Protein 3-Oriented Rational Design and Discovery of Novel Jasmonate Derivatives as Potential Aphid-Repellent Agents. Journal of Agricultural and Food Chemistry, 2022, 70, 11792-11803.	2.4	4
4426	MetaboAnnotator: an efficient toolbox to annotate metabolites in genome-scale metabolic reconstructions. Bioinformatics, 2022, 38, 4831-4832.	1.8	2
4427	The AhR ligand phthiocol and vitamin K analogs as Pseudomonas aeruginosa quorum sensing inhibitors. Frontiers in Microbiology, 0, 13, .	1.5	2
4428	One of the 5-aminosalicylates drug, mesalamine as a drug repurposing lead against breast cancer. Bulletin of the National Research Centre, 2022, 46, .	0.7	0
4429	Calcium dobesilate efficiency in the treatment of diabetic kidney disease through suppressing MAPK and chemokine signaling pathways based on clinical evaluation and network pharmacology. Frontiers in Pharmacology, 0, 13, .	1.6	2
4431	Crystal structure of the Rho-associated coiled-coil kinase 2 inhibitor belumosudil bound to CK2Î±. Acta Crystallographica Section F, Structural Biology Communications, 2022, 78, 348-353.	0.4	1
4432	Exploring the mechanism of Shexiang Tongxin dropping pill in the treatment of microvascular angina through network pharmacology and molecular docking. Annals of Translational Medicine, 2022, 10, 983-983.	0.7	2
4434	Computational model predicts protein binding sites of a luminescent ligand equipped with guanidiniocarbonyl-pyrrole groups. Beilstein Journal of Organic Chemistry, 0, 18, 1322-1331.	1.3	2
4435	Molecular docking study of various Enterovirusâ€”A71 3C protease proteins and their potential inhibitors. Frontiers in Microbiology, 0, 13, .	1.5	0
4436	ASBase: The universal database for aggregate science. Aggregate, 2023, 4, .	5.2	15
4437	Ligand-based prediction of hERG-mediated cardiotoxicity based on the integration of different machine learning techniques. Frontiers in Pharmacology, 0, 13, .	1.6	7
4438	Identification of New Carbonic Anhydrase VII Inhibitors by Structure-Based Virtual Screening. Journal of Chemical Information and Modeling, 2022, 62, 4760-4770.	2.5	1
4440	A Potential Anticancer Mechanism of Finger Root (Boesenbergia rotunda) Extracts against a Breast Cancer Cell Line. Scientifica, 2022, 2022, 1-17.	0.6	5
4441	Screening of potential inhibitors targeting the main protease structure of SARS-CoV-2 via molecular docking. Frontiers in Pharmacology, 0, 13, .	1.6	3
4442	Comparative inhibitory screening of phytoconstituents from Capparis decidua against various ailments targets: a novel In-silico semblance ADME/Tox profiling studies. Advances in Traditional Medicine, 0, , .	1.0	2
4443	In Vitro Antioxidant and Antimicrobial Potency of Mimosa pudica of Nepalese Terai Region: Insight into L-Mimosine as an Antibacterial Agent. Evidence-based Complementary and Alternative Medicine, 2022, 2022, 1-11.	0.5	1
4444	Pangenome and subtractive genomic analysis of Clostridioides difficile reveals putative drug targets. Journal of Proteins and Proteomics, 0, , .	1.0	0

#	Article	IF	Citations
4445	Advanced simulations and screening to repurposing a 3C protease inhibitor against the rupintrivir-resistant human norovirus-induced gastroenteritis. Journal of Molecular Graphics and Modelling, 2022, , 108345.	1.3	2
4446	Molecular docking of phyto-compounds against VP1 and VP2 proteins of IPNV (Infectious Pancreatic) Tj ETQq1 1 0.784314 rgBT /Ove	0.9	0
4447	Targeting human thymidylate synthase: Ensemble-based virtual screening for drug repositioning and the role of water. Journal of Molecular Graphics and Modelling, 2023, 118, 108348.	1.3	2
4448	In silico evaluation of Philippine Natural Products against SARS-CoV-2 Main Protease. Journal of Molecular Modeling, 2022, 28, .	0.8	0
4449	Identification of natural inhibitor against L1 Î²-lactamase present in Stenotrophomonas maltophilia. Journal of Molecular Modeling, 2022, 28, .	0.8	1
4450	Multi-target direct-acting SARS-CoV-2 antivirals against the nucleotide-binding pockets of virus-specific proteins. Virology, 2022, 577, 1-15.	1.1	6
4451	Evaluation of wound healing effect of Mallotus philippensis (Lam.) Mull. Arg. by in silico multitargets directed for multiligand approach. In Silico Pharmacology, 2022, 10, .	1.8	2
4452	Bioactive phytosteroids from Araucaria columnaris (G. Forst.) Hook.: RP-HPLC-DAD analysis, in-vitro antioxidant potential, in-silico computational study and molecular docking against 3MNG and 1N3U. Steroids, 2022, 188, 109116.	0.8	1
4453	Combining machine learning and quantum chemical calculations for high-throughput virtual screening of thermally activated delayed fluorescence molecular materials: the impact of selection strategy and structural mutations. RSC Advances, 2022, 12, 30962-30975.	1.7	4
4454	Design, synthesis and biological evaluation of novel substituted indazole-1,2,3-triazolyl-1,3,4-oxadiazoles: Antimicrobial activity evaluation and docking study. Results in Chemistry, 2022, 4, 100605.	0.9	8
4455	OSCAR: an extensive repository of chemically and functionally diverse organocatalysts. Chemical Science, 2022, 13, 13782-13794.	3.7	11
4456	Identification of Diosmin and Flavin Adenine Dinucleotide as Repurposing Treatments for Monkeypox Virus: A Computational Study. International Journal of Molecular Sciences, 2022, 23, 11570.	1.8	11
4457	Design, Synthesis, and Biological Evaluation of Fluoroquinolones Linked to 4-Thiazolidinone Moieties as Potent Antimicrobial Agents: Docking Analysis. Russian Journal of General Chemistry, 2022, 92, 1749-1760.	0.3	0
4458	In silico and invitro Antidiabetic Characterization and ADME Studies of Rhus parviflora. Research Journal of Pharmacy and Technology, 2022, , 3919-3923.	0.2	1
4460	Complementary Dual Approach for In Silico Target Identification of Potential Pharmaceutical Compounds in Cystic Fibrosis. International Journal of Molecular Sciences, 2022, 23, 12351.	1.8	1
4461	Exploring the druggability of the binding site of aurovertin, an exogenous allosteric inhibitor of FOF1-ATP synthase. Frontiers in Pharmacology, 0, 13, .	1.6	2
4462	An Evaluation of the Novel Biological Properties of Diterpenes Isolated from Plectranthus ornatus Codd. In Vitro and In Silico. Cells, 2022, 11, 3243.	1.8	3
4463	Transition state search and geometry relaxation throughout chemical compound space with quantum machine learning. Journal of Chemical Physics, 2022, 157, .	1.2	7

#	Article	IF	Citations
4464	Computational and Biophysical Characterization of Heterocyclic Derivatives of Anthraquinone against Human Aurora Kinase A. ACS Omega, 2022, 7, 39603-39618.	1.6	4
4465	Stereochemical editing logic powered by the epimerization of unactivated tertiary stereocenters. Science, 2022, 378, 383-390.	6.0	25
4466	Theoretical Investigation of Key Properties of the Pyrolysis of Methyl, Ethyl, and Dimethyl Dioxolane Isomers. Journal of Physical Chemistry A, 2022, 126, 8326-8336.	1.1	2
4467	MeDBA: the Metalloenzyme Data Bank and Analysis platform. Nucleic Acids Research, 2023, 51, D593-D602.	6.5	12
4468	PacDOCK: A Web Server for Positional Distance-Based and Interaction-Based Analysis of Docking Results. Molecules, 2022, 27, 6884.	1.7	7
4469	Computational Analysis of Bacopa monnieri (L.) Wettst. Compounds for Drug Development against Neurodegenerative Disorders. Current Computer-Aided Drug Design, 2023, 19, 24-36.	0.8	3
4470	Pharmacophore Modeling Using Machine Learning for Screening the Bloodâ€“Brain Barrier Permeation of Xenobiotics. International Journal of Environmental Research and Public Health, 2022, 19, 13471.	1.2	5
4471	Is Caperatic Acid the Only Compound Responsible for Activity of Lichen Platismatia glauca within the Nervous System?. Antioxidants, 2022, 11, 2069.	2.2	8
4472	Nrf2-regulated antioxidant response ameliorating ionizing radiation-induced damages explored throughinÂvitroand molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2023, 41, 8472-8484.	2.0	1
4473	Papaya Leaf Extracts as Potential Dengue Treatment: An In-Silico Study. International Journal of Molecular Sciences, 2022, 23, 12310.	1.8	5
4474	CAT: A Compound Attachment Tool for the Construction of Composite Chemical Compounds. Journal of Chemical Information and Modeling, 0, , .	2.5	0
4475	Virtual Screening and Quantitative Structureâ€“Activity Relationship of Moringa oleifera with Melanoma Antigen A (MAGE-A) Genes against the Therapeutics of Non-Small Cell Lung Cancers (NSCLCs). Cancers, 2022, 14, 5052.	1.7	2
4476	Thiadiazole Functionalized Salicylaldehyde-Schiff Base as a pH-responsive and chemo-reversible â€œTurn-Offâ€•fluorescent probe for selective cu (II) detection: Logic Gate Behaviour and Molecular Docking Studies. Journal of Fluorescence, 2023, 33, 25-41.	1.3	4
4477	Compound C Inhibits Ovarian Cancer Progression via PI3K-AKT-mTOR-NFÎºB Pathway. Cancers, 2022, 14, 5099.	1.7	3
4479	DrugRep: an automatic virtual screening server for drug repurposing. Acta Pharmacologica Sinica, 2023, 44, 888-896.	2.8	21
4480	Computational Studies of Allylpyrocatechol from Piper betle L. as Inhibitor Against Superoxide Dismutase, Catalase, and Glutathione peroxidase as Antioxidant Enzyme. Letters in Drug Design and Discovery, 2024, 21, 559-567.	0.4	0
4481	Identification of Novel Antimicrobial Resistance Genes Using Machine Learning, Homology Modeling, and Molecular Docking. Microorganisms, 2022, 10, 2102.	1.6	4
4482	cardioToxCSM: A Web Server for Predicting Cardiotoxicity of Small Molecules. Journal of Chemical Information and Modeling, 2022, 62, 4827-4836.	2.5	12

#	Article	IF	Citations
4483	Computational prediction and analysis of targeting 17-beta-hydroxysteroid dehydrogenase (17-beta-HSD1) with natural products for colorectal cancer treatment. Journal of Biomolecular Structure and Dynamics, 2023, 41, 7966-7974.	2.0	1
4484	Quantum-based machine learning and AI models to generate force field parameters for drug-like small molecules. Frontiers in Molecular Biosciences, 0, 9, .	1.6	2
4485	In silicostructural elucidation of Nipah virus L protein and targeting RNA-dependent RNA polymerase domain by nucleoside analogs. Journal of Biomolecular Structure and Dynamics, 2023, 41, 8215-8229.	2.0	6
4486	Computational approach to attenuate virulence of Pseudomonas aeruginosa through bioinspired silver nanoparticles. 3 Biotech, 2022, 12, .	1.1	1
4487	Virus-CKB 2.0: Viral-Associated Disease-Specific Chemogenomics Knowledgebase. ACS Omega, 2022, 7, 37476-37484.	1.6	0
4488	Ligand additivity relationships enable efficient exploration of transition metal chemical space. Journal of Chemical Physics, 2022, 157, .	1.2	6
4489	The NORMAN Suspect List Exchange (NORMAN-SLE): facilitating European and worldwide collaboration on suspect screening in high resolution mass spectrometry. Environmental Sciences Europe, 2022, 34, .	2.6	37
4490	Protocol for iterative optimization of modified peptides bound to protein targets. Journal of Computer-Aided Molecular Design, 2022, 36, 825-835.	1.3	3
4491	Identification of essential oil phytocompounds as natural inhibitors of Odorant-binding protein to prevent malaria throughin silicoapproach. Journal of Biomolecular Structure and Dynamics, 2023, 41, 8323-8333.	2.0	0
4492	Liposomal Formulations Loaded with a Eugenol Derivative for Application as Insecticides: Encapsulation Studies and In Silico Identification of Protein Targets. Nanomaterials, 2022, 12, 3583.	1.9	4
4493	Systematic Investigation of Docking Failures in Large-Scale Structure-Based Virtual Screening. ACS Omega, 2022, 7, 39417-39428.	1.6	6
4494	In Silico Identification of New Anti-SARS-CoV-2 Main Protease (Mpro) Molecules with Pharmacokinetic Properties from Natural Sources Using Molecular Dynamics (MD) Simulations and Hierarchical Virtual Screening. Journal of Tropical Medicine, 2022, 2022, 1-22.	0.6	10
4495	An open-source molecular builder and free energy preparation workflow. Communications Chemistry, 2022, 5, .	2.0	2
4496	Adenylate cyclase activity of TIR1/AFB auxin receptors in plants. Nature, 2022, 611, 133-138.	13.7	53
4497	Knema retusa is antibacterial and antibiofilm against antibiotic resistant Staphylococcus aureus and S. haemolyticus isolated in bovine mastitis. Veterinary Research Communications, 2023, 47, 523-538.	0.6	3
4500	Complexation, Antifungal, Antioxidant Activities, and In Silico Studies of Metals Cu(II), Co(II), and Mn(II) with 3,5-Dinitrobenzoic Acid. Russian Journal of Bioorganic Chemistry, 0, , .	0.3	0
4501	Hydroxy-3-Phenylcoumarins as Multitarget Compounds for Skin Aging Diseases: Synthesis, Molecular Docking and Tyrosinase, Elastase, Collagenase and Hyaluronidase Inhibition, and Sun Protection Factor. Molecules, 2022, 27, 6914.	1.7	6
4502	DeepBLI: A Transferable Multichannel Model for Detecting Î²-Lactamase-Inhibitor Interaction. Journal of Chemical Information and Modeling, 2022, 62, 5830-5840.	2.5	3

#	Article	IF	Citations
4503	In-Silico Exploration of Plant Metabolites as Potential Remedies of Norovirus. Advances in Virology, 2022, 2022, 1-13.	0.5	0
4504	Spectroscopic and Molecular Docking Analysis of Ï€-Acceptor Complexes with the Drug Barbital. Applied Sciences (Switzerland), 2022, 12, 10130.	1.3	2
4505	Speed vs Accuracy: Effect on Ligand Pose Accuracy of Varying Box Size and Exhaustiveness in AutoDock Vina. Molecular Informatics, 2023, 42, .	1.4	15
4506	Discovery of a Dual SENP1 and SENP2 Inhibitor. International Journal of Molecular Sciences, 2022, 23, 12085.	1.8	1
4507	Identification of defactinib derivatives targeting focal adhesion kinase using ensemble docking, molecular dynamics simulations and binding free energy calculations. Journal of Biomolecular Structure and Dynamics, 2023, 41, 8654-8670.	2.0	2
4508	Virtual screening and molecular dynamics simulation study of abyssomicins as potential inhibitors of COVIDâ€19 virus main protease and spike protein. Journal of Biomolecular Structure and Dynamics, 2023, 41, 8961-8977.	2.0	1
4509	Molecular Docking and Molecular Dynamics Studies Reveal Secretory Proteins as Novel Targets of Temozolomide in Glioblastoma Multiforme. Molecules, 2022, 27, 7198.	1.7	14
4510	DrugTax: package for drug taxonomy identification and explainable feature extraction. Journal of Cheminformatics, 2022, 14, .	2.8	2
4511	Identifying Potential p53â€MDM2 Interaction Antagonists: An Integrated Approach of Pharmacophoreâ€Based Virtual Screening, Interaction Fingerprinting, MDÂSimulation and DFT Studies. ChemistrySelect, 2022, 7, .	0.7	4
4512	In Silico Investigations into the Selectivity of Psychoactive and New Psychoactive Substances in Monoamine Transporters. ACS Omega, 2022, 7, 38311-38321.	1.6	0
4513	Computational study of potential inhibitors for fat mass and obesity-associated protein from seaweed and plant compounds. PeerJ, 0, 10, e14256.	0.9	1
4514	Pharmacophore modeling, docking and molecular dynamics simulation for identification of novel human protein kinase C beta (PKCI2) inhibitors. Structural Chemistry, 2023, 34, 1157-1171.	1.0	3
4515	Virtual screening for potential discoidin domain receptor 1 (DDR1) inhibitors based on structural assessment. Molecular Diversity, 2023, 27, 2297-2314.	2.1	2
4516	Structure and inhibition of SARS-CoV-1 and SARS-CoV-2 main proteases by oral antiviral compound AG7404. Antiviral Research, 2022, 208, 105458.	1.9	7
4517	Phytochemical study of Lantana camara flowers, ecotoxicity, antioxidant, inÂvitro and in silico acetylcholinesterase: molecular docking, MD, and MM/GBSA calculations. Journal of Biomolecular Structure and Dynamics, 2023, 41, 9282-9296.	2.0	1
4518	Screening the possible anti-cancer constituents of Hibiscus rosa-sinensis flower to address mammalian target of rapamycin: an in silico molecular docking, HYDE scoring, dynamic studies, and pharmacokinetic prediction. Molecular Diversity, 2023, 27, 2273-2296.	2.1	6
4519	Integrated Bioinformatics-Based Subtractive Genomics Approach to Decipher the Therapeutic Drug Target and Its Possible Intervention against Brucellosis. Bioengineering, 2022, 9, 633.	1.6	9
4520	Sulforaphane prevents and reverses allergic airways disease in mice via anti-inflammatory, antioxidant, and epigenetic mechanisms. Cellular and Molecular Life Sciences, 2022, 79, .	2.4	5

#	Article	IF	Citations
4521	Ebola and Marburg virus VP35 coiled-coil validated as antiviral target by tripartite split-GFP complementation. IScience, 2022, 25, 105354.	1.9	5
4522	DyScore: A Boosting Scoring Method with Dynamic Properties for Identifying True Binders and Nonbinders in Structure-Based Drug Discovery. Journal of Chemical Information and Modeling, 2022, 62, 5550-5567.	2.5	4
4523	Smooth polymers charge negatively: Controlling contact electrification polarity in polymers. Nano Energy, 2022, 104, 107914.	8.2	24
4524	Structural insights into conformational stability and binding of thiazolo-[2,3-b] quinazolinone derivatives with EGFR-TKD and in-vitro study. Saudi Journal of Biological Sciences, 2022, 29, 103478.	1.8	10
4525	Cross-category prediction of corrosion inhibitor performance based on molecular graph structures via a three-level message passing neural network model. Corrosion Science, 2022, 209, 110780.	3.0	3
4526	Pharmacophore model-aided virtual screening combined with comparative molecular docking and molecular dynamics for identification of marine natural products as SARS-CoV-2 papain-like protease inhibitors. Arabian Journal of Chemistry, 2022, 15, 104334.	2.3	9
4527	Unveiling the potential of Lichtheimia ramosa AJP11 for myco-transformation of polystyrene sulfonate and its driving molecular mechanism. Journal of Environmental Management, 2023, 325, 116579.	3.8	1
4528	Structurally diverse polycyclic polyprenylated acylphloroglucinols with protective effect on human vein endothelial cells injured by high-glucose from Hypericum acmosepalum N. Robson. Phytochemistry, 2023, 205, 113482.	1.4	3
4529	Sappanin-type homoisoflavonoids from Scilla bisotunensis Speta.: Cytotoxicity, molecular docking, and chemotaxonomic significance. Journal of Molecular Structure, 2023, 1273, 134326.	1.8	0
4530	Investigation of embelin synthetic hybrids as potential COVID-19 and COX inhibitors: Synthesis, spectral analysis, DFT calculations and molecular docking studies. Journal of Molecular Structure, 2023, 1273, 134356.	1.8	14
4531	Purification, identification and in silico models of alkaloids from Nardostachys jatamansi â€" bioactive compounds for neurodegenerative diseases. Biomass Conversion and Biorefinery, 2023, 13, 14889-14900.	2.9	5
4532	Computational studies on PLK1 delta gene in cancer diseases. Journal of Applied Pharmaceutical Science, 0, , 74-79.	0.7	0
4533	An In- Silico Studies for Immunomodulatory Potential of Phytoconstituents from a Naturally Occurring Herb Nigella Sativa. Pharmacophore, 2022, 13, 14-26.	0.2	1
4534	Predicting Drug-Target Interactions Over Heterogeneous Information Network. IEEE Journal of Biomedical and Health Informatics, 2023, 27, 562-572.	3.9	12
4535	Interactive deciphering electron-shuttling characteristics of Coffea arabica leaves and potential bioenergy-steered anti-SARS-CoV-2 RdRp inhibitor via microbial fuel cells. Industrial Crops and Products, 2023, 191, 115944.	2.5	7
4536	Biomolecular Topology: Modelling and Analysis. Acta Mathematica Sinica, English Series, 2022, 38, 1901-1938.	0.2	1
4537	Effectiveness of Quercetin and Its Derivatives Against SARS CoV2 -In silico Approach. Journal of Experimental Biology and Agricultural Sciences, 2022, 10, 1003-1015.	0.1	0
4538	Biscarbazole Derivatives: Synthesis, Characterization, Antimicrobial and Antitumor Activity, and Molecular Docking Study. Russian Journal of General Chemistry, 2022, 92, 2145-2160.	0.3	2

#	Article	IF	Citations
4539	In Silico Targeting of influenza virus haemagglutinin receptor protein using Diosmetin, Tangeritin, and Anthocyanidins as potential drugs. Journal of Experimental Biology and Agricultural Sciences, 2022, 10, 995-1002.	0.1	1
4540	Development of Novel Small Antitumor Compounds Inhibiting PD-1/PD-L1 Binding. Anticancer Research, 2022, 42, 5233-5247.	0.5	3
4541	Dimethylmyricacene: An In Vitro and In Silico Study of a Semisynthetic Non-Camptothecin Derivative Compound, Targeting Human DNA Topoisomerase 1B. Cells, 2022, 11, 3486.	1.8	1
4543	Structure-guided product determination of the bacterial type II diterpene synthase Tpn2. Communications Chemistry, 2022, 5, .	2.0	4
4544	Investigations on a novel biologically active organic molecule of 5-Chloro-1-(4-piperidyl)-2-benzimidazolinone by spectroscopic, molecular docking, and quantum chemical approach. Journal of Molecular Structure, 2023, 1274, 134544.	1.8	2
4545	Molecular Docking and Dynamics Simulation Studies of Ginsenosides with SARS-CoV-2 Host and Viral Entry Protein Targets. Natural Product Communications, 2022, 17, 1934578X2211343.	0.2	3
4546	Linoleic acid binds to SARS-CoV-2 RdRp and represses replication of seasonal human coronavirus OC43. Scientific Reports, 2022, 12, .	1.6	4
4547	Systems biology reveals anatabine to be an NRF2 activator. Frontiers in Pharmacology, 0, 13, .	1.6	2
4548	Guava Leaf Essential Oil as a Potent Antioxidant and Anticancer Agent: Validated through Experimental and Computational Study. Antioxidants, 2022, 11, 2204.	2.2	7
4549	Dietary Diindolylmethane Enhances the Therapeutic Effect of Centchroman in Breast Cancer by Inhibiting Neoangiogenesis. Nutrition and Cancer, 2023, 75, 734-749.	0.9	4
4550	Screening and Identification of Natural Productâ€Like Compounds as Potential Antibacterial Agents Targeting FemC of Staphylococcus aureus: An inâ€Silico Approach. ChemistrySelect, 2022, 7, .	0.7	15
4551	Proteome-Based Investigation Identified Potential Drug Repurposable Small Molecules Against Monkeypox Disease. Molecular Biotechnology, 0, , .	1.3	1
4553	Mechanisms of Electron Transfer Rate Modulations in Cytochrome P450 BM3. Journal of Physical Chemistry B, 2022, 126, 9737-9747.	1.2	1
4554	Anti-biofilm activity of caffeine against uropathogenic E. coli is mediated by curli biogenesis. Scientific Reports, 2022, 12, .	1.6	5
4555	WLLP: A weighted reconstruction-based linear label propagation algorithm for predicting potential therapeutic agents for COVID-19. Frontiers in Microbiology, 0, 13, .	1.5	0
4556	Scaffold Generator: a Java library implementing molecular scaffold functionalities in the Chemistry Development Kit (CDK). Journal of Cheminformatics, 2022, 14, .	2.8	2
4557	Chemical Profiling and Molecular Docking Study of Agathophora alopecuroides. Life, 2022, 12, 1852.	1.1	5
4558	Building a Torsional Potential between Thiophene Rings to Illustrate the Basics of Molecular Modeling. Journal of Chemical Education, 2023, 100, 395-401.	1.1	1

#	Article	IF	Citations
4559	Lubeluzole Repositioning as Chemosensitizing Agent on Multidrug-Resistant Human Ovarian A2780/DX3 Cancer Cells. Molecules, 2022, 27, 7870.	1.7	1
4560	Virtual screening based on the structure of more than 105 compounds against four key proteins of SARS-CoV-2: MPro, SRBD, RdRp, and PLpro. Informatics in Medicine Unlocked, 2022, 35, 101134.	1.9	3
4561	Identification of potential inhibitors of brain-specific CYP46A1 from phytoconstituents in Indian traditional medicinal plants. Journal of Proteins and Proteomics, 0, , .	1.0	0
4562	Deciphering deamidation and isomerization in therapeutic proteins: Effect of neighboring residue. MAbs, 2022, 14, .	2.6	7
4563	Conserved Water Networks Identification for Drug Design Using Density Clustering Approaches on Positional and Orientational Data. Journal of Chemical Information and Modeling, 2022, 62, 6105-6117.	2.5	5
4564	Friedelin, a novel inhibitor of CYP17A1 in prostate cancer from Cassia tora. Journal of Biomolecular Structure and Dynamics, 2023, 41, 9695-9720.	2.0	4
4565	A structural biology community assessment of AlphaFold2 applications. Nature Structural and Molecular Biology, 2022, 29, 1056-1067.	3.6	261
4566	Study of the anticancer effect of new quinazolinone hydrazine derivatives as receptor tyrosine kinase inhibitors. Frontiers in Chemistry, 0, 10, .	1.8	2
4567	Radical scavenging capacity, UV activity, and molecular docking studies of 2Ê¹, 5Ê¹, 3, 4-Tetrahydroxychalcone: An insight into the photoprotection. Chemical Physics Impact, 2022, 5, 100126.	1.7	1
4568	Target Prediction of 5,10,15,20-Tetrakis(4â€²-Sulfonatophenyl)-Porphyrin Using Molecular Docking. Pharmaceutics, 2022, 14, 2390.	2.0	4
4569	MILCDock: Machine Learning Enhanced Consensus Docking for Virtual Screening in Drug Discovery. Journal of Chemical Information and Modeling, 2022, 62, 5342-5350.	2.5	6
4570	Berberine enhances the sensitivity of radiotherapy in ovarian cancer cell line (SKOV-3). Saudi Pharmaceutical Journal, 2023, 31, 110-118.	1.2	1
4571	Identification of Antiviral Compounds against Monkeypox Virus Profilin-like Protein A42R from Plantago lanceolata. Molecules, 2022, 27, 7718.	1.7	6
4572	Structure-based virtual screening and molecular dynamics of potential inhibitors targeting sodium-bile acid co-transporter of carcinogenic liver fluke Clonorchis sinensis. PLoS Neglected Tropical Diseases, 2022, 16, e0010909.	1.3	0
4573	The Charge Transfer Complex between 2, 3-diamino-5-bromopyridine and Chloranilic acid: Preparation, Spectroscopic Characterization, DNA binding, and DFT/PCM analysis. Journal of the Indian Chemical Society, 2022, 99, 100799.	1.3	3
4574	Bioactive metabolites of edible mushrooms efficacious against androgenic alopecia: Targeting SRD5A2 using computational approach. Journal of Herbal Medicine, 2022, 36, 100611.	1.0	1
4575	Linalool reduces the virulence of Pseudomonas syringae pv. tomato DC 3000 by modulating the PsyI/PsyR quorum-sensing system. Microbial Pathogenesis, 2022, 173, 105884.	1.3	4
4576	A pilot reverse virtual screening study suggests toxic exposures caused long-term epigenetic changes in Gulf War Illness. Computational and Structural Biotechnology Journal, 2022, 20, 6206-6213.	1.9	2

#	Article	IF	Citations
4577	Discovery of anticancer agents with c-Met inhibitory potential by virtual and experimental screening of a chemical library. European Journal of Pharmacology, 2023, 938, 175395.	1.7	3
4578	Network pharmacology and molecular docking-based analysis of protective mechanism of MLIF in ischemic stroke. Frontiers in Cardiovascular Medicine, 0, 9, .	1.1	0
4579	Identification of NRAS Diagnostic Biomarkers and Drug Targets for Endometrial Cancerâ€"An Integrated in Silico Approach. International Journal of Molecular Sciences, 2022, 23, 14285.	1.8	1
4580	In Silico Analysis of Tetrodotoxin Binding in Voltage-Gated Sodium Ion Channels from Toxin-Resistant Animal Lineages. Marine Drugs, 2022, 20, 723.	2.2	1
4581	Molecular simulations of liquid aliphatic carboxylic acids (C1-C6) using the 3D-RISM-KH molecular solvation theory. Journal of Molecular Liquids, 2022, 368, 120825.	2.3	0
4582	Analysis of Network Pharmacology and Molecular Docking on Radix Pseudostellariae for Its Active Components on Gastric Cancer. Applied Biochemistry and Biotechnology, 0, , .	1.4	1
4583	Expression of IRAK1 in Hepatocellular Carcinoma, Its Clinical Significance, and Docking Characteristics with Selected Natural Compounds. Current Oncology, 2022, 29, 8904-8916.	0.9	2
4584	<scp>PocketOptimizer</scp> 2.0: A modular framework for computerâ€aided ligandâ€binding design. Protein Science, 2023, 32, .	3.1	2
4585	Evaluating GPCR modeling and docking strategies in the era of deep learning-based protein structure prediction. Computational and Structural Biotechnology Journal, 2023, 21, 158-167.	1.9	15
4586	CSAlign and CSAlign-Dock: Structure alignment of ligands considering full flexibility and application to proteinâ€"ligand docking. Computational and Structural Biotechnology Journal, 2023, 21, 1-10.	1.9	2
4587	Data-driven ligand field exploration of Fe(<scp>iv</scp>)â€"oxo sites for Câ€"H activation. Inorganic Chemistry Frontiers, 2023, 10, 1062-1075.	3.0	3
4588	Accurately predicting solvation free energy in aqueous and organic solvents beyond 298 K by combining deep learning and the 1D reference interaction site model. , 0, , .		1
4589	Anticancer potential of phytochemicals from Oroxylum indicum targeting Lactate Dehydrogenase A through bioinformatic approach. Toxicology Reports, 2023, 10, 56-75.	1.6	7
4590	Design, synthesis and molecular docking of novel substituted azepines as inhibitors of PI3K/Akt/TSC2/mTOR signaling pathway in colorectal carcinoma. Bioorganic Chemistry, 2023, 131, 106299.	2.0	11
4591	Strepyrrolins Aâ€"E, five pyrroleâ€"sesquiterpene hybrids from Streptomyces sp. KIB 015, revealing a new formation logic of pyrroles by isotope labeling. Organic Chemistry Frontiers, 2023, 10, 880-889.	2.3	2
4592	Design, synthetic approach,in silicomolecular docking and antibacterial activity of quinazolin-2,4-dione hybrids bearing bioactive scaffolds. RSC Advances, 2022, 13, 292-308.	1.7	4
4593	Chemo diversity of ginger-a potent crop in Manipur and its acetylcholinesterase (AChE) inhibitory potential. Biochemical Systematics and Ecology, 2023, 106, 104560.	0.6	0
4594	Insect galectin stimulates the human CD4+ T cell proliferation by regulating inflammation (T cell and) Tj ETQq1 1 0.784314 rgBT /Ove	1.8	1

#	Article	IF	Citations
4595	Molecular recognition of some novel mTOR kinase inhibitors to develop anticancer leads by drug-likeness, molecular docking and molecular dynamics based virtual screening strategy. Computational Toxicology, 2023, 25, 100257.	1.8	3
4596	In silico investigation of acyclovir derivatives potency against herpes simplex virus. Scientific African, 2023, 19, e01461.	0.7	0
4597	Computational and experimental investigation on biological and photophysical properties of high yielded novel aryl-substituted pyrazolone analogue. Journal of Molecular Structure, 2023, 1276, 134790.	1.8	2
4598	Sampling theory perspective on tomographic tilt increment schemes. Ultramicroscopy, 2023, 245, 113669.	0.8	2
4599	AutoDock Koto: A Gradient Boosting Differential Evolution for Molecular Docking. IEEE Transactions on Evolutionary Computation, 2023, 27, 1648-1662.	7.5	1
4600	A MOLECULAR DOCKING STUDY: TARGETING COVID-19 (SARS-COV-2) MAIN PROTEASE USING ACTIVE PHYTOCOMPOUNDS FROM TERMINALIA ARJUNA. Innovare Journal of Medical Sciences, 0, , 9-14.	0.2	3
4601	Study on the Antiâ€inflammatory activity of Saponin from Dioscorea bulbifera using in vitro and in silico methods. Research Journal of Pharmacy and Technology, 2022, , 4434-4438.	0.2	0
4602	Identification of Novel Arachidonic Acid 15-Lipoxygenase Inhibitors Based on the Bayesian Classifier Model and Computer-Aided High-Throughput Virtual Screening. Pharmaceuticals, 2022, 15, 1440.	1.7	4
4603	In Silico Molecular Interaction Analysis and Pharmacokinetic Profiling of Flavonoids from Catharanthus roseus (Flower) Against TXNIP Protein. Trends in Sciences, 2023, 20, 6394.	0.2	3
4604	Molecular Docking and Dynamics Simulation Revealed the Potential Inhibitory Activity of New Drugs against Human Topoisomerase I Receptor. International Journal of Molecular Sciences, 2022, 23, 14652.	1.8	5
4605	Potential Disruption of Systemic Hormone Transport by Tobacco Alkaloids Using Computational Approaches. Toxics, 2022, 10, 727.	1.6	1
4606	Benzo[d]thiazole-2-carboxamides as new antituberculosis chemotypes inhibiting mycobacterial ATP phosphoribosyl transferase. Future Medicinal Chemistry, 2022, 14, 1847-1864.	1.1	2
4607	Assessing How Residual Errors of Scoring Functions Correlate to Ligand Structural Features. International Journal of Molecular Sciences, 2022, 23, 15018.	1.8	2
4608	Ligand-Based Discovery of a Small Molecule as Inhibitor of Î±-Synuclein Amyloid Formation. International Journal of Molecular Sciences, 2022, 23, 14844.	1.8	4
4609	In silico evaluation of flavonoids as potential inhibitors of SARS-CoV-2 main nonstructural proteins (Nsps)â€"amentoflavone as a multitarget candidate. Journal of Molecular Modeling, 2022, 28, .	0.8	2
4610	Spiro heterocycles bearing piperidine moiety as potential scaffold for antileishmanial activity: synthesis, biological evaluation, and in silico studies. Journal of Enzyme Inhibition and Medicinal Chemistry, 2023, 38, 330-342.	2.5	7
4611	Graph neural networks for materials science and chemistry. Communications Materials, 2022, 3, .	2.9	90
4613	Synthesis and biological activity evaluation of pyrazoleâ€"1,2,4â€"triazole hybrids: A computer-aided docking studies. Current Drug Discovery Technologies, 2022, 20, .	0.6	1

#	Article	IF	Citations
4614	In silico Identification of Putative Drug Targets in Mycobacterium ulcerans Virulence Proteins. Letters in Drug Design and Discovery, 2022, 20, .	0.4	0
4615	Spectroscopic Analysis and ADME prediction of Phytochemicals in Methanolic Leaves Extract of Avicennia marina. Research Journal of Pharmacognosy and Phytochemistry, 2022, , 231-239.	0.1	1
4616	Construction of an In Silico Structural Profiling Tool Facilitating Mechanistically Grounded Classification of Aquatic Toxicants. Environmental Science & Technology, 2022, 56, 17805-17814.	4.6	1
4617	Phosphorylation of <scp>S11</scp> in <scp>PHR1</scp> negatively controls its transcriptional activity. Physiologia Plantarum, 2022, 174, .	2.6	2
4618	Identification of novel inhibitors against Escherichia coli utilizing HisC as a target from histidine biosynthesis pathway. Journal of Biomolecular Structure and Dynamics, 2023, 41, 9907-9914.	2.0	1
4619	Toward Reliable and Insightful Entropy Calculations on Flexible Molecules. Journal of Chemical Theory and Computation, 2022, 18, 7166-7178.	2.3	2
4620	Testing Serum Albumins and Cyclodextrins as Potential Binders of the Mycotoxin Metabolites Alternariol-3-Sulfate, Alternariol-9-Monomethylether and Alternariol-9-Monomethylether-3-Sulfate. International Journal of Molecular Sciences, 2022, 23, 14353.	1.8	4
4621	N-[1,3-Dialkyl(aryl)-2-oxoimidazolidin-4-ylidene]-aryl(alkyl)sulphonamides as Novel Selective Human Cannabinoid Type 2 Receptor (hCB2R) Ligands; Insights into the Mechanism of Receptor Activation/Deactivation. Molecules, 2022, 27, 8152.	1.7	2
4622	In Silico Drug Repurposing Framework Predicts Repaglinide, Agomelatine and Protokylol as TRPV1 Modulators with Analgesic Activity. Pharmaceutics, 2022, 14, 2563.	2.0	5
4623	Efficient Computation of the Interaction Energies of Very Large Non-covalently Bound Complexes. Synlett, 2023, 34, 1135-1146.	1.0	2
4624	Theoretical Studies of Leu-Pro-Arg-Asp-Ala Pentapeptide (LPRDA) Binding to Sortase A of Staphylococcus aureus. Molecules, 2022, 27, 8182.	1.7	3
4626	Pharmacophore Synergism in Diverse Scaffold Clinches in Aurora Kinase B. International Journal of Molecular Sciences, 2022, 23, 14527.	1.8	0
4627	Interfacial Distribution of Nafion Ionomer Thin Films on Nitrogen-Modified Carbon Surfaces. ACS Applied Materials & Interfaces, 2022, 14, 53744-53754.	4.0	7
4628	Screening of Hub Genes in Hepatocellular Carcinoma Based on Network Analysis and Machine Learning. Computational and Mathematical Methods in Medicine, 2022, 2022, 1-32.	0.7	0
4629	R-SIM: A Database of Binding Affinities for RNA-small Molecule Interactions. Journal of Molecular Biology, 2023, 435, 167914.	2.0	2
4630	The Potential of ZICURMA Herbal Supplement in Inhibiting Pro-Inflammatory Cytokines as Therapeutic Agents in SARS-CoV2 Infection. Trends in Sciences, 2023, 20, 4146.	0.2	1
4631	Interactions of Apigenin and Safranal with the 5HT1A and 5HT2A Receptors and Behavioral Effects in Depression and Anxiety: A Molecular Docking, Lipid-Mediated Molecular Dynamics, and In Vivo Analysis. Molecules, 2022, 27, 8658.	1.7	6
4632	ADMETboost: a web server for accurate ADMET prediction. Journal of Molecular Modeling, 2022, 28, .	0.8	20

#	Article	IF	Citations
4634	Applications of Bond Energyâ€Based Thermodynamic Analysis to the Feasibility of Unfunctionalized Câ^'C Crossâ€Coupling Reactions. ChemistrySelect, 2022, 7, .	0.7	0
4635	In silico mapping of the dynamic interactions and structure-activity relationship of flavonoid compounds against the immune checkpoint programmed-cell death 1 pathway. Frontiers in Drug Discovery, 0, 2, .	1.1	0
4637	Trifluoromethylcinnamanilide Michael Acceptors for Treatment of Resistant Bacterial Infections. International Journal of Molecular Sciences, 2022, 23, 15090.	1.8	1
4638	A New Flavanone from Chromolaena tacotana (Klatt) R. M. King and H. Rob, Promotes Apoptosis in Human Breast Cancer Cells by Downregulating Antiapoptotic Proteins. Molecules, 2023, 28, 58.	1.7	2
4639	Diyabet HastalÄ±ÄŸÄ±nÄ±n Tedavisinde KullanÄ±labilecek Alfa-Amilaz Ä°nhibitÃ¶rÃ¼ Olarak Kuersetin ve Umbelliferonun Etkisinin In Silico KanÄ±tÄ±. Journal of Forestry Faculty of Kastamonu University, 2022, 22, 202-216.	0.1	2
4640	Conjugates of Chloramphenicol Amine and Berberine as Antimicrobial Agents. Antibiotics, 2023, 12, 15.	1.5	7
4641	SARS-CoV-2 proteases Mpro and PLpro: Design of inhibitors with predicted high potency and low mammalian toxicity using artificial neural networks, ligand-protein docking, molecular dynamics simulations, and ADMET calculations. Computers in Biology and Medicine, 2023, 153, 106449.	3.9	9
4642	Development of N-(1-Adamantyl)benzamides as Novel Anti-Inflammatory Multitarget Agents Acting as Dual Modulators of the Cannabinoid CB2 Receptor and Fatty Acid Amide Hydrolase. Journal of Medicinal Chemistry, 2023, 66, 235-250.	2.9	3
4643	Investigation into the Use of Encorafenib to Develop Potential PROTACs Directed against BRAFV600E Protein. Molecules, 2022, 27, 8513.	1.7	4
4644	Brewersâ€™ spent hop revalorization for the production of high added-value cosmetics ingredients with elastase inhibition capacity. Scientific Reports, 2022, 12, .	1.6	0
4645	Pharmacoinformatic approach to identify potential phytochemicals against SARS-CoV-2 spike receptor-binding domain in native and variants of concern. Molecular Diversity, 0, , .	2.1	0
4646	Insights Into Resveratrol as an Inhibitor Against Aβ1-42 Peptide Aggregation: A Molecu-lar Dynamics Simulation Study. Current Chemical Biology, 2022, 17, .	0.2	0
4647	ATESA: An Automated Aimless Shooting Workflow. Journal of Chemical Theory and Computation, 0, , .	2.3	1
4648	(E)-3-([2,2â€™-bithiophen]-5-yl)-1-(4-fluorophenyl)prop-2-en-1-one: Synthesis and structural elucidation of chalcone derivatives for potential antioxidant activity. Molecular Crystals and Liquid Crystals, 0, , 1-14.	0.4	0
4649	Knowledge Engineering in Chemistry: From Expert Systems to Agents of Creation. Accounts of Chemical Research, 2023, 56, 128-139.	7.6	6
4650	In-silico molecular interactions among the secondary metabolites of Caulerpa spp. and colorectal cancer targets. Frontiers in Chemistry, 0, 10, .	1.8	2
4651	Phenols, antioxidant and anticancer properties of Tagetes minuta, Euphorbia granulata and Galinsoga parviflora: in vitro and in silico evaluation. , 2023, 9, 15-28.		2
4652	A Reactive Molecular Dynamics Study of Chlorinated Organic Compounds. Part II: A ChemTraYzer Study of Chlorinated Dibenzofuran Formation and Decomposition Processes. ChemPhysChem, 0, , .	1.0	2

#	Article	IF	Citations
4653	In silico prediction of siRNA ionizable-lipid nanoparticles In vivo efficacy: Machine learning modeling based on formulation and molecular descriptors. Frontiers in Molecular Biosciences, 0, 9, .	1.6	4
4654	Apo2ph4: A Versatile Workflow for the Generation of Receptor-based Pharmacophore Models for Virtual Screening. Journal of Chemical Information and Modeling, 0, , .	2.5	3
4655	Design, synthesis and molecular docking studies of 5-fluoro 1-aryl/alkyl sulfonyl benzimidazole derivatives for treatment of Parkinsonâ€™s disease. Phosphorus, Sulfur and Silicon and the Related Elements, 2023, 198, 336-344.	0.8	2
4656	An In-Silico Evaluation of Anthraquinones as Potential Inhibitors of DNA Gyrase B of Mycobacterium tuberculosis. Microorganisms, 2022, 10, 2434.	1.6	5
4657	ATP-citrate lyase inhibitor improves ectopic lipid accumulation in the kidney in a db/db mouse model. Frontiers in Endocrinology, 0, 13, .	1.5	2
4659	Prediction of the Contribution Ratio of a Target Metabolic Enzyme to Clearance from Chemical Structure Information. Molecular Pharmaceutics, 2023, 20, 419-426.	2.3	3
4660	Gene expression, molecular docking, and molecular dynamics studies to identify potential antifungal compounds targeting virulence proteins/genes VelB and THR as possible drug targets against Curvularia lunata. Frontiers in Molecular Biosciences, 0, 9, .	1.6	3
4662	Hepatoprotective Activity of Lignin-Derived Polyphenols Dereplicated Using High-Resolution Mass Spectrometry, In Vivo Experiments, and Deep Learning. International Journal of Molecular Sciences, 2022, 23, 16025.	1.8	2
4663	LIDeB Tools: A Latin American resource of freely available, open-source cheminformatics apps. Artificial Intelligence in the Life Sciences, 2022, 2, 100049.	1.6	2
4664	Using Network Pharmacology and Molecular Docking to Explore the Mechanism of Qiju Dihuang Pill against Dry Eye Disease. Computational and Mathematical Methods in Medicine, 2022, 2022, 1-13.	0.7	1
4665	Genomic Insight into Shimazuella Soli Sp. Nov. Isolated from Soil and Its Putative Novel Class II Lasso Peptide. Bioengineering, 2022, 9, 812.	1.6	0
4666	iADRGSE: A Graph-Embedding and Self-Attention Encoding for Identifying Adverse Drug Reaction in the Earlier Phase of Drug Development. International Journal of Molecular Sciences, 2022, 23, 16216.	1.8	2
4667	Novel 1,2,3-Triazole-Based Benzothiazole Derivatives: Efficient Synthesis, DFT, Molecular Docking, and ADMET Studies. Molecules, 2022, 27, 8555.	1.7	6
4668	Benchmarking biomolecular force fieldâ€based Zn²⁺ for monoâ€and bimetallic ligand binding sites. Journal of Computational Chemistry, 2023, 44, 912-926.	1.5	8
4669	Identification of allosteric inhibitor against AKT1 through structure-based virtual screening. Molecular Diversity, 2023, 27, 2803-2822.	2.1	3
4670	Computational Exploration of Anti-cancer Potential of Flavonoids against Cyclin-Dependent Kinase 8: An In Silico Molecular Docking and Dynamic Approach. ACS Omega, 2023, 8, 391-409.	1.6	19
4671	Rosetta FlexPepDock to predict peptide-MHC binding: An approach for non-canonical amino acids. PLoS ONE, 2022, 17, e0275759.	1.1	7
4672	Metal chelation ability of Protocatechuic acid anion with 210Po84; a theoretical insight. Computational and Theoretical Chemistry, 2023, 1220, 113996.	1.1	9

#	Article	IF	Citations
4673	The integrative bioinformatics approaches to predict the xanthohumol as anti-breast cancer molecule: Targeting cancer cells signaling PI3K and AKT kinase pathway. Frontiers in Oncology, 0, 12, .	1.3	2
4674	SOMAS: a platform for data-driven material discovery in redox flow battery development. Scientific Data, 2022, 9, .	2.4	4
4675	What the Heck?â”€Automated Regioselectivity Calculations of Palladium-Catalyzed Heck Reactions Using Quantum Chemistry. ACS Omega, 2022, 7, 45617-45623.	1.6	2
4676	Destabilizers of the thymidylate synthase homodimer accelerate its proteasomal degradation and inhibit cancer growth. ELife, 0, 11, .	2.8	1
4677	Potential inhibitors of FemC to combat Staphylococcus aureus: virtual screening, molecular docking, dynamics simulation, and MM-PBSA analysis. Journal of Biomolecular Structure and Dynamics, 0, , 1-12.	2.0	1
4678	Automated handling of complex chemical structures in Zâ€matrix coordinatesâ€”The chemcoord library. Journal of Computational Chemistry, 2023, 44, 710-726.	1.5	4
4679	Detection of ryanodine receptor G4911E and I4754M mutation sites and analysis of binding modes of diamide insecticides with RyR on Galeruca daurica (Coleoptera: Chrysomelidae). Frontiers in Physiology, 0, 13, .	1.3	3
4680	Modelling the Anticancer Activity of 4-Alkoxy Cinnamic Analogues using 3D-Descriptors and Genetic Algorithm-Multiple Linear Regression (GA-MLR) Method. Journal of King Saud University - Science, 2023, 35, 102514.	1.6	1
4681	Molecular interaction studies of thymol via molecular dynamic simulations and free energy calculations using multi-target approach against Aedes aegypti proteome to decipher its role as mosquito repellent. Molecular Simulation, 2023, 49, 325-340.	0.9	6
4682	Pyrido-pyrimido-thiadiazinones: green synthesis, molecular docking studies and biological investigation as obesity inhibitors. Journal of Taibah University for Science, 2022, 16, 1275-1286.	1.1	2
4683	iORbase: A database for the prediction of the structures and functions of insect olfactory receptors. Insect Science, 2023, 30, 1245-1254.	1.5	2
4684	Fusing 2D and 3D molecular graphs as unambiguous molecular descriptors for conformational and chiral stereoisomers. Briefings in Bioinformatics, 2023, 24, .	3.2	2
4685	Andrographolide-based potential anti-inflammatory transcription inhibitors against nuclear factor NF-kappa-B p50 subunit (NF-ÎºB p50): an integrated molecular and quantum mechanical approach. 3 Biotech, 2023, 13, .	1.1	1
4686	Evaluation of <scp>AlphaFold2</scp> structures as docking targets. Protein Science, 2023, 32, .	3.1	26
4687	In silico analysis decodes transthyretin (TTR) binding and thyroid disrupting effects of per- and polyfluoroalkyl substances (PFAS). Archives of Toxicology, 2023, 97, 755-768.	1.9	7
4688	Insights from incorporating quantum computing into drug designÂworkflows. Bioinformatics, 2023, 39, .	1.8	9
4689	Identification of novel natural product inhibitors of BRD4 using high throughput virtual screening and MD simulation. Journal of Biomolecular Structure and Dynamics, 0, , 1-13.	2.0	1
4690	In silico and inÂvitro studies of potential inhibitors against Dengue viral protein NS5 Methyl Transferase from Ginseng and Notoginseng. Journal of Traditional and Complementary Medicine, 2023, 13, 1-10.	1.5	6

#	Article	IF	Citations
4691	On TAML Catalyst Resting State Lifetimes: Kinetic, Mechanistic, and Theoretical Insight into Phosphate-Induced Demetalation of an Iron(III) Bis(sulfonamido)bis(amido)-TAML Catalyst. Inorganic Chemistry, 2023, 62, 639-647.	1.9	1
4692	Crystal structure of toceranib, C₂₂H₂₅FN₄O₂. Powder Diffraction, 0, , 1-6.	0.4	0
4693	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. Journal of Biomolecular Structure and Dynamics, 2023, 41, 11578-11597.	2.0	4
4695	Variational Subspace Valence Bond. , 2024, , 424-440.		0
4696	A Comparative Analytical Review on Machine Learning Methods in Drugtarget Interactions Prediction. Current Computer-Aided Drug Design, 2023, 19, 325-355.	0.8	0
4697	Discovery of new inhibitors of Mycobacterium tuberculosis EPSP synthase - A computational study. Journal of Molecular Graphics and Modelling, 2023, , 108404.	1.3	1
4698	Species-selective nanoreactor molecular dynamics simulations based on linear-scaling tight-binding quantum chemical calculations. Journal of Chemical Physics, 2023, 158, .	1.2	3
4699	Cyto-Genotoxic and Behavioral Effects of Flubendiamide in Allium cepa Root Cells, Drosophila melanogaster and Molecular Docking Studies. International Journal of Molecular Sciences, 2023, 24, 1565.	1.8	4
4700	PETrans: De Novo Drug Design with Protein-Specific Encoding Based on Transfer Learning. International Journal of Molecular Sciences, 2023, 24, 1146.	1.8	8
4701	OntoPESScan: An Ontology for Potential Energy Surface Scans. ACS Omega, 2023, 8, 2462-2475.	1.6	5
4702	In-silico Prediction of Maximum Binding Affinity of Disease-Modifying Antirheumatic Drugs with Homo sapiens Acrosomal Protein SP-10. International Journal of Pharmaceutical Research and Allied Sciences, 2023, 12, 59-65.	0.1	0
4703	Structure-based pharmacophore modeling, virtual screening, and molecular dynamics simulation studies for identification of Plasmodium falciparum 5-aminolevulinate synthase inhibitors. Frontiers in Medicine, 0, 9, .	1.2	2
4704	A gene signature driven by abnormally methylated DEGs was developed for TP53 wild-type ovarian cancer samples by integrative omics analysis of DNA methylation and gene expression data. Annals of Translational Medicine, 2023, 11, 20-20.	0.7	1
4705			

#	Article	IF	Citations
4710	Papyrus: a large-scale curated dataset aimed at bioactivity predictions. Journal of Cheminformatics, 2023, 15, .	2.8	13
4711	Dual Role of a Fluorescent Small Molecule as a Sensor and Inhibitor of Protein Fibrillation. Chemistry - an Asian Journal, 2023, 18, .	1.7	2
4712	Inhibitory effects of Ephedra alte on IL-6, hybrid TLR4, TNF-Î±, IL-1Î², and extracted TLR4 receptors: in silico molecular docking. Heliyon, 2023, 9, e12730.	1.4	5
4713	Latonduine-1-Amino-Hydantoin Hybrid, Triazole-Fused Latonduine Schiff Bases and Their Metal Complexes: Synthesis, X-ray and Electron Diffraction, Molecular Docking Studies and Antiproliferative Activity. Inorganics, 2023, 11, 30.	1.2	3
4714	A drug repurposing approach to identify therapeutics by screening pathogen box exploiting SARSâ€CoVâ€2 main protease. Chemistry and Biodiversity, 0, , .	1.0	3
4715	The Effect of Arginine on the Phase Stability of Aqueous Hen Egg-White Lysozyme Solutions. International Journal of Molecular Sciences, 2023, 24, 1197.	1.8	3
4717	Similarity Downselection: Finding the n Most Dissimilar Molecular Conformers for Reference-Free Metabolomics. Metabolites, 2023, 13, 105.	1.3	1
4718	Synthesis, X-Ray Crystal Structure, and Identification of Potential Drug Candidate against COVID-19 Main Protease through Structure-Guided Modeling and Simulation Approach. Polycyclic Aromatic Compounds, 0, , 1-18.	1.4	0
4719	Multi Stimuli-Responsive Aggregation-Induced Emission Active Polymer Platform Based on Tetraphenylethylene-Appended Maleic Anhydride Terpolymers. ACS Applied Materials & Interfaces, 2023, 15, 3543-3557.	4.0	4
4720	Interactions of fentanyl with blood platelets and plasma proteins: platelet sensitivity to prasugrel metabolite is not affected by fentanyl under in vitro conditions. Pharmacological Reports, 0, , .	1.5	0
4721	In silico Study, Molecular Docking and Synthesis of 2-Amino thiazole Derivatives using Green Chemistry Approach as Antioxidant Agent. Asian Journal of Organic & Medicinal Chemistry, 2023, 7, 280-286.	0.1	0
4722	Comparative Computational Screening of Natural-based Partial Agonists for PPARÎ³ Receptor. Medicinal Chemistry, 2023, 19, 594-618.	0.7	0
4723	Catalytic Oxidation of Benzoins by Hydrogen Peroxide on Nanosized HKUST-1: Influence of Substituents on the Reaction Rates and DFT Modeling of the Reaction Path. Molecules, 2023, 28, 747.	1.7	2
4724	In Vitro and In Vivo Studies of Heraclenol as a Novel Bacterial Histidine Biosynthesis Inhibitor against Invasive and Biofilm-Forming Uropathogenic Escherichia coli. Antibiotics, 2023, 12, 110.	1.5	0
4725	Structure of the Sec14 domain of Kalirin reveals a distinct class of lipid-binding module in RhoGEFs. Nature Communications, 2023, 14, .	5.8	0
4726	Structural homology between 11 beta-hydroxysteroid dehydrogenase and Mycobacterium tuberculosis Inh-A enzyme: Dehydroepiandrosterone as a potential co-adjuvant treatment in diabetes-tuberculosis comorbidity. Frontiers in Endocrinology, 0, 13, .	1.5	1
4727	Structure-Based Identification of Natural-Product-Derived Compounds with Potential to Inhibit HIV-1 Entry. Molecules, 2023, 28, 474.	1.7	3
4728	In silico prediction of the possible antidiabetic and anti-inflammatory targets of Nymphaea lotus -derived phytochemicals and mechanistic insights by molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2023, 41, 12225-12241.	2.0	1

#	Article	IF	Citations
4729	Marmesin and Marmelosin Interact with the Heparan Sulfatase-2 Active Site: Potential Mechanism for Phytochemicals from Bael Fruit Extract as Antitumor Therapeutics. Oxidative Medicine and Cellular Longevity, 2023, 2023, 1-19.	1.9	0
4730	Computational design of prospective molecular targets for Burkholderia cepacia complex by molecular docking and dynamic simulation studies. Proteins: Structure, Function and Bioinformatics, 0, , .	1.5	1
4731	Conformational Sampling Deciphers the Chameleonic Properties of a VHL-Based Degrader. Pharmaceutics, 2023, 15, 272.	2.0	5
4732	Metabolite profiling, in vitro and in silico assessment of antibacterial and anticancer activities of Alternaria alternata endophytic in Jatropha heynei. Archives of Microbiology, 2023, 205, .	1.0	5
4733	Targeting RNA:protein interactions with an integrative approach leads to the identification of potent YBX1 inhibitors. ELife, 0, 12, .	2.8	3
4735	Antioxidant and Anti-inflammatory Activity of Sea Cucumber (Holothuria scabra) Active Compounds against KEAP1 and iNOS Protein. Bioinformatics and Biology Insights, 2023, 17, 117793222211496.	1.0	1
4736	Antihypertensive effects of pentacyclic triterpenoid from Convolvulus pluricaulis and its plausible mechanism of action hypothesizing its selectivity targeting Mineralocorticoid receptor of RAAS.. Phytomedicine Plus, 2023, 3, 100408.	0.9	3
4737	Machine intelligence-guided selection of optimized inhibitor for human immunodeficiency virus (HIV) from natural products. Computers in Biology and Medicine, 2023, 153, 106525.	3.9	2
4738	Antibiotic resistance and drug modification: Synthesis, characterization and bioactivity of newly modified potent pleuromutilin derivatives with a substituted piperazine moiety. Bioorganic Chemistry, 2023, 132, 106353.	2.0	6
4739	Development of predictive QSAR models for the substrates/inhibitors of OATP1B1 by deep neural networks. Toxicology Letters, 2023, 376, 20-25.	0.4	1
4740	Molecular interactions of resveratrol with AÎ² 42 peptide and fibril during in-vitro AÎ² 42 aggregation. Advances in Redox Research, 2023, 7, 100060.	0.9	1
4741	Pan-genome analysis and molecular docking unveil the biocontrol potential of Bacillus velezensis VB7 against Phytophthora infestans. Microbiological Research, 2023, 268, 127277.	2.5	11
4742	IN SILICO ANALYSIS AND DOCKING STUDY OF THE ACTIVE PHYTO COMPOUNDS OF MORINGA OLEIFERA AGAINST MARBURG VIRUS VP35 PROTEIN. Innovare Journal of Science, 0, , 5-12.	0.0	0
4743	CAT-Site: Predicting Protein Binding Sites Using a Convolutional Neural Network. Pharmaceutics, 2023, 15, 119.	2.0	3
4744	Phytochemical analysis and evaluation of antibacterial activity of Moringa oleifera extracts against gram-negative bacteria: an in vitro and molecular docking studies. Current Issues in Pharmacy and Medical Sciences, 2022, .	0.1	0
4745	Integrated approach for studying bioactive compounds from Cladosporium spp. against estrogen receptor alpha as breast cancer drug target. Scientific Reports, 2022, 12, .	1.6	9
4746	An In Vitro and In Silico Investigation about Monteverdia ilicifolia Activity against Helicobacter pylori. Antibiotics, 2023, 12, 46.	1.5	0
4747	Revisiting the South Indian Traditional Plants against Several Targets of SARS-CoV-2 - An in silico Approach. Current Computer-Aided Drug Design, 2023, 19, 202-233.	0.8	1

#	Article	IF	Citations
4748	PandoraRL: DQN and Graph Convolution based ligand pose learning for SARS-COV1 Mprotease. , 2022, , .		2
4749	Design and Synthesis of Conformationally Flexible Scaffold as Bitopic Ligands for Potent D3-Selective Antagonists. International Journal of Molecular Sciences, 2023, 24, 432.	1.8	4
4751	Ultrasound-assisted green synthesis of triazole-based azomethine/thiazolidin-4-one hybrid inhibitors for cancer therapy through targeting dysregulation signatures of some Rab proteins. Green Chemistry Letters and Reviews, 2023, 16, .	2.1	5
4752	Inâ€Silico Device Performance Prediction of Cosensitizer Dye Pairs for Dyeâ€Sensitized Solar Cells. Advanced Energy Materials, 2023, 13, .	10.2	1
4753	Dronabinol as an answer to flavivirus infections: an in-silico investigation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 11219-11230.	2.0	0
4754	Exploring the possibility of drug repurposing for cancer therapy targeting human lactate dehydrogenase A: a computational approach. Journal of Biomolecular Structure and Dynamics, 2023, 41, 9967-9976.	2.0	5
4755	Identification of potential death-associated protein kinase-1 (DAPK1) inhibitors by an integrated ligand-based and structure-based computational drug design approach. Journal of Biomolecular Structure and Dynamics, 2023, 41, 10785-10797.	2.0	5
4756	Non-Nucleoside Inhibitors Decrease Foot-and-Mouth Disease Virus Replication by Blocking the Viral 3Dpol. Viruses, 2023, 15, 124.	1.5	2
4757	Nifuroxazide Activates the Parthanatos to Overcome TMPRSS2:ERG Fusion-Positive Prostate Cancer. Molecular Cancer Therapeutics, 2023, 22, 306-316.	1.9	1
4758	Elucidating the toxicity mechanism of AFM2 and the protective role of quercetin in albino mice. Scientific Reports, 2023, 13, .	1.6	4
4759	Deciphering the interaction mechanism of natural actives against larval proteins of Aedes aegypti to identify potential larvicides: a computational biology analysis. Journal of Biomolecular Structure and Dynamics, 2023, 41, 12480-12502.	2.0	1
4760	DFT calculation and molecular docking of lawsone and its derivatives as antibacterial. AIP Conference Proceedings, 2023, , .	0.3	0
4761	Quantitative Target-specific Toxicity Prediction Modeling (QTTPM): Coupling Machine Learning with Dynamic Proteinâ€“Ligand Interaction Descriptors (DyPLIDs) to Predict Androgen Receptor-mediated Toxicity. Computational Methods in Engineering & the Sciences, 2023, , 263-295.	0.3	1
4762	Systematically Investigating the Pharmacological Mechanism of Momordica grosvenori in the Treatment of Spinal Cord Injury by Network Pharmacology and Experimental Verification. Evidence-based Complementary and Alternative Medicine, 2023, 2023, 1-13.	0.5	1
4763	High-Accuracy Heats of Formation for Alkane Oxidation: From Small to Large via the Automated CBH-ANL Method. Journal of Physical Chemistry A, 2023, 127, 1512-1531.	1.1	10
4764	Identification of potent EGFR-TKD inhibitors from NPACT database through combined computational approaches. Journal of Biomolecular Structure and Dynamics, 2023, 41, 12063-12076.	2.0	7
4765	In Silico Targeting of Fascin Protein for Cancer Therapy: Benchmarking, Virtual Screening and Molecular Dynamics Approaches. Molecules, 2023, 28, 1296.	1.7	2
4766	In silico Structure Prediction, Molecular Docking, and Dynamic Simulation of Plasmodium falciparum AP2-I Transcription Factor. Bioinformatics and Biology Insights, 2023, 17, 117793222211496.	1.0	5

#	Article	IF	Citations
4767	Molecular Docking, ADMET Analysis and Molecular Dynamics (MD) Simulation to Identify Synthetic Isoquinolines as Potential Inhibitors of SARS-CoV-2 MPRO. Current Computer-Aided Drug Design, 2023, 19, 391-404.	0.8	1
4768	Surrogate Based Genetic Algorithm Method for Efficient Identification of Low-Energy Peptide Structures. Journal of Chemical Theory and Computation, 2023, 19, 1080-1097.	2.3	2
4769	New approaches in developing medicinal herbs databases. Database: the Journal of Biological Databases and Curation, 2023, 2023, .	1.4	4
4770	COMA: efficient structure-constrained molecular generation using contractive and margin losses. Journal of Cheminformatics, 2023, 15, .	2.8	1
4771	Potential of plant extracts in targeting SARS-CoV-2 main protease: an inÂvitro and in silico study. Journal of Biomolecular Structure and Dynamics, 0, , 1-10.	2.0	3
4772	A Data-Driven Approach to Construct a Molecular Map of Trypanosoma cruzi to Identify Drugs and Vaccine Targets. Vaccines, 2023, 11, 267.	2.1	2
4773	Highlights in TMPRSS2 inhibition mechanism with guanidine derivatives approved drugs for COVID-19 treatment. Journal of Biomolecular Structure and Dynamics, 2023, 41, 12908-12922.	2.0	1
4774	Influencing Molecular Dynamics Simulations of Ion-Exchange Membranes by Considering Comonomer Propagation. Macromolecules, 2023, 56, 1263-1277.	2.2	1
4775	QDÏ€: A Quantum Deep Potential Interaction Model for Drug Discovery. Journal of Chemical Theory and Computation, 2023, 19, 1261-1275.	2.3	6
4776	Molecular docking and simulation studies against nucleoside diphosphate kinase (NDK) of Pseudomonas aeruginosa with secondary metabolite identified by genome mining from paenibacillusehimensis. Journal of Biomolecular Structure and Dynamics, 2023, 41, 12610-12619.	2.0	1
4777	Polyphenolic Profile of Herniaria hemistemon Aerial Parts Extract and Assessment of Its Anti-Cryptosporidiosis in a Murine Model: In Silico Supported In Vivo Study. Pharmaceutics, 2023, 15, 415.	2.0	8
4778	Machine Learning Identification of Active Sites in Graphite-Conjugated Catalysts. Journal of Physical Chemistry C, 2023, 127, 2303-2313.	1.5	3
4779	Coronavirus Inhibitors Targeting nsp16. Molecules, 2023, 28, 988.	1.7	6
4780	Inhibition of Neutral Sphingomyelinase 2 by Novel Small Molecule Inhibitors Results in Decreased Release of Extracellular Vesicles by Vascular Smooth Muscle Cells and Attenuated Calcification. International Journal of Molecular Sciences, 2023, 24, 2027.	1.8	3
4781	Systematic Analysis of the Mechanism of Polygoni Multiflori Caulis in Improving Depressive Disorder in Mice via Network Pharmacology Combined with Ultra-High Performance Liquid Chromatography Coupled with Quadrupole Exactive Orbitrap Mass Spectrometer. Combinatorial Chemistry and High Throughput Screening, 2023, 26, .	0.6	0
4782	Itraconazole Confers Cytoprotection Against Neurodegenerative Disease-Associated Abnormal Protein Aggregation. Molecular Neurobiology, 2023, 60, 2397-2412.	1.9	2
4783	CAPLA: improved prediction of proteinâ€“ligand binding affinity by a deep learning approach based on a cross-attention mechanism. Bioinformatics, 2023, 39, .	1.8	13
4784	Re-Routing Drugs to Blood Brain Barrier: A Comprehensive Analysis of Machine Learning Approaches With Fingerprint Amalgamation and Data Balancing. IEEE Access, 2023, 11, 9890-9906.	2.6	8

#	Article	IF	Citations
4786	Evaluating the Antimicrobial and Anti-Hemolytic Activity of Synthesized Pseudopeptide against Leptospiral Species: In Silico and In Vitro Approach. Molecules, 2023, 28, 1106.	1.7	0
4787	In Silico Study on the Interactions, Molecular Docking, Dynamics and Simulation of Potential Compounds from WithaniaÂsomnifera (L.) Dunal Root against Cancer by Targeting KAT6A. Molecules, 2023, 28, 1117.	1.7	6
4788	Structural Insights into Plasticity and Discovery of Flavonoid Allosteric Inhibitors of Flavivirus NS2Bâ€“NS3 Protease. Biophysica, 2023, 3, 71-92.	0.6	1
4790	In silico Investigation of Immulina Glycosidic Residues as Immunostimulants by Targeting Penaeus monodon Shrimp Toll-Receptor 9. , 2022, , .		0
4791	Prediction of Aqueous Solubility of Drug Molecules by Embedding Spatial Conformers Using Graph Neural Networks. , 2022, , .		0
4792	Screening of Secondary Metabolite Compounds of Gorontalo Traditional Medicinal Plants Using the In Silico Method as a Candidate for SARS-CoV-2 Antiviral. Jurnal Kimia Sains Dan Aplikasi, 2023, 25, 382-393.	0.1	0
4793	Solvation entropy, enthalpy and free energy prediction using a multi-task deep learning functional in 1D-RISM. Physical Chemistry Chemical Physics, 2023, 25, 6944-6954.	1.3	1
4795	Definition and exploration of realistic chemical spaces using the connectivity and cyclic features of ChEMBL and ZINC. , 2023, 2, 736-747.		1
4796	Deep Learning Methods for Small Molecule Drug Discovery: A Survey. IEEE Transactions on Artificial Intelligence, 2024, 5, 459-479.	3.4	0
4797	Virtual Screening for SARS-COV-2 Entry Inhibitors by Dual Targeting of TMPRSS2 and CTSL. Pharmacophore, 2023, 14, 9-18.	0.2	0
4798	S-Adenosyl-<scp>l</scp>-Homocysteine Exhibits Potential Antiviral Activity Against Dengue Virus Serotype-3 (DENV-3) in Bangladesh: A Viroinformatics-Based Approach. Bioinformatics and Biology Insights, 2023, 17, 117793222311582.	1.0	2
4799	Quantum chemical data generation as fill-in for reliability enhancement of machine-learning reaction and retrosynthesis planning. , 2023, 2, 663-673.		2
4800	Syntheses and Molecular Docking Analysis of Some New Thiazole and Thiazine Derivatives as Three Armed Molecules with a Triazine Ring as a Core Component: A Search for anti-Obesity Agents. Polycyclic Aromatic Compounds, 2024, 44, 275-293.	1.4	3
4801	In silico screening of phenylethanoid glycosides, a class of pharmacologically active compounds as natural inhibitors of SARS-CoV-2 proteases. Computational and Structural Biotechnology Journal, 2023, 21, 1461-1472.	1.9	3
4802	Scalable Inhibitors of the Nsp3â€“Nsp4 Coupling in SARS-CoV-2. ACS Omega, 2023, 8, 5349-5360.	1.6	4
4803	Identification of novel inhibitors against hantaviruses through 2D fingerprinting and molecular modeling approaches. Frontiers in Immunology, 0, 14, .	2.2	1
4804	Quantifying Functional-Group-like Structural Fragments in Molecules and Its Applications in Drug Design. Journal of Chemical Information and Modeling, 2023, 63, 2073-2083.	2.5	2
4805	In Silico Prediction of Antidiabetic Activity of Phytoconstituents of Pterocarpus Marsupium Targeting Î±-Amylase Enzyme. Biosciences, Biotechnology Research Asia, 2023, 20, 147-162.	0.2	0

#	Article	IF	Citations
4806	Artificial intelligence based virtual screening study for competitive and allosteric inhibitors of the SARS-CoV-2 main protease. Journal of Biomolecular Structure and Dynamics, 2023, 41, 15286-15304.	2.0	3
4807	Structure and function of the metagenomic plastic-degrading polyester hydrolase PHL7 bound to its product. Nature Communications, 2023, 14, .	5.8	20
4809	Discovery of novel dual acetylcholinesterase and butyrylcholinesterase inhibitors using machine learning and structure-based drug design. Journal of Molecular Structure, 2023, 1286, 135517.	1.8	4
4810	Discovery of 3CLpro inhibitor of SARS-CoV-2 main protease. Future Science OA, 2023, 9, .	0.9	3
4811	Recombinant production, purification, and biochemical characterization of a novel L-lactate dehydrogenase from Bacillus cereus NRC1 and inhibition study of mangiferin. Frontiers in Bioengineering and Biotechnology, 0, 11, .	2.0	1
4812	EDC-Predictor: A Novel Strategy for Prediction of Endocrine-Disrupting Chemicals by Integrating Pharmacological and Toxicological Profiles. Environmental Science & Technology, 2023, 57, 18013-18025.	4.6	7
4813	Mechanistic insights into the deformation and degradation of a 2D metal organic framework. Npj 2D Materials and Applications, 2023, 7, .	3.9	1
4815	New ferrocene integrated amphiphilic guanidines: Synthesis, spectroscopic elucidation, DFT calculation and in vitro Î±-amylase and Î±-glucosidase inhibition combined with molecular docking approach. Heliyon, 2023, 9, e14919.	1.4	1
4816	Evaluation the selectivity of three lipases in the synthesis of 1-oleoyl-2-palmitoyl-3-linoleoylglycerol, an asymmetric triacylglycerol. LWT - Food Science and Technology, 2023, 181, 114754.	2.5	1
4817	Dock-able linear and homodetic di, tri, tetra and pentapeptide library from canonical amino acids: SARS-CoV-2 Mpro as a case study. Journal of Pharmaceutical Analysis, 2023, 13, 523-534.	2.4	0
4818	Computational probing of Nigella sativa bioactive metabolites against chickungunya nsP2 cysteine protease. Journal of King Saud University - Science, 2023, 35, 102651.	1.6	0
4819	Ovatodiolide inhibits SARS-CoV-2 replication and ameliorates pulmonary fibrosis through suppression of the TGF-Î²/TÎ²Rs signaling pathway. Biomedicine and Pharmacotherapy, 2023, 161, 114481.	2.5	5
4820	Multi-model in silico characterization of 3-benzamidobenzoic acid derivatives as partial agonists of Farnesoid X receptor in the management of NAFLD. Computers in Biology and Medicine, 2023, 157, 106789.	3.9	1
4821	Phytochemical investigation of Scutellaria scordiifolia and its trypanocidal activity. Phytochemistry, 2023, 209, 113615.	1.4	0
4822	Isolation and characterization of novel hydroxyflavone from Kigelia africana (Lam.) Benth. fruit ethyl acetate fraction against CHO 1 and HeLa cancer cell lines: In vitro and in silico studies. Journal of Molecular Structure, 2023, 1282, 135180.	1.8	5
4823	A novel thermostable and salt-tolerant carboxylesterase involved in the initial aerobic degradation pathway for pyrethroids in Glycomyces salinus. Journal of Hazardous Materials, 2023, 451, 131128.	6.5	6
4824	Bioassay guided isolation of caffeoylquinic acids from the leaves of Ilex pubescens Hook. et Arn. and investigation of their anti-influenza mechanism. Journal of Ethnopharmacology, 2023, 309, 116322.	2.0	0
4825	Identification of Potent Small-Molecule PCSK9 Inhibitors Based on Quantitative Structure-Activity Relationship, Pharmacophore Modeling, and Molecular Docking Procedure. Current Problems in Cardiology, 2023, 48, 101660.	1.1	2

#	Article	IF	Citations
4826	Molecular electrostatics and pKa shifts calculations with the Generalized Born model. A tutorial through examples with Bluues2. Computer Physics Communications, 2023, 287, 108716.	3.0	1
4827	Bisbenzylisoquinolines from Cissampelos pareira L. as antimalarial agents: Molecular docking, pharmacokinetics analysis, and molecular dynamic simulation studies. Computational Biology and Chemistry, 2023, 104, 107826.	1.1	9
4828	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. Journal of Molecular Structure, 2023, 1284, 135404.	1.8	12
4829	Synthesis, Insecticidal Activity and Computational Studies of Eugenol-Based Insecticides. , 0, , .		0
4830	What Makes a Good Proteinâ€“Protein Interaction Stabilizer: Analysis and Application of the Dual-Binding Mechanism. ACS Central Science, 2023, 9, 969-979.	5.3	9
4832	Antioxidant activity and enzymatic of lichen substances: A study based on cyclic voltammetry and theoretical. Chemico-Biological Interactions, 2023, 372, 110357.	1.7	5
4833	Mechanisms Contributing to Acquired Activated Protein C Resistance in Patients Treated with Thalidomide: A Molecular Dynamics Study. Cardiovascular & Hematological Disorders Drug Targets, 2022, 22, 237-244.	0.2	0
4834	â€œHitâ€•to lead optimization and chemoinformatic studies for a new series of Autotaxin inhibitors. European Journal of Medicinal Chemistry, 2023, 249, 115130.	2.6	2
4835	Study of a High-Voltage NMC Interphase in the Presence of a Thiophene Additive Realized by Operando SHINERS. ACS Applied Materials & Interfaces, 2023, 15, 6676-6686.	4.0	7
4836	New Dual Inhibitors of SARS-CoV-2 Based on Metal Complexes with Schiff-Base 4-Chloro-3-Methyl Phenyl Hydrazine: Synthesis, DFT, Antibacterial Properties and Molecular Docking Studies. Inorganics, 2023, 11, 63.	1.2	7
4838	Tumor-associated nonmyelinating Schwann cellâ€“expressed PVT1 promotes pancreatic cancer kynurenine pathway and tumor immune exclusion. Science Advances, 2023, 9, .	4.7	10
4839	Exportin 1â€•mediated nuclear/cytoplasmic trafficking controls drug sensitivity of classical Hodgkin's lymphoma. Molecular Oncology, 2023, 17, 2546-2564.	2.1	0
4840	Design, Synthesis, Antimicrobial Evaluation, Antioxidant Studies, and Molecular Docking of Some New 1Hâ€Benzimidazole Derivatives. ChemistrySelect, 2023, 8, .	0.7	0
4841	Towards an Understanding of the Lipophilicity of Non-Coded Amino Acids: Computational Simulations of Proline Analogs. , 2022, , .		0
4842	The prognostic gene CRABP2 affects drug sensitivity by regulating docetaxel-induced apoptosis in breast invasive carcinoma: A pan-cancer analysis. Chemico-Biological Interactions, 2023, 373, 110372.	1.7	3
4843	Novel polyvinyl-alcohol microsphere for everolimus delivery for subependymal giant cell astrocytoma. Journal of Drug Delivery Science and Technology, 2023, 81, 104204.	1.4	2
4844	Toxicological impacts and likely protein targets of bisphenol a in Paramecium caudatum. European Journal of Protistology, 2023, 88, 125958.	0.5	0
4845	Investigation of the Impact of High Concentration LiTFSI Electrolytes on Silicon Anodes with Reactive Force Field Simulations. Liquids, 2023, 3, 132-158.	0.8	1

#	Article	IF	Citations
4846	Shu-Xie decoction alleviates oxidative stress and colon injury in acute sleep-deprived mice by suppressing p62/KEAP1/NRF2/HO1/NQO1 signaling. Frontiers in Pharmacology, 0, 14, .	1.6	2
4847	RGD and Scutellarin Conjugate (WK001) Targeting Platelet Glycoprotein IIb/IIIa Receptor Protects from Myocardial Ischemia/Reperfusion Injury: Synthesis, Characterization, and Bioactivity Evaluation. Bioconjugate Chemistry, 2023, 34, 477-488.	1.8	0
4848	Integrated use of ligand and structure-based virtual screening, molecular dynamics, free energy calculation and ADME prediction for the identification of potential PTP1B inhibitors. Molecular Diversity, 0, , .	2.1	1
4849	Quantum-Mechanical Approach to Predicting the Carcinogenic Potency of N-Nitroso Impurities in Pharmaceuticals. Chemical Research in Toxicology, 2023, 36, 291-304.	1.7	6
4850	High-throughput property-driven generative design of functional organic molecules. Nature Computational Science, 2023, 3, 139-148.	3.8	15
4851	Comprehensive Automated Routine Implementation, Validation, and Benchmark of the Anisotropic Force Field (AUA4) Using Python and GROMACS. Journal of Physical Chemistry A, 2023, 127, 1555-1563.	1.1	0
4852	Computational Modeling for the Prediction of Hepatotoxicity Caused by Drugs and Chemicals. Computational Methods in Engineering & the Sciences, 2023, , 541-561.	0.3	1
4853	Cholesterolâ€Aminoâ€Phosphate (CAP) Derived Lipid Nanoparticles for Delivery of Selfâ€Amplifying RNA and Restoration of Spermatogenesis in Infertile Mice. Advanced Science, 2023, 10, .	5.6	13
4854	Nucleoside Analogs That Inhibit SARS-CoV-2 Replication by Blocking Interaction of Virus Polymerase with RNA. International Journal of Molecular Sciences, 2023, 24, 3361.	1.8	3
4855	In Silico study and design of some new potent threonine tyrosine kinase inhibitors using molecular docking simulation. Molecular Simulation, 2023, 49, 517-524.	0.9	2
4856	Identification of AHL Synthase in Desulfovibrio vulgaris Hildenborough Using an In-Silico Methodology. Catalysts, 2023, 13, 364.	1.6	1
4857	Design, Synthesis, and Molecular Docking Study of 6-Aryl-3-(quinolin-3-yl)-7H-[1,2,4]triazolo[3,4-b][1,3,4]thiaÂdiazines as Novel Antimicrobial Agents. Russian Journal of Organic Chemistry, 2022, 58, 1851-1860.	0.3	0
4858	Inhibiting the transcription and replication of Ebola viruses by disrupting the nucleoprotein and VP30 protein interaction with small molecules. Acta Pharmacologica Sinica, 2023, 44, 1487-1499.	2.8	1
4859	DNMG: Deep molecular generative model by fusion of 3D information for de novo drug design. Methods, 2023, 211, 10-22.	1.9	6
4860	Synergism of mixed cationic collectors in the flotation of quartz unveiled by AFM, solution chemistry and quantum chemical calculations. Journal of Molecular Liquids, 2023, 376, 121397.	2.3	3
4861	Theoretical and Experimental Investigation of Autoxidation Propensity of Selected Drugs in Solution State. Molecular Pharmaceutics, 2023, 20, 1768-1778.	2.3	4
4862	Interaction of Some Asymmetrical Porphyrins with U937 Cell Membranesâ€“In Vitro and In Silico Studies. Molecules, 2023, 28, 1640.	1.7	2
4863	Blinded Predictions and Post Hoc Analysis of the Second Solubility Challenge Data: Exploring Training Data and Feature Set Selection for Machine and Deep Learning Models. Journal of Chemical Information and Modeling, 2023, 63, 1099-1113.	2.5	5

#	Article	IF	Citations
4864	Challenging breast cancer through novel sulfonamideâ€“pyridine hybrids: design, synthesis, carbonic anhydrase IX inhibition and induction of apoptosis. Future Medicinal Chemistry, 2023, 15, 147-166.	1.1	2
4865	Machine learning facilitated structural activity relationship approach for the discovery of novel inhibitors targeting EGFR. Journal of Biomolecular Structure and Dynamics, 2023, 41, 12445-12463.	2.0	1
4866	Computer-assisted discovery of safe and effective DprE1/ aaRSs Inhibitors against TB utilizing Drug Repurposing approach. Journal of Infection and Public Health, 2023, 16, 554-572.	1.9	3
4867	Bioactive compounds from four Indian medicinal plants have different potency to induce sex reversal in Nile tilapia: A chromatographic, molecular docking and in silico analysis. Journal of Ethnopharmacology, 2023, 307, 116263.	2.0	2
4868	Chemical and Biological Review of Endophytic Fungi Associated with Morus sp. (Moraceae) and In Silico Study of Their Antidiabetic Potential. Molecules, 2023, 28, 1718.	1.7	5
4869	Virtual Screening of Hepatitis B Virus Pre-Genomic RNA as a Novel Therapeutic Target. Molecules, 2023, 28, 1803.	1.7	2
4870	Ligand binding free energy evaluation by Monte Carlo Recursion. Computational Biology and Chemistry, 2023, 103, 107830.	1.1	0
4872	Synthesis and In Vitro and In Vivo Evaluation of ¹⁸F-Labeled Positron Emission Tomography Tracers for Imaging AÎ² Plaques. ACS Chemical Neuroscience, 2023, 14, 988-1003.	1.7	3
4873	Complexation between rice starch and cellulose nanocrystal from black tea residues: Gelatinization properties and digestibility in vitro. International Journal of Biological Macromolecules, 2023, 234, 123695.	3.6	7
4874	Artificial intelligence for drug discovery: Resources, methods, and applications. Molecular Therapy - Nucleic Acids, 2023, 31, 691-702.	2.3	27
4876	Interaction of Jania rubens Polyphenolic Extract as an Antidiabetic Agent with Î±-Amylase, Lipase, and Trypsin: In Vitro Evaluations and In Silico Studies. Catalysts, 2023, 13, 443.	1.6	9
4877	Identification of and Mechanistic Insights into SARS-CoV-2 Main Protease Non-Covalent Inhibitors: An In-Silico Study. International Journal of Molecular Sciences, 2023, 24, 4237.	1.8	1
4878	ï»¿An in silico investigation of 1,2,4-triazole derivatives as potential antioxidant agents using molecular docking, MD simulations, MM-PBSA free energy calculations and ADME predictions. Pharmacia, 2023, 70, 139-153.	0.4	4
4879	Dihydroisocoumarins and Phenylglycosides from Scorzonera longiana, Their Antimicrobial Activities and Molecular Docking Studies. Chemistry and Biodiversity, 2023, 20, .	1.0	0
4880	Coâ€Assembly of Carbon Nanotube Porins into Biomimetic Peptoid Membranes. Small, 2023, 19, .	5.2	3
4881	Antibacterial and Antioxidant Superoxide Anion Radical Inhibitors from Myrmecodia pendans: An In Silico Study. Natural Products Journal, 2023, 13, .	0.1	0
4882	Isolation, characterization and in silico study of propenamide alkaloids from Hymenoepmecis bicolor poison against active Î¼ -opioid receptor. Journal of Biomolecular Structure and Dynamics, 2023, 41, 14621-14637.	2.0	0
4883	IMPPAT 2.0: An Enhanced and Expanded Phytochemical Atlas of Indian Medicinal Plants. ACS Omega, 2023, 8, 8827-8845.	1.6	29

#	Article	IF	Citations
4884	Graph isomorphism-based algorithm for cross-checking chemical and crystallographic descriptions. Journal of Cheminformatics, 2023, 15, .	2.8	25
4885	Sterol Structural Featuresâ€™ Impact on the Spontaneous Membrane Insertion of CLIC1 into Artificial Lipid Membranes. Langmuir, 2023, 39, 3286-3300.	1.6	2
4886	Development and test of highly accurate endpoint free energy methods. 2: Prediction of logarithm of nâ€octanolâ€“water partition coefficient (<scp>logP</scp>) for druglike molecules using <scp>MMâ€PBSA</scp> method. Journal of Computational Chemistry, 2023, 44, 1300-1311.	1.5	3
4887	BEAR: A Novel Virtual Screening Method Based on Large-Scale Bioactivity Data. Journal of Chemical Information and Modeling, 2023, 63, 1429-1437.	2.5	3
4888	Identification of novel C-15 fluoro isosteviol derivatives for GABA-AT inhibition by in silico investigations. Journal of Molecular Modeling, 2023, 29, .	0.8	3
4889	Investigating a Library of Flavonoids as Potential Inhibitors of a Cancer Therapeutic Target MEK2 Using in Silico Methods. International Journal of Molecular Sciences, 2023, 24, 4446.	1.8	5
4890	Identifying novel and potent inhibitors of EGFR protein for the drug development against the breast cancer. Journal of Biomolecular Structure and Dynamics, 0, , 1-13.	2.0	2
4891	QSAR Models for the Prediction of Dietary Biomagnification Factor in Fish. Toxics, 2023, 11, 209.	1.6	2
4892	Beware of Simple Methods for Structure-Based Virtual Screening: The Critical Importance of Broader Comparisons. Journal of Chemical Information and Modeling, 2023, 63, 1401-1405.	2.5	7
4893	Machine Learning Models for Predicting Molecular UVâ€“Vis Spectra with Quantum Mechanical Properties. Journal of Chemical Information and Modeling, 2023, 63, 1462-1471.	2.5	13
4894	Response and Resistance to Trametinib in MAP2K1-Mutant Triple-Negative Melanoma. International Journal of Molecular Sciences, 2023, 24, 4520.	1.8	2
4895	Identification of novel Î±-glucosidase inhibitory peptides in rice wine and their antioxidant activities using in silico and in vitro analyses. LWT - Food Science and Technology, 2023, 178, 114629.	2.5	11
4896	In vitro and in vivo suppression of SARSâ€CoVâ€2 replication by a modified, short, cellâ€penetrating peptide targeting the Câ€terminal domain of the viral spike protein. Journal of Medical Virology, 2023, 95, .	2.5	8
4897	An approach combining deep learning and molecule docking for drug discovery of cathepsin L. Expert Opinion on Drug Discovery, 2023, 18, 347-356.	2.5	0
4898	Automatic and accurate ligand structure determination guided by cryo-electron microscopy maps. Nature Communications, 2023, 14, .	5.8	2
4899	IN SILICO LIBRARY SCREENING TO FIND NOVEL ANTICANCER AGENT WITH CHEMOSENSITIZING PROPERTIES: FOCUS ON TARGETING ATAXIA TELANGIECTASIA AND Rad3 RELATED KINASE. Military Medical Science Letters (Vojenske Zdravotnicke Listy), 2024, 93, 68-83.	0.2	0
4900	Imidazole-Based Alkaloids from Marine Sponges (Leucetta and Clathrina) as Potential Inhibitors Targeting SARS-CoV-2 Main Protease: An In Silico Approach. Polycyclic Aromatic Compounds, 0, , 1-16.	1.4	0
4901	Electronically excited states of closed-shell azabenzene and purine anion structures: Is 2ÂD enough for dipole-bound excited states?. Journal of Chemical Physics, 2023, 158, 124302.	1.2	0

#	Article	IF	Citations
4902	Molecular Design and In-Silico Analysis of Trisubstituted Benzimidazole Derivatives as Ftsz Inhibitor. Journal of Chemistry, 2023, 2023, 1-9.	0.9	6
4903	Discovery of novel acetylcholinesterase inhibitors through integration of machine learning with genetic algorithm based in silico screening approaches. Frontiers in Neuroscience, 0, 16, .	1.4	1
4904	Structural Characterization of the Chlorophyllide a Oxygenase (CAO) Enzyme Through an In Silico Approach. Journal of Molecular Evolution, 2023, 91, 225-235.	0.8	0
4905	Effects of synonymous mutations on kinetic properties and structure of firefly luciferase: Molecular dynamics simulation, molecular docking, RNA folding, and experimental study. International Journal of Biological Macromolecules, 2023, 235, 123835.	3.6	1
4906	Design and Synthesis of New Acyl Urea Analogs as Potential Ïƒ1R Ligands. Molecules, 2023, 28, 2319.	1.7	1
4907	Novel phytochemical inhibitors targeting monkeypox virus thymidine and serine/threonine kinase: integrating computational modeling and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 13679-13695.	2.0	6
4908	The Efficient Activity of Glabridin and its Derivatives Against EGFR-mediated Inhibition of Breast Cancer. Current Medicinal Chemistry, 2023, 30, .	1.2	3
4909	Identification of Dietary Bioflavonoids as Potential Inhibitors against KRAS G12D Mutantâ€"Novel Insights from Computer-Aided Drug Discovery. Current Issues in Molecular Biology, 2023, 45, 2136-2156.	1.0	5
4910	Understanding Passive Membrane Permeation of Peptides: Physical Models and Sampling Methods Compared. International Journal of Molecular Sciences, 2023, 24, 5021.	1.8	1
4911	An Impedimetric Biosensor for Detection of Volatile Organic Compounds in Food. Biosensors, 2023, 13, 341.	2.3	5
4912	Interaction of the nanobio-based reagent with sodium fluorescein and lipids via bioinformatics for forensic fingerprint visualisations. Journal of Biomolecular Structure and Dynamics, 2023, 41, 15045-15052.	2.0	2
4913	Photovoltaic characteristics of organic heterocyclic 2,9-dimethyl quinacridone in different solvents using DFT approach. Journal of Photochemistry and Photobiology A: Chemistry, 2023, 441, 114664.	2.0	9
4914	In silico targeting enterotoxin from Staphylococcus aureus with selected flavonoids: Hope for the discovery of natural anti-mastitis agents. Journal of Experimental Biology and Agricultural Sciences, 2023, 11, 132-139.	0.1	1
4915	Exploration of potent antiviral phytomedicines from Lauraceae family plants against SARS-CoV-2 RNA-dependent RNA polymerase. Journal of Biomolecular Structure and Dynamics, 2023, 41, 15085-15105.	2.0	1
4916	Integrating in vivo and in silico approaches to investigate the potential of Zingiber roseum rhizome extract against pyrexia, inflammation and pain. Saudi Journal of Biological Sciences, 2023, 30, 103624.	1.8	2
4917	Interaction of tacrine-coumarin derivatives with double stranded DNA: spectroscopic and molecular docking study. Chemical Papers, 2023, 77, 3993-4006.	1.0	1
4918	Computational Analysis to Predict Drug Targets for the Therapeutic Management of Mycobacterium avium sub. Paratuberculosis. Current Drug Discovery Technologies, 2023, 20, .	0.6	0
4919	SAMPL9 blind predictions for toluene/water partition coefficients using nonequilibrium alchemical approaches. Journal of Chemical Physics, 2023, 158, .	1.2	2

#	Article	IF	Citations
4920	In silico analysis of natural inhibitors against HPV E6 protein. Current Computer-Aided Drug Design, 2023, 19, .	0.8	1
4921	Assessment of lipid metabolismâ€disrupting effects of nonâ€phthalate plasticizer diisobutyl adipate through in silico and in vitro approaches. Environmental Toxicology, 0, , .	2.1	1
4922	In Silico and In Vitro Approach for Validating the Inhibition of Matrix Metalloproteinase-9 by Quercetin. Eye and Contact Lens, 2023, 49, 193-198.	0.8	1
4924	Study on Lowering the Group 1 Protease Allergens from House Dust Mites by Exposing to Todomatsu Oil Atmosphere. Atmosphere, 2023, 14, 548.	1.0	1
4925	Effect of inÂvitro simulated digestion on the anti- Helicobacter Pylori activity of different Propolis extracts. Journal of Enzyme Inhibition and Medicinal Chemistry, 2023, 38, .	2.5	2
4927	Effects of 4â€²-Demethylnobiletin and 4â€²-Demethyltangeretin on Osteoclast Differentiation In Vitro and in a Mouse Model of Estrogen-Deficient Bone Resorption. Nutrients, 2023, 15, 1403.	1.7	0
4928	Synthesis of Esterâ€Linked Ursolic Acidâ€Based Hybrid Compounds: Potential Antibacterial and Anticancer Agents. Chemistry and Biodiversity, 2023, 20, .	1.0	2
4929	High throughput screening of a new fluorescent G-quadruplex ligand having telomerase inhibitory activity in human A549 cells. Nucleosides, Nucleotides and Nucleic Acids, 2023, 42, 696-717.	0.4	0
4930	Free Energy Differences from Molecular Simulations: Exact Confidence Intervals from Transition Counts. Journal of Chemical Theory and Computation, 2023, 19, 2102-2108.	2.3	1
4931	New Fluoroquinoloneâ€1,2,4â€triazoles as Potent Antibacterial Agents: Design, Synthesis, Docking Studies and in Silico ADME Profiles. Chemistry and Biodiversity, 2023, 20, .	1.0	3
4932	A hybrid structure determination approach to investigate the druggability of the nucleocapsid protein of SARS-CoV-2. Nucleic Acids Research, 2023, 51, 4555-4571.	6.5	8
4933	Engineering Saccharomyces cerevisiae for the de novo Production of Halogenated Tryptophan and Tryptamine Derivatives. ChemistryOpen, 2023, 12, .	0.9	3
4934	MolTaut: A Tool for the Rapid Generation of Favorable Tautomer in Aqueous Solution. Journal of Chemical Information and Modeling, 2023, 63, 1833-1840.	2.5	3
4935	Preparation and Evaluation of 6-Gingerol Derivatives as Novel Antioxidants and Antiplatelet Agents. Antioxidants, 2023, 12, 744.	2.2	2
4936	Molecular docking and dynamics simulation study of quinones and pyrones from Alternaria solani and Alternaria alternata with HSP90: an important therapeutic target of cancer. Journal of Biomolecular Structure and Dynamics, 2023, 41, 14744-14756.	2.0	0
4938	Differentiating Toxic and Nontoxic Tricresyl Phosphate Isomers Using Ionâ€“Molecule Reactions with Oxygen. Journal of the American Society for Mass Spectrometry, 2023, 34, 640-648.	1.2	0
4939	Structure-Based Virtual Screening of Helicobacter pylori SecA Inhibitors. IEEE Transactions on Nanobioscience, 2023, , 1-1.	2.2	0
4940	Ligand-based pharmacophore modelling, virtual screening and docking studies to identify potential compounds against FtsZ of Mycobacterium tuberculosis. Indian Journal of Tuberculosis, 2023, , .	0.3	0

#	Article	IF	Citations
4941	Calculated Physicochemical Properties of Glycerol-Derived Solvents to Drive Plastic Waste Recycling. Industrial & Engineering Chemistry Research, 0, , .	1.8	4
4942	Drug repurposing for Mpox: Discovery of small molecules as potential inhibitors against DNAâ€dependent RNA polymerase using molecular modeling approach. Journal of Cellular Biochemistry, 2023, 124, 701-715.	1.2	9
4943	GutBug: A Tool for Prediction of Human Gut Bacteria Mediated Biotransformation of Biotic and Xenobiotic Molecules Using Machine Learning. Journal of Molecular Biology, 2023, 435, 168056.	2.0	4
4944	The impact of low-cost molecular geometry optimization in property prediction via graph neural network. , 2022, , .		0
4945	Finite-Temperature Mechanical Properties of Organic Molecular Crystals from Classical Molecular Simulation. Crystal Growth and Design, 2023, 23, 2155-2168.	1.4	4
4946	Synthesis and antiviral activity of 1,2,3-triazolyl nucleoside analogues with N-acetyl-<scp>d</scp>-glucosamine residue. Nucleosides, Nucleotides and Nucleic Acids, 0, , 1-23.	0.4	0
4947	Molecular modeling and simulations of some antiviral drugs, benzylisoquinoline alkaloid, and coumarin molecules to investigate the effects on Mpro main viral protease inhibition. Biochemistry and Biophysics Reports, 2023, 34, 101459.	0.7	5
4949	In silico characterization of cysteine-stabilized Î±Î² defensins from neglected unicellular microeukaryotes. BMC Microbiology, 2023, 23, .	1.3	0
4950	Computational Approaches for the Structure-Based Identification of Novel Inhibitors Targeting Nucleoid-Associated Proteins in Mycobacterium Tuberculosis. Molecular Biotechnology, 0, , .	1.3	0
4951	Complexation behaviour of piceatannol ligand with Ti(IV) and Zr(IV) metal ions: a combined DFT and deep learning investigation. Structural Chemistry, 2023, 34, 2139-2152.	1.0	3
4952	Design of new reversible and selective inhibitors of monoamine oxidase A and a comparison with drugs already approved. Bulletin of the National Research Centre, 2023, 47, .	0.7	2
4953	Exploring biogenic chalcones as DprE1 inhibitors for antitubercular activity via in silico approach. Journal of Molecular Modeling, 2023, 29, .	0.8	9
4954	Dopamine Fluorescent Sensor Based on Green Synthesized Copper Oxide Nanoparticles and Tyrosinase. , 2023, 2, 183-189.		1
4955	Evaluation of piperine analogs against prostate cancer targeting AKT1 kinase domain through network pharmacological analysis. In Silico Pharmacology, 2023, 11, .	1.8	0
4956	Screening Efficient Tandem Organic Solar Cells with Machine Learning and Genetic Algorithms. Journal of Physical Chemistry C, 2023, 127, 6179-6191.	1.5	4
4957	Potent and selective covalent inhibition of the papain-like protease from SARS-CoV-2. Nature Communications, 2023, 14, .	5.8	16
4958	SARS-CoV2 billion-compound docking. Scientific Data, 2023, 10, .	2.4	4
4959	Repurposing FIASMAs against Acid Sphingomyelinase for COVID-19: A Computational Molecular Docking and Dynamic Simulation Approach. Molecules, 2023, 28, 2989.	1.7	4

#	Article	IF	Citations
4960	Cheminformatics-Based Study Identifies Potential Ebola VP40 Inhibitors. International Journal of Molecular Sciences, 2023, 24, 6298.	1.8	8
4961	Interleukin-10 as Covid-19 biomarker targeting KSK and its analogues: Integrated network pharmacology. PLoS ONE, 2023, 18, e0282263.	1.1	0
4962	Probing the Interactions of 31 Mycotoxins with Xanthine Oxidase: Alternariol, Alternariol-3-Sulfate, and Î±-Zearalenol Are Allosteric Inhibitors of the Enzyme. Toxins, 2023, 15, 250.	1.5	2
4963	Discovery of Mycobacterium tuberculosis CYP121 New Inhibitor via Structure-based Drug Repurposing. Pertanika Journal of Science and Technology, 2023, 31, 1503-1521.	0.3	2
4964	Synthesis of Novel 2,9-Disubstituted-6-morpholino Purine Derivatives Assisted by Virtual Screening and Modelling of Class I PI3K Isoforms. Polymers, 2023, 15, 1703.	2.0	1
4965	A network pharmacology and molecular docking approach in the exploratory investigation of the biological mechanisms of lagundi (Vitex negundo L.) compounds against COVID-19. Genomics and Informatics, 2023, 21, e4.	0.4	0
4967	In silico screening of phytochemicals from Dissotis rotundifolia against Plasmodium falciparum Dihydrofolate Reductase. Phytomedicine Plus, 2023, 3, 100447.	0.9	3
4968	Development of New Targeted Nanotherapy Combined with Magneto-Fluorescent Nanoparticles against Colorectal Cancer. International Journal of Molecular Sciences, 2023, 24, 6612.	1.8	1
4969	Molecular Docking Studies for Evaluation of Amaranth Grain Squalene for Treatment of Melanoma Skin Cancer in Human Beings. Letters in Organic Chemistry, 2023, 20, .	0.2	0
4970	CDGCN: Conditional de novo Drug Generative Model Using Graph Convolution Networks. Lecture Notes in Computer Science, 2023, , 104-119.	1.0	1
4971	Insight into Tyrosine-Containing Pharmaceuticals as Potential Inhibitors of SARS-CoV-2 3CLpro and NSP16: Structural Analysis, Docking Studies, Molecular Dynamics Simulations, and Density Functional Theory Investigations. Chemistry, 2023, 5, 762-777.	0.9	0
4972	Deciphering Houttuynia cordata extract as electron shuttles with anti-COVID-19 activity and its performance in microbial fuel cells. Journal of the Taiwan Institute of Chemical Engineers, 2023, 145, 104838.	2.7	2
4973	Automated reaction kinetics and network exploration (Arkane): A statistical mechanics, thermodynamics, transition state theory, and master equationÂsoftware. International Journal of Chemical Kinetics, 2023, 55, 300-323.	1.0	8
4974	Curcumin and Plumbagin Synergistically Target the PI3K/Akt/mTOR Pathway: A Prospective Role in Cancer Treatment. International Journal of Molecular Sciences, 2023, 24, 6651.	1.8	13
4975	Digital research environments: a requirements analysis. , 0, , .		0
4976	Green Tea Catechins as Potential Drug Scaffolding Molecules in Structural Studies with Diverse Protein Targets. Current Physical Chemistry, 2023, 13, .	0.1	0
4977	Identifying novel selective PPO inhibitors through structure-based virtual screening and bio-evaluation. RSC Advances, 2023, 13, 10873-10883.	1.7	2
4978	Evaluation of Antimalarial Activity of Ethanolic Extract of Annona muricata L.: An in vivo and an in silico Approach. Journal of Evidence-based Integrative Medicine, 2023, 28, 2515690X2311651.	1.4	1

#	Article	IF	Citations
4979	Reorganization Energy Predictions with Graph Neural Networks Informed by Low-Cost Conformers. Journal of Physical Chemistry A, 2023, 127, 3484-3489.	1.1	4
4980	Surfactin-like lipopeptides from Bacillus clausii efficiently bind to spike glycoprotein of SARS-CoV-2. Journal of Biomolecular Structure and Dynamics, 0, , 1-12.	2.0	2
4981	Machine Learning for Ionization Potentials and Photoionization Cross Sections of Volatile Organic Compounds. ACS Earth and Space Chemistry, 2023, 7, 863-875.	1.2	2
4982	Drug Repurposing of FDA Compounds against Î±-Glucosidase for the Treatment of Type 2 Diabetes: Insights from Molecular Docking and Molecular Dynamics Simulations. Pharmaceuticals, 2023, 16, 555.	1.7	2
4983	Artificial intelligence assisted identification of potential tau aggregation inhibitors: ligand- and structure-based virtual screening, in silico ADME, and molecular dynamics study. Molecular Diversity, 0, , .	2.1	3
4984	Searching for the analogues of 1,1-dinitro-2,2-diamino ethylene (FOX-7) by high-throughput computation and machine learning. FirePhysChem, 2023, , .	1.5	2
4985	A good and bad aggregation: Effect of imidazolium- and cholinium-based ionic liquids on the thermal stability of bovine serum albumin. Journal of Molecular Liquids, 2023, 381, 121787.	2.3	2
4986	QSAR and molecular docking studies of isatin and indole derivatives as SARS 3CLpro inhibitors. BMC Chemistry, 2023, 17, .	1.6	2
4988	Tadalafil Rescues the p.M325T Mutant of Best1 Chloride Channel. Molecules, 2023, 28, 3317.	1.7	0
4989	Exploring polyamine interactions and binding pockets in SARS-CoV-2 ORF3a. Journal of Molecular Graphics and Modelling, 2023, 122, 108487.	1.3	0
4990	Using genetic algorithms to discover novel ground-state triplet conjugated polymers. Physical Chemistry Chemical Physics, 2023, 25, 11278-11285.	1.3	1
4991	An immunoinformatic approach to assessing the immunogenic capacity of alpha-neurotoxins in elapid snake venoms. Frontiers in Pharmacology, 0, 14, .	1.6	3
4992	Mapping Protein Targets of Carnosol, a Molecule Identified in Rosmarinus officinalis: In Silico Docking Studies and Network Pharmacology. Scientia Pharmaceutica, 2023, 91, 19.	0.7	0
4994	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. Journal of Molecular Structure, 2023, 1286, 135562.	1.8	6
4995	Molecular modeling, simulation and docking of Rv1250 protein from Mycobacterium tuberculosis. Frontiers in Bioinformatics, 0, 3, .	1.0	3
4996	The role of ETFS amino acids on the stability and inhibition of p53-MDM2 complex of anticancer p53-derivatives peptides: Density functional theory and molecular docking studies. Journal of Molecular Graphics and Modelling, 2023, 122, 108472.	1.3	2
4997	Amorphous Pterostilbene Delivery Systems Preparationâ€"Innovative Approach to Preparation Optimization. Pharmaceutics, 2023, 15, 1231.	2.0	9
4998	In-silico approaches for identification of compounds inhibiting SARS-CoV-2 3CL protease. PLoS ONE, 2023, 18, e0284301.	1.1	2

#	Article	IF	Citations
4999	In silico Exploration of Phytochemical based Thiazolidinone- Caffeic Acid- Indole New Chemical Entities for Simultaneous Management of Diabetes and Hypertension- A Fascinating Study. Cardiovascular & Hematological Disorders Drug Targets, 2023, 23, 21-30.	0.2	0
5000	AI-Driven Discovery of SARS-CoV-2 Main Protease Fragment-like Inhibitors with Antiviral Activity In Vitro. Journal of Chemical Information and Modeling, 2023, 63, 2866-2880.	2.5	4
5001	Gibberellin 2-Oxidases in Potato (Solanum tuberosum L.): Cloning, Characterization, In Silico Analysis and Molecular Docking. Molecular Biotechnology, 0, , .	1.3	1
5002	Computer-aided de novo design and optimization of novel potential inhibitors of HIV-1 Nef protein. Computational Biology and Chemistry, 2023, 104, 107871.	1.1	1
5003	Identification of Potential p38Î³ Inhibitors via In Silico Screening, In Vitro Bioassay and Molecular Dynamics Simulation Studies. International Journal of Molecular Sciences, 2023, 24, 7360.	1.8	2
5004	Ligand-based 3D pharmacophore modeling, virtual screening, and molecular dynamic simulation of potential smoothened inhibitors. Journal of Molecular Modeling, 2023, 29, .	0.8	1
5005	An in silico approach to unveil peptides from Acheta domesticus with potential bioactivity against hypertension, diabetes, cardiac and pulmonary fibrosis. Food Research International, 2023, 169, 112847.	2.9	4
5006	In-silico studies to recognize repurposing therapeutics toward arginase-I inhibitors as a potential onco-immunomodulators. Frontiers in Pharmacology, 0, 14, .	1.6	1
5007	Screening of Inhibitors against Idiopathic Pulmonary Fibrosis: Few-shot Machine Learning and Molecule Docking based Drug Repurposing. Current Computer-Aided Drug Design, 2024, 20, 134-144.	0.8	2
5008	Bayesian optimization for ternary complex prediction (BOTCP). Artificial Intelligence in the Life Sciences, 2023, 3, 100072.	1.6	0
5009	Novel Molecular Representations Using Neumann-Cayley Orthogonal Gated Recurrent Unit. Journal of Chemical Information and Modeling, 0, , .	2.5	0
5010	Co-aggregation between whey proteins and carotenoids from yellow mombin (Spondias mombin): Impact of carotenoidsâ€™ self-aggregation. Food Research International, 2023, 169, 112855.	2.9	0
5012	Anti-Biofilm: Machine Learning Assisted Prediction of IC50 Activity of Chemicals Against Biofilms of Microbes Causing Antimicrobial Resistance and Implications in Drug Repurposing. Journal of Molecular Biology, 2023, 435, 168115.	2.0	3
5013	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. Computers in Biology and Medicine, 2023, , 106965.	3.9	0
5014	Crystal structure of butenafine hydrochloride, C₂₃H₂₈NCl. Powder Diffraction, 2023, 38, 30-36.	0.4	1
5015	Antiviral Activity of Quercetin Hydrate against Zika Virus. International Journal of Molecular Sciences, 2023, 24, 7504.	1.8	3
5016	Polymer-Unit Fingerprint (PUFp): An Accessible Expression of Polymer Organic Semiconductors for Machine Learning. ACS Applied Materials & Interfaces, 2023, 15, 21537-21548.	4.0	0
5017	Principles of computational drug designing and drug repurposingâ€"An algorithmic approach. , 2023, , 129-146.		0

#	Article	IF	Citations
5019	In Silico Interactions of Natural and Synthetic Compounds with Key Proteins Involved in Alzheimerâ€™s Disease: Prospects for Designing New Therapeutics Compound. Neurotoxicity Research, 2023, 41, 408-430.	1.3	3
5050	Receptor-Based Virtual Screening of Large Libraries in a Multi-Level In Silico Approach. Methods in Molecular Biology, 2023, , 261-267.	0.4	0
5097	Bridging the Monomer to Polymer Gap in Radical Polymer Design. ACS Macro Letters, 2023, 12, 801-807.	2.3	2
5106	Aggregation of phospholipid self-assembled structures with addition of cholesterol and curcumin based on coarse-grained molecular dynamics simulations. AIP Conference Proceedings, 2023, , .	0.3	0
5112	Free tools and databases in ligand and structure-based drug design. , 2023, , 701-727.		1
5114	Chemical space and molecular descriptors for QSAR studies. , 2023, , 303-327.		0
5115	Deep learning methodologies in drug design. , 2023, , 361-392.		0
5131	CORAL: Predictions of Quality of Rice Based on Retention Index Using a Combination of Correlation Intensity Index and Consensus Modelling. Challenges and Advances in Computational Chemistry and Physics, 2023, , 421-462.	0.6	0
5153	De Novo Drug Design of Potential Inhibitors of SARS-CoV-2 Papain-like Protease. , 0, , .		0
5154	De Novo Drug Design of Potential Inhibitors of the Receptor-Binding Domain of SARS-CoV-2 Variants. , 0, , .		0
5214	Discovery of Novel Photocatalysts Using Machine Learning Approach. , 2023, , 233-261.		0
5220	Advances in Computational and Bioinformatics Tools and Databases for Designing and Developing a Multi-Epitope-Based Peptide Vaccine. International Journal of Peptide Research and Therapeutics, 2023, 29, .	0.9	6
5235	Drug Repositioning for Drug Disease Association in Meta-paths. Studies in Computational Intelligence, 2023, , 39-51.	0.7	0
5241	Web Services for the Prediction of ADMET Parameters Relevant to the Design of Neuroprotective Drugs. Neuromethods, 2023, , 465-485.	0.2	0
5243	SBDD and Its Challenges. Challenges and Advances in Computational Chemistry and Physics, 2023, , 1-24.	0.6	0
5299	Methods for computer-assisted PROTAC design. Methods in Enzymology, 2023, , 311-340.	0.4	1
5314	Open-Source Machine Learning in Computational Chemistry. Journal of Chemical Information and Modeling, 2023, 63, 4505-4532.	2.5	3
5380	DIY Virtual Chemical Libraries - Novel Starting Points for Drug Discovery. ACS Medicinal Chemistry Letters, 0, , .	1.3	0

#	Article	IF	Citations
5428	Identification of Potential Hits against Fungal Lysine Deacetylase Rpd3 via Molecular Docking, Molecular Dynamics Simulation, DFT, In-Silico ADMET and Drug-Likeness Assessment. Chemistry Africa, 2024, 7, 1151-1164.	1.2	3
5464	In-silico analysis of phytochemical profile of Capparis decidua evince substitutive approach against inhibition of acetylcholinesterase in Alzheimer's. , 2023, , .		0
5469	In silico network pharmacology analysis and molecular docking validation of Swasa Kudori tablet for screening druggable phytoconstituents of asthma. Advances in Protein Chemistry and Structural Biology, 2023, , .	1.0	0
5486	AI-Driven Enhancements in Drug Screening and Optimization. Methods in Molecular Biology, 2024, , 269-294.	0.4	2
5488	Proteinâ€“Ligand Blind Docking Using CB-Dock2. Methods in Molecular Biology, 2024, , 113-125.	0.4	1
5523	Physics-Guided Deep Generative Model For New Ligand Discovery. , 2023, , .		0
5569	MPerformer: An SE(3) Transformer-based Molecular Perceptron. , 2023, , .		0
5674	In Silico Prediction and Screening of Potential Immunomodulators Using Autodock Vina. , 2024, , 567-578.		0
5751	In Silico Analysis of Cyanotoxin Using Computational Tools. , 2023, , 273-281.		0
5833	Finding for New Drugs in Nature for Neglected Tropical Diseases: In Silico Study of Homolycorine Alkaloids Against Chagas Disease. , 2023, , .		0
5857	PandoraRLO: Unveiling Protein-Ligand Interactions with Reinforcement Learning for Optimized Pose Prediction. , 2023, , .		0
5858	Integrative Drug Discovery Platform: A Modular Approach for Efficient and Automated Virtual Screening. , 2023, , .		0
5860	ADMEOOD: Out-of-Distribution Benchmark for Drug Property Prediction. , 2023, , .		0
5867	Mining Large-Scale Knowledge Graphs for Chemical Reaction Fingerprints. , 2023, , .		0
5876	Bioinformatics Approaches in Studying the Fungal Endophyte-Derived Bioactive Compounds with Pharmacological Relevance. Fungal Biology, 2024, , 191-208.	0.3	0
5885	A Scaling Analysis of Post-Detonation Mixing With Detailed Chemical Kinetics. , 2024, , .		0
5886	Generation of Deep Learning Models and Structural Alerts for Accurate Prediction of Eye Irritants. , 2023, , .		0
5887	Three-Dimensional Study of Prompt and Delayed Ignition and Combustion of Explosively Dispersed Aluminum Powder. , 2024, , .		0

#	Article	IF	Citations
5897	Molecular fragmentation as a crucial step in the AI-based drug development pathway. Communications Chemistry, 2024, 7, .	2.0	0
5911	Exploring the Chemical Diversity of Moroccan Medicinal Plants Through MoroChem: A Valuable Resource for Drug Discovery and Traditional Medicine. Lecture Notes in Networks and Systems, 2024, , 465-476.	0.5	0
6027	In Silico Models on Algal Cultivation and Processing. , 2023, , 989-1016.		0