

Surflex: A Fully Automatic Flexible Molecular Docking Search Engine

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Citation Report

#	ARTICLE	IF	CITATIONS
5	Comparative molecular surface analysis: A novel tool for drug design and molecular diversity studies. <i>Molecular Diversity</i> , 2003, 7, 45-59.	3.9	8
6	Inhibition of carbonic anhydrase II by steroidal and non-steroidal sulphamates. <i>Biochemical and Biophysical Research Communications</i> , 2003, 305, 909-914.	2.1	72
7	Modeling and Mutagenesis of the Binding Site of Calhex 231, a Novel Negative Allosteric Modulator of the Extracellular Ca ²⁺ -sensing Receptor. <i>Journal of Biological Chemistry</i> , 2003, 278, 49487-49494.	3.4	115
8	Positive and Negative Allosteric Modulators of the Ca ²⁺ -sensing Receptor Interact within Overlapping but Not Identical Binding Sites in the Transmembrane Domain. <i>Journal of Biological Chemistry</i> , 2004, 279, 18990-18997.	3.4	191
9	A pharmacophore-based evolutionary approach for screening estrogen receptor antagonists. , 0, , .		1
10	Glide: A New Approach for Rapid, Accurate Docking and Scoring. 1. Method and Assessment of Docking Accuracy. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 1739-1749.	6.4	7,428
11	ProPose: a docking engine based on a fully configurable protein-ligand interaction model. <i>Journal of Molecular Modeling</i> , 2004, 10, 342-357.	1.8	23
12	GasDock: a new approach for rapid flexible docking based on an improved multi-population genetic algorithm. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2004, 14, 4671-4676.	2.2	56
13	Comparative evaluation of eight docking tools for docking and virtual screening accuracy. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 57, 225-242.	2.6	496
14	Relative free energy of binding and binding mode calculations of HIV-1 RT inhibitors based on dock-MM-PB/GS. <i>Proteins: Structure, Function and Bioinformatics</i> , 2004, 57, 493-503.	2.6	35
15	Hierarchical analysis of promolecular full electron-density distributions: description of protein structure fragments. <i>Acta Crystallographica Section D: Biological Crystallography</i> , 2004, 60, 1254-1265.	2.5	10
16	Virtual Screening with Flexible Docking and COMBINE-Based Models. Application to a Series of Factor Xa Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 805-820.	6.4	54
17	Glide: A New Approach for Rapid, Accurate Docking and Scoring. 2. Enrichment Factors in Database Screening. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 1750-1759.	6.4	3,982
18	CoMFA 3D-QSAR Analysis of HIV-1 RT Nonnucleoside Inhibitors, TIBO Derivatives Based on Docking Conformation and Alignment. <i>Journal of Chemical Information and Computer Sciences</i> , 2004, 44, 2167-2178.	2.8	45
19	Ligand-Based Structural Hypotheses for Virtual Screening. <i>Journal of Medicinal Chemistry</i> , 2004, 47, 947-961.	6.4	189
20	An Evolutionary Approach with Pharmacophore-Based Scoring Functions for Virtual Database Screening. <i>Lecture Notes in Computer Science</i> , 2004, , 481-492.	1.3	2
21	Design, synthesis, and biological evaluation of novel naphthoquinone derivatives with CDC25 phosphatase inhibitory activity. <i>Bioorganic and Medicinal Chemistry</i> , 2005, 13, 4871-4879.	3.0	51
22	Fast Structure-Based Virtual Ligand Screening Combining FRED, DOCK, and Surflex. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 6012-6022.	6.4	106

#	ARTICLE	IF	CITATIONS
23	A scoring function for docking ligands to low-resolution protein structures. <i>Journal of Computational Chemistry</i> , 2005, 26, 374-383.	3.3	27
24	Yucca: An Efficient Algorithm for Small-Molecule Docking. <i>Chemistry and Biodiversity</i> , 2005, 2, 1517-1524.	2.1	15
25	Design of Ligand Binding to an Engineered Protein Cavity Using Virtual Screening and Thermal Up-shift Evaluation. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 421-443.	2.9	1
26	Influence of conformation on the representation of small flexible molecules at low resolution: alignment of endothiapsin ligands. <i>Journal of Computer-Aided Molecular Design</i> , 2005, 19, 525-549.	2.9	10
27	A pharmacophore-based evolutionary approach for screening selective estrogen receptor modulators. <i>Proteins: Structure, Function and Bioinformatics</i> , 2005, 59, 205-220.	2.6	87
28	Hierarchical Docking of Databases of Multiple Ligand Conformations. <i>Current Topics in Medicinal Chemistry</i> , 2005, 5, 739-749.	2.1	139
29	Docking: Successes and Challenges. <i>Current Pharmaceutical Design</i> , 2005, 11, 323-333.	1.9	203
30	Consensus Scoring Criteria for Improving Enrichment in Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2005, 45, 1134-1146.	5.4	220
31	Modeling Water Molecules in Protein-Ligand Docking Using GOLD. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 6504-6515.	6.4	354
32	Design of Small-Sized Libraries by Combinatorial Assembly of Linkers and Functional Groups to a Given Scaffold: Application to the Structure-Based Optimization of a Phosphodiesterase 4 Inhibitor. <i>Journal of Medicinal Chemistry</i> , 2005, 48, 3816-3822.	6.4	58
33	Do Structurally Similar Ligands Bind in a Similar Fashion?. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 6716-6725.	6.4	171
34	Protein-ligand docking: Current status and future challenges. <i>Proteins: Structure, Function and Bioinformatics</i> , 2006, 65, 15-26.	2.6	761
35	Structure-Based Design, Synthesis, and Biological Evaluation of Novel Inhibitors of Human Cyclophilin A. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 900-910.	6.4	57
36	Parallelized-over-parts computation of absolute binding free energy with docking and molecular dynamics. <i>Journal of Chemical Physics</i> , 2006, 125, 084901.	3.0	92
37	Robust Ligand-Based Modeling of the Biological Targets of Known Drugs. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 2921-2938.	6.4	97
38	Parameter Estimation for Scoring Protein-Ligand Interactions Using Negative Training Data. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 5856-5868.	6.4	139
39	N1-Benzoyl-N2-[1-(1-naphthyl)ethyl]-trans-1,2-diaminocyclohexanes: Development of 4-Chlorophenylcarboxamide (Calhex 231) as a New Calcium Sensing Receptor Ligand Demonstrating Potent Calcilytic Activity. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 5119-5128.	6.4	50
40	Benchmarking Sets for Molecular Docking. <i>Journal of Medicinal Chemistry</i> , 2006, 49, 6789-6801.	6.4	1,184

#	ARTICLE	IF	CITATIONS
41	Leadhopping “ and beyond. Expert Opinion on Drug Discovery, 2006, 1, 311-321.	5.0	8
42	Design of nevirapine derivatives insensitive to the K103N and Y181C HIV-1 reverse transcriptase mutants. SAR and QSAR in Environmental Research, 2006, 17, 183-194.	2.2	5
43	Chapter 11 Recent Advances in Design of Small-Molecule Ligands to Target Protein-Protein Interactions. Annual Reports in Computational Chemistry, 2006, , 197-219.	1.7	1
44	Dock around the Clock “ Current Status of Small Molecule Docking and Scoring. QSAR and Combinatorial Science, 2006, 25, 605-615.	1.4	41
45	Effective handling of induced-fit motion in flexible docking. Proteins: Structure, Function and Bioinformatics, 2006, 63, 878-891.	2.6	53
46	Critical assessment of the automated AutoDock as a new docking tool for virtual screening. Proteins: Structure, Function and Bioinformatics, 2006, 65, 549-554.	2.6	160
47	Challenges facing the biologist doing chemical genetics. Nature Chemical Biology, 2006, 2, 55-58.	8.0	8
48	MolDock: A New Technique for High-Accuracy Molecular Docking. Journal of Medicinal Chemistry, 2006, 49, 3315-3321.	6.4	1,879
49	Chapter 16 Recent Evaluations of High Throughput Docking Methods for Pharmaceutical Lead Finding “ Consensus and Caveats. Annual Reports in Computational Chemistry, 2006, 2, 297-323.	1.7	6
50	Crystal structure of Bacillus subtilis TrmB, the tRNA (m7G46) methyltransferase. Nucleic Acids Research, 2006, 34, 1925-1934.	14.5	36
51	Estrogen Receptors: Molecular Interactions, Virtual Screening and Future Prospects. Current Topics in Medicinal Chemistry, 2006, 6, 217-243.	2.1	29
52	Receptor-Based Computational Screening of Compound Databases: The Main Docking-Scoring Engines. Current Protein and Peptide Science, 2006, 7, 369-393.	1.4	47
53	Scoring Functions for Protein-Ligand Docking. Current Protein and Peptide Science, 2006, 7, 407-420.	1.4	218
54	Curcumin induces caspase-3-dependent apoptotic pathway but inhibits DNA fragmentation factor 40/caspase-activated DNase endonuclease in human Jurkat cells. Molecular Cancer Therapeutics, 2006, 5, 927-934.	4.1	74
55	Critical Role for Polar Residues in Coupling Leukotriene B4 Binding to Signal Transduction in BLT1. Journal of Biological Chemistry, 2007, 282, 10005-10017.	3.4	32
56	Critical Role of Desolvation in the Binding of 20-Hydroxyecdysone to the Ecdysone Receptor. Journal of Biological Chemistry, 2007, 282, 32924-32934.	3.4	66
57	The Structure of the R184A Mutant of the Inositol Monophosphatase Encoded by <i>suH</i> and Implications for Its Functional Interactions in Escherichia coli. Journal of Biological Chemistry, 2007, 282, 26989-26996.	3.4	20
58	Computational Identification of Inhibitors of Protein-Protein Interactions. Current Topics in Medicinal Chemistry, 2007, 7, 63-82.	2.1	86

#	ARTICLE	IF	CITATIONS
59	ParDOCK: An All Atom Energy Based Monte Carlo Docking Protocol for Protein-Ligand Complexes. <i>Protein and Peptide Letters</i> , 2007, 14, 632-646.	0.9	120
60	From Drug Target to Leads-Sketching A Physicochemical Pathway for Lead Molecule Design In Silico. <i>Current Pharmaceutical Design</i> , 2007, 13, 3454-3470.	1.9	61
61	Free Resources to Assist Structure-Based Virtual Ligand Screening Experiments. <i>Current Protein and Peptide Science</i> , 2007, 8, 381-411.	1.4	104
62	Structure-Based Drug Design: Docking and Scoring. <i>Current Protein and Peptide Science</i> , 2007, 8, 312-328.	1.4	279
63	Protein-Ligand Docking with Evolutionary Algorithms. , 0, , 167-195.		3
64	Overview: Differentiating Issues in the Development of Macromolecules Compared with Small Molecules. , 0, , 89-123.		7
65	Structure and ligand-binding site characteristics of the human P2Y11 nucleotide receptor deduced from computational modelling and mutational analysis. <i>Biochemical Journal</i> , 2007, 405, 277-286.	3.7	48
66	Phosphorylation-dependent structure of ATF4 peptides derived from a human ATF4 protein, a member of the family of transcription factors. <i>Peptides</i> , 2007, 28, 2253-2267.	2.4	17
67	Evaluations of Molecular Docking Programs for Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1609-1618.	5.4	138
68	Anaesthetic binding sites for etomidate and propofol on a GABAA receptor model. <i>Neuroscience Letters</i> , 2007, 418, 28-33.	2.1	32
69	Discovery of a Highly Active Ligand of Human Pregnane X Receptor: A Case Study from Pharmacophore Modeling and Virtual Screening to <i>in Vivo</i> Biological Activity. <i>Molecular Pharmacology</i> , 2007, 72, 572-581.	2.3	54
70	Improving Docking Accuracy through Molecular Mechanics Generalized Born Optimization and Scoring. <i>Journal of Chemical Theory and Computation</i> , 2007, 3, 1106-1119.	5.3	45
71	Highly Efficient Ligands for Dihydrofolate Reductase from <i>Cryptosporidium hominis</i> and <i>Toxoplasma gondii</i> Inspired by Structural Analysis. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 940-950.	6.4	72
72	Design of protein-membrane interaction inhibitors by virtual ligand screening, proof of concept with the C2 domain of factor V. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2007, 104, 12697-12702.	7.1	50
73	GlamDock: Development and Validation of a New Docking Tool on Several Thousand Protein-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1657-1672.	5.4	60
74	Impact of Ligand Protonation on Virtual Screening against β -Secretase (BACE1). <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 2366-2373.	5.4	37
75	Comparative Performance of Several Flexible Docking Programs and Scoring Functions: Enrichment Studies for a Diverse Set of Pharmaceutically Relevant Targets. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1599-1608.	5.4	148
76	Identification of Nonpeptide CCR5 Receptor Agonists by Structure-based Virtual Screening. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 1294-1303.	6.4	117

#	ARTICLE	IF	CITATIONS
77	Supervised Scoring Models with Docked Ligand Conformations for Structure-Based Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 1858-1867.	5.4	12
78	Docking and Scoring for Structure-based Drug Design. , 0, , 541-599.		5
79	Supervised Consensus Scoring for Docking and Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 526-534.	5.4	88
80	Tagged Fragment Method for Evolutionary Structure-Based De Novo Lead Generation and Optimization. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 5392-5402.	6.4	35
81	Synthesis and Biological Properties of Novel 2-Aminopyrimidin-4(3H)-ones Highly Potent against HIV-1 Mutant Strains. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 5412-5424.	6.4	55
82	De NovoParallel Design, Synthesis and Evaluation of Inhibitors against the Reverse Transcriptase of Human Immunodeficiency Virus Type-1 and Drug-Resistant Variants. <i>Journal of Medicinal Chemistry</i> , 2007, 50, 2370-2384.	6.4	34
84	Fragment-Based Synthesis and SAR of Modified FKBP Ligands: Influence of Different Linking on Binding Affinity. <i>ChemMedChem</i> , 2007, 2, 1054-1070.	3.2	23
85	Virtual screening strategies in drug discovery. <i>Current Opinion in Chemical Biology</i> , 2007, 11, 494-502.	6.1	372
86	Structure-based virtual ligand screening with LigandFit: Pose prediction and enrichment of compound collections. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 68, 712-725.	2.6	45
87	A novel approach to local similarity of protein binding sites substantially improves computational drug design results. <i>Proteins: Structure, Function and Bioinformatics</i> , 2007, 69, 349-357.	2.6	23
88	ICAM-1 Peptide Inhibitors of T-cell Adhesion bind to the allosteric site of LFA-1. An NMR Characterization. <i>Chemical Biology and Drug Design</i> , 2007, 70, 347-353.	3.2	23
89	Optimizing Fragment and Scaffold Docking by Use of Molecular Interaction Fingerprints. <i>Journal of Chemical Information and Modeling</i> , 2007, 47, 195-207.	5.4	357
90	Surflex-Dock 2.1: Robust performance from ligand energetic modeling, ring flexibility, and knowledge-based search. <i>Journal of Computer-Aided Molecular Design</i> , 2007, 21, 281-306.	2.9	517
91	Bias, reporting, and sharing: computational evaluations of docking methods. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 201-212.	2.9	137
92	A knowledge-based approach to generating diverse but energetically representative ensembles of ligand conformers. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 681-691.	2.9	19
93	Evaluation of the performance of 3D virtual screening protocols: RMSD comparisons, enrichment assessments, and decoy selection—What can we learn from earlier mistakes?. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 213-228.	2.9	330
94	Customizing scoring functions for docking. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 269-286.	2.9	51
95	A ligand's-eye view of protein binding. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 507-521.	2.9	19

#	ARTICLE	IF	CITATIONS
96	High quality binding modes in docking ligands to proteins. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 1373-1386.	2.6	39
97	A phospho-εsugar binding domain homologous to NagB enzymes regulates the activity of the central glycolytic genes repressor. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008, 71, 2038-2050.	2.6	10
98	Virtual Screening and Experimental Verification to Identify Potential Inhibitors of the ErmC Methyltransferase Responsible for Bacterial Resistance against Macrolide Antibiotics. <i>ChemMedChem</i> , 2008, 3, 316-322.	3.2	31
99	Is it possible to increase hit rates in structure-based virtual screening by pharmacophore filtering? An investigation of the advantages and pitfalls of post-filtering. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 26, 1237-1251.	2.4	57
100	N-1H-Benzimidazol-5-ylbenzenesulfonamide derivatives as potent hPXR agonists. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 3537-3549.	3.0	7
101	Diarylmethyloxime and hydrazone derivatives with 5-indolyl moieties as potent inhibitors of tubulin polymerization. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 5952-5961.	3.0	33
102	Naphthylphenstatins as tubulin ligands: Synthesis and biological evaluation. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 8999-9008.	3.0	32
103	CYP19 (aromatase): Exploring the scaffold flexibility for novel selective inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2008, 16, 8349-8358.	3.0	23
104	Lead Finder: An Approach To Improve Accuracy of Protein-Ligand Docking, Binding Energy Estimation, and Virtual Screening. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2371-2385.	5.4	187
105	Biarylpyrazolyl Oxadiazole as Potent, Selective, Orally Bioavailable Cannabinoid-1 Receptor Antagonists for the Treatment of Obesity. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 7216-7233.	6.4	55
106	Virtual screening of the estrogen receptor. <i>Expert Opinion on Drug Discovery</i> , 2008, 3, 853-866.	5.0	3
107	Towards the development of universal, fast and highly accurate docking/scoring methods: a long way to go. <i>British Journal of Pharmacology</i> , 2008, 153, S7-26.	5.4	416
108	Virtual Screening, Identification, and Biochemical Characterization of Novel Inhibitors of the Reverse Transcriptase of Human Immunodeficiency Virus Type-1. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 5702-5713.	6.4	25
109	A novel druglike spleen tyrosine kinase binder prevents anaphylactic shock when administered orally. <i>Journal of Allergy and Clinical Immunology</i> , 2008, 122, 188-194.e3.	2.9	27
110	Theoretical Studies on the Structure and Symmetry of the Transmembrane Region of Glutamatergic GluR5 Receptor. <i>Journal of Medicinal Chemistry</i> , 2008, 51, 3765-3776.	6.4	11
111	Virtual screening of chemical libraries for drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2008, 3, 1011-1026.	5.0	29
112	Molecular Docking of Intercalators and Groove-Binders to Nucleic Acids Using Autodock and Surflex. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1602-1615.	5.4	178
113	Structure-Based Approach to the Development of Potent and Selective Inhibitors of Dihydrofolate Reductase from <i>Cryptosporidium</i> . <i>Journal of Medicinal Chemistry</i> , 2008, 51, 6839-6852.	6.4	39

#	ARTICLE	IF	CITATIONS
114	An amino acid at position 142 in nitrilase from <i>Rhodococcus rhodochrous</i> ATCC 33278 determines the substrate specificity for aliphatic and aromatic nitriles. <i>Biochemical Journal</i> , 2008, 415, 401-407.	3.7	35
115	Structure-based virtual screening for glycosyltransferase51. <i>Molecular Simulation</i> , 2008, 34, 849-856.	2.0	21
116	Mechanism of Inhibition of HIV-1 Reverse Transcriptase by the Novel Broad-Range DNA Polymerase Inhibitor <i>N</i> -[2-[4-(Aminosulfonyl)phenyl]ethyl]-2-(2-thienyl)acetamide. <i>Biochemistry</i> , 2008, 47, 490-502.	2.5	17
117	Evaluation of Different Virtual Screening Programs for Docking in a Charged Binding Pocket. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2010-2020.	5.4	28
118	Receptor-Based Modeling and 3D-QSAR for a Quantitative Prediction of the Butyrylcholinesterase Inhibitors Based on Genetic Algorithm. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1092-1103.	5.4	37
119	Hidden Active Information in a Random Compound Library: Extraction Using a Pseudo-Structure-Activity Relationship Model. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 575-582.	5.4	10
120	Transfer-NMR and Docking Studies Identify the Binding of the Peptide Derived from Activating Transcription Factor 4 to Protein Ubiquitin Ligase \hat{I}^2 -TrCP. Competition STD-NMR with \hat{I}^2 -Catenin. <i>Biochemistry</i> , 2008, 47, 14-29.	2.5	28
121	Structure of the Complex between Phosphorylated Substrates and the SCF \hat{I}^2 -TrCP Ubiquitin Ligase Receptor: A Combined NMR, Molecular Modeling, and Docking Approach. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2350-2361.	5.4	9
122	Information Theory-Based Scoring Function for the Structure-Based Prediction of Protein-Ligand Binding Affinity. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1990-1998.	5.4	18
123	An Anchor-Dependent Molecular Docking Process for Docking Small Flexible Molecules into Rigid Protein Receptors. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 1638-1655.	5.4	8
124	ASEDock-Docking Based on Alpha Spheres and Excluded Volumes. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 583-590.	5.4	132
125	Receptor-Based Virtual Ligand Screening for the Identification of Novel CDC25 Phosphatase Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 157-165.	5.4	43
126	Bootstrap-Based Consensus Scoring Method for Protein-Ligand Docking. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 988-996.	5.4	14
127	Predicting the Accuracy of Ligand Overlay Methods with Random Forest Models. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 2386-2394.	5.4	8
128	Similarity Based Docking. <i>Journal of Chemical Information and Modeling</i> , 2008, 48, 186-196.	5.4	26
129	CYP2E1 Substrate Inhibition. <i>Journal of Biological Chemistry</i> , 2008, 283, 3487-3496.	3.4	64
130	Capsiate, a Nonpungent Capsaicin-Like Compound, Inhibits Angiogenesis and Vascular Permeability via a Direct Inhibition of Src Kinase Activity. <i>Cancer Research</i> , 2008, 68, 227-235.	0.9	79
131	Virtual Screening and Its Integration with Modern Drug Design Technologies. <i>Current Medicinal Chemistry</i> , 2008, 15, 37-46.	2.4	189

#	ARTICLE	IF	CITATIONS
132	Molecular Docking Algorithms. <i>Current Drug Targets</i> , 2008, 9, 1040-1047.	2.1	180
133	How to Efficiently Include Receptor Flexibility During Computational Docking. <i>Current Computer-Aided Drug Design</i> , 2008, 4, 143-153.	1.2	19
134	Small Molecule Docking. , 2008, , 469-500.		2
135	Steroid substrate-induced epimerase mechanism in the active site of the human 11 β -hydroxysteroid dehydrogenase type 1. <i>Nature Precedings</i> , 2008, , .	0.1	0
136	Discovery of novel triple helical DNA intercalators by an integrated virtual and actual screening platform. <i>Nucleic Acids Research</i> , 2009, 37, 1280-1287.	14.5	39
137	Novel synthetic inhibitors of 3-hydroxy-3-methylglutaryl-coenzyme A (HMG-CoA) reductase activity that inhibit tumor cell proliferation and are structurally unrelated to existing statins. <i>International Journal of Molecular Medicine</i> , 2009, 24, 633-43.	4.0	18
138	Modeling Reality for Optimal Docking of Small Molecules to Biological Targets. <i>Current Computer-Aided Drug Design</i> , 2009, 5, 241-263.	1.2	13
139	Bioinformatics Tools for Screening of Antiparasitic Drugs. <i>Current Drug Targets</i> , 2009, 10, 232-239.	2.1	12
140	Molecular Genetic PET Imaging Using an HSV1-tk Mutant Reporter Gene with Enhanced Specificity to Acycloguanosine Nucleoside Analogs. <i>Journal of Nuclear Medicine</i> , 2009, 50, 409-416.	5.0	29
141	Structure-based drug design: From nucleic acid to membrane protein targets. <i>Experimental and Molecular Pathology</i> , 2009, 86, 141-150.	2.1	54
142	Scoring ligand similarity in structure-based virtual screening. <i>Journal of Molecular Recognition</i> , 2009, 22, 280-292.	2.1	32
143	Peptidic modulators of protein-protein interactions: Progress and challenges in computational design. <i>Biopolymers</i> , 2009, 91, 505-513.	2.4	93
144	In vitro biological activity and structural analysis of 2,4-diamino-5-(2-arylpropargyl)pyrimidine inhibitors of <i>Candida albicans</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 4866-4872.	3.0	15
145	An improved adaptive genetic algorithm for protein-ligand docking. <i>Journal of Computer-Aided Molecular Design</i> , 2009, 23, 1-12.	2.9	35
146	Effects of protein conformation in docking: improved pose prediction through protein pocket adaptation. <i>Journal of Computer-Aided Molecular Design</i> , 2009, 23, 355-374.	2.9	88
147	A novel conformation optimization model and algorithm for structure-based drug design. <i>Journal of Mathematical Chemistry</i> , 2009, 46, 182-198.	1.5	3
148	Molecular docking: theoretical background, practical applications and perspectives. <i>Mendeleev Communications</i> , 2009, 19, 237-242.	1.6	22
149	Mechanism-based inhibitors of serine proteases with high selectivity through optimization of S ₁ ' subsite binding. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 3536-3542.	3.0	18

#	ARTICLE	IF	CITATIONS
150	A library of novel allosteric inhibitors against fructose 1,6-bisphosphatase. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 3916-3922.	3.0	82
151	The marine natural-derived inhibitors of glycogen synthase kinase-3 β phenylmethylene hydantoin: In vitro and in vivo activities and pharmacophore modeling. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 6032-6039.	3.0	47
152	Isocombretastatins A: 1,1-Diarylethenes as potent inhibitors of tubulin polymerization and cytotoxic compounds. <i>Bioorganic and Medicinal Chemistry</i> , 2009, 17, 6422-6431.	3.0	50
153	Identification of small molecules that inhibit GSK-3 β through virtual screening. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 533-537.	2.2	11
154	Insight into the effects of chiral isomers quinidine and quinine on CYP2D6 inhibition. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2009, 19, 803-806.	2.2	27
155	Comparison of Several Molecular Docking Programs: Pose Prediction and Virtual Screening Accuracy. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1455-1474.	5.4	387
156	GARD: A Generally Applicable Replacement for RMSD. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1889-1900.	5.4	44
157	Identification of Novel Non-Hydroxamate Anthrax Toxin Lethal Factor Inhibitors by Topomeric Searching, Docking and Scoring, and in Vitro Screening. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2726-2734.	5.4	26
158	Influence of Protonation, Tautomeric, and Stereoisomeric States on Protein-Ligand Docking Results. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1535-1546.	5.4	139
159	Docking and scoring: applications to drug discovery in the interactomics era. <i>Expert Opinion on Drug Discovery</i> , 2009, 4, 673-686.	5.0	13
160	X-ray structure of the ternary MTX-NADPH complex of the anthrax dihydrofolate reductase: A pharmacophore for dual-site inhibitor design. <i>Journal of Structural Biology</i> , 2009, 166, 162-171.	2.8	25
161	Physical Binding Pocket Induction for Affinity Prediction. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 6107-6125.	6.4	17
162	Carborane Clusters in Computational Drug Design: A Comparative Docking Evaluation Using AutoDock, FlexX, Glide, and Surflex. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1581-1589.	5.4	93
163	Modeling of Glutamate GluR6 Receptor and Its Interactions with Novel Noncompetitive Antagonists. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1094-1104.	5.4	14
164	Rational Design and Semisynthesis of Betulinic Acid Analogues as Potent Topoisomerase Inhibitors. <i>Journal of Natural Products</i> , 2009, 72, 1643-1650.	3.0	55
165	Validation of Molecular Docking Programs for Virtual Screening against Dihydropteroate Synthase. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 444-460.	5.4	367
166	Comparative Assessment of Scoring Functions on a Diverse Test Set. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1079-1093.	5.4	444
167	Massively parallel computation of absolute binding free energy with well-equilibrated states. <i>Physical Review E</i> , 2009, 79, 021914.	2.1	84

#	ARTICLE	IF	CITATIONS
168	Combined Virtual Screening Strategies. <i>Current Computer-Aided Drug Design</i> , 2009, 5, 23-37.	1.2	31
169	Novel Method for Generating Structure-Based Pharmacophores Using Energetic Analysis. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2356-2368.	5.4	279
170	Scoring Ensembles of Docked Protein:Ligand Interactions for Virtual Lead Optimization. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 2813-2819.	5.4	37
171	Discovery of Leukotriene A4 Hydrolase Inhibitors Using Metabolomics Biased Fragment Crystallography. <i>Journal of Medicinal Chemistry</i> , 2009, 52, 4694-4715.	6.4	114
172	Protein-Protein Interaction Inhibition (2P2I): Fewer and Fewer Undruggable Targets. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009, 12, 968-983.	1.1	11
173	How Computational Methods Try to Disclose the Estrogen Receptor Secrecy - Modeling the Flexibility. <i>Current Medicinal Chemistry</i> , 2009, 16, 2987-3027.	2.4	15
174	Protein-Drug Interaction Studies for Development of Drugs Against Plasmodium falciparum. <i>Current Drug Targets</i> , 2009, 10, 271-278.	2.1	21
175	Exploring Novel Target Space: A Need to Partner High Throughput Docking and Ligand-Based Similarity Searches?. <i>Combinatorial Chemistry and High Throughput Screening</i> , 2009, 12, 984-999.	1.1	6
176	Novel Organic Proteasome Inhibitors Identified by Virtual and in Vitro Screening. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 509-513.	6.4	42
177	Human spleen tyrosine kinase (Syk) recombinant expression systems for high-throughput assays. <i>Biotechnology Journal</i> , 2010, 5, 201-212.	3.5	4
178	Novel Potent Orally Active Multitargeted Receptor Tyrosine Kinase Inhibitors: Synthesis, Structure-Activity Relationships, and Antitumor Activities of 2-Indolinone Derivatives. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 8140-8149.	6.4	47
179	Homology modeling and atomic level binding study of GABAA receptor with novel enaminone amides. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 3595-3600.	5.5	9
180	Docking and 3D QSAR study of thiourea analogs as potent inhibitors of influenza virus neuraminidase. <i>Journal of Molecular Modeling</i> , 2010, 16, 1809-1818.	1.8	13
181	Mutational analysis of the active site residues of a d-psicose 3-epimerase from <i>Agrobacterium tumefaciens</i> . <i>Biotechnology Letters</i> , 2010, 32, 261-268.	2.2	11
182	A knowledge-guided strategy for improving the accuracy of scoring functions in binding affinity prediction. <i>BMC Bioinformatics</i> , 2010, 11, 193.	2.6	18
183	Druggable pockets and binding site centric chemical space: a paradigm shift in drug discovery. <i>Drug Discovery Today</i> , 2010, 15, 656-667.	6.4	249
184	Comparison of Structure- and Ligand-Based Virtual Screening Protocols Considering Hit List Complementarity and Enrichment Factors. <i>ChemMedChem</i> , 2010, 5, 148-158.	3.2	106
185	Semisynthetic Latrunculin Derivatives as Inhibitors of Metastatic Breast Cancer: Biological Evaluations, Preliminary Structure-Activity Relationship and Molecular Modeling Studies. <i>ChemMedChem</i> , 2010, 5, 274-285.	3.2	34

#	ARTICLE	IF	CITATIONS
186	Evaluation of the performance of four molecular docking programs on a diverse set of protein-ligand complexes. <i>Journal of Computational Chemistry</i> , 2010, 31, 2109-2125.	3.3	277
187	SKATE: A docking program that decouples systematic sampling from scoring. <i>Journal of Computational Chemistry</i> , 2010, 31, 2540-2554.	3.3	13
188	tieredScreen™ – Layered Virtual Screening Tool for the Identification of Novel Estrogen Receptor Alpha Modulators. <i>Molecular Informatics</i> , 2010, 29, 421-430.	2.5	7
189	Determining the binding affinity and binding site of bensulfuron-methyl to human serum albumin by quenching of the intrinsic tryptophan fluorescence. <i>Journal of Luminescence</i> , 2010, 130, 2013-2021.	3.1	59
190	Sulfometuron-methyl binding to human serum albumin: Evidence that sulfometuron-methyl binds at the Sudlow's site I. <i>Journal of Molecular Structure</i> , 2010, 968, 59-66.	3.6	28
191	Benchmarking docking and scoring protocol for the identification of potential acetylcholinesterase inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2010, 28, 870-882.	2.4	25
192	Fluorescence and circular dichroism studies of conjugates between metsulfuron-methyl and human serum albumin. <i>Colloids and Surfaces B: Biointerfaces</i> , 2010, 76, 441-448.	5.0	27
193	Design and pharmacophore modeling of biaryl methyl eugenol analogs as breast cancer invasion inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 496-507.	3.0	40
194	Utilization of the 1,2,3,5-thiazolidin-3-one 1,1-dioxide scaffold in the design of potential inhibitors of human neutrophil proteinase 3. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 1093-1102.	3.0	20
195	An integrative in silico methodology for the identification of modulators of macrophage migration inhibitory factor (MIF) tautomerase activity. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 5425-5440.	3.0	19
196	NMR spectroscopy and computational analysis of interaction between <i>Serratia marcescens</i> chitinase B and a dipeptide derived from natural-product cyclopentapeptide chitinase inhibitor argifin. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 5835-5844.	3.0	9
197	Building a MCHR1 homology model provides insight into the receptor-antagonist contacts that are important for the development of new anti-obesity agents. <i>Bioorganic and Medicinal Chemistry</i> , 2010, 18, 7365-7379.	3.0	8
198	Discovery of cannabinoid-1 receptor antagonists by virtual screening. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2010, 20, 5130-5132.	2.2	7
199	Comparison of current docking tools for the simulation of inhibitor binding by the transmembrane domain of the sarco/endoplasmic reticulum calcium ATPase. <i>Biophysical Chemistry</i> , 2010, 150, 88-97.	2.8	38
200	Exploring the effect of 2,3,4-trimethoxy-phenyl moiety as a component of indolephenstatins. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 588-597.	5.5	29
201	Docking and 3D-QSAR studies of influenza neuraminidase inhibitors using three-dimensional holographic vector of atomic interaction field analysis. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 1008-1014.	5.5	43
202	3D-QSAR studies of latrunculin-based actin polymerization inhibitors using CoMFA and CoMSIA approaches. <i>European Journal of Medicinal Chemistry</i> , 2010, 45, 3662-3668.	5.5	16
203	DynaDock: A new molecular dynamics-based algorithm for protein-peptide docking including receptor flexibility. <i>Proteins: Structure, Function and Bioinformatics</i> , 2010, 78, 1084-1104.	2.6	147

#	ARTICLE	IF	CITATIONS
204	Molecular Docking and QSAR Studies on Substituted Acyl(thio)urea and Thiadiazolo [2,3- α] Pyrimidine Derivatives as Potent Inhibitors of Influenza Virus Neuraminidase. <i>Chemical Biology and Drug Design</i> , 2010, 76, 245-254.	3.2	19
205	Structure-based virtual screening for novel inhibitors of Japanese encephalitis virus NS3 helicase/nucleoside triphosphatase. <i>FEMS Immunology and Medical Microbiology</i> , 2010, 58, 91-101.	2.7	9
206	Mechanism of Entecavir Resistance of Hepatitis B Virus with Viral Breakthrough as Determined by Long-Term Clinical Assessment and Molecular Docking Simulation. <i>Antimicrobial Agents and Chemotherapy</i> , 2010, 54, 882-889.	3.2	31
207	Structural basis for the methylation of G1405 in 16S rRNA by aminoglycoside resistance methyltransferase Sgm from an antibiotic producer: a diversity of active sites in m ⁷ G methyltransferases. <i>Nucleic Acids Research</i> , 2010, 38, 4120-4132.	14.5	34
208	Protein sequence alignment of target for entanyl analgesics μ-opioid receptor and its analysis. , 2010, , .		0
209	Mammary carcinogen-protein binding potentials: novel and biologically relevant structure-activity relationship model descriptors. <i>SAR and QSAR in Environmental Research</i> , 2010, 21, 463-479.	2.2	2
210	Exploring the binding features of polybrominated diphenyl ethers as estrogen receptor antagonists: docking studies. <i>SAR and QSAR in Environmental Research</i> , 2010, 21, 351-367.	2.2	21
211	Capture Compound Mass Spectrometry Sheds Light on the Molecular Mechanisms of Liver Toxicity of Two Parkinson Drugs. <i>Toxicological Sciences</i> , 2010, 113, 243-253.	3.1	34
212	In Silico Prediction of Estrogen Receptor Subtype Binding Affinity and Selectivity Using Statistical Methods and Molecular Docking with 2-Arylnaphthalenes and 2-Arylquinolines. <i>International Journal of Molecular Sciences</i> , 2010, 11, 3434-3458.	4.1	32
213	Reverse Pharmacognosy: Another Way to Harness the Generosity of Nature. <i>Current Pharmaceutical Design</i> , 2010, 16, 1682-1696.	1.9	31
214	MolDock Applied to Structure-Based Virtual Screening. <i>Current Drug Targets</i> , 2010, 11, 327-334.	2.1	89
215	Natural Products in Structure-Assisted Design of Molecular Cancer Therapeutics. <i>Current Pharmaceutical Design</i> , 2010, 16, 1718-1741.	1.9	20
216	Studies of Benzothiadiazine Derivatives as Hepatitis C Virus NS5B Polymerase Inhibitors Using 3D-QSAR, Molecular Docking and Molecular Dynamics. <i>Current Medicinal Chemistry</i> , 2010, 17, 2788-2803.	2.4	39
217	Advances and Challenges in Protein-Ligand Docking. <i>International Journal of Molecular Sciences</i> , 2010, 11, 3016-3034.	4.1	418
218	Cheminformatic Tools for Medicinal Chemists. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 4830-4841.	6.4	72
219	Structural Conservation in Band 4.1, Ezrin, Radixin, Moesin (FERM) Domains as a Guide To Identify Inhibitors of the Proline-Rich Tyrosine Kinase 2. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 669-677.	6.4	11
220	Structural Studies of Pterin-Based Inhibitors of Dihydropteroate Synthase. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 166-177.	6.4	81
221	Herbal Compound Farnesiferol C Exerts Antiangiogenic and Antitumor Activity and Targets Multiple Aspects of VEGFR1 (Flt1) or VEGFR2 (Flk1) Signaling Cascades. <i>Molecular Cancer Therapeutics</i> , 2010, 9, 389-399.	4.1	57

#	ARTICLE	IF	CITATIONS
222	Effects of 7-O Substitutions on Estrogenic and Anti-Estrogenic Activities of Daidzein Analogues in MCF-7 Breast Cancer Cells. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 6153-6163.	6.4	47
223	Rapid Context-Dependent Ligand Desolvation in Molecular Docking. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1561-1573.	5.4	276
226	ParaDockS: A Framework for Molecular Docking with Population-Based Metaheuristics. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 879-889.	5.4	47
227	Total Synthesis and Evaluation of C26-Hydroxyepothilone D Derivatives for Photoaffinity Labeling of β -Tubulin. <i>Journal of Organic Chemistry</i> , 2010, 75, 86-94.	3.2	14
228	Discovery of Novel GSK-3 β Inhibitors with Potent in Vitro and in Vivo Activities and Excellent Brain Permeability Using Combined Ligand- and Structure-Based Virtual Screening. <i>Journal of Medicinal Chemistry</i> , 2010, 53, 8534-8545.	6.4	63
229	Scoring functions and their evaluation methods for protein-ligand docking: recent advances and future directions. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 12899.	2.8	380
230	Molecular Interaction Fields and 3D-QSAR Studies of p53 β -MDM2 Inhibitors Suggest Additional Features of Ligand-Target Interaction. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1451-1465.	5.4	12
231	Molecular Modeling Studies of 4,5-Dihydro-1H-pyrazolo[4,3-h]quinazoline Derivatives as Potent CDK2/Cyclin A Inhibitors Using 3D-QSAR and Docking. <i>International Journal of Molecular Sciences</i> , 2010, 11, 3705-3724.	4.1	21
232	Computational Study on the Interaction of N1 Substituted Pyrazole Derivatives with B-Raf Kinase: An Unusual Water Wire Hydrogen-Bond Network and Novel Interactions at the Entrance of the Active Site. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 1101-1112.	5.4	33
233	Interaction of Morphine With a New μ -Adrenoceptor Agonist in Mice. <i>Journal of Pain</i> , 2010, 11, 71-78.	1.4	31
234	Anacardic Acid Inhibits Estrogen Receptor α -DNA Binding and Reduces Target Gene Transcription and Breast Cancer Cell Proliferation. <i>Molecular Cancer Therapeutics</i> , 2010, 9, 594-605.	4.1	46
235	Comparative Evaluation of 3D Virtual Ligand Screening Methods: Impact of the Molecular Alignment on Enrichment. <i>Journal of Chemical Information and Modeling</i> , 2010, 50, 992-1004.	5.4	52
236	The Geometric and Electrostatic Properties of Binding Cavities and Their Usage in Protein-Ligand Docking. , 2010, , .		0
237	Automatic clustering of docking poses in virtual screening process using self-organizing map. <i>Bioinformatics</i> , 2010, 26, 53-60.	4.1	63
238	Tackling the challenges posed by target flexibility in drug design. <i>Expert Opinion on Drug Discovery</i> , 2010, 5, 347-359.	5.0	38
239	Molecular modelling studies of new potential human DNA polymerase β inhibitors. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2011, 26, 270-279.	5.2	6
240	Investigation on the binding mode of benzothiophene analogues as potent factor IXa (FIXa) inhibitors in thrombosis by CoMFA, docking and molecular dynamic studies. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2011, 26, 792-804.	5.2	9
241	A novel pH-sensitive (α)- β -tocopherol-5-fluorouracil adduct with antioxidant and anticancer properties. <i>Chemical Communications</i> , 2011, 47, 10713.	4.1	10

#	ARTICLE	IF	CITATIONS
242	Titanocene anticancer complexes and their binding mode of action to human serum albumin: A computational study. <i>Metallomics</i> , 2011, 3, 152.	2.4	18
243	($\hat{\alpha}$)-Oleocanthal as a c-Met Inhibitor for the Control of Metastatic Breast and Prostate Cancers. <i>Planta Medica</i> , 2011, 77, 1013-1019.	1.3	115
244	Molecular Docking with Ligand Attached Water Molecules. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 909-917.	5.4	67
245	<i>AADS</i> - An Automated Active Site Identification, Docking, and Scoring Protocol for Protein Targets Based on Physicochemical Descriptors. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2515-2527.	5.4	113
246	Using Computational Techniques in Fragment-Based Drug Discovery. <i>Methods in Enzymology</i> , 2011, 493, 137-155.	1.0	11
247	Preparation and Refinement of Model Protein-Ligand Complexes. <i>Methods in Molecular Biology</i> , 2011, 857, 351-373.	0.9	12
249	FRED Pose Prediction and Virtual Screening Accuracy. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 578-596.	5.4	606
250	Combined 3D-QSAR, Molecular Docking, and Molecular Dynamics Study on Piperazinyl-Glutamate-Pyridines/Pyrimidines as Potent P2Y12 Antagonists for Inhibition of Platelet Aggregation. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2560-2572.	5.4	38
251	<i>DSX</i> : A Knowledge-Based Scoring Function for the Assessment of Protein-Ligand Complexes. <i>Journal of Chemical Information and Modeling</i> , 2011, 51, 2731-2745.	5.4	249
253	Screening Informatics and Cheminformatics. , 0, , 137-156.		0
254	Structure Based 3D-QSAR Studies on Cholinesterase Inhibitors. , 2011, , .		1
255	Computational Perspectives into Plasmeppsins Structure-Function Relationship: Implications to Inhibitors Design. <i>Journal of Tropical Medicine</i> , 2011, 2011, 1-15.	1.7	8
256	Virtual screening strategies in drug design - methods and applications. <i>Biotechnologia</i> , 2011, 3, 249-264.	0.9	36
257	Computational Approaches for the Discovery of Natural Lead Structures. , 2011, , 97-132.		1
258	Survey of public domain software for docking simulations and virtual screening. <i>Human Genomics</i> , 2011, 5, 497.	2.9	48
259	Synthesis and <i>in vitro</i> antibacterial activity of a series of novel gatifloxacin derivatives. <i>European Journal of Medicinal Chemistry</i> , 2011, 46, 4267-4273.	5.5	39
260	Thiosemicarbazones derived from 1-indanones as new anti-Trypanosoma cruzi agents. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 6818-6826.	3.0	50
261	Targeting the Proangiogenic VEGF-VEGFR Protein-Protein Interface with Drug-like Compounds by <i>In Silico</i> and <i>In vitro</i> Screening. <i>Chemistry and Biology</i> , 2011, 18, 1631-1639.	6.0	38

#	ARTICLE	IF	CITATIONS
262	Insights into the structural and conformational requirements of polybrominated diphenyl ethers and metabolites as potential estrogens based on molecular docking. <i>Chemosphere</i> , 2011, 84, 328-335.	8.2	10
263	Design, Synthesis, and Qualitative Structure-Activity Evaluations of Novel β -Secretase Inhibitors as Potential Alzheimer's Drug Leads. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 8373-8385.	6.4	46
265	Update 1 of: Computational Modeling Approaches to Structure-Function Analysis of G Protein-Coupled Receptors. <i>Chemical Reviews</i> , 2011, 111, PR438-PR535.	47.7	71
266	Integrating structure-based and ligand-based approaches for computational drug design. <i>Future Medicinal Chemistry</i> , 2011, 3, 735-750.	2.3	132
267	Docking Performance of Fragments and Druglike Compounds. <i>Journal of Medicinal Chemistry</i> , 2011, 54, 5422-5431.	6.4	109
268	Protein-ligand docking. <i>Frontiers in Bioscience - Landmark</i> , 2011, 16, 2289.	3.0	17
269	Outstanding challenges in protein-ligand docking and structure-based virtual screening. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 229-259.	14.6	94
270	Influence of P-glycoprotein on embryotoxicity of the antifouling biocides to sea urchin (<i>Strongylocentrotus intermedius</i>). <i>Ecotoxicology</i> , 2011, 20, 419-428.	2.4	12
271	Molecular motions in drug design: the coming age of the metadynamics method. <i>Journal of Computer-Aided Molecular Design</i> , 2011, 25, 395-402.	2.9	38
272	Increased d-allose production by the R132E mutant of ribose-5-phosphate isomerase from <i>Clostridium thermocellum</i> . <i>Applied Microbiology and Biotechnology</i> , 2011, 89, 1859-1866.	3.6	24
273	A python-based docking program utilizing a receptor bound ligand shape: PythDock. <i>Archives of Pharmacal Research</i> , 2011, 34, 1451-1458.	6.3	16
274	vsLab: An implementation for virtual high-throughput screening using AutoDock and VMD. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 1208-1212.	2.0	28
275	Challenges and advances in computational docking: 2009 in review. <i>Journal of Molecular Recognition</i> , 2011, 24, 149-164.	2.1	273
276	Identification of Small-Molecule Inhibitors of the XendoU Endoribonucleases Family. <i>ChemMedChem</i> , 2011, 6, 1797-1805.	3.2	8
277	Synthesis and Anti-HIV Activity of Aryl-[(4-cyanophenyl)amino]-4-pyrimidinone hydrazones as Potent Non-nucleoside Reverse Transcriptase Inhibitors. <i>ChemMedChem</i> , 2011, 6, 2225-2232.	3.2	31
278	VoteDock: Consensus docking method for prediction of protein-ligand interactions. <i>Journal of Computational Chemistry</i> , 2011, 32, 568-581.	3.3	82
279	Can we trust docking results? Evaluation of seven commonly used programs on PDBbind database. <i>Journal of Computational Chemistry</i> , 2011, 32, 742-755.	3.3	308
280	Synthesis and biological evaluation of (\pm)-benzhydrol derivatives as potent non-nucleoside HIV-1 reverse transcriptase inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2011, 19, 4704-4709.	3.0	6

#	ARTICLE	IF	CITATIONS
281	2,4-Diamino-5-(2-arylpropargyl)pyrimidine derivatives as new nonclassical antifolates for human dihydrofolate reductase inhibition. <i>Journal of Molecular Graphics and Modelling</i> , 2011, 29, 608-613.	2.4	17
282	Characterization of Alizarin Red S binding sites and structural changes on human serum albumin: A biophysical study. <i>Journal of Hazardous Materials</i> , 2011, 186, 352-359.	12.4	77
283	Complexation of insecticide chlorantraniliprole with human serum albumin: Biophysical aspects. <i>Journal of Luminescence</i> , 2011, 131, 1327-1335.	3.1	12
284	Development of Anti-Viral Agents Using Molecular Modeling and Virtual Screening Techniques. <i>Infectious Disorders - Drug Targets</i> , 2011, 11, 64-93.	0.8	43
285	Bio-Inspired Algorithms Applied to Molecular Docking Simulations. <i>Current Medicinal Chemistry</i> , 2011, 18, 1339-1352.	2.4	68
286	Anti-Inflammatory and Antioxidant Properties of a New Arylidene-Thiazolidinedione in Macrophages. <i>Current Medicinal Chemistry</i> , 2011, 18, 3351-3360.	2.4	27
287	NMR Applications for Identifying β-TrCP Protein-Ligand Interactions. <i>Mini-Reviews in Medicinal Chemistry</i> , 2011, 11, 283-297.	2.4	4
288	Methysticin and 7,8-Dihydromethysticin are Two Major Kavalactones in Kava Extract to Induce CYP1A1. <i>Toxicological Sciences</i> , 2011, 124, 388-399.	3.1	30
289	An Extensible Database Management System for Large-Scale Virtual Screening. , 2011, , .		2
290	Characterization of a Mannose-6-Phosphate Isomerase from <i>Thermus thermophilus</i> and Increased α -Ribose Production by Its R142N Mutant. <i>Applied and Environmental Microbiology</i> , 2011, 77, 762-767.	3.1	20
291	Identification and Validation of Novel Human Pregnane X Receptor Activators among Prescribed Drugs via Ligand-Based Virtual Screening. <i>Drug Metabolism and Disposition</i> , 2011, 39, 337-344.	3.3	42
292	Combined 3D-QSAR, Molecular Docking and Molecular Dynamics Study on Derivatives of Peptide Epoxyketone and Tyropeptin-Boronic Acid as Inhibitors Against the β 5 Subunit of Human 20S Proteasome. <i>International Journal of Molecular Sciences</i> , 2011, 12, 1807-1835.	4.1	34
293	Development of molecular docking-based binding energy to predict the joint effect of BPA and its analogs. <i>Human and Experimental Toxicology</i> , 2011, 30, 318-327.	2.2	10
294	On modeling peptidomimetics in complex with the SH2 domain of Stat3. , 2011, 2011, 3229-32.		3
295	Drug design for cardiovascular disease: The effect of solvation energy on Rac1-ligand interactions. , 2011, 2011, 3237-40.		3
296	Combined 3D-QSAR Modeling and Molecular Docking Studies on Pyrrole-Indolin-2-ones as Aurora A Kinase Inhibitors. <i>International Journal of Molecular Sciences</i> , 2011, 12, 1605-1624.	4.1	17
297	In Silico Identification of Structure Requirement for Novel Thiazole and Oxazole Derivatives as Potent Fructose 1,6-Bisphosphatase Inhibitors. <i>International Journal of Molecular Sciences</i> , 2011, 12, 8161-8180.	4.1	7
298	 Structural Requirements of N-Substituted Spiropiperidine Analogues as Agonists of Nociceptin/Orphanin FQ Receptor. <i>International Journal of Molecular Sciences</i> , 2011, 12, 8961-8981.	4.1	3

#	ARTICLE	IF	CITATIONS
299	A Novel Chemometric Method for the Prediction of Human Oral Bioavailability. <i>International Journal of Molecular Sciences</i> , 2012, 13, 6964-6982.	4.1	668
300	Modelación por homologación de la proteína LuxS de <i>Porphyromonas gingivalis</i> cepa W83. <i>Revista Clínica De Periodoncia Implantología Y Rehabilitación Oral</i> , 2012, 5, 105-113.	0.1	1
301	Production of <i>l</i> -Ribose from <i>l</i> -Ribulose by a Triple-Site Variant of Mannose-6-Phosphate Isomerase from <i>Geobacillus thermodenitrificans</i> . <i>Applied and Environmental Microbiology</i> , 2012, 78, 3880-3884.	3.1	21
302	Global structure-activity relationship model for nonmutagenic carcinogens using virtual ligand-protein interactions as model descriptors. <i>Carcinogenesis</i> , 2012, 33, 1940-1945.	2.8	3
303	Computational Tools for In Silico Fragment-Based Drug Design. <i>Current Topics in Medicinal Chemistry</i> , 2012, 12, 1935-1943.	2.1	25
304	Insight into the Structural Determinants of Imidazole Scaffold-Based Derivatives as P38 MAP Kinase Inhibitors by Computational Explorations. <i>Current Medicinal Chemistry</i> , 2012, 19, 4024-4037.	2.4	8
305	Perspectives on Developing Small Molecule Inhibitors Targeting HIV-1 Integrase. <i>Mini-Reviews in Medicinal Chemistry</i> , 2012, 12, 875-889.	2.4	7
306	Steered Molecular Dynamics-A Promising Tool for Drug Design. <i>Current Bioinformatics</i> , 2012, 7, 342-351.	1.5	73
307	Structural and Functional Characterization of Nrf2 Degradation by the Glycogen Synthase Kinase 3 β -TrCP Axis. <i>Molecular and Cellular Biology</i> , 2012, 32, 3486-3499.	2.3	338
308	Virtual Screening in Structure-Based Drug Discovery. <i>Mini-Reviews in Medicinal Chemistry</i> , 2012, 4, 779-91.	2.4	41
309	GAMESS As a Free Quantum-Mechanical Platform for Drug Research. <i>Current Topics in Medicinal Chemistry</i> , 2012, 12, 2013-2033.	2.1	118
310	Recent Progress of Molecular Docking Simulations Applied to Development of Drugs. <i>Current Bioinformatics</i> , 2012, 7, 352-365.	1.5	50
311	From Laptop to Benchtop to Bedside: Structure-based Drug Design on Protein Targets. <i>Current Pharmaceutical Design</i> , 2012, 18, 1217-1239.	1.9	64
312	Protein Bioinformatics Applied to Virology. <i>Current Protein and Peptide Science</i> , 2012, 13, 547-559.	1.4	2
313	Screening of a Chemical Library by HT-G4-FID for Discovery of Selective G-quadruplex Binders. <i>Current Pharmaceutical Design</i> , 2012, 18, 1992-2001.	1.9	18
314	From Laptop to Benchtop to Bedside: Structure-based Drug Design on Protein Targets. <i>Current Drug Metabolism</i> , 2012, 18, 1217-1239.	1.2	7
315	Molecular Modeling on Pyrimidine-Urea Inhibitors of TNF- α Production: An Integrated Approach Using a Combination of Molecular Docking, Classification Techniques, and 3D-QSAR CoMSIA. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 711-723.	5.4	57
316	Synthesis, structure-activity relationships, and docking studies of N-phenylarylformamide derivatives (PAFAs) as non-nucleoside HIV reverse transcriptase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2012, 58, 504-512.	5.5	4

#	ARTICLE	IF	CITATIONS
317	In Silico Discovery of Androgen Receptor Antagonists with Activity in Castration Resistant Prostate Cancer. <i>Molecular Endocrinology</i> , 2012, 26, 1836-1846.	3.7	22
318	On Setting Up and Assessing Docking Simulations for Virtual Screening. <i>Methods in Molecular Biology</i> , 2012, 928, 1-16.	0.9	3
319	From the protein's perspective: the benefits and challenges of protein structure-based pharmacophore modeling. <i>MedChemComm</i> , 2012, 3, 28-38.	3.4	81
320	Structures of cytochrome P450 17A1 with prostate cancer drugs abiraterone and TOK-001. <i>Nature</i> , 2012, 482, 116-119.	27.8	284
321	Identification of Non-Macrocyclic Small Molecule Inhibitors against the NS3/4A Serine Protease of Hepatitis C Virus through in Silico Screening. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2245-2256.	5.4	12
322	Structure-Based Virtual Screening for Drug Discovery: a Problem-Centric Review. <i>AAPS Journal</i> , 2012, 14, 133-141.	4.4	461
323	Integrating Ligand-Based and Protein-Centric Virtual Screening of Kinase Inhibitors Using Ensembles of Multiple Protein Kinase Genes and Conformations. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2501-2515.	5.4	26
324	A novel halogen bond and a better-known hydrogen bond cooperation of neonicotinoid and insect nicotinic acetylcholine receptor recognition. <i>Journal of Molecular Modeling</i> , 2012, 18, 3867-3875.	1.8	20
325	Small molecules containing hetero-bicyclic ring systems compete with UDP-Glc for binding to WaaG glycosyltransferase. <i>Glycoconjugate Journal</i> , 2012, 29, 491-502.	2.7	12
326	A combined 3D-QSAR and molecular docking strategy to understand the binding mechanism of V600EB-RAF inhibitors. <i>Molecular Diversity</i> , 2012, 16, 771-785.	3.9	6
327	Synthesis and SAR of 2,3-bis-O-substituted N ⁶ , 5-bis-ureidoadenosine derivatives: Implications for prodrug delivery and mechanism of action. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 6067-6071.	2.2	12
328	An improved LGA for protein-ligand docking prediction. , 2012, , .		2
329	Synthesis, Biological Evaluation, and Radioiodination of Halogenated <i>closo</i> -Carboranylthymidine Analogues. <i>Inorganic Chemistry</i> , 2012, 51, 629-639.	4.0	30
330	Receptor-Ligand Interaction-Based Virtual Screening for Novel Eg5/Kinesin Spindle Protein Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2012, 55, 2561-2573.	6.4	32
331	Identification and Characterization of Human Apurinic/Apyrimidinic Endonuclease-1 Inhibitors. <i>Biochemistry</i> , 2012, 51, 6246-6259.	2.5	36
332	Leveraging Structural Information for the Discovery of New Drugs: Computational Methods. <i>Methods in Molecular Biology</i> , 2012, 841, 209-234.	0.9	0
333	In silico prediction of inhibitory effects of pyrazol-5-one and indazole derivatives on GSK3 β kinase enzyme. <i>Journal of Molecular Structure</i> , 2012, 1024, 94-103.	3.6	2
334	Molecular dynamics and free energy studies on the carboxypeptidases complexed with peptide/small molecular inhibitor: Mechanism for drug resistance. <i>Insect Biochemistry and Molecular Biology</i> , 2012, 42, 583-595.	2.7	8

#	ARTICLE	IF	CITATIONS
335	Inhibitors of Dengue virus and West Nile virus proteases based on the aminobenzamide scaffold. <i>Bioorganic and Medicinal Chemistry</i> , 2012, 20, 4140-4148.	3.0	43
336	Potential toxicity and affinity of triphenylmethane dye malachite green to lysozyme. <i>Ecotoxicology and Environmental Safety</i> , 2012, 78, 41-49.	6.0	41
337	Exploring the binding of BACE-1 inhibitors using comparative binding energy analysis (COMBINE). <i>BMC Structural Biology</i> , 2012, 12, 21.	2.3	25
339	Discovery of Novel Vascular Endothelial Growth Factor Receptor 2 Inhibitors: A Virtual Screening Approach. <i>Chemical Biology and Drug Design</i> , 2012, 80, 893-901.	3.2	6
340	Computational drug discovery. <i>Acta Pharmacologica Sinica</i> , 2012, 33, 1131-1140.	6.1	238
341	Molecular docking, molecular dynamics simulation, and structure-based 3D-QSAR studies on estrogenic activity of hydroxylated polychlorinated biphenyls. <i>Science of the Total Environment</i> , 2012, 441, 230-238.	8.0	60
342	In silico virtual screening approaches for anti-viral drug discovery. <i>Drug Discovery Today: Technologies</i> , 2012, 9, e219-e225.	4.0	67
343	A Hadoop-based Massive Molecular Data Storage Solution for Virtual Screening. , 2012, , .		2
344	Pyrrolo[3,2-d]pyrimidine Derivatives as Type II Kinase Insert Domain Receptor (KDR) Inhibitors: CoMFA and CoMSIA Studies. <i>International Journal of Molecular Sciences</i> , 2012, 13, 2387-2404.	4.1	9
345	A hierarchical method for molecular docking using cloud computing. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2012, 22, 6568-6572.	2.2	4
347	Medicinal Chemistry and Ligand Profiling for Evaluation of Promising Marine Bioactive Molecules. , 2012, , 173-206.		1
348	Computational Drug Discovery and Design. <i>Methods in Molecular Biology</i> , 2012, , .	0.9	30
349	Sanjeevini: a freely accessible web-server for target directed lead molecule discovery. <i>BMC Bioinformatics</i> , 2012, 13, S7.	2.6	169
350	Local functional descriptors for surface comparison based binding prediction. <i>BMC Bioinformatics</i> , 2012, 13, 314.	2.6	3
351	Molecular Basis of Inhibitory Activities of Berberine against Pathogenic Enzymes in Alzheimer's Disease. <i>Scientific World Journal, The</i> , 2012, 2012, 1-4.	2.1	46
352	Using Molecular Modelling to Study Interactions Between Molecules with Biological Activity. , 0, , .		3
353	Synthesis and in silico screening of a library of β^2 -carboline-containing compounds. <i>Beilstein Journal of Organic Chemistry</i> , 2012, 8, 1048-1058.	2.2	10
354	Protein flexibility in docking and surface mapping. <i>Quarterly Reviews of Biophysics</i> , 2012, 45, 301-343.	5.7	108

#	ARTICLE	IF	CITATIONS
355	Binding Free Energy Calculation and Scoring in Small-Molecule Docking. RSC Drug Discovery Series, 2012, , 195-222.	0.3	5
356	Surflex-Dock: Docking benchmarks and real-world application. Journal of Computer-Aided Molecular Design, 2012, 26, 687-699.	2.9	215
357	Binding Conformation of 2-Oxoamide Inhibitors to Group IVA Cytosolic Phospholipase A ₂ Determined by Molecular Docking Combined with Molecular Dynamics. Journal of Chemical Information and Modeling, 2012, 52, 243-254.	5.4	20
358	Modeling Chemical Interaction Profiles: II. Molecular Docking, Spectral Data-Activity Relationship, and Structure-Activity Relationship Models for Potent and Weak Inhibitors of Cytochrome P450 CYP3A4 Isozyme. Molecules, 2012, 17, 3407-3460.	3.8	22
359	Development of a Comprehensive, Validated Pharmacophore Hypothesis for Anthrax Toxin Lethal Factor (LF) Inhibitors Using Genetic Algorithms, Pareto Scoring, and Structural Biology. Journal of Chemical Information and Modeling, 2012, 52, 1886-1897.	5.4	14
360	Efficient Hit-Finding Approaches for Histone Methyltransferases: The Key Parameters. Journal of Biomolecular Screening, 2012, 17, 85-98.	2.6	5
361	Application of Binding Free Energy Calculations to Prediction of Binding Modes and Affinities of MDM2 and MDMX Inhibitors. Journal of Chemical Information and Modeling, 2012, 52, 1821-1832.	5.4	41
362	Molecular modeling of the Toxoplasma gondii adenosine kinase inhibitors. Medicinal Chemistry Research, 2012, 21, 590-600.	2.4	23
363	Pharmacophore modeling and structure-based virtual screening for a novel "switch region" target of bacterial RNA polymerase. Medicinal Chemistry Research, 2012, 21, 642-652.	2.4	3
364	QSAR analysis on PfPK7 inhibitors using HQSAR, CoMFA, and CoMSIA. Medicinal Chemistry Research, 2012, 21, 681-693.	2.4	9
365	Variability in docking success rates due to dataset preparation. Journal of Computer-Aided Molecular Design, 2012, 26, 775-786.	2.9	338
366	Algorithmic challenges in structure-based drug design and NMR structural biology. Frontiers of Electrical and Electronic Engineering, 2012, 7, 69-84.	0.5	1
367	Structural requirements of pyrimidine, thienopyridine and ureido thiophene carboxamide-based inhibitors of the checkpoint kinase 1: QSAR, docking, molecular dynamics analysis. Journal of Molecular Modeling, 2012, 18, 3227-3242.	1.8	6
368	3D-QSAR Studies of JNK1 Inhibitors Utilizing Various Alignment Methods. Chemical Biology and Drug Design, 2012, 79, 53-67.	3.2	10
369	Design, synthesis and molecular docking studies of some novel spiro[indoline-3, 4'-piperidine]-2-ones as potential c-Met inhibitors. European Journal of Medicinal Chemistry, 2012, 50, 370-375.	5.5	33
370	Chiral resolution, absolute configuration assignment and biological activity of racemic diarylpyrimidine CH(OH)-DAPY as potent nonnucleoside HIV-1 reverse transcriptase inhibitors. European Journal of Medicinal Chemistry, 2012, 53, 229-234.	5.5	28
371	Inhibition of Dengue virus and West Nile virus proteases by click chemistry-derived benz[d]isothiazol-3(2H)-one derivatives. Bioorganic and Medicinal Chemistry, 2012, 20, 1213-1221.	3.0	67
372	Adamantyl N-benzylbenzamide: New series of depigmentation agents with tyrosinase inhibitory activity. Bioorganic and Medicinal Chemistry Letters, 2012, 22, 2110-2113.	2.2	26

#	ARTICLE	IF	CITATIONS
373	Docking and 3D-QSAR investigations of pyrrolidine derivatives as potent neuraminidase inhibitors. <i>Chemical Biology and Drug Design</i> , 2012, 79, 863-868.	3.2	7
374	Generation of Receptor Structural Ensembles for Virtual Screening Using Binding Site Shape Analysis and Clustering. <i>Chemical Biology and Drug Design</i> , 2012, 80, 182-193.	3.2	71
375	Features of the complex of food additive hesperidin to hemoglobin. <i>Journal of Photochemistry and Photobiology B: Biology</i> , 2012, 106, 53-60.	3.8	11
376	Analysis of conjugation of chloramphenicol and hemoglobin by fluorescence, circular dichroism and molecular modeling. <i>Journal of Molecular Structure</i> , 2012, 1007, 81-87.	3.6	24
377	Comparative modeling of human kappa opioid receptor and docking analysis with the peptide YFa. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 33, 44-51.	2.4	3
378	Exploring the structure requirement for PKC δ inhibitory activity of pyridinecarbonitrile derivatives: an in silico analysis. <i>Journal of Molecular Graphics and Modelling</i> , 2012, 34, 76-88.	2.4	2
379	An NMR-based scoring function improves the accuracy of binding pose predictions by docking by two orders of magnitude. <i>Journal of Biomolecular NMR</i> , 2012, 52, 23-30.	2.8	18
380	Probing the structural requirements of A-type Aurora kinase inhibitors using 3D-QSAR and molecular docking analysis. <i>Journal of Molecular Modeling</i> , 2012, 18, 1107-1122.	1.8	10
381	Ab initio parameterization of YFF1, a universal force field for drug-design applications. <i>Journal of Molecular Modeling</i> , 2012, 18, 663-673.	1.8	14
382	Molecular docking and 3D-QSAR study on 4-(1H-indazol-4-yl) phenylamino and aminopyrazolopyridine urea derivatives as kinase insert domain receptor (KDR) inhibitors. <i>Journal of Molecular Modeling</i> , 2012, 18, 1207-1218.	1.8	16
383	Binding site analysis, 3D-QSAR studies, and molecular design of flavonoids derivatives as potent neuraminidase inhibitors. <i>Medicinal Chemistry Research</i> , 2013, 22, 606-614.	2.4	8
384	Fragment Informatics and Computational Fragment-Based Drug Design: An Overview and Update. <i>Medicinal Research Reviews</i> , 2013, 33, 554-598.	10.5	56
385	Aminopyridyl/Pyrazinyl Spiro[indoline-3,4-piperidine]-2-ones As Highly Selective and Efficacious c-Met/ALK Inhibitors. <i>ACS Medicinal Chemistry Letters</i> , 2013, 4, 806-810.	2.8	31
386	Design, synthesis and docking-based 3D-QSAR study of novel 2-substituted 2-aminopropane-1,3-diols as potent and selective agonists of sphingosine-1-phosphate 1 (S1P1) receptor. <i>MedChemComm</i> , 2013, 4, 1267.	3.4	19
387	Structure-Based Design and Synthesis of Novel Dual-Target Inhibitors against Cyanobacterial Fructose-1,6-Bisphosphate Aldolase and Fructose-1,6-Bisphosphatase. <i>Journal of Agricultural and Food Chemistry</i> , 2013, 61, 7453-7461.	5.2	24
388	Alzheimer's Disease: Identification and Development of β -Secretase (BACE1) Binding Fragments and Inhibitors by Dynamic Ligand Screening (DLS). <i>ChemMedChem</i> , 2013, 8, 1041-1056.	3.2	14
389	Discovery of 4-amino-2-(thio)phenol derivatives as novel protein kinase and angiogenesis inhibitors for the treatment of cancer: Synthesis and biological evaluation. Part II. <i>European Journal of Medicinal Chemistry</i> , 2013, 69, 191-200.	5.5	12
390	SimG: An Alignment Based Method for Evaluating the Similarity of Small Molecules and Binding Sites. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2103-2115.	5.4	6

#	ARTICLE	IF	CITATIONS
391	Discovery of New Inhibitors of <i>Mycobacterium tuberculosis</i> InhA Enzyme Using Virtual Screening and a 3D-Pharmacophore-Based Approach. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 2390-2401.	5.4	72
392	New tungstenocenes containing 3-hydroxy-4-pyrone ligands: antiproliferative activity on HT-29 and MCF-7 cell lines and binding to human serum albumin studied by fluorescence spectroscopy and molecular modeling methods. <i>Journal of Biological Inorganic Chemistry</i> , 2013, 18, 195-209.	2.6	10
393	Message passing interface and multithreading hybrid for parallel molecular docking of large databases on petascale high performance computing machines. <i>Journal of Computational Chemistry</i> , 2013, 34, 915-927.	3.3	69
395	In Silico Models for Drug Discovery. <i>Methods in Molecular Biology</i> , 2013, , .	0.9	8
396	Fragment-Based Identification of a Locus in the Sec7 Domain of Arno for the Design of Protein-Protein Interaction Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2013, 56, 8497-8511.	6.4	20
397	Structural analysis of the active sites of dihydrofolate reductase from two species of <i>Candida</i> uncovers ligand-induced conformational changes shared among species. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 1279-1284.	2.2	16
398	Molecular docking simulation studies on potent butyrylcholinesterase inhibitors obtained from microbial transformation of dihydrotestosterone. <i>Chemistry Central Journal</i> , 2013, 7, 164.	2.6	8
399	Selective growth inhibition of human malignant melanoma cells by syringic acid-derived proteasome inhibitors. <i>Cancer Cell International</i> , 2013, 13, 82.	4.1	31
400	Combined QSAR and molecule docking studies on predicting P-glycoprotein inhibitors. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 1067-1073.	2.9	28
401	Raltegravir flexibility and its impact on recognition by the HIV-1 IN targets. <i>Journal of Molecular Recognition</i> , 2013, 26, 383-401.	2.1	4
402	Binding interaction of hypocrellin B to myoglobin: A spectroscopic and computational study. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2013, 115, 337-344.	3.9	5
403	A rapid identification of hit molecules for target proteins via physico-chemical descriptors. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 9107.	2.8	44
404	Rational questing for inhibitors of endothelin converting enzyme-1 from <i>Salvia miltiorrhiza</i> by combining ligand- and structure-based virtual screening. <i>Canadian Journal of Chemistry</i> , 2013, 91, 448-456.	1.1	13
405	7-((5-Nitrothiophen-2-yl)methoxy)-3H-phenoxazin-3-one as a spectroscopic off-on probe for highly sensitive and selective detection of nitroreductase. <i>Chemical Communications</i> , 2013, 49, 5859.	4.1	69
406	Olive secoiridoids and semisynthetic bioisostere analogues for the control of metastatic breast cancer. <i>Bioorganic and Medicinal Chemistry</i> , 2013, 21, 2117-2127.	3.0	42
407	A shortcut organic dye-based staining method for the detection of DNA both in agarose and polyacrylamide gel electrophoresis. <i>Analyst</i> , The, 2013, 138, 1187.	3.5	4
408	Are predicted protein structures of any value for binding site prediction and virtual ligand screening?. <i>Current Opinion in Structural Biology</i> , 2013, 23, 191-197.	5.7	29
409	In silico simulations of STAT1 and STAT3 inhibitors predict SH2 domain cross-binding specificity. <i>European Journal of Pharmacology</i> , 2013, 720, 38-48.	3.5	26

#	ARTICLE	IF	CITATIONS
410	Encoding Protein-Ligand Interaction Patterns in Fingerprints and Graphs. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 623-637.	5.4	139
411	Development of a Natural Products Database from the Biodiversity of Brazil. <i>Journal of Natural Products</i> , 2013, 76, 439-444.	3.0	137
412	From Heptahelical Bundle to Hits from the Haystack. <i>Methods in Enzymology</i> , 2013, 522, 279-336.	1.0	47
413	Latest developments in molecular docking: 2010-2011 in review. <i>Journal of Molecular Recognition</i> , 2013, 26, 215-239.	2.1	263
414	Rational Design of HIV-1 Entry Inhibitors. <i>Methods in Molecular Biology</i> , 2013, 993, 185-204.	0.9	15
415	Synthesis and biological evaluation of N-(4-hydroxy-3-mercaptanaphthalen-1-yl)amides as inhibitors of angiogenesis and tumor growth. <i>European Journal of Medicinal Chemistry</i> , 2013, 64, 377-388.	5.5	24
416	Design, development and evaluation of novel dual PPAR α /PPAR β agonists. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2013, 23, 873-879.	2.2	12
417	How to Improve Docking Accuracy of AutoDock4.2: A Case Study Using Different Electrostatic Potentials. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 188-200.	5.4	97
418	Identification of Novel Anthrax Toxin Countermeasures Using In Silico Methods. <i>Methods in Molecular Biology</i> , 2013, 993, 177-184.	0.9	1
419	Use of Experimental Design To Optimize Docking Performance: The Case of LiGenDock, the Docking Module of Ligen, a New De Novo Design Program. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1503-1517.	5.4	28
420	Automated docking for novel drug discovery. <i>Expert Opinion on Drug Discovery</i> , 2013, 8, 821-834.	5.0	58
421	Docking Challenge: Protein Sampling and Molecular Docking Performance. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1934-1945.	5.4	194
422	Boosting Virtual Screening Enrichments with Data Fusion: Coalescing Hits from Two-Dimensional Fingerprints, Shape, and Docking. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1531-1542.	5.4	67
423	Synthesis and in-silico studies of some diaryltriazole derivatives as potential cyclooxygenase inhibitors. <i>Archives of Pharmacal Research</i> , 2013, 36, 553-563.	6.3	4
424	Docking and 3-D QSAR studies on the binding of tetrahydropyrimid-2-one HIV-1 protease inhibitors. <i>Journal of Molecular Structure</i> , 2013, 1042, 86-103.	3.6	3
425	Indazoles as potential c-met inhibitors: Design, synthesis and molecular docking studies. <i>European Journal of Medicinal Chemistry</i> , 2013, 65, 112-118.	5.5	24
426	Multiple Structures for Virtual Ligand Screening: Defining Binding Site Properties-Based Criteria to Optimize the Selection of the Query. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 293-311.	5.4	33
427	CSAR Benchmark Exercise 2011-2012: Evaluation of Results from Docking and Relative Ranking of Blinded Congeneric Series. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 1853-1870.	5.4	124

#	ARTICLE	IF	CITATIONS
428	FINDSITE ^{comb} : A Threading/Structure-Based, Proteomic-Scale Virtual Ligand Screening Approach. <i>Journal of Chemical Information and Modeling</i> , 2013, 53, 230-240.	5.4	59
429	Docking-based three-dimensional quantitative structure-activity relationship (3D-QSAR) predicts binding affinities to aryl hydrocarbon receptor for polychlorinated dibenzodioxins, dibenzofurans, and biphenyls. <i>Environmental Toxicology and Chemistry</i> , 2013, 32, 1453-1458.	4.3	14
430	A structure-guided approach for protein pocket modeling and affinity prediction. <i>Journal of Computer-Aided Molecular Design</i> , 2013, 27, 917-934.	2.9	8
431	Nitroreductase Detection and Hypoxic Tumor Cell Imaging by a Designed Sensitive and Selective Fluorescent Probe, 7-[(5-Nitrofuran-2-yl)methoxy]-3-phenoxazin-3-one. <i>Analytical Chemistry</i> , 2013, 85, 3926-3932.	6.5	194
432	Computational insight into novel molecular recognition mechanism of different bioactive GAs and the Arabidopsis receptor GID1A. <i>Journal of Molecular Modeling</i> , 2013, 19, 4613-4624.	1.8	2
433	FIPSDock: A new molecular docking technique driven by fully informed swarm optimization algorithm. <i>Journal of Computational Chemistry</i> , 2013, 34, 67-75.	3.3	62
434	Identification of Five Structurally Unrelated Quorum-Sensing Inhibitors of <i>Pseudomonas aeruginosa</i> from a Natural-Derivative Database. <i>Antimicrobial Agents and Chemotherapy</i> , 2013, 57, 5629-5641.	3.2	113
435	Disarming Bacterial Virulence through Chemical Inhibition of the DNA Binding Domain of an AraC-like Transcriptional Activator Protein. <i>Journal of Biological Chemistry</i> , 2013, 288, 31115-31126.	3.4	23
436	State-of-the-art and dissemination of computational tools for drug-design purposes: a survey among Italian academics and industrial institutions. <i>Future Medicinal Chemistry</i> , 2013, 5, 907-927.	2.3	5
437	Fluorescent staining of protein in SDS polyacrylamide gels by salicylaldehyde azine. <i>Electrophoresis</i> , 2013, 34, 3171-3179.	2.4	2
438	Insight into the Structural Requirements of Protoporphyrinogen Oxidase Inhibitors: Molecular Docking and CoMFA of Diphenyl Ether, Isoxazole Phenyl, and Pyrazole Phenyl Ether. <i>Chinese Journal of Chemistry</i> , 2013, 31, 1153-1158.	4.9	10
439	Identification of Pharmacological Targets Combining Docking and Molecular Dynamics Simulations. <i>American Journal of Agricultural and Biological Science</i> , 2013, 8, 89-106.	0.4	6
440	Insights into an Original Pocket-Ligand Pair Classification: A Promising Tool for Ligand Profile Prediction. <i>PLoS ONE</i> , 2013, 8, e63730.	2.5	18
441	Isozyme-Specific Ligands for O-acetylserine sulfhydrylase, a Novel Antibiotic Target. <i>PLoS ONE</i> , 2013, 8, e77558.	2.5	43
442	Combining Machine Learning Systems and Multiple Docking Simulation Packages to Improve Docking Prediction Reliability for Network Pharmacology. <i>PLoS ONE</i> , 2013, 8, e83922.	2.5	268
443	Nonsteroidal Aromatase Inhibitors for the Treatment of Breast Cancer: An Update. <i>Anti-Cancer Agents in Medicinal Chemistry</i> , 2014, 14, 54-65.	1.7	27
444	Insight into the Interactions between Novel Isoquinolin-1,3-Dione Derivatives and Cyclin-Dependent Kinase 4 Combining QSAR and Molecular Docking. <i>PLoS ONE</i> , 2014, 9, e93704.	2.5	6
445	CMHX008, a Novel Peroxisome Proliferator-Activated Receptor δ Partial Agonist, Enhances Insulin Sensitivity In Vitro and In Vivo. <i>PLoS ONE</i> , 2014, 9, e102102.	2.5	12

#	ARTICLE	IF	CITATIONS
446	Structure-Based Virtual Screening for Drug Discovery: Principles, Applications and Recent Advances. Current Topics in Medicinal Chemistry, 2014, 14, 1923-1938.	2.1	706
447	PL-PatchSurfer: A Novel Molecular Local Surface-Based Method for Exploring Protein-Ligand Interactions. International Journal of Molecular Sciences, 2014, 15, 15122-15145.	4.1	22
448	Computational Analysis of Amiloride Analogue Inhibitors of Coxsackie Virus B3 RNA Polymerase. Journal of Proteomics and Bioinformatics, 2014, s9, 004.	0.4	2
449	Conformational analysis of a polyconjugated protein-binding ligand by joint quantum chemistry and polarizable molecular mechanics. Addressing the issues of anisotropy, conjugation, polarization, and multipole transferability. Journal of Molecular Modeling, 2014, 20, 2472.	1.8	7
450	Purification and characterization of guanylate kinase, a nucleoside monophosphate kinase of <i>Brugia malayi</i> . Parasitology, 2014, 141, 1341-1352.	1.5	3
451	LXR- β antagonist meso-dihydroguaiaretic acid attenuates high-fat diet-induced nonalcoholic fatty liver. Biochemical Pharmacology, 2014, 90, 414-424.	4.4	32
452	Crystal Structure of the Vaccinia Virus DNA Polymerase Holoenzyme Subunit D4 in Complex with the A20 N-Terminal Domain. PLoS Pathogens, 2014, 10, e1003978.	4.7	27
453	A force fields-based multi-scale docking method in drug molecular design. , 2014, , .		0
454	Structure-Dependent Binding of Arylimidamides to the DNA Minor Groove. ChemBioChem, 2014, 15, 68-79.	2.6	20
455	A survey of pyrethroid-resistant populations of <i>Meligethes aeneus</i> ... in Poland indicates the incidence of numerous substitutions in the pyrethroid target site of voltage-sensitive sodium channels in individual beetles. Insect Molecular Biology, 2014, 23, 682-693.	2.0	11
456	Rational Design and Screening Study of Novel Lead Compound Based on Acetohydroxyacid Synthase Structure. Chemical Biology and Drug Design, 2014, 84, 316-324.	3.2	4
457	Optimization of Compound Ranking for Structure-Based Virtual Ligand Screening Using an Established FRED-Surflex Consensus Approach. Chemical Biology and Drug Design, 2014, 83, 37-51.	3.2	10
458	Drug-Like Protein-Protein Interaction Modulators: Challenges and Opportunities for Drug Discovery and Chemical Biology. Molecular Informatics, 2014, 33, 414-437.	2.5	93
460	EFFICIENCY OF A HIERARCHICAL DOCKING PROTOCOL FOR COMPUTATIONAL LIGAND SCREENING AGAINST HOMOLOGY MODELS. Biomedical Engineering - Applications, Basis and Communications, 2014, 26, 1450024.	0.6	1
461	Experimental validation of FINDSITEcomb virtual ligand screening results for eight proteins yields novel nanomolar and micromolar binders. Journal of Cheminformatics, 2014, 6, 16.	6.1	23
462	3D-QSAR study on 2,3-dihydroimidazo[4,5]-pyridin-2-one derivatives with a meta substitution pattern as V600EBRAF inhibitors. Medicinal Chemistry Research, 2014, 23, 587-602.	2.4	3
463	In vitro studies on the interaction between human serum albumin and fosfomycin disodium salt, an antibiotic drug by multi-spectroscopic and molecular docking methods. Molecular Biology Reports, 2014, 41, 2377-2387.	2.3	5
464	Protein function annotation by local binding site surface similarity. Proteins: Structure, Function and Bioinformatics, 2014, 82, 679-694.	2.6	8

#	ARTICLE	IF	CITATIONS
465	3-Hydroxybutanolide derivatives and flavonoid glucosides from <i>Anoectochilus roxburghii</i> . <i>Phytochemistry Letters</i> , 2014, 8, 109-115.	1.2	15
466	Water soluble molybdenocene complexes: Synthesis, cytotoxic activity and binding studies to ubiquitin by fluorescence spectroscopy, circular dichroism and molecular modeling. <i>Journal of Inorganic Biochemistry</i> , 2014, 132, 77-91.	3.5	9
467	Discovery of N-(3-((7H-purin-6-yl)thio)-4-hydroxynaphthalen-1-yl)-sulfonamide derivatives as novel protein kinase and angiogenesis inhibitors for the treatment of cancer: Synthesis and biological evaluation. Part III. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 1487-1495.	3.0	16
468	Molecular docking and molecular dynamics studies on β -lactamases and penicillin binding proteins. <i>Molecular BioSystems</i> , 2014, 10, 891-900.	2.9	60
469	Computational Approaches and Resources in Single Amino Acid Substitutions Analysis Toward Clinical Research. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 94, 365-423.	2.3	22
470	Molecular docking- and genetic algorithm-based approaches to produce robust 3D-QSAR models. <i>Medicinal Chemistry Research</i> , 2014, 23, 2198-2206.	2.4	3
471	Discovery of 3-(4-methanesulfonylphenoxy)-N-[1-(2-methoxy-ethoxymethyl)-1H-pyrazol-3-yl]-5-(3-methylpyridin-2-yl)-benzamide as a novel glucokinase activator (GKA) for the treatment of type 2 diabetes mellitus. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 2280-2293.	3.0	23
472	Studies on the isolated mitochondrial damage induced by α -tocopheryl succinate and its interactions with human serum albumin. <i>RSC Advances</i> , 2014, 4, 3913-3919.	3.6	6
473	Molecular docking and molecular dynamics studies on the interactions of hydroxylated polybrominated diphenyl ethers to estrogen receptor alpha. <i>Ecotoxicology and Environmental Safety</i> , 2014, 101, 83-89.	6.0	16
474	Discovery of Tertiary Amine and Indole Derivatives as Potent ROR β Inverse Agonists. <i>ACS Medicinal Chemistry Letters</i> , 2014, 5, 65-68.	2.8	61
475	Design, synthesis, molecular docking and 3D-QSAR studies of potent inhibitors of enoyl-acyl carrier protein reductase as potential antimycobacterial agents. <i>European Journal of Medicinal Chemistry</i> , 2014, 71, 199-218.	5.5	28
476	Computational Methods in Drug Discovery. <i>Pharmacological Reviews</i> , 2014, 66, 334-395.	16.0	1,370
477	Identification of novel drug scaffolds for inhibition of SARS-CoV 3-Chymotrypsin-like protease using virtual and high-throughput screenings. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 167-177.	3.0	48
478	Rational design of novel CYP2A6 inhibitors. <i>Bioorganic and Medicinal Chemistry</i> , 2014, 22, 6655-6664.	3.0	12
479	Protein Ligand Docking Docking in Drug Discovery Drug Discovery. , 2014, , 249-286.		11
480	Design Some New Type β -secretase Inhibitors Based on Molecular Docking and Topomer CoMFA Research. <i>Molecular Informatics</i> , 2014, 33, 536-543.	2.5	11
481	Bypassing Fluoroquinolone Resistance with Quinazolinones: Studies of Drug-Gyrase-DNA Complexes Having Implications for Drug Design. <i>ACS Chemical Biology</i> , 2014, 9, 2895-2904.	3.4	38
482	Using S-adenosyl-L-homocysteine capture compounds to characterize S-adenosyl-L-methionine and S-adenosyl-L-homocysteine binding proteins. <i>Analytical Biochemistry</i> , 2014, 467, 14-21.	2.4	10

#	ARTICLE	IF	CITATIONS
483	Lead Discovery and Lead Modification. , 2014, , 19-122.		7
484	FRODRUG: A Virtual Screening GPU Accelerated Approach for Drug Discovery. , 2014, , .		1
485	Importance of the Pharmacological Profile of the Bound Ligand in Enrichment on Nuclear Receptors: Toward the Use of Experimentally Validated Decoy Ligands. Journal of Chemical Information and Modeling, 2014, 54, 2915-2944.	5.4	8
486	Stabilization of Human Telomeric Gâ€¢Quadruplex and Inhibition of Telomerase Activity by Propellerâ€¢Shaped Trinuclear Pt^{II} Complexes. Chemistry - an Asian Journal, 2014, 9, 2519-2526.	3.3	29
487	Daclatasvir-Like Inhibitors of NS5A Block Early Biogenesis of Hepatitis C Virusâ€¢Induced Membranous Replication Factories, Independent of RNA Replication. Gastroenterology, 2014, 147, 1094-1105.e25.	1.3	135
488	Comparative Normal/Failing Rat Myocardium Cell Membrane Chromatographic Analysis System for Screening Specific Components That Counteract Doxorubicin-Induced Heart Failure from <i>Acontium carmichaeli</i>. Analytical Chemistry, 2014, 86, 4748-4757.	6.5	87
489	SAHA-based novel HDAC inhibitor design by core hopping method. Journal of Molecular Graphics and Modelling, 2014, 54, 10-18.	2.4	20
490	Size does matter! Label-free detection of small moleculeâ€¢protein interaction. Analytical and Bioanalytical Chemistry, 2014, 406, 4033-4051.	3.7	30
491	Autogrid-based clustering of kinases: selection of representative conformations for docking purposes. Molecular Diversity, 2014, 18, 611-619.	3.9	3
492	Molecular dynamics and molecular docking studies on E166A point mutant, R274N/R276N double mutant, and E166A/R274N/R276N triple mutant forms of class A Î²-lactamases. Journal of Biomolecular Structure and Dynamics, 2014, 32, 1953-1968.	3.5	19
493	Beware of Machine Learning-Based Scoring Functionsâ€¢On the Danger of Developing Black Boxes. Journal of Chemical Information and Modeling, 2014, 54, 2807-2815.	5.4	110
494	Synthesis, screening and docking of small heterocycles as Glycogen Phosphorylase inhibitors. European Journal of Medicinal Chemistry, 2014, 84, 584-594.	5.5	12
495	Structure-based discovery of a small non-peptidic Neuropilins antagonist exerting in vitro and in vivo anti-tumor activity on breast cancer model. Cancer Letters, 2014, 349, 120-127.	7.2	46
496	Design, synthesis and docking studies of some novel (R)-2-(4â€¢chlorophenyl)-3-(4â€¢nitrophenyl)-1,2,3,5-tetrahydrobenzo[4,5] imidazo [1,2-c]pyrimidin-4-ol derivatives as antitubercular agents. European Journal of Medicinal Chemistry, 2014, 83, 245-255.	5.5	28
497	A Cresyl Violetâ€¢Based Fluorescent Offâ€¢On Probe for the Detection and Imaging of Hypoxia and Nitroreductase in Living Organisms. Chemistry - an Asian Journal, 2014, 9, 2058-2062.	3.3	28
498	Comparative Assessment of Scoring Functions on an Updated Benchmark: 2. Evaluation Methods and General Results. Journal of Chemical Information and Modeling, 2014, 54, 1717-1736.	5.4	294
499	Docking of anti-HIV-1 oxoquinoline-acylhydrazone derivatives as potential HSV-1 DNA polymerase inhibitors. Journal of Molecular Structure, 2014, 1074, 263-270.	3.6	9
500	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.	5.4	33

#	ARTICLE	IF	CITATIONS
501	AG-690/11026014, a novel PARP-1 inhibitor, protects cardiomyocytes from AngII-induced hypertrophy. <i>Molecular and Cellular Endocrinology</i> , 2014, 392, 14-22.	3.2	29
502	Design and synthesis of a new series of modified CH-diarylpyrimidines as drug-resistant HIV non-nucleoside reverse transcriptase inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2014, 82, 600-611.	5.5	28
504	- Fragment-Based Methods in Drug Design. , 2015, , 370-407.		3
505	In Silico Approaches Assisting the Rational Design of Low Molecular Weight Protein-Protein Interaction Modulators. , 2015, , 441-482.		0
506	Enrichment Assessment of Multiple Virtual Screening Strategies for Toll-Like Receptor 8 Agonists Based on a Maximal Unbiased Benchmarking Data Set. <i>Chemical Biology and Drug Design</i> , 2015, 86, 1226-1241.	3.2	11
507	Structure-Based Analysis of the Ligand-Binding Mechanism for DheselOBP21, a C-minus Odorant Binding Protein, from <i>Dastarcus helophoroides</i> (Fairmaire; Coleoptera: Bothrideridae). <i>International Journal of Biological Sciences</i> , 2015, 11, 1281-1295.	6.4	40
508	Molecular docking, synthesis, and antimycobacterial activities of pyrrolyl hydrazones and their copper complexes. <i>Research and Reports in Medicinal Chemistry</i> , 2015, , 1.	0.3	2
509	Insight into the Structural Determinants of Imidazole Scaffold-Based Derivatives as TNF-Release Inhibitors by in Silico Explorations. <i>International Journal of Molecular Sciences</i> , 2015, 16, 20118-20138.	4.1	4
510	An Investigation of Molecular Docking and Molecular Dynamic Simulation on Imidazopyridines as B-Raf Kinase Inhibitors. <i>International Journal of Molecular Sciences</i> , 2015, 16, 27350-27361.	4.1	16
511	S4MPLE-Sampler for Multiple Protein-Ligand Entities: Methodology and Rigid-Site Docking Benchmarking. <i>Molecules</i> , 2015, 20, 8997-9028.	3.8	25
512	Molecular Docking and Structure-Based Drug Design Strategies. <i>Molecules</i> , 2015, 20, 13384-13421.	3.8	1,255
513	Identification of STAT1 and STAT3 Specific Inhibitors Using Comparative Virtual Screening and Docking Validation. <i>PLoS ONE</i> , 2015, 10, e0116688.	2.5	32
514	Structure-Based Virtual Screening and Discovery of New PPAR γ / β Dual Agonist and PPAR γ and β Agonists. <i>PLoS ONE</i> , 2015, 10, e0118790.	2.5	21
515	3D Structure Prediction of Human β 1-Adrenergic Receptor via Threading-Based Homology Modeling for Implications in Structure-Based Drug Designing. <i>PLoS ONE</i> , 2015, 10, e0122223.	2.5	10
516	Computational drug design strategies applied to the modelling of human immunodeficiency virus-1 reverse transcriptase inhibitors. <i>Memorias Do Instituto Oswaldo Cruz</i> , 2015, 110, 847-864.	1.6	23
518	Identification of small-molecule inhibitors against SecA by structure-based virtual ligand screening. <i>Journal of Antibiotics</i> , 2015, 68, 666-673.	2.0	14
519	MRT β 2 inhibits Hedgehog signaling by blocking overlapping binding sites in the transmembrane domain of the Smoothed receptor. <i>FASEB Journal</i> , 2015, 29, 1817-1829.	0.5	48
520	Benchmarking Data Sets for the Evaluation of Virtual Ligand Screening Methods: Review and Perspectives. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 1297-1307.	5.4	67

#	ARTICLE	IF	CITATIONS
521	Effective virtual screening strategy focusing on the identification of novel Bruton's tyrosine kinase inhibitors. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 60, 142-154.	2.4	12
522	Design, synthesis and molecular docking analysis of some novel 7-[(quinolin-6-yl)methyl] purines as potential c-Met inhibitors. <i>Medicinal Chemistry Research</i> , 2015, 24, 3327-3333.	2.4	8
523	Synthesis and affinities of C3-symmetric thioglycoside-containing trimannosides. <i>Carbohydrate Research</i> , 2015, 412, 56-65.	2.3	4
524	3D-QSAR and docking studies on piperidine-substituted diarylpyrimidine analogues as HIV-1 reverse transcriptase inhibitors. <i>Medicinal Chemistry Research</i> , 2015, 24, 3314-3326.	2.4	11
525	Pyrrolyl thiaziazoles as Mycobacterium tuberculosis inhibitors and their in silico analyses. <i>Research and Reports in Medicinal Chemistry</i> , 0, , 1.	0.3	2
526	Predictiveness curves in virtual screening. <i>Journal of Cheminformatics</i> , 2015, 7, 52.	6.1	73
527	A systems chemical biology approach to identify targets of antibacterial agents: A case study of Chelerythrine and Rhein. , 2015, , .		0
528	CAVSâ€”Novel in silico selection strategy of specific STAT inhibitory compounds. <i>Journal of Computational Science</i> , 2015, 10, 186-194.	2.9	5
529	Discovery of Small Molecule CD40â€”TRAF6 Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2015, 55, 294-307.	5.4	58
530	Activity of Quinolone CP-115,955 Against Bacterial and Human Type II Topoisomerases Is Mediated by Different Interactions. <i>Biochemistry</i> , 2015, 54, 1278-1286.	2.5	22
531	Discovery of Small Molecule Inhibitors to KrÃ¼ppel-like Factor 10 (KLF10): Implications for Modulation of T Regulatory Cell Differentiation. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 1466-1478.	6.4	10
532	Design and Synthesis of Acetylenyl Benzamide Derivatives as Novel Glucokinase Activators for the Treatment of T2DM. <i>ACS Medicinal Chemistry Letters</i> , 2015, 6, 296-301.	2.8	28
533	Combined Molecular Docking, 3Dâ€”QSAR, and Pharmacophore Model: Design of Novel Tubulin Polymerization Inhibitors by Binding to Colchicineâ€”binding Site. <i>Chemical Biology and Drug Design</i> , 2015, 86, 731-745.	3.2	17
534	Chemical and protein structural basis for biological crosstalk between PPARÎ± and COX enzymes. <i>Journal of Computer-Aided Molecular Design</i> , 2015, 29, 101-112.	2.9	9
535	Comparative Molecular Modeling and Docking Analysis of Î²-galactosidase Enzymes from Commercially Important Starter Cultures Used in the Dairy Industry. <i>Food Biotechnology</i> , 2015, 29, 248-262.	1.5	4
536	Identification of PPARÎ³ Agonists from Natural Sources Using Different In Silico Approaches. <i>Planta Medica</i> , 2015, 81, 488-494.	1.3	17
537	How to Valorize Biodiversity? Let's Go Hashing, Extracting, Filtering, Mining, Fishing. <i>Planta Medica</i> , 2015, 81, 436-449.	1.3	11
538	Engineering substrate specificity of succinic semialdehyde reductase (AKR7A5) for efficient conversion of levulinic acid to 4-hydroxyvaleric acid. <i>Journal of Biotechnology</i> , 2015, 210, 38-43.	3.8	4

#	ARTICLE	IF	CITATIONS
539	Receptor-based virtual screening protocol for drug discovery. Archives of Biochemistry and Biophysics, 2015, 582, 56-67.	3.0	98
540	Binding Activity Prediction of Cyclin-Dependent Inhibitors. Journal of Chemical Information and Modeling, 2015, 55, 1469-1482.	5.4	10
541	Hybrid chemistry. Part 4: Discovery of etravirineâ€“VRX-480773 hybrids as potent HIV-1 non-nucleoside reverse transcriptase inhibitors. Bioorganic and Medicinal Chemistry, 2015, 23, 4248-4255.	3.0	25
542	Novel lead compound optimization and synthesized based on the target structure of Xanthomonas oryzae pv. oryzae GlmU. Pesticide Biochemistry and Physiology, 2015, 122, 22-28.	3.6	5
543	MoDock: A multi-objective strategy improves the accuracy for molecular docking. Algorithms for Molecular Biology, 2015, 10, 8.	1.2	12
544	Identification of Novel Inhibitors of <i>Mycobacterium tuberculosis</i> PknG Using Pharmacophore Based Virtual Screening, Docking, Molecular Dynamics Simulation, and Their Biological Evaluation. Journal of Chemical Information and Modeling, 2015, 55, 1120-1129.	5.4	51
545	Synthesis, evaluation and in silico molecular modeling of pyrrolyl-1,3,4-thiadiazole inhibitors of InhA. Bioorganic Chemistry, 2015, 59, 151-167.	4.1	15
546	Enhancing the Sensitivity of Pharmacophore-Based Virtual Screening by Incorporating Customized ZBC Features: A Case Study Using Histone Deacetylase 8. Journal of Chemical Information and Modeling, 2015, 55, 861-871.	5.4	40
547	Exploring quercetin and luteolin derivatives as antiangiogenic agents. European Journal of Medicinal Chemistry, 2015, 97, 259-274.	5.5	47
548	HQSAR and topomer CoMFA for predicting melanocortin-4 receptor binding affinities of trans-4-(4-chlorophenyl) pyrrolidine-3-carboxamides. Chemometrics and Intelligent Laboratory Systems, 2015, 146, 34-41.	3.5	32
549	Discovery of piperidin-4-yl-aminopyrimidine derivatives as potent non-nucleoside HIV-1 reverse transcriptase inhibitors. European Journal of Medicinal Chemistry, 2015, 97, 1-9.	5.5	23
550	In-silico identification of the binding mode of synthesized adamantyl derivatives inside cholinesterase enzymes. Acta Pharmacologica Sinica, 2015, 36, 879-886.	6.1	12
551	Knowledge-guided docking: accurate prospective prediction of bound configurations of novel ligands using Surflex-Dock. Journal of Computer-Aided Molecular Design, 2015, 29, 485-509.	2.9	42
552	Discovery of target based novel pyrrolyl phenoxy derivatives as antimycobacterial agents: An in silico approach. European Journal of Medicinal Chemistry, 2015, 94, 317-339.	5.5	15
553	Tubulin Inhibitor Identification by Bioactive Conformation Alignment Pharmacophoreâ€“Guided Virtual Screening. Chemical Biology and Drug Design, 2015, 86, 998-1016.	3.2	6
554	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
555	Mutation-Guided Unbiased Modeling of the Fat Sensor GPR119 for High-Yield Agonist Screening. Structure, 2015, 23, 2377-2386.	3.3	6
556	Catecholic amides as potential selective phosphodiesterase 4D inhibitors: Design, synthesis, pharmacological evaluation and structureâ€“activity relationships. Bioorganic and Medicinal Chemistry, 2015, 23, 7332-7339.	3.0	15

#	ARTICLE	IF	CITATIONS
557	Probing the S2â€² Subsite of the Anthrax Toxin Lethal Factor Using Novel N-Alkylated Hydroxamates. <i>Journal of Medicinal Chemistry</i> , 2015, 58, 8723-8733.	6.4	6
558	Cancer Chemoprevention Effects of Ginger and its Active Constituents: Potential for New Drug Discovery. <i>The American Journal of Chinese Medicine</i> , 2015, 43, 1351-1363.	3.8	48
559	An efficient one-pot conversion of Boc-protected adenines to N6-ureas. <i>Tetrahedron Letters</i> , 2015, 56, 6574-6576.	1.4	3
560	Design, synthesis of quinolinyl Schiff bases and azetidinones as enoyl ACP-reductase inhibitors. <i>Medicinal Chemistry Research</i> , 2015, 24, 3892-3911.	2.4	18
561	Pyrimidine sulfonylacetanilides with improved potency against key mutant viruses of HIV-1 by specific targeting of a highly conserved residue. <i>European Journal of Medicinal Chemistry</i> , 2015, 102, 215-222.	5.5	23
562	Synthesis, biological evaluation and 3D-QSAR studies of imidazolidine-2,4-dione derivatives as novel protein tyrosine phosphatase 1B inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2015, 103, 91-104.	5.5	28
563	A novel family of diarylpyrimidines (DAPYs) featuring a diatomic linker: Design, synthesis and anti-HIV activities. <i>Bioorganic and Medicinal Chemistry</i> , 2015, 23, 6587-6593.	3.0	23
564	Computational analysis reveal inhibitory action of nimbin against dengue viral envelope protein. <i>VirusDisease</i> , 2015, 26, 243-254.	2.0	12
565	Virtual screening strategies: Recent advances in the identification and design of anti-cancer agents. <i>Methods</i> , 2015, 71, 64-70.	3.8	41
566	<i>in silico</i> analysis reveals the anti-malarial potential of quinolinyl chalcone derivatives. <i>Journal of Biomolecular Structure and Dynamics</i> , 2015, 33, 961-977.	3.5	27
567	Benchmarking methods and data sets for ligand enrichment assessment in virtual screening. <i>Methods</i> , 2015, 71, 146-157.	3.8	40
568	Exploiting ChEMBL database to identify indole analogs as HCV replication inhibitors. <i>Methods</i> , 2015, 71, 4-13.	3.8	20
569	3D-QSAR modeling and molecular docking study on Mer kinase inhibitors of pyridine-substituted pyrimidines. <i>Molecular Diversity</i> , 2015, 19, 135-147.	3.9	17
570	Adaptive molecular docking method based on information entropy genetic algorithm. <i>Applied Soft Computing Journal</i> , 2015, 26, 299-302.	7.2	46
571	Molecular dynamics-based discovery of novel phosphodiesterase-9A inhibitors with non-pyrazolopyrimidinone scaffolds. <i>Molecular BioSystems</i> , 2015, 11, 115-125.	2.9	21
572	<i>in vivo</i> imaging and detection of nitroreductase in zebrafish by a new near-infrared fluorescence offâ€œon probe. <i>Biosensors and Bioelectronics</i> , 2015, 63, 112-116.	10.1	159
573	Predicting dual-targeting anti-influenza agents using multi-models. <i>Molecular Diversity</i> , 2015, 19, 123-134.	3.9	5
574	Comparative Evaluation of Different Docking Tools for Kinases Against Cancerous (Malignant) Cells. <i>Archives in Cancer Research</i> , 2016, 04, .	0.3	0

#	ARTICLE	IF	CITATIONS
575	Virtual Screening Approaches towards the Discovery of Toll-Like Receptor Modulators. <i>International Journal of Molecular Sciences</i> , 2016, 17, 1508.	4.1	32
576	Targeted inhibition of STATs and IRFs as a potential treatment strategy in cardiovascular disease. <i>Oncotarget</i> , 2016, 7, 48788-48812.	1.8	60
577	Steroid-Functionalized Titanocenes: Docking Studies with Estrogen Receptor Alpha. <i>Inorganics</i> , 2016, 4, 38.	2.7	8
578	Fucoxanthin, a Marine Carotenoid, Reverses Scopolamine-Induced Cognitive Impairments in Mice and Inhibits Acetylcholinesterase in Vitro. <i>Marine Drugs</i> , 2016, 14, 67.	4.6	100
579	Molecular Modeling Studies of 11 β -Hydroxysteroid Dehydrogenase Type 1 Inhibitors through Receptor-Based 3D-QSAR and Molecular Dynamics Simulations. <i>Molecules</i> , 2016, 21, 1222.	3.8	9
580	Three-Dimensional Biologically Relevant Spectrum (BRS-3D): Shape Similarity Profile Based on PDB Ligands as Molecular Descriptors. <i>Molecules</i> , 2016, 21, 1554.	3.8	19
581	AutoSite: an automated approach for pseudo-ligands prediction from ligand-binding sites identification to predicting key ligand atoms. <i>Bioinformatics</i> , 2016, 32, 3142-3149.	4.1	59
582	Novel Scaffold Identification of mGlu1 Receptor Negative Allosteric Modulators Using a Hierarchical Virtual Screening Approach. <i>Chemical Biology and Drug Design</i> , 2016, 87, 239-256.	3.2	21
583	Amiloride Analogs as ASIC1a Inhibitors. <i>CNS Neuroscience and Therapeutics</i> , 2016, 22, 468-476.	3.9	38
584	A Molecular Docking and Dynamics Study to Screen Potent Anti-Staphylococcal Compounds Against Cefaroline Resistant MRSA. <i>Journal of Cellular Biochemistry</i> , 2016, 117, 542-548.	2.6	13
585	DOX: A new computational protocol for accurate prediction of the protein-ligand binding structures. <i>Journal of Computational Chemistry</i> , 2016, 37, 336-344.	3.3	24
586	Docking and three-dimensional quantitative structure-activity relationship analyses of imidazole and thiazolidine derivatives as Aurora A kinase inhibitors. <i>Archives of Pharmacal Research</i> , 2016, 39, 1635-1643.	6.3	2
587	Benchmark of four popular virtual screening programs: construction of the active/decoy dataset remains a major determinant of measured performance. <i>Journal of Cheminformatics</i> , 2016, 8, 56.	6.1	71
588	Predicted structure of a Minus-C OBP from <i>Batocera horsfieldi</i> (Hope) suggests an intermediate structure in evolution of OBPs. <i>Scientific Reports</i> , 2016, 6, 33981.	3.3	41
589	Binding interaction and conformational changes of human serum albumin with ranitidine studied by spectroscopic and time-resolved fluorescence methods. <i>Journal of the Iranian Chemical Society</i> , 2016, 13, 1325-1338.	2.2	35
590	Discovery of vascular endothelial growth factor receptor tyrosine kinase inhibitors by quantitative structure-activity relationships, molecular dynamics simulation and free energy calculation. <i>RSC Advances</i> , 2016, 6, 35402-35415.	3.6	6
591	Molecular Docking and Molecular Dynamics Studies to Identify Potential OXA-10 Extended Spectrum β -Lactamase Non-hydrolysing Inhibitors for <i>Pseudomonas aeruginosa</i> . <i>Cell Biochemistry and Biophysics</i> , 2016, 74, 141-155.	1.8	19
592	Computational approaches in target identification and drug discovery. <i>Computational and Structural Biotechnology Journal</i> , 2016, 14, 177-184.	4.1	270

#	ARTICLE	IF	CITATIONS
593	Sunitinib, a Clinically Used Anticancer Drug, Is a Potent AChE Inhibitor and Attenuates Cognitive Impairments in Mice. <i>ACS Chemical Neuroscience</i> , 2016, 7, 1047-1056.	3.5	34
594	Comprehensive evaluation of ten docking programs on a diverse set of protein-ligand complexes: the prediction accuracy of sampling power and scoring power. <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 12964-12975.	2.8	669
595	WScore: A Flexible and Accurate Treatment of Explicit Water Molecules in Ligand-Receptor Docking. <i>Journal of Medicinal Chemistry</i> , 2016, 59, 4364-4384.	6.4	75
596	New insight into the binding modes of TNP-AMP to human liver fructose-1,6-bisphosphatase. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 165, 155-160.	3.9	11
597	Polydatin ameliorates lipid and glucose metabolism in type 2 diabetes mellitus by downregulating proprotein convertase subtilisin/kexin type 9 (PCSK9). <i>Cardiovascular Diabetology</i> , 2016, 15, 19.	6.8	61
598	Computational analysis of binding between benzamide-based derivatives and Abl wt and T315I mutant kinases. <i>RSC Advances</i> , 2016, 6, 85355-85366.	3.6	5
599	Identification of potential CCR5 inhibitors through pharmacophore-based virtual screening, molecular dynamics simulation and binding free energy analysis. <i>Molecular BioSystems</i> , 2016, 12, 3396-3406.	2.9	13
600	Integrated machine learning, molecular docking and 3D-QSAR based approach for identification of potential inhibitors of trypanosomal N-myristoyltransferase. <i>Molecular BioSystems</i> , 2016, 12, 3711-3723.	2.9	21
601	Development of highly potent phosphodiesterase 4 inhibitors with anti-neuroinflammation potential: Design, synthesis, and structure-activity relationship study of catecholamides bearing aromatic rings. <i>European Journal of Medicinal Chemistry</i> , 2016, 124, 372-379.	5.5	27
602	The dopamine D2 receptor dimer and its interaction with homobivalent antagonists: homology modeling, docking and molecular dynamics. <i>Journal of Molecular Modeling</i> , 2016, 22, 203.	1.8	28
603	Preselection of A- and B- modified d-homo lactone and d-seco androstane derivatives as potent compounds with antiproliferative activity against breast and prostate cancer cells - QSAR approach and molecular docking analysis. <i>European Journal of Pharmaceutical Sciences</i> , 2016, 93, 107-113.	4.0	11
604	In Silico Investigation of the Neurotensin Receptor 1 Binding Site: Overlapping Binding Modes for Small Molecule Antagonists and the Endogenous Peptide Agonist. <i>Molecular Informatics</i> , 2016, 35, 19-24.	2.5	8
605	Structure-guided discovery of thiazolidine-2,4-dione derivatives as a novel class of <i>Leishmania major</i> pteridine reductase 1 inhibitors. <i>European Journal of Medicinal Chemistry</i> , 2016, 123, 639-648.	5.5	39
606	Design, synthesis and SAR study of novel sulfonylureas containing an alkenyl moiety. <i>Organic and Biomolecular Chemistry</i> , 2016, 14, 8356-8366.	2.8	22
607	Structural basis for the substrate specificity of 3-hydroxybutyrate dehydrogenase. <i>Biotechnology and Bioprocess Engineering</i> , 2016, 21, 364-372.	2.6	9
608	Discovery and characterization of novel small-molecule CXCR4 receptor agonists and antagonists. <i>Scientific Reports</i> , 2016, 6, 30155.	3.3	51
609	Novel Podophyllotoxin Derivatives as Partial PPAR γ Agonists and their Effects on Insulin Resistance and Type 2 Diabetes. <i>Scientific Reports</i> , 2016, 6, 37323.	3.3	6
610	How does curcumin work with poor bioavailability? Clues from experimental and theoretical studies. <i>Scientific Reports</i> , 2016, 6, 20872.	3.3	102

#	ARTICLE	IF	CITATIONS
611	Mechanism of metamifop inhibition of the carboxyltransferase domain of acetyl-coenzyme A carboxylase in <i>Echinochloa crus-galli</i> . <i>Scientific Reports</i> , 2016, 6, 34066.	3.3	29
612	Predicting Subtype Selectivity for Adenosine Receptor Ligands with Three-Dimensional Biologically Relevant Spectrum (BRS-3D). <i>Scientific Reports</i> , 2016, 6, 36595.	3.3	15
613	Screening Explorer—An Interactive Tool for the Analysis of Screening Results. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 2281-2286.	5.4	53
614	Prediction and evaluation of the lipase inhibitory activities of tea polyphenols with 3D-QSAR models. <i>Scientific Reports</i> , 2016, 6, 34387.	3.3	18
615	Novel ligands of Choline Acetyltransferase designed by in silico molecular docking, hologram QSAR and lead optimization. <i>Scientific Reports</i> , 2016, 6, 31247.	3.3	24
616	3D-QSAR and docking studies on 1-hydroxypyridin-2-one compounds as mutant isocitrate dehydrogenase 1 inhibitors. <i>Journal of Molecular Structure</i> , 2016, 1123, 335-343.	3.6	6
617	Ethyl 4-(4-methylphenyl)-4-pentenoate from <i>Vetiveria zizanioides</i> Inhibits Dengue NS2B—NS3 Protease and Prevents Viral Assembly: A Computational Molecular Dynamics and Docking Study. <i>Cell Biochemistry and Biophysics</i> , 2016, 74, 337-351.	1.8	10
618	Identification of phenoxyacetamide derivatives as novel DOT1L inhibitors via docking screening and molecular dynamics simulation. <i>Journal of Molecular Graphics and Modelling</i> , 2016, 68, 128-139.	2.4	13
619	Novel synthesised flavone derivatives provide significant insight into the structural features required for enhanced anti-proliferative activity. <i>RSC Advances</i> , 2016, 6, 64544-64556.	3.6	26
620	vSDC: a method to improve early recognition in virtual screening when limited experimental resources are available. <i>Journal of Cheminformatics</i> , 2016, 8, 1.	6.1	110
621	Computer-aided rational design of novel EBF analogues with an aromatic ring. <i>Journal of Molecular Modeling</i> , 2016, 22, 144.	1.8	7
622	Insight into the <i>Meligethes aeneus</i> voltage-sensitive sodium channel structure and an attempt to select the best pyrethroid ligands. <i>Pest Management Science</i> , 2016, 72, 162-171.	3.4	0
623	LEADS-PEP: A Benchmark Data Set for Assessment of Peptide Docking Performance. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 188-200.	5.4	76
624	Building a virtual ligand screening pipeline using free software: a survey. <i>Briefings in Bioinformatics</i> , 2016, 17, 352-366.	6.5	74
625	PatchSurfers: Two methods for local molecular property-based binding ligand prediction. <i>Methods</i> , 2016, 93, 41-50.	3.8	8
626	Applying the designed multiple ligands approach to inhibit dihydrofolate reductase and thioredoxin reductase for anti-proliferative activity. <i>European Journal of Medicinal Chemistry</i> , 2016, 115, 63-74.	5.5	32
627	Extrapolative prediction using physically-based QSAR. <i>Journal of Computer-Aided Molecular Design</i> , 2016, 30, 127-152.	2.9	3
628	Design, synthesis and anti-HIV evaluation of novel diarylpyridine derivatives targeting the entrance channel of NNRTI binding pocket. <i>European Journal of Medicinal Chemistry</i> , 2016, 109, 294-304.	5.5	28

#	ARTICLE	IF	CITATIONS
629	Molecular modeling studies to characterize N-phenylpyrimidin-2-amine selectivity for CDK2 and CDK4 through 3D-QSAR and molecular dynamics simulations. <i>Molecular BioSystems</i> , 2016, 12, 1250-1268.	2.9	53
630	Synthesis and biological evaluation of novel inhibitors against 1,3,8-trihydroxynaphthalene reductase from <i>Magnaporthe grisea</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2016, 24, 1225-1230.	3.0	10
631	Prediction and characterization of P-glycoprotein substrates potentially bound to different sites by emerging chemical pattern and hierarchical cluster analysis. <i>International Journal of Pharmaceutics</i> , 2016, 502, 61-69.	5.2	15
632	Threading the Needle: Small-Molecule Targeting of a Xenobiotic Receptor to Ablate <i>Escherichia coli</i> Polysaccharide Capsule Expression Without Altering Antibiotic Resistance. <i>Journal of Infectious Diseases</i> , 2016, 213, 1330-1339.	4.0	14
633	A Rational Design, Synthesis, Biological Evaluation and Structure-Activity Relationship Study of Novel Inhibitors against Cyanobacterial Fructose-1,6-bisphosphate Aldolase. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 73-81.	5.4	14
634	An Automated Strategy for Binding-Pose Selection and Docking Assessment in Structure-Based Drug Design. <i>Journal of Chemical Information and Modeling</i> , 2016, 56, 54-72.	5.4	46
635	Molecular simulation studies on the binding selectivity of 2-anilino-4-(thiazol-5-yl)-pyrimidines in complexes with CDK2 and CDK7. <i>Molecular BioSystems</i> , 2016, 12, 145-161.	2.9	36
636	BindingDB in 2015: A public database for medicinal chemistry, computational chemistry and systems pharmacology. <i>Nucleic Acids Research</i> , 2016, 44, D1045-D1053.	14.5	1,002
637	Synthesis, antimycobacterial screening and ligand-based molecular docking studies on novel pyrrole derivatives bearing pyrazoline, isoxazole and phenyl thiourea moieties. <i>European Journal of Medicinal Chemistry</i> , 2016, 107, 133-152.	5.5	79
638	New 1(2H)-phthalazinone derivatives as potent nonpeptidic HIV-1 protease inhibitors: molecular docking studies, molecular dynamics simulation, oral bioavailability and ADME prediction. <i>Molecular Simulation</i> , 2016, 42, 628-641.	2.0	3
639	Theoretical study of binding affinity for diamidine with DNA. <i>Structural Chemistry</i> , 2016, 27, 681-696.	2.0	3
640	FGF2 Prevents Sunitinib-Induced Cardiotoxicity in Zebrafish and Cardiomyoblast H9c2 Cells. <i>Cardiovascular Toxicology</i> , 2016, 16, 46-53.	2.7	28
641	Synthesis, Characterization, and Antimicrobial Activities of Novel <i>N</i> -substituted β -Hydroxy Amines and β -Hydroxy Ethers that Contained <i>o</i> -Methoxy Fluoroquinolones. <i>Journal of Heterocyclic Chemistry</i> , 2016, 53, 284-293.	2.6	7
642	Appliance Recognition Unit for Home Energy Management System With UPnP Network. <i>IEEE Systems Journal</i> , 2017, 11, 2794-2803.	4.6	11
643	Novel anti-cancer agents based on germacrone: design, synthesis, biological activity, docking studies and MD simulations. <i>RSC Advances</i> , 2017, 7, 3760-3767.	3.6	13
644	Software for molecular docking: a review. <i>Biophysical Reviews</i> , 2017, 9, 91-102.	3.2	880
645	An enantiomer-based virtual screening approach: Discovery of chiral organophosphates as acetyl cholinesterase inhibitors. <i>Ecotoxicology and Environmental Safety</i> , 2017, 138, 215-222.	6.0	7
646	Efficient Approximation of Ligand Rotational and Translational Entropy Changes upon Binding for Use in MM-PBSA Calculations. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 170-189.	5.4	46

#	ARTICLE	IF	CITATIONS
647	Interaction of phenolic acids with trypsin: Experimental and molecular modeling studies. Food Chemistry, 2017, 228, 1-6.	8.2	34
648	Insights from molecular modeling into the selective inhibition of cathepsin S by its inhibitor. Journal of Molecular Modeling, 2017, 23, 92.	1.8	12
649	Transition metal complexes of 2-(2-(1H-benzo[d]imidazol-2-yl)hydrazono)propan-1-ol: Synthesis, characterization, crystal structures and anti-tuberculosis assay with docking studies. Polyhedron, 2017, 127, 225-237.	2.2	10
650	Structural modifications of diarylpyrimidines (DAPYs) as HIV-1 NNRTIs: Synthesis, anti-HIV activities and SAR. Bioorganic and Medicinal Chemistry, 2017, 25, 2491-2497.	3.0	26
651	Theoretical analysis of somatostatin receptor 5 with antagonists and agonists for the treatment of neuroendocrine tumors. Molecular Diversity, 2017, 21, 367-384.	3.9	6
652	Heterologous expression of <i>Helicoverpa armigera</i> cytochrome P450 CYP6B7 in <i>Pichia pastoris</i> and interactions of CYP6B7 with insecticides. Pest Management Science, 2017, 73, 1866-1872.	3.4	18
653	Exploring the Potential of Herbal Ligands Toward Multidrug-Resistant Bacterial Pathogens by Computational Drug Discovery. Translational Medicine Research, 2017, , 89-117.	0.0	1
654	Bioresources and Bioprocess in Biotechnology. , 2017, , .		1
655	Pyrrole-indolinone SU11652 targets the nucleoside diphosphate kinase from Leishmania parasites. Biochemical and Biophysical Research Communications, 2017, 488, 461-465.	2.1	10
656	3D-QSAR modeling and molecular docking studies on a series of 2,5 disubstituted 1,3,4-oxadiazoles. Journal of Molecular Structure, 2017, 1145, 278-284.	3.6	22
657	Structure-Based Rational Design of Novel Inhibitors Against Fructose-1,6-Bisphosphate Aldolase from <i>Candida albicans</i> . Journal of Chemical Information and Modeling, 2017, 57, 1426-1438.	5.4	28
658	Identification of an in vivo orally active dual-binding protein-protein interaction inhibitor targeting TNF α through combined in silico/in vitro/in vivo screening. Scientific Reports, 2017, 7, 3424.	3.3	14
659	Triptolide-Assisted Phosphorylation of p53 Suppresses Inflammation-Induced NF- κ B Survival Pathways in Cancer Cells. Molecular and Cellular Biology, 2017, 37, .	2.3	28
660	Simple Tetrahydroisoquinolines Are Potent and Selective Kappa Opioid Receptor Antagonists. ACS Medicinal Chemistry Letters, 2017, 8, 742-745.	2.8	9
661	Discovery of novel inhibitors for Leishmania nucleoside diphosphatase kinase (NDK) based on its structural and functional characterization. Journal of Computer-Aided Molecular Design, 2017, 31, 547-562.	2.9	21
662	A molecular docking study of the interactions between human transferrin and seven metallocene dichlorides. Journal of Molecular Graphics and Modelling, 2017, 75, 250-265.	2.4	13
663	Conformational analysis of capsaicin using ¹³ C, ¹⁵ N MAS NMR, GIAO DFT and GA calculations. Journal of Molecular Structure, 2017, 1146, 773-781.	3.6	13
664	Novel aryl piperazines for alleviation of α -andropause™ associated prostatic disorders and depression. European Journal of Medicinal Chemistry, 2017, 132, 204-218.	5.5	5

#	ARTICLE	IF	CITATIONS
665	ForceGen 3D structure and conformer generation: from small lead-like molecules to macrocyclic drugs. <i>Journal of Computer-Aided Molecular Design</i> , 2017, 31, 419-439.	2.9	45
666	Structure-Based Discovery of Small Molecules Binding to RNA. <i>Topics in Medicinal Chemistry</i> , 2017, , 47-77.	0.8	8
667	Identification of Novel Inhibitors of <i>Leishmania donovani</i> β -Glutamylcysteine Synthetase Using Structure-Based Virtual Screening, Docking, Molecular Dynamics Simulation, and in Vitro Studies. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 815-825.	5.4	21
668	Discovery of novel dual VEGFR2 and Src inhibitors using a multistep virtual screening approach. <i>Future Medicinal Chemistry</i> , 2017, 9, 7-24.	2.3	11
669	Model of the Interaction between the NF- κ B Inhibitory Protein p100 and the E3 Ubiquitin Ligase β -TrCP based on NMR and Docking Experiments. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 223-233.	5.4	7
670	Computational evaluation of glutamine synthetase as drug target against infectious diseases: molecular modeling, substrate-binding analysis, and molecular dynamics simulation studies. <i>Medicinal Chemistry Research</i> , 2017, 26, 450-460.	2.4	7
671	Molecular modeling study of CP-690550 derivatives as JAK3 kinase inhibitors through combined 3D-QSAR, molecular docking, and dynamics simulation techniques. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 72, 178-186.	2.4	20
672	Discovery of Novel Phosphodiesterase-2A Inhibitors by Structure-Based Virtual Screening, Structural Optimization, and Bioassay. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 355-364.	5.4	40
673	Exploring the resistance mechanism of imipenem in carbapenem hydrolysing class D beta-lactamases OXA-143 and its variant OXA-231 (D224A) expressing <i>Acinetobacter baumannii</i> : An in-silico approach. <i>Computational Biology and Chemistry</i> , 2017, 67, 1-8.	2.3	18
674	ProSelection: A Novel Algorithm to Select Proper Protein Structure Subsets for in Silico Target Identification and Drug Discovery Research. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2686-2698.	5.4	12
675	Leachable diphenylguanidine from rubber closures used in pre-filled syringes: A case study to understand solid and solution interactions with oxytocin. <i>International Journal of Pharmaceutics</i> , 2017, 532, 491-501.	5.2	9
676	Chemical synthesis and in silico molecular modeling of novel pyrrolyl benzohydrazide derivatives: Their biological evaluation against enoyl ACP reductase (InhA) and <i>Mycobacterium tuberculosis</i> . <i>Bioorganic Chemistry</i> , 2017, 75, 181-200.	4.1	5
677	New molecular insights into the tyrosyl-tRNA synthase inhibitors: CoMFA, CoMSIA analyses and molecular docking studies. <i>Scientific Reports</i> , 2017, 7, 11525.	3.3	13
678	6-Nitrotriazolo[1,5-a]pyrimidines as promising structures for pharmacotherapy of septic conditions. <i>Russian Journal of Bioorganic Chemistry</i> , 2017, 43, 421-428.	1.0	30
679	Virtual screening of B-Raf kinase inhibitors: A combination of pharmacophore modelling, molecular docking, 3D-QSAR model and binding free energy calculation studies. <i>Computational Biology and Chemistry</i> , 2017, 70, 186-190.	2.3	7
680	Discriminating Agonist from Antagonist Ligands of the Nuclear Receptors Using Different Chemoinformatics Approaches. <i>Molecular Informatics</i> , 2017, 36, 1700020.	2.5	8
681	Structure-based development of novel triazoles and related thiazolotriazoles as anticancer agents and Cdc25A/B phosphatase inhibitors. Synthesis, in vitro biological evaluation, molecular docking and in silico ADME-T studies. <i>European Journal of Medicinal Chemistry</i> , 2017, 139, 263-279.	5.5	21
682	Discovery of 9H-purins as potential tubulin polymerization inhibitors: Synthesis, biological evaluation and structure-activity relationships. <i>European Journal of Medicinal Chemistry</i> , 2017, 138, 1126-1134.	5.5	10

#	ARTICLE	IF	CITATIONS
684	In silico identification of milk antihypertensive di- and tripeptides involved in angiotensin converting enzyme inhibitory activity. <i>Nutrition Research</i> , 2017, 46, 22-30.	2.9	26
685	Superior Performance of the SQM/COSMO Scoring Functions in Native Pose Recognition of Diverse Protein-Ligand Complexes in Cognate Docking. <i>ACS Omega</i> , 2017, 2, 4022-4029.	3.5	22
686	Identification of an intraspecific alarm pheromone and two conserved odorant-binding proteins associated with (E)- β -farnesene perception in aphid <i>Rhopalosiphum padi</i> . <i>Journal of Insect Physiology</i> , 2017, 101, 151-160.	2.0	32
687	In silico structure-based approaches to discover protein-protein interaction-targeting drugs. <i>Methods</i> , 2017, 131, 22-32.	3.8	69
688	Research on Controllable Degradation of Novel Sulfonylurea Herbicides in Acidic and Alkaline Soils. <i>Journal of Agricultural and Food Chemistry</i> , 2017, 65, 7661-7668.	5.2	10
689	Investigating the Importance of the Pocket Estimation Method in Pocket-based Approaches: An Illustration Using Pocket-Ligand Classification. <i>Molecular Informatics</i> , 2017, 36, 1700025.	2.5	2
690	Discovery of Novel Pyrazolopyrimidinone Derivatives as Phosphodiesterase 9A Inhibitors Capable of Inhibiting Butyrylcholinesterase for Treatment of Alzheimer's Disease. <i>ACS Chemical Neuroscience</i> , 2017, 8, 2522-2534.	3.5	29
691	Identification of insulin-sensitizing molecules acting by disrupting the interaction between the Insulin Receptor and Grb14. <i>Scientific Reports</i> , 2017, 7, 16901.	3.3	4
692	Discovery of novel choline acetyltransferase inhibitors using structure-based virtual screening. <i>Scientific Reports</i> , 2017, 7, 16287.	3.3	29
693	Key site residues of pheromone-binding protein 1 involved in interacting with sex pheromone components of <i>Helicoverpa armigera</i> . <i>Scientific Reports</i> , 2017, 7, 16859.	3.3	15
695	Autonomic Identity Framework for the Internet of Things. , 2017, , .		35
696	Modulation of Quorum Sensing in a Gram-Positive Pathogen by Linear Molecularly Imprinted Polymers with Anti-infective Properties. <i>Angewandte Chemie</i> , 2017, 129, 16782-16785.	2.0	10
697	Selectivity and ligand-based molecular modeling of an odorant-binding protein from the leaf beetle <i>Ambrostoma quadriimpressum</i> (Coleoptera: Chrysomelidae) in relation to habitat-related volatiles. <i>Scientific Reports</i> , 2017, 7, 15374.	3.3	13
698	Modulation of Quorum Sensing in a Gram-Positive Pathogen by Linear Molecularly Imprinted Polymers with Anti-infective Properties. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 16555-16558.	13.8	39
699	Efficient conformational sampling and weak scoring in docking programs? Strategy of the wisdom of crowds. <i>Journal of Cheminformatics</i> , 2017, 9, 37.	6.1	44
700	Combined HQSAR, topomer CoMFA, homology modeling and docking studies on triazole derivatives as SGLT2 inhibitors. <i>Future Medicinal Chemistry</i> , 2017, 9, 847-858.	2.3	10
701	Insecticidal activity of an essential oil of <i>Tagetes patula</i> L. (Asteraceae) on common bed bug <i>Cimex lectularius</i> L. and molecular docking of major compounds at the catalytic site of ClAChE1. <i>Parasitology Research</i> , 2017, 116, 415-424.	1.6	34
702	Discovery of <i>N</i> -Alkyl Catecholamides as Selective Phosphodiesterase-4 Inhibitors with Anti-neuroinflammation Potential Exhibiting Antidepressant-like Effects at Non-emetic Doses. <i>ACS Chemical Neuroscience</i> , 2017, 8, 135-146.	3.5	27

#	ARTICLE	IF	CITATIONS
703	Improving scoring-docking-screening powers of protein-ligand scoring functions using random forest. <i>Journal of Computational Chemistry</i> , 2017, 38, 169-177.	3.3	201
704	Synthesis and molecular modeling studies of novel pyrrole analogs as antimycobacterial agents. <i>Journal of Saudi Chemical Society</i> , 2017, 21, 42-57.	5.2	18
706	Recent Advances and Applications of Molecular Docking to G Protein-Coupled Receptors. <i>Molecules</i> , 2017, 22, 340.	3.8	51
707	Assessing the Risk for Resistance and Elucidating the Genetics of <i>Colletotrichum truncatum</i> That Is Only Sensitive to Some DMI Fungicides. <i>Frontiers in Microbiology</i> , 2017, 8, 1779.	3.5	38
708	Free Energy Calculation Guided Virtual Screening of Synthetically Feasible Ligand R-Group and Scaffold Modifications: An Emerging Paradigm for Lead Optimization. <i>Annual Reports in Medicinal Chemistry</i> , 2017, 50, 237-262.	0.9	4
709	Insights into cytochrome bc ₁ complex binding mode of antimalarial 2-hydroxy-1,4-naphthoquinones through molecular modelling. <i>Memorias Do Instituto Oswaldo Cruz</i> , 2017, 112, 299-308.	1.6	15
710	Computational investigation of the molecular conformation-dependent binding mode of (E)- β -farnesene analogs with a heterocycle to aphid odorant-binding proteins. <i>Journal of Molecular Modeling</i> , 2018, 24, 70.	1.8	16
711	Assessing protein-ligand interaction scoring functions with the CASF-2013 benchmark. <i>Nature Protocols</i> , 2018, 13, 666-680.	12.0	79
712	The discovery of novel diarylpyridine derivatives with high level activity against a wide variety of HIV-1 strains as well as against HIV-2. <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 2051-2060.	3.0	10
713	In-vitro evaluation and in-silico studies applied on newly synthesized amide derivatives of N-phthaloylglycine as Butyrylcholinesterase (BChE) inhibitors. <i>Computational Biology and Chemistry</i> , 2018, 74, 212-217.	2.3	12
714	Molecular modelling insights into a physiologically favourable approach to eicosanoid biosynthesis inhibition through novel thieno[2,3-b]pyridine derivatives. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018, 33, 755-767.	5.2	19
715	New selective cyclooxygenase-2 inhibitors from cyclocoumarol: Synthesis, characterization, biological evaluation and molecular modeling. <i>European Journal of Medicinal Chemistry</i> , 2018, 146, 577-587.	5.5	13
716	Optimization of reverse chemical ecology method: false positive binding of <i>Aenasius bambawalei</i> odorant binding protein 1 caused by uncertain binding mechanism. <i>Insect Molecular Biology</i> , 2018, 27, 305-318.	2.0	30
717	Structure-based discovery of cytotoxic dimeric tetrahydroxanthones as potential topoisomerase I inhibitors from a marine-derived fungus. <i>European Journal of Medicinal Chemistry</i> , 2018, 148, 268-278.	5.5	29
718	Furanone derivatives as new inhibitors of CDC7 kinase: development of structure activity relationship model using 3D QSAR, molecular docking, and in silico ADMET. <i>Structural Chemistry</i> , 2018, 29, 1031-1043.	2.0	23
719	Benchmark Study Based on 2P2I _{DB} to Gain Insights into the Discovery of Small-Molecule PPI Inhibitors. <i>Journal of Physical Chemistry B</i> , 2018, 122, 2544-2555.	2.6	12
720	Importance of protein flexibility in molecular recognition: a case study on Type-I1/2 inhibitors of ALK. <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 4851-4863.	2.8	22
721	Discovery of novel PDE9A inhibitors with antioxidant activities for treatment of Alzheimer's disease. <i>Journal of Enzyme Inhibition and Medicinal Chemistry</i> , 2018, 33, 260-270.	5.2	19

#	ARTICLE	IF	CITATIONS
722	A new point mutation in β -tubulin confers resistance to carbendazim in <i>Fusarium asiaticum</i> . <i>Pesticide Biochemistry and Physiology</i> , 2018, 145, 15-21.	3.6	31
723	<i>K</i>_{DEEP}: Proteinâ€“Ligand Absolute Binding Affinity Prediction via 3D-Convolutional Neural Networks. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 287-296.	5.4	586
724	Discovery of biphenyl-substituted diarylpyrimidines as non-nucleoside reverse transcriptase inhibitors with high potency against wild-type and mutant HIV-1. <i>European Journal of Medicinal Chemistry</i> , 2018, 145, 726-734.	5.5	42
725	Molecular modeling study, synthesis and biological evaluation of combretastatin A-4 analogues as anticancer agents and tubulin inhibitors. <i>MedChemComm</i> , 2018, 9, 316-327.	3.4	15
726	Proteinâ€“peptide docking: opportunities and challenges. <i>Drug Discovery Today</i> , 2018, 23, 1530-1537.	6.4	212
727	Eckmaxol, a Phlorotannin Extracted from <i>Ecklonia maxima</i>, Produces Anti- β -amyloid Oligomer Neuroprotective Effects Possibly via Directly Acting on Glycogen Synthase Kinase 3 β . <i>ACS Chemical Neuroscience</i> , 2018, 9, 1349-1356.	3.5	41
728	Application of molecular docking for the degradation of organic pollutants in the environmental remediation: A review. <i>Chemosphere</i> , 2018, 203, 139-150.	8.2	111
729	A novel interaction fingerprint derived from per atom score contributions: exhaustive evaluation of interaction fingerprint performance in docking based virtual screening. <i>Journal of Cheminformatics</i> , 2018, 10, 15.	6.1	32
730	Structure-based design, synthesis, and biological evaluation of novel pyrimidinone derivatives as PDE9 inhibitors. <i>Acta Pharmaceutica Sinica B</i> , 2018, 8, 615-628.	12.0	20
731	3D QSAR studies, molecular docking and ADMET evaluation, using thiazolidine derivatives as template to obtain new inhibitors of PIM1 kinase. <i>Computational Biology and Chemistry</i> , 2018, 74, 201-211.	2.3	15
732	Research on controllable alkaline soil degradation of 5-substituted chlorsulfuron. <i>Chinese Chemical Letters</i> , 2018, 29, 945-948.	9.0	7
733	Ligand-biased ensemble receptor docking (LigBEnD): a hybrid ligand/receptor structure-based approach. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 187-198.	2.9	39
734	Molecular Docking and Molecular Dynamics Simulation to Evaluate Compounds That Avoid the Amyloid Beta 1-42 Aggregation. <i>Neuromethods</i> , 2018, , 229-248.	0.3	6
735	Enhancing large-scale docking simulation on heterogeneous systems: An MPI vs rCUDA study. <i>Future Generation Computer Systems</i> , 2018, 79, 26-37.	7.5	12
736	Methods for Virtual Screening of GPCR Targets: Approaches and Challenges. <i>Methods in Molecular Biology</i> , 2018, 1705, 233-264.	0.9	3
737	Enhanced Turnover for the P450 119 Peroxygenaseâ€“Catalyzed Asymmetric Epoxidation of Styrenes by Random Mutagenesis. <i>Chemistry - A European Journal</i> , 2018, 24, 2741-2749.	3.3	16
738	Discovery of novel purine nucleoside derivatives as phosphodiesterase 2 (PDE2) inhibitors: Structure-based virtual screening, optimization and biological evaluation. <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 119-133.	3.0	11
739	Design, synthesis, molecular modeling, and ADMET studies of some pyrazoline derivatives as shikimate kinase inhibitors. <i>Medicinal Chemistry Research</i> , 2018, 27, 546-559.	2.4	15

#	ARTICLE	IF	CITATIONS
740	MurB as a target in an alternative approach to tackle the <i>Vibrio cholerae</i> resistance using molecular docking and simulation study. <i>Journal of Cellular Biochemistry</i> , 2018, 119, 1726-1732.	2.6	25
741	Molecular Modeling and Design Studies of Purine Derivatives as Novel CDK2 Inhibitors. <i>Molecules</i> , 2018, 23, 2924.	3.8	9
742	Analysis of docking algorithms by HPC methods generated in bioinformatics studies. <i>ITM Web of Conferences</i> , 2018, 16, 02009.	0.5	0
743	Computational Issues of Protein-Ligand Docking. <i>Journal of Biomolecular Research & Therapeutics</i> , 2018, 07, .	0.2	0
744	3D QSAR Modeling and Molecular Docking Studies on a Series of Triazole Analogues as Antibacterial Agents. <i>Journal of Structural Chemistry</i> , 2018, 59, 1544-1554.	1.0	1
745	DESIGNING OF COUMARIN DERIVATIVES AS SQUALENE SYNTHASE INHIBITORS. <i>Asian Journal of Pharmaceutical and Clinical Research</i> , 2018, 11, 200.	0.3	1
746	Repellency, Toxicity, Gene Expression Profiling and In Silico Studies to Explore Insecticidal Potential of <i>Melaleuca alternifolia</i> Essential Oil against <i>Myzus persicae</i> . <i>Toxins</i> , 2018, 10, 425.	3.4	6
747	PotentialNet for Molecular Property Prediction. <i>ACS Central Science</i> , 2018, 4, 1520-1530.	11.3	278
748	Genome-Wide Inhibition of Pro-atherogenic Gene Expression by Multi-STAT Targeting Compounds as a Novel Treatment Strategy of CVDs. <i>Frontiers in Immunology</i> , 2018, 9, 2141.	4.8	7
749	Energy-based tuning of metaheuristics for molecular docking on multi-GPUs. <i>Concurrency Computation Practice and Experience</i> , 2018, 30, e4684.	2.2	6
750	The emerging chemical patterns applied in predicting human toll-like receptor 8 agonists. <i>MedChemComm</i> , 2018, 9, 1961-1971.	3.4	4
751	Identification of protoberberine alkaloids as novel histone methyltransferase G9a inhibitors by structure-based virtual screening. <i>Journal of Computer-Aided Molecular Design</i> , 2018, 32, 917-928.	2.9	12
752	Pharmacophore mapping, molecular docking, chemical synthesis of some novel pyrrolyl benzamide derivatives and evaluation of their inhibitory activity against enoyl-ACP reductase (InhA) and <i>Mycobacterium tuberculosis</i> . <i>Bioorganic Chemistry</i> , 2018, 81, 440-453.	4.1	20
753	Structural basis of pyrazolopyrimidine derivatives as CAMKII β kinase inhibitors: insights from 3D QSAR, docking studies and in silico ADMET evaluation. <i>Chemical Papers</i> , 2018, 72, 2833-2847.	2.2	4
754	Identification of natural product compounds as quorum sensing inhibitors in <i>Pseudomonas fluorescens</i> P07 through virtual screening. <i>Bioorganic and Medicinal Chemistry</i> , 2018, 26, 4088-4099.	3.0	28
755	L-Captopril and its derivatives as potential inhibitors of microbial enzyme DapE: A combined approach of drug repurposing and similarity screening. <i>Journal of Molecular Graphics and Modelling</i> , 2018, 84, 82-89.	2.4	12
756	G-quadruplex virtual drug screening: A review. <i>Biochimie</i> , 2018, 152, 134-148.	2.6	42
757	Dimeric chalcones derivatives from <i>Myracrodruon urundeuva</i> act as cathepsin V inhibitors. <i>Phytochemistry</i> , 2018, 154, 31-38.	2.9	10

#	ARTICLE	IF	CITATIONS
758	Binding Affinity via Docking: Fact and Fiction. <i>Molecules</i> , 2018, 23, 1899.	3.8	292
759	Fast Green FCF Alleviates Pain Hypersensitivity and Down-Regulates the Levels of Spinal P2X4 Expression and Pro-inflammatory Cytokines in a Rodent Inflammatory Pain Model. <i>Frontiers in Pharmacology</i> , 2018, 9, 534.	3.5	19
760	New Oxadiazole Derivatives: Synthesis and Appraisal of Their Potential as Antimicrobial Agents. <i>Letters in Drug Design and Discovery</i> , 2018, 15, 21-30.	0.7	4
761	Novel Consensus Docking Strategy to Improve Ligand Pose Prediction. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1662-1668.	5.4	30
762	Biologically active azolo-1,2,4-triazines and azolopyrimidines. <i>Russian Chemical Bulletin</i> , 2018, 67, 573-599.	1.5	79
763	In Silico Analysis of the Association Relationship between Neuroprotection and Flavors of Traditional Chinese Medicine Based on the mGluRs. <i>International Journal of Molecular Sciences</i> , 2018, 19, 163.	4.1	5
764	Computational Simulation Studies on the Binding Selectivity of 1-(1H-Benzimidazol-5-yl)-5-aminopyrazoles in Complexes with FGFR1 and FGFR4. <i>Molecules</i> , 2018, 23, 767.	3.8	6
765	Molecular Docking: From Lock and Key to Combination Lock. <i>Journal of Molecular Medicine and Clinical Applications</i> , 2018, 2, .	0.4	48
766	Human Topopoisons From Weeds : A Review. <i>Current Traditional Medicine</i> , 2018, 4, 4-15.	0.4	2
767	Structure-Based Design, Synthesis, Biological Evaluation, and Molecular Docking of Novel PDE10 Inhibitors With Antioxidant Activities. <i>Frontiers in Chemistry</i> , 2018, 6, 167.	3.6	9
768	Cheminformatics Driven Development of Novel Therapies for Drug Resistant Prostate Cancer. <i>Molecular Informatics</i> , 2018, 37, e1800043.	2.5	8
769	Vasodilator effects and putative guanylyl cyclase stimulation by 2-nitro-1-phenylethanone and 2-nitro-2-phenyl-propane-1,3-diol on rat aorta. <i>European Journal of Pharmacology</i> , 2018, 830, 105-114.	3.5	3
770	Hierarchical Flexible Peptide Docking by Conformer Generation and Ensemble Docking of Peptides. <i>Journal of Chemical Information and Modeling</i> , 2018, 58, 1292-1302.	5.4	53
771	Accelerating Drugs Discovery with Deep Reinforcement Learning. , 2018, , .		4
772	Computational Design of Multi-Target Drugs Against Breast Cancer. <i>Methods in Pharmacology and Toxicology</i> , 2018, , 443-458.	0.2	2
773	Selection of protein conformations for structure-based polypharmacology studies. <i>Drug Discovery Today</i> , 2018, 23, 1889-1896.	6.4	22
774	Toward Expanded Diversity of Host-Guest Interactions via Synthesis and Characterization of Cyclodextrin Derivatives. <i>Journal of Solution Chemistry</i> , 2018, 47, 1597-1608.	1.2	14
775	Investigation of indirubin derivatives: a combination of 3D-QSAR, molecular docking, and ADMET towards the design of new DRAX2 inhibitors. <i>Structural Chemistry</i> , 2018, 29, 1609-1622.	2.0	14

#	ARTICLE	IF	CITATIONS
776	Drug Repurposing and Multi-Target Therapies. , 2019, , 780-791.		1
777	Toward a better understanding of the interaction between somatostatin receptor 2 and its ligands: a structural characterization study using molecular dynamics and conceptual density functional theory. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 3081-3102.	3.5	9
778	Mechanism of imipenem resistance in metallo-β-lactamases expressing pathogenic bacterial spp. and identification of potential inhibitors: An in silico approach. <i>Journal of Cellular Biochemistry</i> , 2019, 120, 584-591.	2.6	4
779	Combined approach of homology modeling, molecular dynamics, and docking: computer-aided drug discovery. <i>Physical Sciences Reviews</i> , 2019, 4, .	0.8	2
780	Chemical synthesis, molecular modeling and pharmacophore mapping of new pyrrole derivatives as inhibitors of InhA enzyme and <i>Mycobacterium tuberculosis</i> growth. <i>Medicinal Chemistry Research</i> , 2019, 28, 1838-1863.	2.4	9
781	Design, synthesis, and preliminary biological evaluation of catalpol propionates as antiaging drugs. <i>BMC Chemistry</i> , 2019, 13, 109.	3.8	6
783	Parallel cascade selection molecular dynamics to screen for protein complexes generated by rigid docking. <i>Journal of Molecular Graphics and Modelling</i> , 2019, 92, 94-99.	2.4	1
784	Subtle differences in chemical pattern between human toll-like receptor 8 agonists and antagonists: Emerging chemical patterns analysis. <i>Chemical Biology and Drug Design</i> , 2019, 94, 1824-1834.	3.2	2
785	Systems Pharmacology for Investigation of the Mechanisms of Action of Traditional Chinese Medicine in Drug Discovery. <i>Frontiers in Pharmacology</i> , 2019, 10, 743.	3.5	123
786	Binding of iodinated contrast media (ICM) and their transformation products with hormone receptors: Are ICM the new EDCs?. <i>Science of the Total Environment</i> , 2019, 692, 32-36.	8.0	9
787	Discovery of Potent Inhibitors of 11β-Hydroxysteroid Dehydrogenase Type 1 Using a Novel Growth-Based Protocol of <i>in Silico</i> Screening and Optimization in CONTOUR. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3422-3436.	5.4	5
788	Extensive benchmark of rDock as a peptide-protein docking tool. <i>Journal of Computer-Aided Molecular Design</i> , 2019, 33, 613-626.	2.9	12
789	Essentials of Bioinformatics, Volume II. , 2019, , .		1
790	Learning from the ligand: using ligand-based features to improve binding affinity prediction. <i>Bioinformatics</i> , 2020, 36, 758-764.	4.1	60
791	Molecular Characterization and Key Binding Sites of Sex Pheromone-Binding Proteins from the Meadow Moth, <i>Loxostege sticticalis</i> . <i>Journal of Agricultural and Food Chemistry</i> , 2019, 67, 12685-12695.	5.2	19
792	Insights into the c-Jun N-terminal kinase 3 (JNK3) inhibitors: CoMFA, CoMSIA analyses and molecular docking studies. <i>Medicinal Chemistry Research</i> , 2019, 28, 1796-1805.	2.4	2
793	Ligand- and Structure-Based Approaches of <i>Escherichia coli</i> FabI Inhibition by Triclosan Derivatives: From Chemical Similarity to Protein Dynamics Influence. <i>ChemMedChem</i> , 2019, 14, 1995-2004.	3.2	7
794	Inhibition of Hepatic CYP2D6 by the Active N-Oxide Metabolite of Sorafenib. <i>AAPS Journal</i> , 2019, 21, 107.	4.4	2

#	ARTICLE	IF	CITATIONS
795	Integration of multiscale molecular modeling approaches with the design and discovery of fusidic acid derivatives. <i>Future Medicinal Chemistry</i> , 2019, 11, 1427-1442.	2.3	10
796	Hidden bias in the DUD-E dataset leads to misleading performance of deep learning in structure-based virtual screening. <i>PLoS ONE</i> , 2019, 14, e0220113.	2.5	144
797	Theoretical Molecular Dynamics Simulation of the DIF-1 Receptor Activation. <i>Bulletin of the Chemical Society of Japan</i> , 2019, 92, 1436-1443.	3.2	1
798	Predicting Drug-Target Interaction Using a Novel Graph Neural Network with 3D Structure-Embedded Graph Representation. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3981-3988.	5.4	244
799	Discovery of Novel Inhibitors Targeting Human O-GlcNAcase: Docking-Based Virtual Screening, Biological Evaluation, Structural Modification, and Molecular Dynamics Simulation. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4374-4382.	5.4	19
800	In Silico Exploration of Aryl Halides Analogues as CheckpointKinase 1 Inhibitors by Using 3D QSAR, Molecular Docking Study, and ADMET Screening. <i>Advanced Pharmaceutical Bulletin</i> , 2019, 9, 84-92.	1.4	17
801	Niclosamide, an anthelmintic drug, enhances efficacy of PD-1/PD-L1 immune checkpoint blockade in non-small cell lung cancer. , 2019, 7, 245.		66
802	Ensemble docking-based virtual screening toward identifying inhibitors against Wee1 kinase. <i>Future Medicinal Chemistry</i> , 2019, 11, 1889-1906.	2.3	7
803	Transcriptome Analysis of <i>Sogatella furcifera</i> (Homoptera: Delphacidae) in Response to Sulfoxaflor and Functional Verification of Resistance-Related P450 Genes. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4573.	4.1	16
804	Key Topics in Molecular Docking for Drug Design. <i>International Journal of Molecular Sciences</i> , 2019, 20, 4574.	4.1	245
805	Structural Perspective on Revealing and Altering Molecular Functions of Genetic Variants Linked with Diseases. <i>International Journal of Molecular Sciences</i> , 2019, 20, 548.	4.1	20
806	Molecular modelling studies of quinazolinone derivatives as MMP-13 inhibitors by QSAR, molecular docking and molecular dynamics simulations techniques. <i>MedChemComm</i> , 2019, 10, 101-115.	3.4	16
807	Catalase inhibition by two Schiff base derivatives. Kinetics, thermodynamic and molecular docking studies. <i>Journal of Molecular Liquids</i> , 2019, 287, 111003.	4.9	33
808	Fragment-Based Ligand-Protein Contact Statistics: Application to Docking Simulations. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2499.	4.1	7
809	AGL-Score: Algebraic Graph Learning Score for Protein-Ligand Binding Scoring, Ranking, Docking, and Screening. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3291-3304.	5.4	145
810	Random Forest Refinement of Pairwise Potentials for Protein-Ligand Decoy Detection. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 3305-3315.	5.4	14
811	Design, synthesis, biological activities, and dynamic simulation study of novel thiourea derivatives with gibberellin activity towards <i>Arabidopsis thaliana</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2019, 27, 114969.	3.0	5
812	Fast Green FCF Attenuates Lipopolysaccharide-Induced Depressive-Like Behavior and Downregulates TLR4/Myd88/NF- κ B Signal Pathway in the Mouse Hippocampus. <i>Frontiers in Pharmacology</i> , 2019, 10, 501.	3.5	32

#	ARTICLE	IF	CITATIONS
813	Conformation Search Across Multiple-Level Potential-Energy Surfaces (CSAMP): A Strategy for Accurate Prediction of Protein-Ligand Binding Structures. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 4264-4279.	5.3	17
814	Ecological toxicity reduction of dinotefuran to honeybee: New perspective from an enantiomeric level. <i>Environment International</i> , 2019, 130, 104854.	10.0	69
815	Evaluating the effect of aminoglycosides on the interaction between bovine serum albumins by atomic force microscopy. <i>International Journal of Biological Macromolecules</i> , 2019, 134, 28-35.	7.5	8
816	Synthesis and biological evaluation of dihydroquinazoline-2-amines as potent non-nucleoside reverse transcriptase inhibitors of wild-type and mutant HIV-1 strains. <i>European Journal of Medicinal Chemistry</i> , 2019, 176, 11-20.	5.5	11
817	Identifying the Antiproliferative Effect of Astragalus Polysaccharides on Breast Cancer: Coupling Network Pharmacology With Targetable Screening From the Cancer Genome Atlas. <i>Frontiers in Oncology</i> , 2019, 9, 368.	2.8	27
818	A Comprehensive Review on Current Advances in Peptide Drug Development and Design. <i>International Journal of Molecular Sciences</i> , 2019, 20, 2383.	4.1	413
819	Assessing the performance of MM/PBSA and MM/GBSA methods. 9. Prediction reliability of binding affinities and binding poses for protein-peptide complexes. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 10135-10145.	2.8	96
820	Molecular Docking: A Structure-Based Approach for Drug Repurposing. , 2019, , 161-189.		22
821	Stalis : A Computational Method for Template-Based Ab Initio Ligand Design. <i>Journal of Computational Chemistry</i> , 2019, 40, 1622-1632.	3.3	4
822	Novel drug candidate for the treatment of several soft-tissue sarcoma histologic subtypes: A computational method using survival-associated gene signatures for drug repurposing. <i>Oncology Reports</i> , 2019, 41, 2241-2253.	2.6	8
823	Molecular dynamics-guided discovery of an ago-allosteric modulator for GPR40/FFAR1. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 7123-7128.	7.1	35
824	An Overview of Scoring Functions Used for Protein-Ligand Interactions in Molecular Docking. <i>Interdisciplinary Sciences, Computational Life Sciences</i> , 2019, 11, 320-328.	3.6	224
825	Computational Prediction of the Site(s) of Metabolism and Binding Modes of Protein Kinase Inhibitors Metabolized by CYP3A4. <i>Drug Metabolism and Disposition</i> , 2019, 47, 616-631.	3.3	10
826	A Molecular Docking Approach to Evaluate the Pharmacological Properties of Natural and Synthetic Treatment Candidates for Use against Hypertension. <i>International Journal of Environmental Research and Public Health</i> , 2019, 16, 923.	2.6	86
827	Comparative Molecular Field Analysis and Molecular Docking Studies on Quinolinone Derivatives Indicate Potential Hepatitis C Virus Inhibitors. <i>Cell Biochemistry and Biophysics</i> , 2019, 77, 139-156.	1.8	3
828	Identification of New Potent Acetylcholinesterase Inhibitors Using Virtual Screening and <i>in vitro</i> Approaches. <i>Molecular Informatics</i> , 2019, 38, e1800118.	2.5	13
829	Benchmarking of different molecular docking methods for protein-peptide docking. <i>BMC Bioinformatics</i> , 2019, 19, 426.	2.6	104
830	Spectroscopic studies on the interaction of a novel porphyrin derivative (PFP) and bovine serum albumin. <i>Medicine in Drug Discovery</i> , 2019, 4, 100015.	4.5	0

#	ARTICLE	IF	CITATIONS
831	Identification of The Fipronil Resistance Associated Mutations in Nilaparvata lugens GABA Receptors by Molecular Modeling. <i>Molecules</i> , 2019, 24, 4116.	3.8	13
832	Survey of the scoring functions for protein-ligand docking. <i>AIP Conference Proceedings</i> , 2019, , .	0.4	17
833	Distinctively complete inhibition of fibrillation of serum albumins by methotrexate <i>in vitro</i> : experimental and modelling studies to understand the tuning of protein misfolding-related aggregations. <i>New Journal of Chemistry</i> , 2019, 43, 18983-18987.	2.8	6
834	Taxifolin prevents postprandial hyperglycemia by regulating the activity of Î±-amylase: Evidence from an <i>in vivo</i> and <i>in silico</i> studies. <i>Journal of Cellular Biochemistry</i> , 2019, 120, 425-438.	2.6	53
835	Chemosensory proteins used as target for screening behaviourally active compounds in the rice pest <i>Cnaphalocrocis medinalis</i> (Lepidoptera: Pyralidae). <i>Insect Molecular Biology</i> , 2019, 28, 123-135.	2.0	39
836	Structural Insights into Characterizing Binding Sites in Epidermal Growth Factor Receptor Kinase Mutants. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 453-462.	5.4	30
837	Discovery of 2-(3,4-dialkoxyphenyl)-(substituted pyridazin-3-yl)acetonitriles as phosphodiesterase 4 inhibitors with anti-neuroinflammation potential based on three-dimensional quantitative structure-activity relationship study. <i>Chemical Biology and Drug Design</i> , 2019, 93, 484-502.	3.2	8
838	Molecules that Inhibit Bacterial Resistance Enzymes. <i>Molecules</i> , 2019, 24, 43.	3.8	25
839	Therapeutic Inhibition of Myc in Cancer. <i>Structural Bases and Computer-Aided Drug Discovery Approaches</i> . <i>International Journal of Molecular Sciences</i> , 2019, 20, 120.	4.1	109
840	Discovery of Nonpeptide, Reversible HER1/HER2 Dual-Targeting Small-Molecule Inhibitors as Near-Infrared Fluorescent Probes for Efficient Tumor Detection, Diagnostic Imaging, and Drug Screening. <i>Analytical Chemistry</i> , 2019, 91, 1507-1515.	6.5	20
841	FtsA as a cidal target for <i>Staphylococcus aureus</i> : Molecular docking and dynamics studies. <i>Journal of Cellular Biochemistry</i> , 2019, 120, 7751-7758.	2.6	31
842	Sorafenib N-Oxide Is an Inhibitor of Human Hepatic CYP3A4. <i>AAPS Journal</i> , 2019, 21, 15.	4.4	10
843	Understanding the structural features of JAK2 inhibitors: a combined 3D-QSAR, DFT and molecular dynamics study. <i>Molecular Diversity</i> , 2019, 23, 845-874.	3.9	11
844	Structure-Based Drug Design with a Special Emphasis on Herbal Extracts. <i>Challenges and Advances in Computational Chemistry and Physics</i> , 2019, , 271-305.	0.6	0
845	Identification of potential inhibitors for <i>Klebsiella pneumoniae</i> carbapenemase-3: a molecular docking and dynamics study. <i>Journal of Biomolecular Structure and Dynamics</i> , 2019, 37, 4601-4613.	3.5	22
846	The epigallocatechin gallate derivative Y6 reverses drug resistance mediated by the ABCB1 transporter both <i>in vitro</i> and <i>in vivo</i> . <i>Acta Pharmaceutica Sinica B</i> , 2019, 9, 316-323.	12.0	20
847	Interaction mechanism of flavonoids and zein in ethanol-water solution based on 3D-QSAR and spectrofluorimetry. <i>Food Chemistry</i> , 2019, 276, 776-781.	8.2	34
848	Antibacterial activity evaluation of synthetic novel pleuromutilin derivatives <i>in vitro</i> and in experimental infection mice. <i>European Journal of Medicinal Chemistry</i> , 2019, 162, 194-202.	5.5	19

#	ARTICLE	IF	CITATIONS
849	Converging a Knowledge-Based Scoring Function: DrugScore ²⁰¹⁸ . Journal of Chemical Information and Modeling, 2019, 59, 509-521.	5.4	48
850	Synthesis, molecular modeling and BACE-1 inhibitory study of tetrahydrobenzo[b] pyran derivatives. Bioorganic Chemistry, 2019, 84, 202-210.	4.1	22
851	<i>In silico</i> identification and design of potent peptide inhibitors against PDZ-3 domain of Postsynaptic Density Protein (PSD-95). Journal of Biomolecular Structure and Dynamics, 2019, 37, 1241-1253.	3.5	16
852	Effective prediction model and determination of binding residues influential for inhibitors targeting HIV-1 integrase-LEDGF/p75 interface by employing solvent accessible surface area energy as key determinant. Journal of Biomolecular Structure and Dynamics, 2020, 38, 460-473.	3.5	2
853	Computational-Aided Discovery of Novel 1,3-Benzodioxole Plant Growth Retardants. Journal of Plant Growth Regulation, 2020, 39, 888-896.	5.1	5
854	Computational prediction and experimental validation of the activator function of C2- ¹² -D-glucopyranosyl-1,3,6,7-tetrahydroxyxanthone on pancreatic and hepatic hexokinase. Journal of Biomolecular Structure and Dynamics, 2020, 38, 2976-2987.	3.5	3
855	Recent developments in molecular docking technology applied in food science: a review. International Journal of Food Science and Technology, 2020, 55, 33-45.	2.7	117
856	Virtual screening of antibacterial compounds by similarity search of Enoyl-ACP reductase (FabI) inhibitors. Future Medicinal Chemistry, 2020, 12, 51-68.	2.3	12
857	Molecular docking, antiproliferative and anticonvulsant activities of swertiamarin isolated from Elicostemma axillare. Bioorganic Chemistry, 2020, 94, 103428.	4.1	9
858	Computer-aided GPCR drug discovery. , 2020, , 283-293.		3
859	Characterization of seaweed hypoglycemic property with integration of virtual screening for identification of bioactive compounds. Journal of Functional Foods, 2020, 64, 103656.	3.4	10
860	Indazolyl-substituted piperidin-4-yl-aminopyrimidines as HIV-1 NNRTIs: Design, synthesis and biological activities. European Journal of Medicinal Chemistry, 2020, 186, 111864.	5.5	21
861	Modeling ligand docking to RNA in the design of RNA-based nanostructures. Current Opinion in Biotechnology, 2020, 63, 16-25.	6.6	8
862	Molecular Docking Analysis of 120 Potential HPV Therapeutic Epitopes Using a New Analytical Method. International Journal of Peptide Research and Therapeutics, 2020, 26, 1847-1861.	1.9	0
863	Discovery of Potent, Reversible, and Competitive Cruzain Inhibitors with Trypanocidal Activity: A Structure-Based Drug Design Approach. Journal of Chemical Information and Modeling, 2020, 60, 1028-1041.	5.4	32
864	The mechanism underlying OBP heterodimer formation and the recognition of odors in <i>Holotrichia obliqua</i> Faldermann. International Journal of Biological Macromolecules, 2020, 152, 957-968.	7.5	13
865	Molecular docking and inhibitory effects of a novel cytotoxic agent with bovine liver catalase. Journal of Molecular Structure, 2020, 1205, 127590.	3.6	27
866	2D- and 3D-QSAR and Molecular Docking of 2-Hydroxyisoquinoline-1,3-Diones as Inhibitors of HIV Reverse Transcriptase. International Journal of Quantitative Structure-Property Relationships, 2020, 5, 32-52.	0.5	0

#	ARTICLE	IF	CITATIONS
867	Two Rationally Identified Novel Glitazones Reversed the Behavioral Dysfunctions and Exhibited Neuroprotection Through Ameliorating Brain Cytokines and Oxy-Radicals in ICV-LPS Neuroinflammatory Rat Model. <i>Frontiers in Neuroscience</i> , 2020, 14, 530148.	2.8	8
868	Synthesis, biological evaluation and molecular docking studies of Combretastatin A-4 phosphoramidates as novel anticancer prodrugs. <i>Medicinal Chemistry Research</i> , 2020, 29, 2192-2202.	2.4	6
869	Esomeprazole reduces sperm motility index by targeting the spermic cholinergic machinery: A mechanistic study for the association between use of proton pump inhibitors and reduced sperm motility index. <i>Biochemical Pharmacology</i> , 2020, 182, 114212.	4.4	7
870	Phytochemical profiling, antioxidant and antiproliferation potential of <i>Euphorbia milii</i> var.: Experimental analysis and in-silico validation. <i>Saudi Journal of Biological Sciences</i> , 2020, 27, 3025-3034.	3.8	8
871	Gallic acid attenuates blood-spinal cord barrier disruption by inhibiting Jmjd3 expression and activation after spinal cord injury. <i>Neurobiology of Disease</i> , 2020, 145, 105077.	4.4	23
872	Combining fragment docking with graph theory to improve ligand docking for homology model structures. <i>Journal of Computer-Aided Molecular Design</i> , 2020, 34, 1237-1259.	2.9	4
873	Computational methods-guided design of modulators targeting protein-protein interactions (PPIs). <i>European Journal of Medicinal Chemistry</i> , 2020, 207, 112764.	5.5	26
874	Structural Insights into the Binding Modes of Viral RNA-Dependent RNA Polymerases Using a Function-Site Interaction Fingerprint Method for RNA Virus Drug Discovery. <i>Journal of Proteome Research</i> , 2020, 19, 4698-4705.	3.7	19
875	Two Point Mutations on CYP51 Combined With Induced Expression of the Target Gene Appeared to Mediate Pyrisoxazole Resistance in <i>Botrytis cinerea</i> . <i>Frontiers in Microbiology</i> , 2020, 11, 1396.	3.5	18
876	Identification of Hub Genes in Protective Effect of Astragaloside IV on Aconitine-Induced Cardiac Damage in Zebrafish Based on Bioinformatics Analysis. <i>Frontiers in Pharmacology</i> , 2020, 11, 957.	3.5	8
877	A drug-biomarker interaction model to predict the key targets of <i>Scutellaria barbata</i> D. Don in adverse-risk acute myeloid leukaemia. <i>Molecular Diversity</i> , 2020, 25, 2351-2365.	3.9	1
878	Development of disulfide-derived fructose-1,6-bisphosphatase (FBPase) covalent inhibitors for the treatment of type 2 diabetes. <i>European Journal of Medicinal Chemistry</i> , 2020, 203, 112500.	5.5	8
879	Novel Positive Allosteric Modulators of μ Opioid Receptor—Insight from In Silico and In Vivo Studies. <i>International Journal of Molecular Sciences</i> , 2020, 21, 8463.	4.1	9
880	Exploring the Interaction Mechanism of Desmethyl-broflanilide in Insect GABA Receptors and Screening Potential Antagonists by <i>In Silico</i> Simulations. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 14768-14780.	5.2	15
881	In Silico Prediction of the Mode of Action of <i>Viola odorata</i> in Diabetes. <i>BioMed Research International</i> , 2020, 2020, 1-13.	1.9	8
882	Fast Rescoring Protocols to Improve the Performance of Structure-Based Virtual Screening Performed on Protein-Protein Interfaces. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3910-3934.	5.4	14
883	The Use of Methods of Computer-Aided Drug Discovery in the Development of Topoisomerase II Inhibitors: Applications and Future Directions. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 3703-3721.	5.4	15
884	Discovery of Rhodanine and Thiazolidinediones as Novel Scaffolds for EGFR Inhibition: Design, Synthesis, Analysis and CoMSIA Studies. <i>Polycyclic Aromatic Compounds</i> , 2022, 42, 2483-2499.	2.6	8

#	ARTICLE	IF	CITATIONS
885	Optimization Rules for SARS-CoV-2 Mpro Antivirals: Ensemble Docking and Exploration of the Coronavirus Protease Active Site. <i>Viruses</i> , 2020, 12, 942.	3.3	34
886	Molecular-Level Understanding of the Somatostatin Receptor 1 (SSTR1)â€™Ligand Binding: A Structural Biology Study Based on Computational Methods. <i>ACS Omega</i> , 2020, 5, 21145-21161.	3.5	9
887	Design, microwave synthesis, and molecular docking studies of catalpol crotonates as potential neuroprotective agent of diabetic encephalopathy. <i>Scientific Reports</i> , 2020, 10, 20415.	3.3	6
888	Computational Insights into Allosteric Conformational Modulation of P-Glycoprotein by Substrate and Inhibitor Binding. <i>Molecules</i> , 2020, 25, 6006.	3.8	9
889	Rational Design of 2-Chloroadenine Derivatives as Highly Selective Phosphodiesterase 8A Inhibitors. <i>Journal of Medicinal Chemistry</i> , 2020, 63, 15852-15863.	6.4	9
890	Adsorption kinetics and mechanism of diâ€™nâ€™butyl phthalate by <i>Leuconostoc mesenteroides</i>. <i>Food Science and Nutrition</i> , 2020, 8, 6153-6163.	3.4	8
891	Advances in Docking. <i>Current Medicinal Chemistry</i> , 2020, 26, 7555-7580.	2.4	66
892	Proton pump inhibitors act with unprecedented potencies as inhibitors of the acetylcholine biosynthesizing enzymeâ€™A plausible missing link for their association with incidence of dementia. <i>Alzheimer's and Dementia</i> , 2020, 16, 1031-1042.	0.8	32
893	TCP1 ^{Î³} Subunit Is Indispensable for Growth and Infectivity of <i>Leishmania donovani</i> . <i>Antimicrobial Agents and Chemotherapy</i> , 2020, 64, .	3.2	6
894	In silico development of quorum sensing inhibitors. , 2020, , 329-357.		1
895	Bioanalytical chiral chromatographic technique and docking studies for enantioselective separation of meclizine hydrochloride: Application to pharmacokinetic study in rabbits. <i>Chirality</i> , 2020, 32, 1091-1106.	2.6	4
896	Computer-Aided Ligand Discovery for Estrogen Receptor Alpha. <i>International Journal of Molecular Sciences</i> , 2020, 21, 4193.	4.1	33
897	New techniques and strategies in drug discovery. <i>Chinese Chemical Letters</i> , 2020, 31, 1695-1708.	9.0	82
898	A machine learning-driven study indicates emodin improves cardiac hypertrophy by modulation of mitochondrial SIRT3 signaling. <i>Pharmacological Research</i> , 2020, 155, 104739.	7.1	30
899	Theoretical investigation of AhR binding property with relevant structural requirements for AhR-mediated toxicity of polybrominated diphenyl ethers. <i>Chemosphere</i> , 2020, 249, 126554.	8.2	14
900	Design, Synthesis, and Biological Activity of Novel Aromatic Amide Derivatives Containing Sulfide and Sulfone Substructures. <i>Engineering</i> , 2020, 6, 553-559.	6.7	25
901	Cov_FB3D: A De Novo Covalent Drug Design Protocol Integrating the BA-SAMP Strategy and Machine-Learning-Based Synthetic Tractability Evaluation. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4388-4402.	5.4	12
902	Computational insight on the binding and selectivity of target-subunit-dependent for neonicotinoid insecticides. <i>Journal of Molecular Graphics and Modelling</i> , 2020, 98, 107586.	2.4	13

#	ARTICLE	IF	CITATIONS
903	Binding of clozapine to the GABAB receptor: clinical and structural insights. <i>Molecular Psychiatry</i> , 2020, 25, 1910-1919.	7.9	52
904	Computational Methods Used in Phytocompound-Based Drug Discovery. , 2020, , 549-573.		0
905	A review of mathematical representations of biomolecular data. <i>Physical Chemistry Chemical Physics</i> , 2020, 22, 4343-4367.	2.8	56
906	CoMFA, CoMSIA, molecular docking and MOLCAD studies of pyrimidinone derivatives to design novel and selective tankyrase inhibitors. <i>Journal of Molecular Structure</i> , 2020, 1221, 128783.	3.6	8
907	Three point mutations in cytochrome <i>b</i> confer resistance to trifloxystrobin in <i>Magnaporthe oryzae</i> . <i>Pest Management Science</i> , 2020, 76, 4258-4267.	3.4	16
908	Binding properties of marine bromophenols with human protein tyrosine phosphatase 1B: Molecular docking, surface plasmon resonance and cellular insulin resistance study. <i>International Journal of Biological Macromolecules</i> , 2020, 163, 200-208.	7.5	8
909	Novel ACE Inhibitory Peptides Derived from Simulated Gastrointestinal Digestion in Vitro of Sesame (<i>Sesamum indicum</i> L.) Protein and Molecular Docking Study. <i>International Journal of Molecular Sciences</i> , 2020, 21, 1059.	4.1	48
910	Discovery and Optimization of Chromone Derivatives as Novel Selective Phosphodiesterase 10 Inhibitors. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1058-1071.	3.5	7
911	Controllable Soil Degradation Rate of 5-Substituted Sulfonylurea Herbicides as Novel AHAS Inhibitors. <i>Journal of Agricultural and Food Chemistry</i> , 2020, 68, 3017-3025.	5.2	12
912	Conjugation of haloperidol to PEG allows peripheral localisation of haloperidol and eliminates CNS extrapyramidal effects. <i>Journal of Controlled Release</i> , 2020, 322, 227-235.	9.9	8
913	Hesperidin improves insulin resistance via down-regulation of inflammatory responses: Biochemical analysis and in silico validation. <i>PLoS ONE</i> , 2020, 15, e0227637.	2.5	20
914	Identification of herbal categories active in pain disorder subtypes by machine learning help reveal novel molecular mechanisms of algisia. <i>Pharmacological Research</i> , 2020, 156, 104797.	7.1	9
915	Structure- and Ligand-Based Virtual Screening on DUD-E: Performance Dependence on Approximations to the Binding Pocket. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 4296-4310.	5.4	33
916	Revealing Acquired Resistance Mechanisms of Kinase-Targeted Drugs Using an on-the-Fly, Function-Site Interaction Fingerprint Approach. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 3152-3161.	5.3	8
917	Design and synthesis of diazine-based panobinostat analogues for HDAC8 inhibition. <i>Beilstein Journal of Organic Chemistry</i> , 2020, 16, 628-637.	2.2	3
918	Pharmacophore modeling and virtual screening for the discovery of biologically active natural products. <i>Studies in Natural Products Chemistry</i> , 2020, 64, 321-364.	1.8	2
919	Rational drug repurposing for cancer by inclusion of the unbiased molecular dynamics simulation in the structure-based virtual screening approach: Challenges and breakthroughs. <i>Seminars in Cancer Biology</i> , 2021, 68, 249-257.	9.6	20
920	Identification of a druggable protein-protein interaction site between mutant p53 and its stabilizing chaperone DNAJA1. <i>Journal of Biological Chemistry</i> , 2021, 296, 100098.	3.4	20

#	ARTICLE	IF	CITATIONS
921	Chemical synthesis and molecular modeling of novel substituted N-1,3-benzoxazol-2-yl benzene sulfonamides as inhibitors of inhA enzyme and Mycobacterium tuberculosis growth. Journal of the Iranian Chemical Society, 2021, 18, 903-920.	2.2	3
922	Bioinformatics and Chemometrics for Discovering Biologically Active Peptides From Food Proteins. , 2021, , 482-494.		3
923	Post-processing of Docking Results: Tools and Strategies. , 2021, , 57-74.		0
924	<i>in silico</i> design of novel FAK inhibitors using integrated molecular docking, 3D-QSAR and molecular dynamics simulation studies. Journal of Biomolecular Structure and Dynamics, 2022, 40, 5965-5982.	3.5	9
925	Advances in structure-based drug design. , 2021, , 55-103.		9
926	Divide-and-Link Peptide Docking: A Fragment-Based Peptide Docking Protocol. Physical Chemistry Chemical Physics, 2021, 23, 22647-22660.	2.8	9
927	Chiral Separation of Oxomemazine Enantiomers by HPLC Technique and Enantiomeric Separation Mechanism via Docking Studies. Current Pharmaceutical Analysis, 2021, 17, 222-230.	0.6	3
928	Resources for Docking-Based Virtual Screening. , 2021, , 179-203.		1
929	3D-QSAR modeling, molecular docking and ADMET properties of benzothiazole derivatives as β -glucosidase inhibitors. Materials Today: Proceedings, 2021, 45, 7643-7652.	1.8	7
930	Structure-Based Virtual Screening: Theory, Challenges and Guidelines. , 2021, , .		0
931	Update and Potential Opportunities in CBP [Cyclic Adenosine Monophosphate (cAMP) Response Element-Binding Protein (CREB)-Binding Protein] Research Using Computational Techniques. Protein Journal, 2021, 40, 19-27.	1.6	4
932	General Purpose Structure-Based Drug Discovery Neural Network Score Functions with Human-Interpretable Pharmacophore Maps. Journal of Chemical Information and Modeling, 2021, 61, 603-620.	5.4	27
934	Three Dimensional Quantitative Structure Activity Relationship and Molecular Docking Studies of Flavonoids as Reverse Transcriptase Inhibitors. Asian Journal of Organic & Medicinal Chemistry, 2021, 6, 33-39.	0.0	0
935	Unprecedented polycyclic polyprenylated acylphloroglucinols with anti-Alzheimer's activity from St. John's wort. Chemical Science, 2021, 12, 11438-11446.	7.4	19
936	An evaluation of combined strategies for improving the performance of molecular docking. Journal of Bioinformatics and Computational Biology, 2021, 19, 2150003.	0.8	4
937	Prediction of potential inhibitors of SARS-CoV-2 using 3D-QSAR, molecular docking modeling and ADMET properties. Heliyon, 2021, 7, e06603.	3.2	16
938	6-amide-2-aryl benzoxazole/benzimidazole derivatives as VEGFR-2 inhibitors in two-and three-dimensional QSAR studies: topomer CoMFA and HQSAR. Chemical Papers, 2021, 75, 3551-3562.	2.2	3
939	Discovery of behaviorally active semiochemicals in <i>Aenasius bambawalei</i> using a reverse chemical ecology approach. Pest Management Science, 2021, 77, 2843-2853.	3.4	5

#	ARTICLE	IF	CITATIONS
940	FRAGSITE: A Fragment-Based Approach for Virtual Ligand Screening. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2074-2089.	5.4	20
941	Predicting Potential Endocrine Disrupting Chemicals Binding to Estrogen Receptor α (ER α) Using a Pipeline Combining Structure-Based and Ligand-Based in Silico Methods. <i>International Journal of Molecular Sciences</i> , 2021, 22, 2846.	4.1	6
942	SMPLIP-Score: predicting ligand binding affinity from simple and interpretable on-the-fly interaction fingerprint pattern descriptors. <i>Journal of Cheminformatics</i> , 2021, 13, 28.	6.1	24
943	Conformational Strain of Macrocyclic Peptides in Ligand-Receptor Complexes Based on Advanced Refinement of Bound-State Conformers. <i>Journal of Medicinal Chemistry</i> , 2021, 64, 3282-3298.	6.4	7
944	MD Simulations on a Well-Built Docking Model Reveal Fine Mechanical Stability and Force-Dependent Dissociation of Mac-1/GPIIb/IIIa Complex. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 638396.	3.5	5
946	Withanolides from dietary tomatillo suppress HT1080 cancer cell growth by targeting mutant IDH1. <i>Bioorganic and Medicinal Chemistry</i> , 2021, 36, 116095.	3.0	8
947	Design, synthesis and anti-rheumatoid arthritis evaluation of double-ring conjugated enones. <i>Bioorganic Chemistry</i> , 2021, 109, 104701.	4.1	14
948	In silico Approaches for the Design and Optimization of Interfering Peptides Against Protein-Protein Interactions. <i>Frontiers in Molecular Biosciences</i> , 2021, 8, 669431.	3.5	38
950	Deep Learning-Based Ligand Design Using Shared Latent Implicit Fingerprints from Collaborative Filtering. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2159-2174.	5.4	5
951	Docking Paradigm in Drug Design. <i>Current Topics in Medicinal Chemistry</i> , 2021, 21, 507-546.	2.1	23
952	Protective Effects of Cocos Nucifera Oil in Paraphenylene Diamine Toxicity. <i>Current Pharmaceutical Biotechnology</i> , 2021, 22, 423-432.	1.6	1
953	A rapid method and mechanism to identify the active compounds in Malus micromalus Makino fruit with spectrum-effect relationship, components knock-out and molecular docking technology. <i>Food and Chemical Toxicology</i> , 2021, 150, 112086.	3.6	16
954	A Review on Molecular Docking. <i>International Research Journal of Pure and Applied Chemistry</i> , 0, , 60-68.	0.2	6
955	Introduction of Advanced Methods for Structure-based Drug Discovery. <i>Current Bioinformatics</i> , 2021, 16, 351-363.	1.5	10
956	An Updated Review of Computer-Aided Drug Design and Its Application to COVID-19. <i>BioMed Research International</i> , 2021, 2021, 1-18.	1.9	95
957	Computational Drug Repurposing Resources and Approaches for Discovering Novel Antifungal Drugs against <i>Candida albicans</i> N-Myristoyl Transferase. <i>Journal of Pure and Applied Microbiology</i> , 2021, 15, 556-579.	0.9	2
958	MOLECULAR DOCKING: AN EXPLANATORY APPROACH IN STRUCTURE-BASED DRUG DESIGNING AND DISCOVERY. <i>International Journal of Pharmacy and Pharmaceutical Sciences</i> , 0, , 6-12.	0.3	1
959	Virtual Screening and Biological Evaluation of Anti-Biofilm Agents Targeting LuxS in the Quorum Sensing System. <i>Natural Product Communications</i> , 2021, 16, 1934578X2110196.	0.5	3

#	ARTICLE	IF	CITATIONS
961	Identification of Novel Inhibitors of Type-I Mycobacterium Tuberculosis Fatty Acid Synthase Using Docking-Based Virtual Screening and Molecular Dynamics Simulation. <i>Applied Sciences (Switzerland)</i> , 2021, 11, 6977.	2.5	2
962	AutoDock Vina 1.2.0: New Docking Methods, Expanded Force Field, and Python Bindings. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3891-3898.	5.4	1,481
963	Virtual screening of potential anticancer drugs based on microbial products. <i>Seminars in Cancer Biology</i> , 2022, 86, 1207-1217.	9.6	6
964	Raphanus sativus Seeds Oil Arrested in vivo Inflammation and Angiogenesis through Down-regulation of TNF- α . <i>Current Pharmaceutical Biotechnology</i> , 2022, 23, 728-739.	1.6	6
965	Phytochemical, pharmacological, and In-silico molecular docking studies of <i>Strobilanthes glutinosus</i> Nees: An unexplored source of bioactive compounds. <i>South African Journal of Botany</i> , 2022, 147, 618-627.	2.5	13
966	Structure-aware Interactive Graph Neural Networks for the Prediction of Protein-Ligand Binding Affinity. , 2021, , .		58
967	Shape-Restrained Modeling of Protein-Small-Molecule Complexes with High Ambiguity Driven DOCKing. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4807-4818.	5.4	11
968	Network Pharmacology and Experimental Evidence: PI3K/AKT Signaling Pathway is Involved in the Antidepressive Roles of Chaihu Shugan San. <i>Drug Design, Development and Therapy</i> , 2021, Volume 15, 3425-3441.	4.3	25
969	Development and Benchmarking of Open Force Field v1.0.0-the Parsley Small-Molecule Force Field. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6262-6280.	5.3	80
970	Design, synthesis and biological evaluation of novel pyrazolopyrimidone derivatives as potent PDE1 inhibitors. <i>Bioorganic Chemistry</i> , 2021, 114, 105104.	4.1	4
971	Clinical insights into topically applied multipronged nanoparticles in subjects with atopic dermatitis. <i>Journal of Drug Delivery Science and Technology</i> , 2021, 65, 102744.	3.0	1
972	A novel multi-objective metaheuristic algorithm for protein-peptide docking and benchmarking on the LEADS-PEP dataset. <i>Computers in Biology and Medicine</i> , 2021, 138, 104896.	7.0	15
973	Structural and functional changes of catalase through interaction with Erlotinib hydrochloride. Use of Chou's 5-steps rule to study mechanisms. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2021, 260, 119940.	3.9	16
974	Identification of bioactive natural compounds as efficient inhibitors against Mycobacterium tuberculosis protein-targets: A molecular docking and molecular dynamics simulation study. <i>Journal of Molecular Liquids</i> , 2021, 341, 117340.	4.9	27
975	Molecular Docking: A Contemporary Story About Food Safety. , 2021, , 479-492.		0
976	Methods for Molecular Modelling of Protein Complexes. <i>Methods in Molecular Biology</i> , 2021, 2305, 53-80.	0.9	7
977	Biased Docking for Protein-Ligand Pose Prediction. <i>Methods in Molecular Biology</i> , 2021, 2266, 39-72.	0.9	9
978	Modern Tools and Techniques in Computer-Aided Drug Design. , 2021, , 1-30.		5

#	ARTICLE	IF	CITATIONS
979	Advanced approaches and in silico tools of chemoinformatics in drug designing. , 2021, , 173-206.		1
981	Structure-Based Drug Design. Biological and Medical Physics Series, 2007, , 135-176.	0.4	3
982	Virtual Screening for RNA-Interacting Small Molecules. , 2012, , 235-252.		2
983	Structure-Based Functional Design of Drugs: From Target to Lead Compound. Methods in Molecular Biology, 2012, 823, 359-366.	0.9	32
984	Guide to Virtual Screening: Application to the Akt Phosphatase PHLPP. Methods in Molecular Biology, 2012, 819, 561-573.	0.9	3
985	Modeling, Docking, and Fitting of Atomic Structures to 3D Maps from Cryo-Electron Microscopy. Methods in Molecular Biology, 2013, 955, 229-241.	0.9	10
986	Design of New Chemoinformatic Tools for the Analysis of Virtual Screening Studies: Application to Tubulin Inhibitors. Advances in Soft Computing, 2009, , 189-196.	0.4	2
987	High-Throughput and In Silico Screening in Drug Discovery. , 2017, , 247-273.		5
988	Comparison of Binding Site of Remdesivir and Its Metabolites with NSP12-NSP7-NSP8, and NSP3 of SARS CoV-2 Virus and Alternative Potential Drugs for COVID-19 Treatment. Protein Journal, 2020, 39, 619-630.	1.6	15
989	Design, synthesis and evaluation of pyrazolopyrimidinone derivatives as novel PDE9A inhibitors for treatment of Alzheimer's disease. Bioorganic and Medicinal Chemistry Letters, 2020, 30, 127254.	2.2	6
990	Pharmacophore-based Virtual Screening in Drug Discovery. , 2008, , 76-119.		10
991	Conformational Analysis, Solvent-Accessible Surface and Geometric Extent of Inhibitors and Substrates. Collection of Czechoslovak Chemical Communications, 2006, 71, 842-858.	1.0	1
992	Potential Molecular Mechanisms and Drugs for Aconitine-Induced Cardiotoxicity in Zebrafish through RNA Sequencing and Bioinformatics Analysis. Medical Science Monitor, 2020, 26, e924092.	1.1	4
993	Some Critical Aspects of Molecular Interactions Between Drugs and Receptors. American Journal of Modeling and Optimization, 2014, 2, 84-102.	0.5	4
995	Combinatorial Computational Approaches to Identify Tetracycline Derivatives as Flavivirus Inhibitors. PLoS ONE, 2007, 2, e428.	2.5	87
996	Application of Consensus Scoring and Principal Component Analysis for Virtual Screening against β -Secretase (BACE-1). PLoS ONE, 2012, 7, e38086.	2.5	42
997	Prediction and Identification of T Cell Epitopes in the H5N1 Influenza Virus Nucleoprotein in Chicken. PLoS ONE, 2012, 7, e39344.	2.5	23
998	A Targeted Library Screen Reveals a New Inhibitor Scaffold for Protein Kinase D. PLoS ONE, 2012, 7, e44653.	2.5	16

#	ARTICLE	IF	CITATIONS
999	A Single Glycine-Alanine Exchange Directs Ligand Specificity of the Elephant Progesterin Receptor. PLoS ONE, 2012, 7, e50350.	2.5	10
1000	Glucose 6P Binds and Activates HlyIIIR to Repress Bacillus cereus Haemolysin hlyII Gene Expression. PLoS ONE, 2013, 8, e55085.	2.5	21
1001	A Novel Transport Mechanism for MOMP in Chlamydomophila pneumoniae and Its Putative Role in Immune-Therapy. PLoS ONE, 2013, 8, e61139.	2.5	6
1002	Template CoMFA Generates Single 3D-QSAR Models that, for Twelve of Twelve Biological Targets, Predict All ChEMBL-Tabulated Affinities. PLoS ONE, 2015, 10, e0129307.	2.5	13
1003	Discovery of a Series of Acridinones as Mechanism-Based Tubulin Assembly Inhibitors with Anticancer Activity. PLoS ONE, 2016, 11, e0160842.	2.5	9
1004	Genomic profiling is predictive of response to cisplatin treatment but not to PI3K inhibition in bladder cancer patient-derived xenografts. Oncotarget, 2016, 7, 76374-76389.	1.8	32
1005	Blockade of the malignant phenotype by β -subunit selective noncovalent inhibition of immuno- and constitutive proteasomes. Oncotarget, 2017, 8, 10437-10449.	1.8	13
1006	Germanone derivatives: synthesis, biological activity, molecular docking studies and molecular dynamics simulations. Oncotarget, 2017, 8, 15149-15158.	1.8	15
1007	Indirubin, a bisindole alkaloid from <i>Isatis indigotica</i> , reduces H1N1 susceptibility in stressed mice by regulating MAVS signaling. Oncotarget, 2017, 8, 105615-105629.	1.8	31
1008	Honokiol inhibits the growth of head and neck squamous cell carcinoma by targeting epidermal growth factor receptor. Oncotarget, 2015, 6, 21268-21282.	1.8	43
1009	Targeting the sugar metabolism of tumors with a first-in-class 6-phosphofructo-2-kinase (PFKFB4) inhibitor. Oncotarget, 2015, 6, 18001-18011.	1.8	37
1010	Dimeric peroxiredoxins are druggable targets in human Burkitt lymphoma. Oncotarget, 2016, 7, 1717-1731.	1.8	48
1011	Protein-Ligand Docking in the New Millennium – A Retrospective of 10 Years in the Field. Current Medicinal Chemistry, 2013, 20, 2296-2314.	2.4	197
1012	Current Approaches in Antiviral Drug Discovery Against the Flaviviridae Family. Current Pharmaceutical Design, 2014, 20, 3428-3444.	1.9	23
1013	In Silico Studies against Viral Sexually Transmitted Diseases. Current Protein and Peptide Science, 2019, 20, 1135-1150.	1.4	1
1014	Molecular Docking: Challenges, Advances and its Use in Drug Discovery Perspective. Current Drug Targets, 2019, 20, 501-521.	2.1	246
1015	Consensus Analyses in Molecular Docking Studies Applied to Medicinal Chemistry. Mini-Reviews in Medicinal Chemistry, 2020, 20, 1322-1340.	2.4	8
1016	Virtual Screening of Natural Products Database. Mini-Reviews in Medicinal Chemistry, 2021, 21, 2657-2730.	2.4	17

#	ARTICLE	IF	CITATIONS
1017	Guided Docking Approaches to Structure-Based Design and Screening. <i>Current Topics in Medicinal Chemistry</i> , 2004, 4, 687-700.	2.1	62
1018	Statistical Analysis, Optimization, and Prioritization of Virtual Screening Parameters for Zinc Enzymes Including the Anthrax Toxin Lethal Factor. <i>Current Topics in Medicinal Chemistry</i> , 2014, 14, 2105-2114.	2.1	1
1019	Application of Computational Techniques to Unravel Structure-Function Relationship and their Role in Therapeutic Development. <i>Current Topics in Medicinal Chemistry</i> , 2018, 18, 1769-1791.	2.1	5
1020	Virtual Screening Techniques in Drug Discovery: Review and Recent Applications. <i>Current Topics in Medicinal Chemistry</i> , 2019, 19, 1751-1767.	2.1	99
1021	In Silico Studies in Drug Research Against Neurodegenerative Diseases. <i>Current Neuropharmacology</i> , 2018, 16, 664-725.	2.9	51
1022	Computer Aided Drug Design and its Application to the Development of Potential Drugs for Neurodegenerative Disorders. <i>Current Neuropharmacology</i> , 2018, 16, 740-748.	2.9	98
1023	3D-QSAR and Molecular Docking Studies on Design Anti-Prostate Cancer Curcumin Analogues. <i>Current Computer-Aided Drug Design</i> , 2020, 16, 245-256.	1.2	9
1024	Screening Outside the Catalytic Site: Inhibition of Macromolecular Interactions Through Structure-Based Virtual Ligand Screening Experiments. <i>The Open Biochemistry Journal</i> , 2008, 2, 29-37.	0.5	17
1025	Pyrryl Pyrazoline Carbaldehydes as Enoyl-ACP Reductase Inhibitors: Design, Synthesis and Antitubercular Activity. <i>Open Medicinal Chemistry Journal</i> , 2017, 11, 92-108.	2.4	4
1026	Integrated Computational Approaches and Tools for Allosteric Drug Discovery. <i>International Journal of Molecular Sciences</i> , 2020, 21, 847.	4.1	73
1027	Different Types of Molecular Docking Based on Variations of Interacting Molecules. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , 2016, , 148-172.	0.3	2
1028	Molecular Docking of Biologically Active Substances to Double Helical Nucleic Acids. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , 2016, , 127-157.	0.3	1
1029	Computational Approaches for the Discovery of Novel Hepatitis C Virus NS3/4A and NS5B Inhibitors. , 2017, , 482-518.		1
1030	Proposal of Dual Inhibitor Targeting ATPase Domains of Topoisomerase II and Heat Shock Protein 90. <i>Biomolecules and Therapeutics</i> , 2016, 24, 453-468.	2.4	14
1031	Modelaci3n por homol3a de la prote3na Luxs de Porphyromonas gingivalis cepa W83. <i>Revista Cl3nica De Periodoncia Implantolog3a Y Rehabilitaci3n Oral</i> , 2012, 5, 105-113.	0.1	1
1032	Docking Efficiency Comparison of Surflex, a Commercial Package and Arguslab, a Licensable Freewar. <i>Journal of Computer Science and Systems Biology</i> , 2008, 01, .	0.0	11
1033	3D-QSAR Analysis and Molecular Docking of Thiosemicarbazone Analogues as a Potent Tyrosinase Inhibitor. <i>Bulletin of the Korean Chemical Society</i> , 2011, 32, 1241-1248.	1.9	7
1034	Flavonoid from Carica papaya inhibits NS2B-NS3 protease and prevents Dengue 2 viral assembly. <i>Bioinformation</i> , 2013, 9, 889-895.	0.5	94

#	ARTICLE	IF	CITATIONS
1035	Docking Studies of Chlorogenic Acid against Aldose Reductase by using Molgro Virtual Docker Software. <i>Journal of Applied Pharmaceutical Science</i> , 0, , .	1.0	6
1036	An antigen display system of GEM nanoparticles based on affinity peptide ligands. <i>International Journal of Biological Macromolecules</i> , 2021, 193, 574-584.	7.5	9
1037	Structure and dynamics of the somatostatin receptor 3 ligand binding in the presence of lipids examined using computational structural biology methods. <i>Proteins: Structure, Function and Bioinformatics</i> , 2022, 90, 704-719.	2.6	2
1038	Parasitological profiling shows 4(1H)-quinolone derivatives as new lead candidates for malaria. <i>European Journal of Medicinal Chemistry Reports</i> , 2021, 3, 100012.	1.4	5
1039	Application of Chemoinformatic Tools for the Analysis of Virtual Screening Studies of Tubulin Inhibitors. <i>Advances in Intelligent and Soft Computing</i> , 2007, , 411-417.	0.2	1
1040	ICAM-1 Peptide Inhibitors of T-cell Adhesion bind to the allosteric site of LFA-1. An NMR Characterization. <i>Chemical Biology and Drug Design</i> , 2007, , .	3.2	0
1042	The Roles of Hydroxyl Substituents in Tyrosinase Inhibitory Activation of Flavone Analogues. <i>Journal of Applied Biological Chemistry</i> , 2011, 54, 56-62.	0.4	0
1043	Prediction of Active Residues of β -galactosidase from <i>Bacteroides thetaiotaomicron</i> . <i>Advances in Intelligent Systems and Computing</i> , 2014, , 65-71.	0.6	0
1044	Depigmenting Effects of Esculetin and Esculin Isolated from <i>Fraxinus rhynchophylla</i> Hance. <i>Journal of the Society of Cosmetic Scientists of Korea</i> , 2014, 40, 89-94.	0.2	0
1045	Comparative Docking Studies of Osthol Derivatives and Sorafenib on BRAF V599E Mutant Protein. <i>Computational Research</i> , 2014, 2, 13-20.	0.2	1
1046	Computational Approaches for the Discovery of Novel Hepatitis C Virus NS3/4A and NS5B Inhibitors. <i>Advances in Chemical and Materials Engineering Book Series</i> , 2015, , 318-353.	0.3	0
1047	Synthesis and Anti Hiv-1 Reverse Transcriptase Evaluation of A Series of N-Mono Substituted Thiourea Derivatives. <i>International Journal of HIV/AIDS and Research</i> , 0, , 19-27.	0.0	0
1048	Combined Pharmacophore and Molecular Docking-based In silico Study of Some Pyrrolyl 1,3,4-oxadiazole benzothioate Derivatives. <i>Rajiv Gandhi University of Health Sciences Journal of Pharmaceutical Sciences</i> , 2015, 5, 69-80.	0.1	0
1049	Molecular Docking at a Glance. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , 2016, , 1-38.	0.3	1
1050	Homology modelling and docking analysis of L-lactate dehydrogenase from <i>Streptococcus thermophilus</i> . <i>Acta Periodica Technologica</i> , 2016, , 241-248.	0.2	0
1051	Role of Molecular Docking in Computer-Aided Drug Design and Development. <i>Advances in Medical Technologies and Clinical Practice Book Series</i> , 2016, , 1-28.	0.3	2
1052	Prediction of kinase-inhibitor binding affinity using energetic parameters. <i>Bioinformation</i> , 2016, 12, 172-181.	0.5	0
1053	Different Types of Molecular Docking Based on Variations of Interacting Molecules. , 2017, , 795-819.		0

#	ARTICLE	IF	CITATIONS
1054	Role of Molecular Docking in Computer-Aided Drug Design and Development. , 2017, , 683-710.		0
1055	Molecular Docking at a Glance. , 2017, , 764-803.		0
1057	Refined Molecular Docking with Multi-objective Optimization Method. Advances in Intelligent Systems and Computing, 2019, , 56-63.	0.6	0
1058	Molecular Modeling and Drug Design Techniques in Microbial Drug Discovery. , 2019, , 185-231.		0
1059	Carbamoyl Imidazoles As Potent, Reversible and Competitive Cruzain Inhibitors with <i>in vitro</i> and <i>in vivo</i> Trypanocidal Activity: A Structure-Based Drug Design Approach. SSRN Electronic Journal, 0, , .	0.4	0
1062	Virtual Screening for Type II B Inhibitors of B-RafV600E Kinase. Current Computer-Aided Drug Design, 2020, 16, 222-230.	1.2	0
1064	Radio-protective efficacy of <i>Gymnema sylvestre</i> on <i>Pangasius sutchi</i> against gamma (60Co) irradiation. International Journal of Radiation Biology, 2021, , 1-43.	1.8	1
1065	Docking and scoring for nucleic acid–ligand interactions: Principles and current status. Drug Discovery Today, 2022, 27, 838-847.	6.4	19
1066	CHAPTER 3. Computational Methods for the Discovery of Chemical Probes. Chemical Biology, 2020, , 39-68.	0.2	0
1067	In Silico and In Vivo: Evaluating the Therapeutic Potential of Kaempferol, Quercetin, and Catechin to Treat Chronic Epilepsy in a Rat Model. Frontiers in Bioengineering and Biotechnology, 2021, 9, 754952.	4.1	13
1069	In vitro anti- <i>Toxoplasma gondii</i> activity evaluation of a new series of quinazolin-4(3H)-one derivatives. Chemistry and Biodiversity, 2021, , e2100687.	2.1	1
1070	<i>In silico</i> data mining of large-scale databases for the virtual screening of human interleukin-2 inhibitors. Acta Pharmaceutica, 2021, 71, 33-56.	2.0	2
1073	Evaluation of the antibacterial activity of patchouli oil. Iranian Journal of Pharmaceutical Research, 2013, 12, 307-16.	0.5	32
1076	Molecular docking and molecular dynamics simulation. , 2022, , 291-304.		25
1077	De Novo Molecular Design of Caspase-6 Inhibitors by a GRU-Based Recurrent Neural Network Combined with a Transfer Learning Approach. Pharmaceuticals, 2021, 14, 1249.	3.8	7
1078	Targeting the Central Pocket of the <i>Pseudomonas aeruginosa</i> Lectin LecA. ChemBioChem, 2021, , .	2.6	12
1079	OUP accepted manuscript. Journal of Chromatographic Science, 2021, , .	1.4	0
1080	Design, Synthesis <i>In Vitro</i> Anticancer Activity and Docking Studies of (ˆ)–Catechin Derivatives. Bulletin of the Korean Chemical Society, 2015, 36, 564-570.	1.9	10

#	ARTICLE	IF	CITATIONS
1081	Structure-Based Virtual Screening for Ligands of G Protein-Coupled Receptors: What Can Molecular Docking Do for You?. <i>Pharmacological Reviews</i> , 2021, 73, 1698-1736.	16.0	61
1082	Advances in structure-based virtual screening for drug discovery. , 2022, , 387-404.		2
1083	DrugDevCovid19: An Atlas of Anti-COVID-19 Compounds Derived by Computer-Aided Drug Design. <i>Molecules</i> , 2022, 27, 683.	3.8	11
1084	3D-QSAR modeling and molecular docking studies on a series of 2, 4, 5-trisubstituted imidazole derivatives as CK2 inhibitors. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 234-248.	3.5	8
1085	Molecular docking-based computational platform for high-throughput virtual screening. <i>CCF Transactions on High Performance Computing</i> , 2022, 4, 63-74.	1.7	23
1086	Evaluation of sustained-release in-situ injectable gels, containing naproxen sodium, using in vitro, in silico and in vivo analysis. <i>International Journal of Pharmaceutics</i> , 2022, 616, 121512.	5.2	10
1087	Application of Reverse Docking in the Research of Small Molecule Drugs and Traditional Chinese Medicine. <i>Biological and Pharmaceutical Bulletin</i> , 2022, 45, 19-26.	1.4	2
1089	A Review on Parallel Virtual Screening Softwares for High-Performance Computers. <i>Pharmaceutics</i> , 2022, 15, 63.	3.8	34
1090	Bio-chemical characterization and in silico computational experimental properties of <i>Trianthema triquetra</i> Rottler & Willd.: A desert medicinal plant for industrial products. <i>Industrial Crops and Products</i> , 2022, 177, 114474.	5.2	1
1091	PIGNet: a physics-informed deep learning model toward generalized drug-target interaction predictions. <i>Chemical Science</i> , 2022, 13, 3661-3673.	7.4	62
1092	Molecular modeling in drug discovery. <i>Informatics in Medicine Unlocked</i> , 2022, 29, 100880.	3.4	81
1093	Docking Ligands into Flexible and Solvated Macromolecules. 8. Forming New Bonds-Challenges and Opportunities. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1061-1077.	5.4	6
1094	Mechanism of inhibition of α -glucosidase activity by bavachalcone. <i>Food Science and Technology</i> , 0, 42, .	1.7	4
1095	Computational Methods for the Interaction between Cyclodextrins and Natural Compounds: Technology, Benefits, Limitations, and Trends. <i>Journal of Agricultural and Food Chemistry</i> , 2022, 70, 2466-2482.	5.2	18
1096	In-Vitro Catalytic and Antibacterial Potential of Green Synthesized CuO Nanoparticles against Prevalent Multiple Drug Resistant Bovine Mastitogen <i>Staphylococcus aureus</i> . <i>International Journal of Molecular Sciences</i> , 2022, 23, 2335.	4.1	15
1098	Cov_DOX: A Method for Structure Prediction of Covalent Protein-Ligand Bindings. <i>Journal of Medicinal Chemistry</i> , 2022, 65, 5528-5538.	6.4	16
1099	Inspiration for COVID-19 Treatment: Network Analysis and Experimental Validation of Baicalin for Cytokine Storm. <i>Frontiers in Pharmacology</i> , 2022, 13, 853496.	3.5	10
1101	Drug targeting Nsp1-ribosomal complex shows antiviral activity against SARS-CoV-2. <i>ELife</i> , 2022, 11, .	6.0	28

#	ARTICLE	IF	CITATIONS
1102	Evaluation of the binding performance of flavonoids to estrogen receptor alpha by Autodock, Autodock Vina and Surflex-Dock. <i>Ecotoxicology and Environmental Safety</i> , 2022, 233, 113323.	6.0	47
1103	Artificial Intelligence Uncovers Natural MMP Inhibitor Crocin as a Potential Treatment of Thoracic Aortic Aneurysm and Dissection. <i>Frontiers in Cardiovascular Medicine</i> , 2022, 9, 871486.	2.4	3
1104	Leveraging nonstructural data to predict structures and affinities of protein–ligand complexes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2021, 118, .	7.1	17
1105	Potent but transient immunosuppression of T-cells is a general feature of CD71+ erythroid cells. <i>Communications Biology</i> , 2021, 4, 1384.	4.4	12
1106	Identification of Potent and Selective JAK1 Lead Compounds Through Ligand-Based Drug Design Approaches. <i>Frontiers in Pharmacology</i> , 2022, 13, 837369.	3.5	10
1123	Biochemical Investigation of Inhibitory Activities of Plant-Derived Bioactive Compounds Against Carbohydrate and Glucagon-Like Peptide-1 Metabolizing Enzymes. <i>Dose-Response</i> , 2022, 20, 155932582210932.	1.6	9
1124	Design and Prediction of ADME/Tox Properties of Novel Magnolol Derivatives as Anticancer Agents for NSCLC Using 3D-QSAR, Molecular Docking, MOLCAD and MM-GBSA Studies. <i>Letters in Drug Design and Discovery</i> , 2023, 20, 545-569.	0.7	12
1125	Structural Optimization for 4-hydroxyphenylpyruvate Dioxygenase Inhibitors based on 3D-QSAR, Molecular Docking, SBP Modeling and MOLCAD Studies. <i>Letters in Drug Design and Discovery</i> , 2022, 19, .	0.7	0
1126	Decoding the protein–ligand interactions using parallel graph neural networks. <i>Scientific Reports</i> , 2022, 12, 7624.	3.3	15
1127	Coumarin derivatives: biomedical properties and interactions with carrier proteins. <i>Studies in Natural Products Chemistry</i> , 2022, , 173-220.	1.8	2
1128	In Silico Drug Discovery for Treatment of Virus Diseases. <i>Advances in Experimental Medicine and Biology</i> , 2022, 1368, 73-93.	1.6	1
1129	Copper-Catalyzed Oxidative [3 + 2]-Annulation of Quinoxalin-2(1 <i>H</i>)-one with Oxime Esters toward Functionalized Pyrazolo[1,5- <i>a</i>]quinoxalin-4(5 <i>H</i>)-ones as Opioid Receptor Modulators. <i>Journal of Organic Chemistry</i> , 2022, 87, 7350-7364.	3.2	8
1130	Structural insights into the interaction between gabazine (SR-95531) and α 1 and α 2 L α delphax striatellus GABA receptors. <i>Journal of Pesticide Sciences</i> , 2022, 47, .	1.4	0
1131	Development of Simple and Accurate in Silico Ligand-Based Models for Predicting ABCG2 Inhibition. <i>Frontiers in Chemistry</i> , 2022, 10, .	3.6	0
1132	Machine-Learning- and Knowledge-Based Scoring Functions Incorporating Ligand and Protein Fingerprints. <i>ACS Omega</i> , 2022, 7, 19030-19039.	3.5	6
1133	History and Present Scenario of Computers in Pharmaceutical Research and Development. , 2022, , 1-38.		1
1134	Chiral Ru(II)–Pt(II) Complexes Inducing Telomere Dysfunction against Cisplatin-Resistant Cancer Cells. <i>Angewandte Chemie - International Edition</i> , 2022, 61, .	13.8	8
1135	Chiral Ru(II)–Pt(II) Complexes Inducing Telomere Dysfunction against Cisplatin-Resistant Cancer Cells. <i>Angewandte Chemie</i> , 0, , .	2.0	0

#	ARTICLE	IF	CITATIONS
1136	AI-Based Protein Structure Prediction in Drug Discovery: Impacts and Challenges. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 3142-3156.	5.4	36
1137	G-quadruplex stabilizer Tetra-Pt(bpy) disrupts telomere maintenance and impairs FAK-mediated migration of telomerase-positive cells. <i>International Journal of Biological Macromolecules</i> , 2022, 213, 858-870.	7.5	3
1138	Ex vivo, in vitro, and in silico approaches to unveil the mechanisms underlying vasorelaxation effect of <i>Mentha Longifolia</i> (L.) in porcine coronary artery. <i>Biomedicine and Pharmacotherapy</i> , 2022, 153, 113298.	5.6	2
1139	Fundamentals of Molecular Docking and Comparative Analysis of Proteinâ€“Small-Molecule Docking Approaches. , 0, , .		1
1140	Halogenated Flavonoid Derivatives Display Antiangiogenic Activity. <i>Molecules</i> , 2022, 27, 4757.	3.8	3
1141	Atherosclerosis fate in the era of tailored functional foods: Evidence-based guidelines elicited from structure- and ligand-based approaches. <i>Trends in Food Science and Technology</i> , 2022, 128, 75-89.	15.1	11
1142	Phytochemical, biological, and in-silico characterization of <i>Portulacaria afra</i> Jacq.: A possible source of natural products for functional food and medicine. <i>South African Journal of Botany</i> , 2022, 150, 139-145.	2.5	5
1143	Identifying the Antitumor Effects of Curcumin on Lung Adenocarcinoma Using Comprehensive Bioinformatics Analysis. <i>Drug Design, Development and Therapy</i> , 0, Volume 16, 2365-2382.	4.3	4
1144	Viral informatics: bioinformatics-based solution for managing viral infections. <i>Briefings in Bioinformatics</i> , 2022, 23, .	6.5	10
1145	Design, synthesis and computational approach to study novel pyrrole scaffolds as active inhibitors of enoyl ACP reductase (InhA) and <i>Mycobacterium tuberculosis</i> antagonists. <i>Journal of the Indian Chemical Society</i> , 2022, 99, 100674.	2.8	3
1146	Tools and techniques for rational designing of antimicrobial peptides for aquaculture. <i>Fish and Shellfish Immunology</i> , 2022, 127, 1033-1050.	3.6	6
1147	Direct Determination of Pyrethroids in Aqueous Samples by a Metal Organic Framework â€œMIL-101(Cr)â€• Sorbent for Solid-Phase Extraction and Thermal Desorption Coupled with GC-FID. <i>Journal of Analytical Chemistry</i> , 2022, 77, 1047-1056.	0.9	0
1148	Z. officinale-doped silver/calcium oxide nanocomposites: Catalytic activity and antimicrobial potential with molecular docking analysis. <i>Process Biochemistry</i> , 2022, 121, 635-646.	3.7	18
1149	Applications of machine learning in computer-aided drug discovery. <i>QRB Discovery</i> , 2022, 3, .	1.6	5
1150	Druggable sites/pockets of the p53-DNAJA1 proteinâ€“protein interaction: In silico modeling and in vitro/in vivo validation. <i>Methods in Enzymology</i> , 2022, , 83-107.	1.0	0
1155	Molecular Modeling Study of Novel Lancifolamide Bioactive Molecule as an Inhibitor of Acetylcholinesterase (AChE), Herpes Simplex Virus (HSV-1), and Anti-proliferative Proteins. <i>Molecules</i> , 2022, 27, 5480.	3.8	1
1158	Synthesis, herbicidal activity and soil degradation of novel <sc>5â€•substituted</sc> sulfonylureas as <sc>AHAS</sc> inhibitors. <i>Pest Management Science</i> , 2022, 78, 5313-5324.	3.4	1
1159	DENVIS: Scalable and High-Throughput Virtual Screening Using Graph Neural Networks with Atomic and Surface Protein Pocket Features. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 4642-4659.	5.4	7

#	ARTICLE	IF	CITATIONS
1160	Can docking scoring functions guarantee success in virtual screening?. Annual Reports in Medicinal Chemistry, 2022, , .	0.9	1
1161	Free Energy Calculations Using the Movable Type Method with Molecular Dynamics Driven Protein-Ligand Sampling. Journal of Chemical Information and Modeling, 2022, 62, 5645-5665.	5.4	7
1162	Discovery of MAO-B Inhibitor with Machine Learning, Topomer CoMFA, Molecular Docking and Multi-Spectroscopy Approaches. Biomolecules, 2022, 12, 1470.	4.0	3
1163	Quality improvement in <i>Scophthalmus maximus</i> fillets during cold storage by coating with polylactic acid/hesperidin electrospun fiber. LWT - Food Science and Technology, 2022, 170, 114080.	5.2	1
1164	Development of Nucleic Acid Targeting Molecules: Molecular Docking Approaches and Recent Advances. , 0, , .		1
1165	Identification and Analysis of Small Molecule Inhibitors of CRISPR-Cas9 in Human Cells. Cells, 2022, 11, 3574.	4.1	1
1166	CADD, AI and ML in drug discovery: A comprehensive review. European Journal of Pharmaceutical Sciences, 2023, 181, 106324.	4.0	30
1167	Design and Synthesis of Novel Double-Ring Conjugated Enones as Potent Anti-rheumatoid Arthritis Agents. ACS Omega, 0, , .	3.5	3
1168	AutoDock Koto: A Gradient Boosting Differential Evolution for Molecular Docking. IEEE Transactions on Evolutionary Computation, 2023, 27, 1648-1662.	10.0	1
1169	Perceiver CPI: a nested cross-attention network for compound-protein interaction prediction. Bioinformatics, 2023, 39, .	4.1	11
1170	Reverse engineering approach: a step towards a new era of vaccinology with special reference to <i>Salmonella</i> . Expert Review of Vaccines, 2022, 21, 1763-1785.	4.4	5
1171	NlugOBP8 in <i>Nilaparvata lugens</i> Involved in the Perception of Two Terpenoid Compounds from Rice Plant. Journal of Agricultural and Food Chemistry, 2022, 70, 16323-16334.	5.2	7
1172	Molecular Characterization, Purification, and Mode of Action of Enterocin KAE01 from Lactic Acid Bacteria and Its In Silico Analysis against MDR/ESBL <i>Pseudomonas aeruginosa</i> . Genes, 2022, 13, 2333.	2.4	3
1173	Identification of Small Inhibitors for Human Metadherin, an Oncoprotein, through in silico Approach. Current Computer-Aided Drug Design, 2023, 19, 278-287.	1.2	3
1174	Congener-specificity, dioxygenation dependency and association with enzyme binding for biodegradation of polybrominated diphenyl ethers by typical aerobic bacteria: Experimental and theoretical studies. Chemosphere, 2023, 314, 137697.	8.2	0
1175	A Guide to In Silico Drug Design. Pharmaceuticals, 2023, 15, 49.	4.5	22
1176	ViTRMSE: a three-dimensional RMSE scoring method for protein-ligand docking models based on Vision Transformer. , 2022, , .		1
1177	Design of novel anti-cancer drugs targeting TRKs inhibitors based 3D QSAR, molecular docking and molecular dynamics simulation. Journal of Biomolecular Structure and Dynamics, 2023, 41, 11657-11670.	3.5	7

#	ARTICLE	IF	CITATIONS
1178	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. <i>International Journal of Molecular Sciences</i> , 2023, 24, 2027.	4.1	3
1179	MetalProGNet: a structure-based deep graph model for metalloproteinâ€“ligand interaction predictions. <i>Chemical Science</i> , 2023, 14, 2054-2069.	7.4	6
1180	In silico studies of interaction of lantibiotics with virulent proteins. , 2023, , 221-239.		0
1181	A novel molecular docking program based on a multi-swarm competitive algorithm. <i>Swarm and Evolutionary Computation</i> , 2023, 78, 101292.	8.1	5
1182	Insight into the phytochemical, biological, and in silico studies of <i>Erythrina suberosa</i> roxb.: A source of novel therapeutic bioactive products from a medicinal plant. <i>Food Bioscience</i> , 2023, 52, 102429.	4.4	3
1183	Molecular modeling study of pyrrolidine derivatives as novel myeloid cell leukemia-1 inhibitors through combined 3D-QSAR, molecular docking, ADME/Tox and MD simulation techniques. <i>Journal of Biomolecular Structure and Dynamics</i> , 2023, 41, 13798-13814.	3.5	8
1184	Alternative biological screening methods. , 2023, , 95-137.		0
1185	High-efficiency drug design research based on virtual high-throughput screening. , 2023, , .		0
1186	Drug repurposing for viral cancers: A paradigm of machine learning, deep learning, and virtual screeningâ€“based approaches. <i>Journal of Medical Virology</i> , 2023, 95, .	5.0	13
1187	Chemical Profiling and Biological Properties of Essential Oils of <i>Lavandula stoechas</i> L. Collected from Three Moroccan Sites: In Vitro and In Silico Investigations. <i>Plants</i> , 2023, 12, 1413.	3.5	8
1188	Design and Identification of a Novel Antiviral Affinity Peptide against Fowl Adenovirus Serotype 4 (FAdV-4) by Targeting Fiber2 Protein. <i>Viruses</i> , 2023, 15, 821.	3.3	0
1189	Structural investigation of Keap1â€“Nrf2 proteinâ€“protein interaction (PPI) inhibitors for treating myocarditis through molecular simulations. <i>New Journal of Chemistry</i> , 2023, 47, 8524-8537.	2.8	1
1190	Decoding Connectivity Map-based drug repurposing for oncotherapy. <i>Briefings in Bioinformatics</i> , 2023, 24, .	6.5	9
1191	Synthesis, Molecular Docking Study, and Biological Evaluation of New 4-(2,5-Dimethyl-1H-pyrrol-1-yl)-Nâ€“(2-(substituted)acetyl)benzohydrazides as Dual Enoyl ACP Reductase and DHFR Enzyme Inhibitors. <i>Antibiotics</i> , 2023, 12, 763.	3.7	2
1192	Probing the combination of erlotinib hydrochloride, an anticancer drug, and human serum albumin: Spectroscopic, molecular docking, and molecular dynamic analyses. <i>Luminescence</i> , 2023, 38, 772-782.	2.9	7
1193	Benzoic-D5 acid as D2 receptor agonist in the treatment of rotenone induced Parkinsonâ€“s disease in mice. <i>Arabian Journal of Chemistry</i> , 2023, 16, 104982.	4.9	0
1194	A multicentric consortium study demonstrates that dimethylarginine dimethylaminohydrolase 2 is not a dimethylarginine dimethylaminohydrolase. <i>Nature Communications</i> , 2023, 14, .	12.8	6
1195	In Silico Studies of Drug Discovery and Design Against COVID-19 Focusing on ACE2 and Spike Protein Virus Receptors: A Systematic Review. , 2023, 2, 73-78.		0

#	ARTICLE	IF	CITATIONS
1196	Exploring the molecular mechanism of Huangqin-Jinyinhua couplet medicines for the treatment of hand-foot and mouth disease using network pharmacology, molecular docking and bioinformatics databases. , 2023, 1, 106-115.		0
1197	ViTScore: A Novel Three-Dimensional Vision Transformer Method for Accurate Prediction of Protein-Ligand Docking Poses. IEEE Transactions on Nanobioscience, 2023, 22, 734-743.	3.3	1
1198	Combined Metabolite Analysis and Network Pharmacology to Elucidate the Mechanisms of Therapeutic Effect of <i>Melastoma dodecandrum</i> Ellagitannins on Abnormal Uterine Bleeding. Chemistry and Biodiversity, 2023, 20, .	2.1	1
1199	Recent Advances in Computational Modeling of Multi-targeting Inhibitors as Anti-Alzheimer Agents. Neuromethods, 2023, , 231-277.	0.3	0
1201	In silico techniques for screening of key secondary metabolites of medicinal plants. , 2024, , 331-347.		0
1202	To explore the effect of kaempferol on non-small cell lung cancer based on network pharmacology and molecular docking. Frontiers in Pharmacology, 0, 14, .	3.5	1
1203	Theoretical and Experimental Studies on Plant Light-Dependent Protochlorophyllide Oxidoreductase as a Novel Target for Searching Potential Herbicides. Journal of Agricultural and Food Chemistry, 0, , .	5.2	0
1204	How Good Are Current Docking Programs at Nucleic Acid-Ligand Docking? A Comprehensive Evaluation. Journal of Chemical Theory and Computation, 2023, 19, 5633-5647.	5.3	5
1205	A Comprehensive Study on the Binding of Anti-cancer Drug (Floxuridine) with Human Serum Albumin. , 2023, 47, 1155-1167.		1
1206	Applying molecular docking to pesticides. Pest Management Science, 2023, 79, 4140-4152.	3.4	3
1207	Design of Tetra-Peptide Ligands of Antibody Fc Regions Using In Silico Combinatorial Library Screening. Pharmaceuticals, 2023, 16, 1170.	3.8	1
1208	An Updated Review on Developing Small Molecule Kinase Inhibitors Using Computer-Aided Drug Design Approaches. International Journal of Molecular Sciences, 2023, 24, 13953.	4.1	5
1209	Structural Bioinformatics and Artificial Intelligence Approaches in De Novo Drug Design. , 2023, , 44-61.		0
1210	Phospholipases as therapeutic targets: Systems biology and bioinformatics approaches. , 2023, , 359-374.		0
1211	A comprehensive assessment of phytochemicals from <i>Phyllanthus nodiflora</i> (L.) Greene as a potential enzyme inhibitor, and their biological potential: An in-silico, in-vivo, and in-vitro approach. Arabian Journal of Chemistry, 2023, 16, 105233.	4.9	0
1212	Discovering potential inhibitors of the YEATS domain of YEATS2 through virtual screening, molecular optimization and molecular dynamics simulations. New Journal of Chemistry, 2023, 47, 19447-19460.	2.8	1
1213	CurvAGN: Curvature-based Adaptive Graph Neural Networks for Predicting Protein-Ligand Binding Affinity. BMC Bioinformatics, 2023, 24, .	2.6	0
1214	Peptide and protein in vaccine delivery. , 2024, , 217-234.		0

#	ARTICLE	IF	CITATIONS
1215	Tracking the binding site of anticancer drug fluxoridin with Fe-related proteins to achieve intelligent drug delivery. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2024, 306, 123569.	3.9	3
1216	Using biologically synthesized TiO ₂ nanoparticles as potential remedy against multiple drug resistant <i>Staphylococcus aureus</i> of bovine mastitis. <i>Scientific Reports</i> , 2023, 13, .	3.3	0
1217	Integrated Molecular Modeling and Machine Learning for Drug Design. <i>Journal of Chemical Theory and Computation</i> , 2023, 19, 7478-7495.	5.3	5
1218	Polyherbal and Multimodal Treatments: Kaempferol- and Quercetin-Rich Herbs Alleviate Symptoms of Alzheimer's Disease. <i>Biology</i> , 2023, 12, 1453.	2.8	1
1219	Mechanistic insights into the selectivity of bicyclophosphorothionate antagonists for housefly <i>versus</i> rat GABA receptors. <i>Pest Management Science</i> , 2024, 80, 1382-1399.	3.4	0
1220	Anticancer Activity of Medicinal Plants Extract and Molecular Docking Studies. , 2023, , 136-158.		0
1221	FRAGSITE2: A structure and fragment-based approach for virtual ligand screening. <i>Protein Science</i> , 2024, 33, .	7.6	0
1222	Exploring azomethine ylides reactivity with acrolein through cycloaddition reaction and computational antiviral activity assessment against hepatitis C virus. <i>Journal of Molecular Modeling</i> , 2024, 30, .	1.8	1
1223	MulinforCPI: enhancing precision of compound-protein interaction prediction through novel perspectives on multi-level information integration. <i>Briefings in Bioinformatics</i> , 2023, 25, .	6.5	0
1224	Aminopyrimidine Derivatives as Multiflavivirus Antiviral Compounds Identified from a Consensus Virtual Screening Approach. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 393-411.	5.4	0
1225	CLICK-chemoproteomics and molecular dynamics simulation reveals pregnenolone targets and their binding conformations in Th2 cells. <i>Frontiers in Immunology</i> , 0, 14, .	4.8	0
1226	A Review on Molecular Docking As an Interpretative Tool for Molecular Targets in Disease Management. <i>Assay and Drug Development Technologies</i> , 2024, 22, 40-50.	1.2	1
1227	Molecular docking and metagenomics assisted mitigation of microplastic pollution. <i>Chemosphere</i> , 2024, 351, 141271.	8.2	0
1229	Machine Learning Methods as a Cost-Effective Alternative to Physics-Based Binding Free Energy Calculations. <i>Molecules</i> , 2024, 29, 830.	3.8	0
1230	TECHNIQUES AND ALGORITHMS FOR STRUCTURE-BASED VIRTUAL SCREENING (SBVS): AN OVERVIEW. <i>Indian Drugs</i> , 2024, 61, 7-17.	0.1	0
1232	Comprehensive Evaluation of 10 Docking Programs on a Diverse Set of Protein-Cyclic Peptide Complexes. <i>Journal of Chemical Information and Modeling</i> , 2024, 64, 2112-2124.	5.4	0
1233	Computational Tools in Drug-Lead Identification and Development. , 2024, , 89-119.		0
1234	Assessing the performance of MM/PBSA and MM/GBSA methods. 10. Prediction reliability of binding affinities and binding poses for RNA-ligand complexes. <i>Physical Chemistry Chemical Physics</i> , 2024, 26, 10323-10335.	2.8	0