Ruben Abagyan

List of Publications by Year
in descending order

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163	12,247	41323	28275
papers	citations	49 h-index	105 g-index

179	179	179	14227
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	ICM?A new method for protein modeling and design: Applications to docking and structure prediction from the distorted native conformation. Journal of Computational Chemistry, 1994, 15, 488-506.	1.5	1,502
2	Biased Probability Monte Carlo Conformational Searches and Electrostatic Calculations for Peptides and Proteins. Journal of Molecular Biology, 1994, 235, 983-1002.	2.0	901
3	Virtual Ligand Screening of the p300/CBP Histone Acetyltransferase: Identification of a Selective Small Molecule Inhibitor. Chemistry and Biology, 2010, 17, 471-482.	6.2	538
4	Flexible ligand docking to multiple receptor conformations: a practical alternative. Current Opinion in Structural Biology, 2008, 18, 178-184.	2.6	456
5	Methods of Protein Structure Comparison. Methods in Molecular Biology, 2011, 857, 231-257.	0.4	378
6	Lanosterol reverses protein aggregation in cataracts. Nature, 2015, 523, 607-611.	13.7	351
7	Pocketome via Comprehensive Identification and Classification of Ligand Binding Envelopes. Molecular and Cellular Proteomics, 2005, 4, 752-761.	2.5	350
8	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	1.5	334
9	Crystal structure of the chemokine receptor CXCR4 in complex with a viral chemokine. Science, 2015, 347, 1117-1122.	6.0	325
10	Docking and scoring with ICM: the benchmarking results and strategies for improvement. Journal of Computer-Aided Molecular Design, 2012, 26, 675-686.	1.3	290
11	Status of GPCR Modeling and Docking as Reflected by Community-wide GPCR Dock 2010 Assessment. Structure, 2011, 19, 1108-1126.	1.6	269
12	Structure-Based Discovery of Novel Chemotypes for Adenosine A_{2A} Receptor Antagonists. Journal of Medicinal Chemistry, 2010, 53, 1799-1809.	2.9	231
13	Structure of CC chemokine receptor 2 with orthosteric and allosteric antagonists. Nature, 2016, 540, 458-461.	13.7	220
14	Optimal docking area: A new method for predicting protein-protein interaction sites. Proteins: Structure, Function and Bioinformatics, 2004, 58, 134-143.	1.5	185
15	ICM-DISCO docking by global energy optimization with fully flexible side-chains. Proteins: Structure, Function and Bioinformatics, 2003, 52, 113-117.	1.5	183
16	Four-Dimensional Docking: A Fast and Accurate Account of Discrete Receptor Flexibility in Ligand Docking. Journal of Medicinal Chemistry, 2009, 52, 397-406.	2.9	172
17	Nuclear Hormone Receptor Targeted Virtual Screening. Journal of Medicinal Chemistry, 2003, 46, 3045-3059.	2.9	170
18	Discovery of diverse thyroid hormone receptor antagonists by high-throughput docking. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 7354-7359.	3.3	170

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19	Type-II Kinase Inhibitor Docking, Screening, and Profiling Using Modified Structures of Active Kinase States. Journal of Medicinal Chemistry, 2008, 51, 7921-7932.	2.9	162
20	Pocketome: an encyclopedia of small-molecule binding sites in 4D. Nucleic Acids Research, 2012, 40, D535-D540.	6.5	149
21	Advances in GPCR Modeling Evaluated by the GPCR Dock 2013 Assessment: Meeting New Challenges. Structure, 2014, 22, 1120-1139.	1.6	149
22	Structure of CC Chemokine Receptor 5 with a Potent Chemokine Antagonist Reveals Mechanisms of Chemokine Recognition and Molecular Mimicry by HIV. Immunity, 2017, 46, 1005-1017.e5.	6.6	148
23	Prediction of the binding energy for small molecules, peptides and proteins. Journal of Molecular Recognition, 1999, 12, 177-190.	1.1	146
24	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	1.5	139
25	Detailed ab initio prediction of lysozymeâ€“antibody complex with 1.6 Ã... accuracy. Nature Structural and Molecular Biology, 1994, 1, 259-263.	3.6	123
26	Adverse Effects of Cholinesterase Inhibitors in Dementia, According to the Pharmacovigilance Databases of the United-States and Canada. PLoS ONE, 2015, 10, e0144337.	1.1	119
27	An electrostatic mechanism for Ca2+-mediated regulation of gap junction channels. Nature Communications, 2016, 7, 8770.	5.8	119
28	Rapid boundary element solvation electrostatics calculations in folding simulations: Successful folding of a 23-residue peptide. Biopolymers, 2001, 60, 124-133.	1.2	115
29	Analysis of full and partial agonists binding to Î²₂â€adrenergic receptor suggests a role of transmembrane helix V in agonistâ€specific conformational changes. Journal of Molecular Recognition, 2009, 22, 307-318.	1.1	113
30	Structural model of nicotinic acetylcholine receptor isotypes bound to acetylcholine and nicotine. BMC Structural Biology, 2002, 2, 1.	2.3	103
31	A receptor-like protein mediates plant immune responses to herbivore-associated molecular patterns. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 31510-31518.	3.3	86
32	Towards a structural understanding of allosteric drugs at the human calcium-sensing receptor. Cell Research, 2016, 26, 574-592.	5.7	85
33	Structural basis of ligand interaction with atypical chemokine receptor 3. Nature Communications, 2017, 8, 14135.	5.8	83
34	Systematic Exploitation of Multiple Receptor Conformations for Virtual Ligand Screening. PLoS ONE, 2011, 6, e18845.	1.1	82
35	Rational Design of Berberine-Based FtsZ Inhibitors with Broad-Spectrum Antibacterial Activity. PLoS ONE, 2014, 9, e97514.	1.1	82
36	Structure based prediction of subtype-selectivity for adenosine receptor antagonists. Neuropharmacology, 2011, 60, 108-115.	2.0	81

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37	SIRT2- and NRF2-Targeting Thiazole-Containing Compound with Therapeutic Activity in Huntington's Disease Models. Cell Chemical Biology, 2016, 23, 849-861.	2.5	71
38	Stoichiometry and geometry of the CXC chemokine receptor 4 complex with CXC ligand 12: Molecular modeling and experimental validation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E5363-72.	3.3	70
39	Identifying ligands at orphan GPCRs: current status using structureâ€based approaches. British Journal of Pharmacology, 2016, 173, 2934-2951.	2.7	70
40	The anthelmintic praziquantel is a human serotoninergic G-protein-coupled receptor ligand. Nature Communications, 2017, 8, 1910.	5.8	66
41	Identification of a New Class of FtsZ Inhibitors by Structure-Based Design and in Vitro Screening. Journal of Chemical Information and Modeling, 2013, 53, 2131-2140.	2.5	65
42	Molecular Properties of Drugs Interacting with SLC22 Transporters OAT1, OAT3, OCT1, and OCT2: A Machine-Learning Approach. Journal of Pharmacology and Experimental Therapeutics, 2016, 359, 215-229.	1.3	60
43	X-ray structures of thioredoxin and thioredoxin reductase from Entamoeba histolytica and prevailing hypothesis of the mechanism of Auranofin action. Journal of Structural Biology, 2016, 194, 180-190.	1.3	60
44	Improved docking, screening and selectivity prediction for small molecule nuclear receptor modulators using conformational ensembles. Journal of Computer-Aided Molecular Design, 2010, 24, 459-471.	1.3	59
45	Recognition of distantly related proteins through energy calculations. Proteins: Structure, Function and Bioinformatics, 1994, 19, 132-140.	1.5	58
46	Homology modeling with internal coordinate mechanics: Deformation zone mapping and improvements of models via conformational search. Proteins: Structure, Function and Bioinformatics, 1997, 29, 29-37.	1.5	58
47	GPCR agonist binding revealed by modeling and crystallography. Trends in Pharmacological Sciences, 2011, 32, 637-643.	4.0	56
48	The Flexible Pocketome Engine for Structural Chemogenomics. Methods in Molecular Biology, 2009, 575, 249-279.	0.4	55
49	Structural basis for activation of trimeric Gi proteins by multiple growth factor receptors via GIV/Girdin. Molecular Biology of the Cell, 2014, 25, 3654-3671.	0.9	54
50	The Pthaladyns: GTP Competitive Inhibitors of Dynamin I and II GTPase Derived from Virtual Screening. Journal of Medicinal Chemistry, 2010, 53, 5267-5280.	2.9	50
51	Analysis of postmarketing safety data for proton-pump inhibitors reveals increased propensity for renal injury, electrolyte abnormalities, and nephrolithiasis. Scientific Reports, 2019, 9, 2282.	1.6	48
52	In silico discovery of novel retinoic acid receptor agonist structures. BMC Structural Biology, 2001, 1, 1.	2.3	47
53	Discovery of novel membrane binding structures and functions. Biochemistry and Cell Biology, 2014, 92, 555-563.	0.9	46
54	Activation of GÎ±i at the Golgi by GIV/Girdin Imposes Finiteness in Arf1 Signaling. Developmental Cell, 2015, 33, 189-203.	3.1	46

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55	CYP51 is an essential drug target for the treatment of primary amoebic meningoencephalitis (PAM). PLoS Neglected Tropical Diseases, 2017, 11, e0006104.	1.3	45
56	Systems Biology Analysis Reveals Eight SLC22 Transporter Subgroups, Including OATs, OCTs, and OCTNs. International Journal of Molecular Sciences, 2020, 21, 1791.	1.8	44
57	Flexible proteinâ€“ligand docking by global energy optimization in internal coordinates. Proteins: Structure, Function and Bioinformatics, 1997, 29, 215-220.	1.5	44
58	Disseminating structural genomics data to the public: from a data dump to an animated story. Trends in Biochemical Sciences, 2006, 31, 76-78.	3.7	42
59	Compound Activity Prediction Using Models of Binding Pockets or Ligand Properties in 3D. Current Topics in Medicinal Chemistry, 2012, 12, 1869-1882.	1.0	42
60	ALiBERO: Evolving a Team of Complementary Pocket Conformations Rather than a Single Leader. Journal of Chemical Information and Modeling, 2012, 52, 2705-2714.	2.5	42
61	Membrane and Protein Interactions of the Pleckstrin Homology Domain Superfamily. Membranes, 2015, 5, 646-663.	1.4	42
62	Proton-pump inhibitor use is associated with a broad spectrum of neurological adverse events including impaired hearing, vision, and memory. Scientific Reports, 2019, 9, 17280.	1.6	42
63	Recommendations for Improving Methods and Models for Aquatic Hazard Assessment of Ionizable Organic Chemicals. Environmental Toxicology and Chemistry, 2020, 39, 269-286.	2.2	42
64	Ligand-Guided Receptor Optimization. Methods in Molecular Biology, 2011, 857, 189-205.	0.4	41
65	Homology modeling with internal coordinate mechanics: Deformation zone mapping and improvements of models via conformational search. Proteins: Structure, Function and Bioinformatics, 1997, 29, 29-37.	1.5	40
66	A new method for modeling large-scale rearrangements of protein domains. , 1997, 27, 410-424.		39
67	An Organic Anion Transporter 1 (OAT1)-centered Metabolic Network. Journal of Biological Chemistry, 2016, 291, 19474-19486.	1.6	39
68	Ligand-biased ensemble receptor docking (LigBEnD): a hybrid ligand/receptor structure-based approach. Journal of Computer-Aided Molecular Design, 2018, 32, 187-198.	1.3	39
69	Unique metabolite preferences of the drug transporters OAT1 and OAT3 analyzed by machine learning. Journal of Biological Chemistry, 2020, 295, 1829-1842.	1.6	39
70	A New Method for Publishing Three-Dimensional Content. PLoS ONE, 2009, 4, e7394.	1.1	37
71	Lapatinib-Binding Protein Kinases in the African Trypanosome: Identification of Cellular Targets for Kinase-Directed Chemical Scaffolds. PLoS ONE, 2013, 8, e56150.	1.1	36
72	In Silico Identification and Pharmacological Evaluation of Novel Endocrine Disrupting Chemicals That Act via the Ligand-Binding Domain of theÂEstrogen Receptor Î±. Toxicological Sciences, 2014, 141, 188-197.	1.4	36

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73	A Thiazole Orange Derivative Targeting the Bacterial Protein FtsZ Shows Potent Antibacterial Activity. Frontiers in Microbiology, 2017, 8, 855.	1.5	36
74	Phenotypic, chemical and functional characterization of cyclic nucleotide phosphodiesterase 4 (PDE4) as a potential anthelmintic drug target. PLoS Neglected Tropical Diseases, 2017, 11, e0005680.	1.3	36
75	Structure-Based Predictions of Activity Cliffs. Journal of Chemical Information and Modeling, 2015, 55, 1062-1076.	2.5	34
76	Retrospective analysis reveals significant association of hypoglycemia with tramadol and methadone in contrast to other opioids. Scientific Reports, 2019, 9, 12490.	1.6	34
77	High-quality and universal empirical atomic charges for chemoinformatics applications. Journal of Cheminformatics, 2015, 7, 59.	2.8	32
78	Hedgehog pathway and smoothened inhibitors in cancer therapies. Anti-Cancer Drugs, 2018, 29, 387-401.	0.7	31
79	Flipping states: a few key residues decide the winning conformation of the only universally conserved transcription factor. Nucleic Acids Research, 2017, 45, 8835-8843.	6.5	28
80	2-Aminothiazole Derivatives as Selective Allosteric Modulators of the Protein Kinase CK2. 1. Identification of an Allosteric Binding Site. Journal of Medicinal Chemistry, 2019, 62, 1803-1816.	2.9	25
81	Crosslinking-guided geometry of a complete CXC receptor-chemokine complex and the basis of chemokine subfamily selectivity. PLoS Biology, 2020, 18, e3000656.	2.6	24
82	Myocarditis occurrence with cancer immunotherapy across indications in clinical trial and post-marketing data. Scientific Reports, 2021, 11, 17324.	1.6	24
83	From Homology Models to a Set of Predictive Binding Pocketsâ€“a 5-HT_{1A} Receptor Case Study. Journal of Chemical Information and Modeling, 2017, 57, 311-321.	2.5	23
84	Population scale data reveals the antidepressant effects of ketamine and other therapeutics approved for non-psychiatric indications. Scientific Reports, 2017, 7, 1450.	1.6	23
85	Elucidation of transient protein-protein interactions within carrier protein-dependent biosynthesis. Communications Biology, 2021, 4, 340.	2.0	23
86	New Method for the Assessment of All Drug-Like Pockets Across a Structural Genome. Journal of Computational Biology, 2008, 15, 231-240.	0.8	21
87	Secretin Occupies a Single Protomer of the Homodimeric Secretin Receptor Complex. Journal of Biological Chemistry, 2010, 285, 9919-9931.	1.6	21
88	A General Method for Site Specific Fluorescent Labeling of Recombinant Chemokines. PLoS ONE, 2014, 9, e81454.	1.1	21
89	Environmental Photochemistry of Altrenogest: Photoisomerization to a Bioactive Product with Increased Environmental Persistence via Reversible Photohydration. Environmental Science & Technology, 2016, 50, 7480-7488.	4.6	21
90	Differential activities of maize plant elicitor peptides as mediators of immune signaling and herbivore resistance. Plant Journal, 2020, 104, 1582-1602.	2.8	21

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91	Revisiting Antipsychotic Drug Actions Through Gene Networks Associated With Schizophrenia. American Journal of Psychiatry, 2018, 175, 674-682.	4.0	20
92	Population scale retrospective analysis reveals distinctive antidepressant and anxiolytic effects of diclofenac, ketoprofen and naproxen in patients with pain. PLoS ONE, 2018, 13, e0195521.	1.1	20
93	Multi-center screening of the Pathogen Box collection for schistosomiasis drug discovery. Parasites and Vectors, 2019, 12, 493.	1.0	20
94	Identification of new benzamide inhibitor against Î±-subunit of tryptophan synthase from Mycobacterium tuberculosis through structure-based virtual screening, anti-tuberculosis activity and molecular dynamics simulations. Journal of Biomolecular Structure and Dynamics, 2019, 37, 1043-1053.	2.0	20
95	Molecular Basis for Benzodiazepine Agonist Action at the Type 1 Cholecystokinin Receptor. Journal of Biological Chemistry, 2013, 288, 21082-21095.	1.6	19
96	Structureâ€based Design, Synthesis, and Biological Evaluation of Isatin Derivatives as Potential Glycosyltransferase Inhibitors. Chemical Biology and Drug Design, 2014, 84, 685-696.	1.5	19
97	Discovery of New Inhibitors of Hepatitis C Virus NS3/4A Protease and Its D168A Mutant. ACS Omega, 2019, 4, 16999-17008.	1.6	19
98	Concomitant drugs associated with increased mortality for MDMA users reported in a drug safety surveillance database. Scientific Reports, 2021, 11, 5997.	1.6	19
99	Shared Ligands Between Organic Anion Transporters (OAT1 and OAT6) and Odorant Receptors. Drug Metabolism and Disposition, 2015, 43, 1855-1863.	1.7	18
100	Discovery of holoenzyme-disrupting chemicals as substrate-selective CK2 inhibitors. Scientific Reports, 2019, 9, 15893.	1.6	18
101	Postmarketing safety surveillance data reveals antidepressant effects of botulinum toxin across various indications and injection sites. Scientific Reports, 2020, 10, 12851.	1.6	18
102	Common osteoporosis drug associated with increased rates of depression and anxiety. Scientific Reports, 2021, 11, 23956.	1.6	18
103	2-Aminothiazole Derivatives as Selective Allosteric Modulators of the Protein Kinase CK2. 2. Structure-Based Optimization and Investigation of Effects Specific to the Allosteric Mode of Action. Journal of Medicinal Chemistry, 2019, 62, 1817-1836.	2.9	17
104	Extended Multitarget Pharmacology of Anticancer Drugs. Journal of Chemical Information and Modeling, 2019, 59, 3006-3017.	2.5	17
105	Hybrid receptor structure/ligand-based docking and activity prediction in ICM: development and evaluation in D3R Grand Challenge 3. Journal of Computer-Aided Molecular Design, 2019, 33, 35-46.	1.3	16
106	Biomimetic Membrane-Structured Nanovesicles Carrying a Supramolecular Enzyme to Cure Lung Cancer. ACS Applied Materials & Interfaces, 2020, 12, 31112-31123.	4.0	16
107	Docking to multiple pockets or ligand fields for screening, activity prediction and scaffold hopping. Future Medicinal Chemistry, 2014, 6, 1741-1755.	1.1	15
108	Molecular Mechanism of Action of Triazolobenzodiazepinone Agonists of the Type 1 Cholecystokinin Receptor. Possible Cooperativity across the Receptor Homodimeric Complex. Journal of Medicinal Chemistry, 2015, 58, 9562-9577.	2.9	15

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109	Protein-RNA Docking Using ICM. Journal of Chemical Theory and Computation, 2018, 14, 4971-4984.	2.3	15
110	Quantum mechanics approaches to drug research in the era of structural chemogenomics. International Journal of Quantum Chemistry, 2013, 113, 1669-1675.	1.0	14
111	Cardiac adverse events associated with chloroquine and hydroxychloroquine exposure in 20Âyears of drug safety surveillance reports. Scientific Reports, 2020, 10, 19199.	1.6	14
112	Biomimetic polysaccharide-cloaked lipidic nanovesicles/microassemblies for improving the enzymatic activity and prolonging the action time for hyperuricemia treatment. Nanoscale, 2020, 12, 15222-15235.	2.8	14
113	PeptiSite: A structural database of peptide binding sites in 4D. Biochemical and Biophysical Research Communications, 2014, 445, 717-723.	1.0	13
114	Multi-targeting Drug Community Challenge. Cell Chemical Biology, 2017, 24, 1434-1435.	2.5	13
115	HMG-CoA Reductase Inhibitors as Drug Leads against Naegleria fowleri. ACS Chemical Neuroscience, 2020, 11, 3089-3096.	1.7	13
116	Cytomembrane-mimicking nanocarriers with a scaffold consisting of a CD44-targeted endogenous component for effective asparaginase supramolecule delivery. Nanoscale, 2020, 12, 12083-12097.	2.8	13
117	Postmarketing safety surveillance data reveals protective effects of botulinum toxin injections against incident anxiety. Scientific Reports, 2021, 11, 24173.	1.6	13
118	SimiCon: a web tool for proteinâ€“ligand model comparison through calculation of equivalent atomic contacts. Bioinformatics, 2010, 26, 2784-2785.	1.8	12
119	Synthesis, Optimization, Antifungal Activity, Selectivity, and CYP51 Binding of New 2-Aryl-3-azolyl-1-indolyl-propan-2-ols. Pharmaceuticals, 2020, 13, 186.	1.7	12
120	Molecular Properties of Drugs Handled by Kidney OATs and Liver OATPs Revealed by Chemoinformatics and Machine Learning: Implications for Kidney and Liver Disease. Pharmaceutics, 2021, 13, 1720.	2.0	12
121	Efficient parallelization of the energy, surface, and derivative calculations for internal coordinate mechanics. Journal of Computational Chemistry, 1994, 15, 1105-1112.	1.5	11
122	Conformational Heterogeneity of Unbound Proteins Enhances Recognition in Proteinâ€“Protein Encounters. Journal of Chemical Theory and Computation, 2016, 12, 3236-3249.	2.3	11
123	In silico discovery of small molecules that inhibit RfaH recruitment to RNA polymerase. Molecular Microbiology, 2018, 110, 128-142.	1.2	11
124	Experiment-Guided Molecular Modeling of Proteinâ€“Protein Complexes Involving GPCRs. Methods in Molecular Biology, 2015, 1335, 295-311.	0.4	11
125	ARN25068, a versatile starting point towards triple GSK-3Î²/FYN/DYRK1A inhibitors to tackle tau-related neurological disorders. European Journal of Medicinal Chemistry, 2022, 229, 114054.	2.6	11
126	Development of a Highly Selective Allosteric Antagonist Radioligand for the Type 1 Cholecystokinin Receptor and Elucidation of Its Molecular Basis of Binding. Molecular Pharmacology, 2015, 87, 130-140.	1.0	10

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127	How Does the Methodology of 3D Structure Preparation Influence the Quality of pK_a Prediction?. Journal of Chemical Information and Modeling, 2015, 55, 1088-1097.	2.5	10
128	Transcriptome and binding data indicate that citral inhibits single strand DNAâ€binding proteins. Physiologia Plantarum, 2020, 169, 99-109.	2.6	10
129	Antineoplastic kinase inhibitors: A new class of potent anti-amoebic compounds. PLoS Neglected Tropical Diseases, 2021, 15, e0008425.	1.3	10
130	Use of Cysteine Trapping to Map Spatial Approximations between Residues Contributing to the Helix N-capping Motif of Secretin and Distinct Residues within Each of the Extracellular Loops of Its Receptor. Journal of Biological Chemistry, 2016, 291, 5172-5184.	1.6	9
131	Mapping the gene network landscape of Alzheimerâ€™s disease through integrating genomics and transcriptomics. PLoS Computational Biology, 2022, 18, e1009903.	1.5	9
132	BioSuper: A web tool for the superimposition of biomolecules and assemblies with rotational symmetry. BMC Structural Biology, 2013, 13, 32.	2.3	8
133	Macrocycle modeling in ICM: benchmarking and evaluation in D3R Grand Challenge 4. Journal of Computer-Aided Molecular Design, 2019, 33, 1057-1069.	1.3	8
134	Structure based design and synthesis of novel Toll-like Receptor 2 (TLR 2) lipid antagonists. Bioorganic and Medicinal Chemistry Letters, 2021, 40, 127861.	1.0	7
135	Crowdsourced identification of multi-target kinase inhibitors for RET- and TAU- based disease: The Multi-Targeting Drug DREAM Challenge. PLoS Computational Biology, 2021, 17, e1009302.	1.5	7
136	Retrospective analysis of clinical trial safety data for pembrolizumab reveals the effect of co-occurring infections on immune-related adverse events. PLoS ONE, 2022, 17, e0263402.	1.1	7
137	Interactive JIMD articles using the iSee concept: turning a new page on structural biology data. Journal of Inherited Metabolic Disease, 2011, 34, 565-567.	1.7	6
138	Computational chemistry in 25Âyears. Journal of Computer-Aided Molecular Design, 2012, 26, 9-10.	1.3	6
139	All-Atom Internal Coordinate Mechanics (ICM) Force Field for Hexopyranoses and Glycoproteins. Journal of Chemical Theory and Computation, 2015, 11, 2167-2186.	2.3	6
140	Inhibition of PDE5A1 guanosine cyclic monophosphate (cGMP) hydrolysing activity by sildenafil analogues that inhibit cellular cGMP efflux. Journal of Pharmacy and Pharmacology, 2017, 69, 675-683.	1.2	6
141	Identification of Four Amoebicidal Nontoxic Compounds by a Molecular Docking Screen of Naegleria fowleri Sterol Î”8â†’Î”7-Isomerase and Phenotypic Assays. ACS Infectious Diseases, 2019, 5, 2029-2038.	1.8	6
142	Population Scale Retrospective Analysis Reveals Potential Risk of Cholestasis in Pregnant Women Taking Omeprazole, Lansoprazole, and Amoxicillin. Interdisciplinary Sciences, Computational Life Sciences, 2019, 11, 273-281.	2.2	6
143	Proteinâ€“protein interaction based substrate control in the E. coli octanoic acid transferase, LipB. RSC Chemical Biology, 2021, 2, 1466-1473.	2.0	6
144	How can proton pump inhibitors damage central and peripheral nervous systems?. Neural Regeneration Research, 2020, 15, 2041.	1.6	6

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145	Reported Cases of Serotonin Syndrome in MDMA Users in FAERS Database. Frontiers in Psychiatry, 2021, 12, 824288.	1.3	6
146	Dexamethasone and Fludrocortisone Inhibit Hedgehog Signaling in Embryonic Cells. ACS Omega, 2018, 3, 12019-12025.	1.6	5
147	Mtor inhibitors associated with higher cardiovascular adverse eventsâ€"A large population database analysis. Clinical Transplantation, 2021, 35, e14228.	0.8	5
148	Analysis of drug binding pockets and repurposing opportunities for twelve essential enzymes of ESKAPE pathogens. PeerJ, 2017, 5, e3765.	0.9	5
149	Discovery of Triple Inhibitors of Both SARS-CoV-2 Proteases and Human Cathepsin L. Pharmaceuticals, 2022, 15, 744.	1.7	5
150	Histidine7.36(305) in the conserved peptide receptor activation domain of the gonadotropin releasing hormone receptor couples peptide binding and receptor activation. Molecular and Cellular Endocrinology, 2015, 402, 95-106.	1.6	4
151	Nilotinib, an approved leukemia drug, inhibits smoothened signaling in Hedgehog-dependent medulloblastoma. PLoS ONE, 2019, 14, e0214901.	1.1	4
152	SCREENED CHARGE ELECTROSTATIC MODEL IN PROTEIN-PROTEIN DOCKING SIMULATIONS. , 2001, , .		4
153	Druggable exosites of the human kino-pocketome. Journal of Computer-Aided Molecular Design, 2020, 34, 219-230.	1.3	2
154	Biomimetic microbioreactor-supramolecular nanovesicles improve enzyme therapy of hepatic cancer. Nanomedicine: Nanotechnology, Biology, and Medicine, 2021, 31, 102311.	1.7	2
155	Control of Unsaturation in De Novo Fatty Acid Biosynthesis by FabA. Biochemistry, 2022, 61, 608-615.	1.2	2
156	Role of 3D Structures in Understanding, Predicting, and Designing Molecular Interactions in the Chemokine Receptor Family. Topics in Medicinal Chemistry, 2014, , 41-85.	0.4	1
157	Prediction of the binding energy for small molecules, peptides and proteins. , 1999, 12, 177.		1
158	Title is missing!. , 2020, 18, e3000656.		0
159	Title is missing!. , 2020, 18, e3000656.		0
160	Title is missing!. , 2020, 18, e3000656.		0
161	Title is missing!. , 2020, 18, e3000656.		0
162	Title is missing!. , 2020, 18, e3000656.		0

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163	Title is missing!. , 2020, 18, e3000656.		0