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List of Publications by Year in descending order

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37
papers

729
citations

623734

14
h-index

580821

25
g-index

38
all docs

38
docs citations

38
times ranked

1010
citing authors

#	ARTICLE	IF	CITATIONS
1	Oral IDN-6556, an antiapoptotic caspase inhibitor, may lower aminotransferase activity in patients with chronic hepatitis C. <i>Hepatology</i> , 2007, 46, 324-329.	7.3	177
2	Correlating hydration shell structure with amino acid hydrophobicity. <i>Journal of the American Chemical Society</i> , 1993, 115, 3336-3337.	13.7	77
3	CUREs in biochemistry—where we are and where we should go. <i>Biochemistry and Molecular Biology Education</i> , 2017, 45, 7-12.	1.2	52
4	Exploiting Atropisomerism to Increase the Target Selectivity of Kinase Inhibitors. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 11754-11759.	13.8	51
5	Computational Intelligence Methods for Docking Scores. <i>Current Computer-Aided Drug Design</i> , 2009, 5, 56-68.	1.2	33
6	A Novel <i>In Silico</i> Approach to Drug Discovery via Computational Intelligence. <i>Journal of Chemical Information and Modeling</i> , 2009, 49, 1105-1121.	5.4	32
7	QSAR using evolved neural networks for the inhibition of mutant PfDHFR by pyrimethamine derivatives. <i>BioSystems</i> , 2008, 92, 10-15.	2.0	31
8	Modeling the structural origins of drug resistance to isoniazid via key mutations in <i>Mycobacterium tuberculosis</i> catalase-peroxidase, KatG. <i>Tuberculosis</i> , 2018, 108, 155-162.	1.9	26
9	Defining hydrophobicity: probing the structure of solute-induced hydration shells by Fourier transform infrared spectroscopy. <i>Journal of the American Chemical Society</i> , 1992, 114, 4336-4339.	13.7	25
10	High-Throughput Ligand Screening via Preclustering and Evolved Neural Networks. <i>IEEE/ACM Transactions on Computational Biology and Bioinformatics</i> , 2007, 4, 476-484.	3.0	20
11	Modeling the inhibition of quadruple mutant <i>Plasmodium falciparum</i> dihydrofolate reductase by pyrimethamine derivatives. <i>Journal of Computer-Aided Molecular Design</i> , 2008, 22, 29-38.	2.9	20
12	In silico screening against wild-type and mutant <i>Plasmodium falciparum</i> dihydrofolate reductase. <i>Journal of Molecular Graphics and Modelling</i> , 2008, 26, 1145-1152.	2.4	20
13	Applications of machine learning and computational intelligence to drug discovery and development. <i>Drug Development Research</i> , 2011, 72, 53-65.	2.9	19
14	Structural-based analysis of dihydrofolate reductase evolution. <i>Molecular Phylogenetics and Evolution</i> , 2011, 61, 212-230.	2.7	14
15	The Preorganization of Atropisomers to Increase Target Selectivity. <i>Synlett</i> , 2016, 27, 977-983.	1.8	11
16	USING SCDL FOR INTEGRATING TOOLS AND DATA FOR COMPLEX BIOMEDICAL APPLICATIONS. <i>International Journal of Semantic Computing</i> , 2008, 02, 291-308.	0.5	10
17	Activity of Selected Nucleoside Analogue ProTides against Zika Virus in Human Neural Stem Cells. <i>Viruses</i> , 2019, 11, 365.	3.3	10
18	On the relationship between GC content and the number of predicted microRNA binding sites by MicroInspector. <i>Computational Biology and Chemistry</i> , 2008, 32, 222-226.	2.3	9

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19	Modeling the evolution of drug resistance in malaria. <i>Journal of Computer-Aided Molecular Design</i> , 2012, 26, 1343-1353.	2.9	9
20	Quantitative structure-property relationships for drug solubility prediction using evolved neural networks. , 2008, , .		7
21	Cefoxitin is both an inhibitor of class A beta-lactamase of <i>Xanthomonas campestris</i> pv. <i>campestris</i> str. 17 and an inducer of its gene. <i>Research in Microbiology</i> , 2012, 163, 550-556.	2.1	6
22	The novel protein homeostatic modulator BTX306 is active in myeloma and overcomes bortezomib and lenalidomide resistance. <i>Journal of Molecular Medicine</i> , 2020, 98, 1161-1173.	3.9	6
23	Docking scores and QSAR using evolved neural networks for the Pan-inhibition of wild-type and mutant PfDHFR by cycloguanil derivatives. , 2009, , .		5
24	Discovery of cyclic guanidine-linked sulfonamides as inhibitors of LMTK3 kinase. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 127108.	2.2	5
25	Machine learning approaches for customized docking scores: Modeling of inhibition of <i>Mycobacterium tuberculosis</i> enoyl acyl carrier protein reductase. , 2010, , .		4
26	Semantic Computing and Drug Discovery - A Preliminary Report. , 2013, , .		4
27	Enhancing the selectivity of kinase inhibitors in oncology: a chemical biology perspective. <i>Future Medicinal Chemistry</i> , 2016, 8, 241-244.	2.3	4
28	Structure-based analysis of Bacilli and plasmid dihydrofolate reductase evolution. <i>Journal of Molecular Graphics and Modelling</i> , 2017, 71, 135-153.	2.4	3
29	Towards predictive structure-based models of evolved drug resistance. , 2012, , .		2
30	BioSemantic System: Applications of Structured Natural Language to Biological and Biochemical Research. , 2008, , .		1
31	SCDL Applications to Drug Discovery. , 2009, , .		1
32	Molecular Modeling Studies of AmpR Mediated AmpC ß-Lactamase Repression. , 2011, , .		1
33	Describing Dynamic Biological Systems in SPDL and SCDL. , 2009, , .		0
34	BioFactory: Semantic Integration of Biomedical Data and Applications. , 2012, , .		0
35	Modeling the evolution of drug resistance in <i>Plasmodium falciparum</i> DHFR. , 2013, , .		0
36	Structure-based design of guanosine analogue inhibitors targeting GTP cyclohydrolase IB towards a new class of antibiotics. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2020, 30, 126818.	2.2	0

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37	Syntheses and Binding Testing of N1-Alkylamino-Substituted 2-Aminobenzimidazole Analogues Targeting the Hepatitis C Virus Internal Ribosome Entry Site. Australian Journal of Chemistry, 2020, 73, 212.	0.9	0