

Rafael Andrade Caceres

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

37
papers

693
citations

15
h-index

25
g-index

37
ext. papers

791
ext. citations

3.2
avg, IF

3.7
L-index

#	Paper	IF	Citations
37	Understanding the role of mTOR-mLst8 binding through coarse-grained simulation approaches. <i>Molecular Simulation</i> , 2021 , 47, 1198-1207	2	
36	Geo-Measures: A PyMOL plugin for protein structure ensembles analysis. <i>Computational Biology and Chemistry</i> , 2020 , 87, 107322	3.6	20
35	Searching for potential mTOR inhibitors: Ligand-based drug design, docking and molecular dynamics studies of rapamycin binding site. <i>Journal of Molecular Graphics and Modelling</i> , 2018 , 80, 251-263 ⁸	2.8	9
34	Prion protein conversion triggered by acidic condition: a molecular dynamics study through different force fields. <i>Journal of Computational Chemistry</i> , 2018 , 39, 2000-2011	3.5	3
33	LiGRO: a graphical user interface for protein-ligand molecular dynamics. <i>Journal of Molecular Modeling</i> , 2017 , 23, 304	2	5
32	Functional New World monkey oxytocin forms elicit an altered signaling profile and promotes parental care in rats. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017 , 114, 9044-9049	11.5	22
31	New potential inhibitors of mTOR: a computational investigation integrating molecular docking, virtual screening and molecular dynamics simulation. <i>Journal of Biomolecular Structure and Dynamics</i> , 2017 , 35, 3555-3568	3.6	11
30	Pathways of cardiac toxicity: comparison between chemotherapeutic drugs doxorubicin and mitoxantrone. <i>Archives of Toxicology</i> , 2016 , 90, 2063-2076	5.8	134
29	Crystal structure and molecular dynamics studies of purine nucleoside phosphorylase from <i>Mycobacterium tuberculosis</i> associated with acyclovir. <i>Biochimie</i> , 2012 , 94, 155-65	4.6	15
28	Role of Serine140 in the mode of action of <i>Mycobacterium tuberculosis</i> β -ketoacyl-ACP Reductase (MabA). <i>BMC Research Notes</i> , 2012 , 5, 526	2.3	7
27	Crystal structure determination and dynamic studies of <i>Mycobacterium tuberculosis</i> Cytidine deaminase in complex with products. <i>Archives of Biochemistry and Biophysics</i> , 2011 , 509, 108-15	4.1	6
26	Crystal structure and molecular dynamics studies of human purine nucleoside phosphorylase complexed with 7-deazaguanine. <i>Journal of Structural Biology</i> , 2010 , 169, 379-88	3.4	5
25	Molecular dynamics studies of a hexameric purine nucleoside phosphorylase. <i>Journal of Molecular Modeling</i> , 2010 , 16, 543-50	2	4
24	Bioinformatics tools for screening of antiparasitic drugs. <i>Current Drug Targets</i> , 2009 , 10, 232-9	3	8
23	Structural studies of shikimate dehydrogenase from <i>Bacillus anthracis</i> complexed with cofactor NADP. <i>Journal of Molecular Modeling</i> , 2009 , 15, 147-55	2	6
22	Molecular modeling and dynamics studies of purine nucleoside phosphorylase from <i>Bacteroides fragilis</i> . <i>Journal of Molecular Modeling</i> , 2009 , 15, 913-22	2	4
21	Molecular modeling and dynamics simulation of human cyclin-dependent kinase 3 complexed with inhibitors. <i>Computers in Biology and Medicine</i> , 2009 , 39, 130-40	7	18

20	Molecular modeling, dynamics and docking studies of purine nucleoside phosphorylase from <i>Streptococcus pyogenes</i> . <i>Biophysical Chemistry</i> , 2009 , 142, 7-16	3.5	9
19	Structural studies of PNP from <i>Toxoplasma gondii</i> . <i>International Journal of Bioinformatics Research and Applications</i> , 2009 , 5, 154-62	0.9	
18	Protein-drug interaction studies for development of drugs against <i>Plasmodium falciparum</i> . <i>Current Drug Targets</i> , 2009 , 10, 271-8	3	15
17	Genomic databases and the search of protein targets for protozoan parasites. <i>Current Drug Targets</i> , 2009 , 10, 240-5	3	9
16	Structural studies of human purine nucleoside phosphorylase: towards a new specific empirical scoring function. <i>Archives of Biochemistry and Biophysics</i> , 2008 , 479, 28-38	4.1	30
15	In silico and in vitro: identifying new drugs. <i>Current Drug Targets</i> , 2008 , 9, 1054-61	3	20
14	Molecular modeling as a tool for drug discovery. <i>Current Drug Targets</i> , 2008 , 9, 1084-91	3	17
13	Structural bioinformatics study of PNP from <i>Listeria monocytogenes</i> . <i>Protein and Peptide Letters</i> , 2008 , 15, 843-9	1.9	5
12	Drug-binding databases. <i>Current Drug Targets</i> , 2008 , 9, 1092-9	3	26
11	Molecular recognition models: a challenge to overcome. <i>Current Drug Targets</i> , 2008 , 9, 1077-83	3	14
10	Molecular modeling and dynamics studies of cytidylate kinase from <i>Mycobacterium tuberculosis</i> H37Rv. <i>Journal of Molecular Modeling</i> , 2008 , 14, 427-34	2	15
9	Structural studies of prephenate dehydratase from <i>Mycobacterium tuberculosis</i> H37Rv by SAXS, ultracentrifugation, and computational analysis. <i>Proteins: Structure, Function and Bioinformatics</i> , 2008 , 72, 1352-62	4.2	6
8	Molecular modeling and dynamics simulations of PNP from <i>Streptococcus agalactiae</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2008 , 16, 4984-93	3.4	32
7	Molecular modeling and dynamics studies of Shikimate Kinase from <i>Bacillus anthracis</i> . <i>Bioorganic and Medicinal Chemistry</i> , 2008 , 16, 8098-108	3.4	19
6	Linear interaction energy (LIE) method in lead discovery and optimization. <i>Current Drug Targets</i> , 2008 , 9, 1100-5	3	27
5	Evaluation of molecular docking using polynomial empirical scoring functions. <i>Current Drug Targets</i> , 2008 , 9, 1062-70	3	35
4	CDK9 a potential target for drug development. <i>Medicinal Chemistry</i> , 2008 , 4, 210-8	1.8	48
3	Protein kinases as targets for antiparasitic chemotherapy drugs. <i>Current Drug Targets</i> , 2007 , 8, 389-98	3	50

2	Molecular Dynamics and Structural Studies of the Ets Domain-DNA Complexes. <i>Current Bioinformatics</i> , 2007 , 2, 222-228	4-7	1
1	Shikimate kinase: a potential target for development of novel antitubercular agents. <i>Current Drug Targets</i> , 2007 , 8, 459-68	3	38