Rafael Andrade Caceres

List of Publications by Citations

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	Pathways of cardiac toxicity: comparison between chemotherapeutic drugs doxorubicin and mitoxantrone. *Archives of Toxicology*, **2016**, 90, 2063-2076	5.8	134
36	Protein kinases as targets for antiparasitic chemotherapy drugs. *Current Drug Targets*, **2007**, 8, 389-98	3	50
35	CDK9 a potential target for drug development. *Medicinal Chemistry*, **2008**, 4, 210-8	1.8	48
34	Shikimate kinase: a potential target for development of novel antitubercular agents. *Current Drug Targets*, **2007**, 8, 459-68	3	38
33	Evaluation of molecular docking using polynomial empirical scoring functions. *Current Drug Targets*, **2008**, 9, 1062-70	3	35
32	Molecular modeling and dynamics simulations of PNP from Streptococcus agalactiae. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 4984-93	3.4	32
31	Structural studies of human purine nucleoside phosphorylase: towards a new specific empirical scoring function. *Archives of Biochemistry and Biophysics*, **2008**, 479, 28-38	4.1	30
30	Linear interaction energy (LIE) method in lead discovery and optimization. *Current Drug Targets*, **2008**, 9, 1100-5	3	27
29	Drug-binding databases. *Current Drug Targets*, **2008**, 9, 1092-9	3	26
28	Functional New World monkey oxytocin forms elicit an altered signaling profile and promotes parental care in rats. *Proceedings of the National Academy of Sciences of the United States of America* , **2017**, 114, 9044-9049	11.5	22
27	Geo-Measures: A PyMOL plugin for protein structure ensembles analysis. *Computational Biology and Chemistry*, **2020**, 87, 107322	3.6	20
26	In silico and in vitro: identifying new drugs. *Current Drug Targets*, **2008**, 9, 1054-61	3	20
25	Molecular modeling and dynamics studies of Shikimate Kinase from Bacillus anthracis. *Bioorganic and Medicinal Chemistry*, **2008**, 16, 8098-108	3.4	19
24	Molecular modeling and dynamics simulation of human cyclin-dependent kinase 3 complexed with inhibitors. *Computers in Biology and Medicine*, **2009**, 39, 130-40	7	18
23	Molecular modeling as a tool for drug discovery. *Current Drug Targets*, **2008**, 9, 1084-91	3	17
22	Crystal structure and molecular dynamics studies of purine nucleoside phosphorylase from Mycobacterium tuberculosis associated with acyclovir. *Biochimie*, **2012**, 94, 155-65	4.6	15
21	Protein-drug interaction studies for development of drugs against Plasmodium falciparum. *Current Drug Targets*, **2009**, 10, 271-8	3	15

20	Molecular modeling and dynamics studies of cytidylate kinase from Mycobacterium tuberculosis H37Rv. *Journal of Molecular Modeling*, **2008**, 14, 427-34	2	15
19	Molecular recognition models: a challenge to overcome. *Current Drug Targets*, **2008**, 9, 1077-83	3	14
18	New potential inhibitors of mTOR: a computational investigation integrating molecular docking, virtual screening and molecular dynamics simulation. *Journal of Biomolecular Structure and Dynamics*, **2017**, 35, 3555-3568	3.6	11
17	Searching for potential mTOR inhibitors: Ligand-based drug design, docking and molecular dynamics studies of rapamycin binding site. *Journal of Molecular Graphics and Modelling*, **2018**, 80, 251-263	2.8	9
16	Molecular modeling, dynamics and docking studies of purine nucleoside phosphorylase from Streptococcus pyogenes. *Biophysical Chemistry*, **2009**, 142, 7-16	3.5	9
15	Genomic databases and the search of protein targets for protozoan parasites. *Current Drug Targets*, **2009**, 10, 240-5	3	9
14	Bioinformatics tools for screening of antiparasitic drugs. *Current Drug Targets*, **2009**, 10, 232-9	3	8
13	Role of Serine140 in the mode of action of Mycobacterium tuberculosis β-ketoacyl-ACP Reductase (MabA). *BMC Research Notes*, **2012**, 5, 526	2.3	7
12	Crystal structure determination and dynamic studies of Mycobacterium tuberculosis Cytidine deaminase in complex with products. *Archives of Biochemistry and Biophysics*, **2011**, 509, 108-15	4.1	6
11	Structural studies of shikimate dehydrogenase from Bacillus anthracis complexed with cofactor NADP. *Journal of Molecular Modeling*, **2009**, 15, 147-55	2	6
10	Structural studies of prephenate dehydratase from Mycobacterium tuberculosis H37Rv by SAXS, ultracentrifugation, and computational analysis. *Proteins: Structure, Function and Bioinformatics*, **2008**, 72, 1352-62	4.2	6
9	LiGRO: a graphical user interface for protein-ligand molecular dynamics. *Journal of Molecular Modeling*, **2017**, 23, 304	2	5
8	Crystal structure and molecular dynamics studies of human purine nucleoside phosphorylase complexed with 7-deazaguanine. *Journal of Structural Biology*, **2010**, 169, 379-88	3.4	5
7	Structural bioinformatics study of PNP from Listeria monocytogenes. *Protein and Peptide Letters*, **2008**, 15, 843-9	1.9	5
6	Molecular modeling and dynamics studies of purine nucleoside phosphorylase from Bacteroides fragilis. *Journal of Molecular Modeling*, **2009**, 15, 913-22	2	4
5	Molecular dynamics studies of a hexameric purine nucleoside phosphorylase. *Journal of Molecular Modeling*, **2010**, 16, 543-50	2	4
4	Prion protein conversion triggered by acidic condition: a molecular dynamics study through different force fields. *Journal of Computational Chemistry*, **2018**, 39, 2000-2011	3.5	3
3	Molecular Dynamics and Structural Studies of the Ets Domain-DNA Complexes. *Current Bioinformatics*, **2007**, 2, 222-228	4.7	1

2	Structural studies of PNP from Toxoplasma gondii. *International Journal of Bioinformatics Research and Applications*, **2009**, 5, 154-62	0.9
1	Understanding the role of mTOR-mLst8 binding through coarse-grained simulation approaches. *Molecular Simulation*, **2021**, 47, 1198-1207	2