Pedro G Pascutti

List of Publications by Year
in descending order

Source: https://exaly.com/author-pdf/5007307/publications.pdf

Version: 2024-02-01

41 papers	750 citations	535685 17 h-index	620720 26 g-index
41 all docs	41 docs citations	41 times ranked	1447 citing authors

#	Article	IF	Citations
1	Enzymatic and structural properties of human glutamine:fructose-6-phosphate amidotransferase 2 (hGFAT2). Journal of Biological Chemistry, 2021, 296, 100180.	1.6	11
2	Improving Blind Docking in DOCK6 through an Automated Preliminary Fragment Probing Strategy. Molecules, 2021, 26, 1224.	1.7	14
3	A novel receptor for plateletâ€activating factor and lysophosphatidylcholine in Trypanosoma cruzi. Molecular Microbiology, 2021, 116, 890-908.	1.2	1
4	Theoretical studies and NMR assay of coumarins and neoflavanones derivatives as potential inhibitors of acetylcholinesterase. Computational Biology and Chemistry, 2020, 87, 107293.	1.1	5
5	Identification of (4-(9H-fluoren-9-yl) piperazin-1-yl) methanone derivatives as falcipain 2 inhibitors active against Plasmodium falciparum cultures. Biochimica Et Biophysica Acta - General Subjects, 2018, 1862, 2911-2923.	1.1	6
6	Dataset showing the impact of the protonation states on molecular dynamics of HIV protease. Data in Brief, 2016, 8, 1144-1150.	0.5	3
7	Unraveling HIV protease flaps dynamics by Constant pH Molecular Dynamics simulations. Journal of Structural Biology, 2016, 195, 216-226.	1.3	15
8	Allosteric regulation of the Plasmodium falciparum cysteine protease falcipain-2 by heme. Archives of Biochemistry and Biophysics, 2015, 573, 92-99.	1.4	13
9	Structural and Functional Analysis of a Platelet-Activating Lysophosphatidylcholine of Trypanosoma cruzi. PLoS Neglected Tropical Diseases, 2014, 8, e3077.	1.3	37
10	Impact of M36I polymorphism on the interaction of HIV-1 protease with its substrates: insights from molecular dynamics. BMC Genomics, 2014, 15, S5.	1.2	13
11	Conformational Changes in Human Hsp70 Induced by High Hydrostatic Pressure Produce Oligomers with ATPase Activity but without Chaperone Activity. Biochemistry, 2014, 53, 2884-2889.	1.2	9
12	Anti-Prion Activity of a Panel of Aromatic Chemical Compounds: In Vitro and In Silico Approaches. PLoS ONE, 2014, 9, e84531.	1.1	41
13	GSAFold: A new application of GSA to protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2012, 80, 2305-2310.	1.5	11
14	The role of helices 5 and 6 on the human Î²1-adrenoceptor activation mechanism. Molecular Simulation, 2012, 38, 236-240.	0.9	8
15	Hybrid QM/MM Molecular Dynamics Study of Benzocaine in a Membrane Environment: How Does a Quantum Mechanical Treatment of Both Anesthetic and Lipids Affect Their Interaction. Journal of Chemical Theory and Computation, 2012, 8, 2197-2203.	2.3	20
16	The Structural Dynamics of the Flavivirus Fusion Peptideâ€“Membrane Interaction. PLoS ONE, 2012, 7, e47596.	1.1	23
17	Conformational Variability of Organophosphorus Hydrolase upon Soman and Paraoxon Binding. Journal of Physical Chemistry B, 2011, 115, 15389-15398.	1.2	9
18	Free Energy Profiles along Consensus Normal Modes Provide Insight into HIV-1 Protease Flap Opening. Journal of Chemical Theory and Computation, 2011, 7, 2348-2352.	2.3	32

#	Article	IF	Citations
19	Dynamical behaviour of the human Î²1-adrenoceptor under agonist binding. Molecular Simulation, 2011, 37, 907-913.	0.9	10
20	Molecular dynamics simulations and QM/MM studies of the reactivation by 2-PAM of tabun inhibited human acethylcolinesterase. Journal of the Brazilian Chemical Society, 2011, 22, 155-165.	0.6	42
21	Computational Perspectives into Plasmepsins Structureâ€"Function Relationship: Implications to Inhibitors Design. Journal of Tropical Medicine, 2011, 2011, 1-15.	0.6	8
22	How does heparin prevent the pH inactivation of cathepsin B? Allosteric mechanism elucidated by docking and molecular dynamics. BMC Genomics, 2010, 11, S5.	1.2	44
23	New parameterization approaches of the LIE method to improve free energy calculations of PlmIIâ€Inhibitors complexes. Journal of Computational Chemistry, 2010, 31, 2723-2734.	1.5	15
24	Understanding the HIV-1 protease nelfinavir resistance mutation D30N in subtypes B and C through molecular dynamics simulations. Journal of Molecular Graphics and Modelling, 2010, 29, 137-147.	1.3	24
25	Solvation of anionic waterâ€soluble porphyrins: A computational study. International Journal of Quantum Chemistry, 2010, 110, 2094-2100.	1.0	5
26	Conformational Analysis of Toxogonine, TMB-4 and HI-6 using PM6 and RM1 methods. Journal of the Brazilian Chemical Society, 2010, 21, 179-184.	0.6	27
27	The Role of Nonbonded Interactions in the Conformational Dynamics of Organophosphorous Hydrolase Adsorbed onto Functionalized Mesoporous Silica Surfaces. Journal of Physical Chemistry B, 2010, 114, 531-540.	1.2	37
28	Dissociation of molecular aggregates under high hydrostatic pressure: the influence of water structure on Benzene cluster solubility. Journal of the Brazilian Chemical Society, 2009, 20, 1227-1234.	0.6	8
29	Predicting functional residues in Plasmodium falciparum plasmepsins by combining sequence and structural analysis with molecular dynamics simulations. Proteins: Structure, Function and Bioinformatics, 2008, 73, 440-457.	1.5	19
30	Molecular Models to Emulate Confinement Effects on the Internal Dynamics of Organophosphorous Hydrolase. Lecture Notes in Computer Science, 2008, , 68-78.	1.0	2
31	Molecular dynamics of the interaction of Plasmodium falciparum and human serine hydroxymethyltransferase with 5-formyl-6-hydrofolic acid analogues: design of new potential antimalarials. Journal of the Brazilian Chemical Society, 2006, 17, 1383-1392.	0.6	24
32	Molecular Dynamics Simulations Applied to the Study of Subtypes of HIV-1 Protease Common to Brazil, Africa, and Asia. Cell Biochemistry and Biophysics, 2006, 44, 395-404.	0.9	39
33	Generalized simulated annealing applied to protein folding studies. Journal of Computational Chemistry, 2006, 27, 1142-1155.	1.5	37
34	A three-dimensional structure of Plasmodium falciparum serine hydroxymethyltransferase in complex with glycine and 5-formyl-tetrahydrofolate. Homology modeling and molecular dynamics. Biophysical Chemistry, 2005, 115, 1-10.	1.5	37
35	The BioPAUÃ•Project: A Portal for Molecular Dynamics Using Grid Environment. Lecture Notes in Computer Science, 2005, , 214-217.	1.0	4
36	Nonspecific interaction forces at water-membrane interface by forced molecular dynamics simulations. Journal of Computational Chemistry, 2003, 24, 328-339.	1.5	3

#	Article	IF	Citations
37	Molecular Modeling and Dynamics of the Sodium Channel Inactivation Gate. Biophysical Journal, 2002, 82, 1207-1215.	0.2	15
38	Polarization effects on peptide conformations at water-membrane interface by molecular dynamics simulation. Journal of Computational Chemistry, 1999, 20, 971-982.	1.5	22
39	On the contribution of electron transfer reactions to the quenching of tryptophan fluorescence. Journal of Chemical Physics, 1995, 103, 10614-10620.	1.2	22
40	Molecular Dynamics Simulations of Signal Sequences at a Membrane/Water Interface. The Journal of Physical Chemistry, 1995, 99, 14885-14892.	2.9	30
41	Kinetic studies of the photodecomposition of dipyridamole in solution: Interaction with lysophosphatidylcholine and bovine serum albumin. Spectrochimica Acta Part A: Molecular Spectroscopy, 1992, 48, 1427-1436.	0.1	5