Rodrigo Casasnovas

List of Publications by Year
in descending order

25 papers	864 citations	516710 16 h-index	610901 24 g-index
26 all docs	26 docs citations	26 times ranked	1233 citing authors

#	Article	IF	Citations
1	Unbinding Kinetics of a p38 MAP Kinase Type II Inhibitor from Metadynamics Simulations. Journal of the American Chemical Society, 2017, 139, 4780-4788.	13.7	187
2	Theoretical pK_a calculations with continuum model solvents, alternative protocols to thermodynamic cycles. International Journal of Quantum Chemistry, 2014, 114, 1350-1363.	2.0	88
3	Avoiding gas-phase calculations in theoretical pK a predictions. Theoretical Chemistry Accounts, 2011, 130, 1-13.	1.4	65
4	Absolute and relative pKa calculations of mono and diprotic pyridines by quantum methods. Computational and Theoretical Chemistry, 2009, 912, 5-12.	1.5	61
5	Chasing the Full Free Energy Landscape of Neuroreceptor/Ligand Unbinding by Metadynamics Simulations. Journal of Chemical Theory and Computation, 2019, 15, 3354-3361.	5.3	53
6	Isodesmic reaction for pK a calculations of common organic molecules. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	50
7	A Coarse-Grained Molecular Dynamics Approach to the Study of the Intrinsically Disordered Protein Î±-Synuclein. Journal of Chemical Information and Modeling, 2019, 59, 1458-1471.	5.4	44
8	Theoretical study on the distribution of atomic charges in the Schiff bases of 3-hydroxypyridine-4-aldehyde and alanine. The effect of the protonation state of the pyridine and imine nitrogen atoms. Chemical Physics, 2009, 355, 149-156.	1.9	42
9	Isodesmic reaction for accurate theoretical pK_a calculations of amino acids and peptides. Physical Chemistry Chemical Physics, 2016, 18, 11202-11212.	2.8	35
10	Theoretical calculations of stability constants and pKa values of metal complexes in solution: application to pyridoxamineâ€“copper(ii) complexes and their biological implications in AGE inhibition. Physical Chemistry Chemical Physics, 2013, 15, 16303.	2.8	34
11	Simplification of the CBSâ€QB3 method for predicting gasâ€phase deprotonation free energies. International Journal of Quantum Chemistry, 2010, 110, 323-330.	2.0	31
12	Câ€“H Activation in Pyridoxal-5â€²-phosphate Schiff Bases: The Role of the Imine Nitrogen. A Combined Experimental and Computational Study. Journal of Physical Chemistry B, 2012, 116, 10665-10675.	2.6	31
13	How Does Pyridoxamine Inhibit the Formation of Advanced Glycation End Products? The Role of Its Primary Antioxidant Activity. Antioxidants, 2019, 8, 344.	5.1	25
14	High- and Low-Spin Fe(III) Complexes of Various AGE Inhibitors. Journal of Physical Chemistry A, 2012, 116, 2961-2971.	2.5	21
15	Rare FLT3 deletion mutants may provide additional treatment options to patients with AML: an approach to individualized medicine. Leukemia, 2015, 29, 2434-2438.	7.2	21
16	Ortho-methylated 3-hydroxypyridines hinder hen egg-white lysozyme fibrillogenesis. Scientific Reports, 2015, 5, 12052.	3.3	18
17	Câ€“H Activation in Pyridoxal-5â€²-phosphate and Pyridoxamine-5â€²-phosphate Schiff Bases: Effect of Metal Chelation. A Computational Study. Journal of Physical Chemistry B, 2013, 117, 2339-2347.	2.6	14
18	Unravelling the effect ofN(Îµ)-(carboxyethyl)lysine on the conformation, dynamics and aggregation propensity of Î±-synuclein. Chemical Science, 2020, 11, 3332-3344.	7.4	13

#	Article	IF	Citations
19	Designing the Sniper: Improving Targeted Human Cytolytic Fusion Proteins for Anti-Cancer Therapy via Molecular Simulation. Biomedicines, 2017, 5, 9.	3.2	8
20	Modelling the repair of carbon-centred protein radicals by the antioxidants glutathione and Trolox. New Journal of Chemistry, 2019, 43, 2085-2097.	2.8	7
21	Does glycation really distort the peptide Î±-helicity?. International Journal of Biological Macromolecules, 2019, 129, 254-266.	7.5	5
22	A density functional theory study of the freeâ€•radical scavenging activity of aminoguanidine. Comparison with its reactive carbonyl compound and metal scavenging activities. International Journal of Quantum Chemistry, 2019, 119, e25911.	2.0	5
23	New insights into human farnesyl pyrophosphate synthase inhibition by second-generation bisphosphonate drugs. Journal of Computer-Aided Molecular Design, 2017, 31, 675-688.	2.9	3
24	Isodesmic reaction for pK a calculations of common organic molecules. Highlights in Theoretical Chemistry, 2014, , 51-58.	0.0	1
25	STUDENTS PROBLEM DESIGN AS A TOOL FOR AUTONOMOUS LEARNING AND FOR STIMULATING CREATIVITY. , 2021, , .		0