Santiago Tolosa

List of Publications by Year
in descending order

11	114	1307594 7	1372567 10
papers	citations	h-index	g-index

11	11	11	105
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Amide-imide tautomerism of acetohydroxamic acid in aqueous solution: quantum calculation and SMD simulations. RSC Advances, 2014, 4, 44757-44768.	3.6	21
2	Mechanisms for guanineâ€“cytosine tautomeric equilibrium in solution via steered molecular dynamic simulations. Journal of Molecular Liquids, 2018, 251, 308-316.	4.9	18
3	Theoretical thermodynamic study of the adenine-thymine tautomeric equilibrium: Electronic structure calculations and steered molecular dynamic simulations. International Journal of Quantum Chemistry, 2017, 117, e25429.	2.0	17
4	Steered molecular dynamic simulations of the tautomeric equilibria in solution of DNA bases. Journal of Molecular Liquids, 2017, 237, 81-88.	4.9	16
5	Theoretical determination of aqueous acidâ€“base pK values: electronic structure calculations and steered molecular dynamic simulations. Theoretical Chemistry Accounts, 2016, 135, 1.	1.4	9
6	Theoretical Study of Adenine to Guanine Transition Assisted by Water and Formic Acid Using Steered Molecular Dynamic Simulations. Frontiers in Chemistry, 2019, 7, 414.	3.6	9
7	Structural and thermodynamic studies of cytosine to thymine conversion in gas and solution phases using steered molecular dynamic simulations. Journal of Molecular Liquids, 2019, 278, 61-69.	4.9	9
8	Mechanisms of the T-A to C-G transition studied by SMD simulations: Deamination vs tautomerisation. Journal of Molecular Liquids, 2020, 308, 113036.	4.9	6
9	Theoretical study of mechanisms for the hydrolytic deamination of cytosine via steered molecular dynamic simulations. RSC Advances, 2018, 8, 34867-34876.	3.6	5
10	Theoretical study of mechanisms for double proton transfer in adenineâ€“uracil base pair via steered molecular dynamic simulations. Journal of Molecular Liquids, 2018, 265, 487-495.	4.9	4
11	A procedure to understanding the C-G to A-T transversion. SMD simulations from guanine oxidation pathways assisted by one H2O2 molecule in the C-G basis pair. Journal of Molecular Liquids, 2020, 319, 114123.	4.9	0