MichaÅ, Rostkowski

List of Publications by Year
in descending order

22 papers	5,146 citations	840776 11 h-index	677142 22 g-index
22 all docs	22 docs citations	22 times ranked	7317 citing authors

#	Article	IF	Citations
1	PROPKA3: Consistent Treatment of Internal and Surface Residues in Empirical p<i>K</i>_a Predictions. Journal of Chemical Theory and Computation, 2011, 7, 525-537.	5.3	3,121
2	Improved Treatment of Ligands and Coupling Effects in Empirical Calculation and Rationalization of p<i>K</i>_a Values. Journal of Chemical Theory and Computation, 2011, 7, 2284-2295.	5.3	1,436
3	Graphical analysis of pH-dependent properties of proteins predicted using PROPKA. BMC Structural Biology, 2011, 11, 6.	2.3	328
4	WhichCyp: prediction of cytochromes P450 inhibition. Bioinformatics, 2013, 29, 2051-2052.	4.1	57
5	The Contribution of Atom Accessibility to Site of Metabolism Models for Cytochromes P450. Molecular Pharmaceutics, 2013, 10, 1216-1223.	4.6	38
6	A Theoretical Investigation of Î±-Carbon Kinetic Isotope Effects and Their Relationship to the Transition-State Structure of SN2 Reactions. Journal of Organic Chemistry, 2005, 70, 4022-4027.	3.2	29
7	A New Interpretation of Chlorine Leaving Group Kinetic Isotope Effects; A Theoretical Approach. Journal of Organic Chemistry, 2004, 69, 4900-4905.	3.2	27
8	Oxidation of ethidium-based probes by biological radicals: mechanism, kinetics and implications for the detection of superoxide. Scientific Reports, 2020, 10, 18626.	3.3	14
9	Calculations of Substituent and Solvent Effects on the Kinetic Isotope Effects of Menshutkin Reactions. Journal of Organic Chemistry, 2003, 68, 8232-8235.	3.2	12
10	Validation of semiempirical methods for modeling of corrinoid systems. Journal of Inorganic Biochemistry, 2004, 98, 1078-1086.	3.5	11
11	Chlorine Isotope Effects on Chemical Reactions. Current Organic Chemistry, 2005, 9, 75-88.	1.6	11
12	Decomposition of Piloty's acid derivatives â€“ Toward the understanding of factors controlling HNO release. Archives of Biochemistry and Biophysics, 2019, 661, 132-144.	3.0	11
13	Enzyme mechanisms from molecular modeling and isotope effects. Archives of Biochemistry and Biophysics, 2008, 474, 274-282.	3.0	9
14	Mechanistic Analysis of the Base-Catalyzed HF Elimination from 4-Fluoro-4-(4â€²-nitrophenyl)butane-2-one Based on Liquid-Phase Kinetic Isotope Effects Calculated by Dynamics Modeling with Multidimensional Tunneling. Journal of Chemical Theory and Computation, 2009, 5, 59-67.	5.3	8
15	Influence of the Solvent Description on the Predicted Mechanism of SN2 Reactions. Journal of Physical Chemistry B, 2008, 112, 12414-12419.	2.6	7
16	Kinetic Study on the Reactivity of Azanone (HNO) toward Cyclic C-Nucleophiles. International Journal of Molecular Sciences, 2021, 22, 12982.	4.1	6
17	Isotope Effects on the Vaporization of Organic Compounds from an Aqueous Solutionâ€“Insight from Experiment and Computations. Journal of Physical Chemistry B, 2021, 125, 13868-13885.	2.6	5
18	PIN3 duplication may be partially responsible for TP53haploinsufficiency. BMC Cancer, 2014, 14, 669.	2.6	4

#	Article	IF	Citations
19	Can Path Integral Molecular Dynamics Make a Good Approximation for Vapor Pressure Isotope Effects Prediction for Organic Solvents? A Comparison to ONIOM QM/MM and QM Cluster Calculation. Journal of Physical Chemistry B, 2018, 122, 7353-7364.	2.6	4
20	Kinetics of Azanone (HNO) Reactions with Thiols: Effect of pH. Cell Biochemistry and Biophysics, 2021, 79, 845-856.	1.8	4
21	Analysis of Conformer Stability for 1,3,8-Trihydroxynaphthalene:Â Natural Substrate of Fungal Trihydroxynaphthalene Reductase. Journal of Physical Chemistry B, 2007, 111, 8314-8320.	2.6	2
22	RNA model evaluation based on MD simulation of four tRNA analogs. RSC Advances, 2016, 6, 101778-101789.	3.6	2