Mats Hm Olsson

List of Publications by Year
in descending order

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33 papers	8,568 citations	201674 27 h-index	414414 32 g-index
33 all docs	33 docs citations	33 times ranked	9554 citing authors

#	Article	IF	Citations
1	Effect of mutations on the thermostability of Aspergillus aculeatus Î²-1,4-galactanase. Computational and Structural Biotechnology Journal, 2015, 13, 256-264.	4.1	14
2	Improving the desolvation penalty in empirical protein pKa modeling. Journal of Molecular Modeling, 2012, 18, 1097-1106.	1.8	7
3	PROPKA3: Consistent Treatment of Internal and Surface Residues in Empirical pK_a Predictions. Journal of Chemical Theory and Computation, 2011, 7, 525-537.	5.3	3,121
4	Improved Treatment of Ligands and Coupling Effects in Empirical Calculation and Rationalization of pK_a Values. Journal of Chemical Theory and Computation, 2011, 7, 2284-2295.	5.3	1,436
5	Graphical analysis of pH-dependent properties of proteins predicted using PROPKA. BMC Structural Biology, 2011, 11, 6.	2.3	328
6	Protein electrostatics and pK_a blind predictions; contribution from empirical predictions of internal ionizable residues. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3333-3345.	2.6	38
7	Progress in the prediction of pK_a values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275.	2.6	229
8	Simulation of Tunneling in Enzyme Catalysis by Combining a Biased Propagation Approach and the Quantum Classical Path Method:Â Application to Lipoxygenaseâ€. Journal of Physical Chemistry B, 2008, 112, 5950-5954.	2.6	41
9	A new paradigm for electrostatic catalysis of radical reactions in vitamin B12 enzymes. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 9661-9666.	7.1	95
10	Exploring pathways and barriers for coupled ET/PT in cytochrome c oxidase: A general framework for examining energetics and mechanistic alternatives. Biochimica Et Biophysica Acta - Bioenergetics, 2007, 1767, 244-260.	1.0	45
11	Electrostatic Basis for Enzyme Catalysis. Chemical Reviews, 2006, 106, 3210-3235.	47.7	1,117
12	Transition state theory can be used in studies of enzyme catalysis: lessons from simulations of tunnelling and dynamical effects in lipoxygenase and other systems. Philosophical Transactions of the Royal Society B: Biological Sciences, 2006, 361, 1417-1432.	4.0	100
13	Dynamical Contributions to Enzyme Catalysis:â€‰ Critical Tests of A Popular Hypothesis. Chemical Reviews, 2006, 106, 1737-1756.	47.7	284
14	Monte Carlo simulations of proton pumps: On the working principles of the biological valve that controls proton pumping in cytochrome c oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2006, 103, 6500-6505.	7.1	82
15	Simulating redox coupled proton transfer in cytochromecoxidase: Looking for the proton bottleneck. FEBS Letters, 2005, 579, 2026-2034.	2.8	53
16	Computer modeling of enzyme catalysis and its relationship to concepts in physical organic chemistry. Advances in Physical Organic Chemistry, 2005, , 201-245.	0.5	10
17	Computer Simulations of Isotope Effects in Enzyme Catalysis. , 2005, , 621-644.		7
18	Simulations of the Large Kinetic Isotope Effect and the Temperature Dependence of the Hydrogen Atom Transfer in Lipoxygenase. Journal of the American Chemical Society, 2004, 126, 2820-2828.	13.7	152

#	Article	IF	Citations
19	Simulating large nuclear quantum mechanical corrections in hydrogen atom transfer reactions in metalloenzymes. Journal of Biological Inorganic Chemistry, 2004, 9, 96-99.	2.6	32
20	Solute Solvent Dynamics and Energetics in Enzyme Catalysis:Â The SN2 Reaction of Dehalogenase as a General Benchmark. Journal of the American Chemical Society, 2004, 126, 15167-15179.	13.7	87
21	Frozen Density Functional Free Energy Simulations of Redox Proteins:Â Computational Studies of the Reduction Potential of Plastocyanin and Rusticyanin. Journal of the American Chemical Society, 2003, 125, 5025-5039.	13.7	236
22	Inner-Sphere Reorganization Energy of Ironâ^'Sulfur Clusters Studied with Theoretical Methods. Inorganic Chemistry, 2001, 40, 2509-2519.	4.0	97
23	Geometry, Reduction Potential, and Reorganization Energy of the Binuclear CuASite, Studied by Density Functional Theory. Journal of the American Chemical Society, 2001, 123, 7866-7876.	13.7	96
24	A Comparison of the Inner-Sphere Reorganization Energies of Cytochromes, Ironâ^'Sulfur Clusters, and Blue Copper Proteins. Journal of Physical Chemistry B, 2001, 105, 5546-5552.	2.6	135
25	A theoretical study of the copper-cysteine bond in blue copper proteins. Theoretical Chemistry Accounts, 2001, 105, 452-462.	1.4	58
26	The structure and function of blue copper proteins. Theoretical and Computational Chemistry, 2001, 9, 1-55.	0.4	24
27	Structure, strain, and reorganization energy of blue copper models in the protein. International Journal of Quantum Chemistry, 2001, 81, 335-347.	2.0	5
28	On the role of strain in blue copper proteins. Journal of Biological Inorganic Chemistry, 2000, 5, 565-574.	2.6	89
29	The influence of axial ligands on the reduction potential of blue copper proteins. Journal of Biological Inorganic Chemistry, 1999, 4, 654-663.	2.6	72
30	On the relative stability of tetragonal and trigonal Cu(II) complexes with relevance to the blue copper proteins. Journal of Biological Inorganic Chemistry, 1998, 3, 109-125.	2.6	60
31	Quantum chemical calculations of the reorganization energy of blueâ€copper proteins. Protein Science, 1998, 7, 2659-2668.	7.6	84
32	Relation between the Structure and Spectroscopic Properties of Blue Copper Proteins. Journal of the American Chemical Society, 1998, 120, 13156-13166.	13.7	158
33	The Cupric Geometry of Blue Copper Proteins is not Strained. Journal of Molecular Biology, 1996, 261, 586-596.	4.2	176