# 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 | PROPKA3: Consistent Treatment of Internal and Surface Residues in Empirical pK<sub>a</sub> 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 pK<sub>a</sub> Values. Journal of Chemical Theory and Computation, 2011, 7, 2284-2295. | 5.3 | 1,436 |
| 3 | Electrostatic Basis for Enzyme Catalysis. Chemical Reviews, 2006, 106, 3210-3235. | 47.7 | 1,117 |
| 4 | Graphical analysis of pH-dependent properties of proteins predicted using PROPKA. BMC Structural Biology, 2011, 11, 6. | 2.3 | 328 |
| 5 | Dynamical Contributions to Enzyme Catalysis:â€‰Critical Tests of A Popular Hypothesis. Chemical Reviews, 2006, 106, 1737-1756. | 47.7 | 284 |
| 6 | 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 |
| 7 | Progress in the prediction of pK<sub>a</sub> values in proteins. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3260-3275. | 2.6 | 229 |
| 8 | The Cupric Geometry of Blue Copper Proteins is not Strained. Journal of Molecular Biology, 1996, 261, 586-596. | 4.2 | 176 |
| 9 | Relation between the Structure and Spectroscopic Properties of Blue Copper Proteins. Journal of the American Chemical Society, 1998, 120, 13156-13166. | 13.7 | 158 |
| 10 | 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 |
| 11 | 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 |
| 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 | Inner-Sphere Reorganization Energy of Ironâ^'Sulfur Clusters Studied with Theoretical Methods. Inorganic Chemistry, 2001, 40, 2509-2519. | 4.0 | 97 |
| 14 | 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 |
| 15 | 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 |
| 16 | On the role of strain in blue copper proteins. Journal of Biological Inorganic Chemistry, 2000, 5, 565-574. | 2.6 | 89 |
| 17 | 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 |
| 18 | Quantum chemical calculations of the reorganization energy of blueâ€copper proteins. Protein Science, 1998, 7, 2659-2668. | 7.6 | 84 |

| # | Article | IF | Citations |
|---|---|---|---|
| 19 | 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 |
| 20 | 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 |
| 21 | 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 |
| 22 | A theoretical study of the copper-cysteine bond in blue copper proteins. Theoretical Chemistry Accounts, 2001, 105, 452-462. | 1.4 | 58 |
| 23 | Simulating redox coupled proton transfer in cytochromecoxidase: Looking for the proton bottleneck. FEBS Letters, 2005, 579, 2026-2034. | 2.8 | 53 |
| 24 | 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 |
| 25 | 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 |
| 26 | Protein electrostatics and pK<sub>a</sub> blind predictions; contribution from empirical predictions of internal ionizable residues. Proteins: Structure, Function and Bioinformatics, 2011, 79, 3333-3345. | 2.6 | 38 |
| 27 | 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 |
| 28 | The structure and function of blue copper proteins. Theoretical and Computational Chemistry, 2001, 9, 1-55. | 0.4 | 24 |
| 29 | 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 |
| 30 | 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 |
| 31 | Improving the desolvation penalty in empirical protein pKa modeling. Journal of Molecular Modeling, 2012, 18, 1097-1106. | 1.8 | 7 |
| 32 | Computer Simulations of Isotope Effects in Enzyme Catalysis. , 2005, , 621-644. | | 7 |
| 33 | Structure, strain, and reorganization energy of blue copper models in the protein. International Journal of Quantum Chemistry, 2001, 81, 335-347. | 2.0 | 5 |