David C Chatfield

List of Publications by Year
in descending order

29 papers	1,137 citations	516215 16 h-index	476904 29 g-index
29 all docs	29 docs citations	29 times ranked	1091 citing authors

#	Article	IF	Citations
1	Proximal Pocket Controls Alkene Oxidation Selectivity of Cytochrome P450 and Chloroperoxidase toward Small, Nonpolar Substrates. Journal of Physical Chemistry B, 2018, 122, 7828-7838.	1.2	7
2	How the Proximal Pocket May Influence the Enantiospecificities of Chloroperoxidase-Catalyzed Epoxidations of Olefins. International Journal of Molecular Sciences, 2016, 17, 1297.	1.8	5
3	Chloroperoxidase-Catalyzed Epoxidation of Cis-Î²-Methylstyrene: NHâ€“S Hydrogen Bonds and Proximal Helix Dipole Change the Catalytic Mechanism and Significantly Lower the Reaction Barrier. Journal of Physical Chemistry B, 2015, 119, 14350-14363.	1.2	8
4	Proximal Pocket Hydrogen Bonds Significantly Influence the Mechanism of Chloroperoxidase Compound I Formation. Journal of Physical Chemistry B, 2015, 119, 12590-12602.	1.2	6
5	A Possible Mechanism for Redox Control of Human Neuroglobin Activity. Journal of Chemical Information and Modeling, 2014, 54, 1997-2003.	2.5	11
6	Theoretical Study of HOCl-Catalyzed Ketoâ€“Enol Tautomerization of Î²-Cyclopentanedione in an Explicit Water Environment. Journal of Physical Chemistry A, 2013, 117, 8437-8448.	1.1	13
7	Paramagnetic Nuclear Magnetic Resonance Relaxation and Molecular Mechanics Studies of the Chloroperoxidaseâ€“Indole Complex: Insights into the Mechanism of Chloroperoxidase-Catalyzed Regioselective Oxidation of Indole. Biochemistry, 2013, 52, 3688-3701.	1.2	18
8	Chloroperoxidase-Catalyzed Epoxidation of cis-Î²-Methylstyrene: Distal Pocket Flexibility Tunes Catalytic Reactivity. Journal of Physical Chemistry B, 2012, 116, 12905-12914.	1.2	16
9	Enantiospecificity of Chloroperoxidase-Catalyzed Epoxidation: Biased Molecular Dynamics Study of a Cis-Î²-Methylstyrene/Chloroperoxidase-Compound I Complex. Biophysical Journal, 2011, 100, 1066-1075.	0.2	14
10	The conformation of end-groups is one determinant of carotenoid topology suitable for high fidelity molecular recognition: A study of Î²- and Îµ-end-groups. Archives of Biochemistry and Biophysics, 2010, 493, 169-174.	1.4	11
11	1,3-Dipolar Cycloadditions of Trimethylsilyldiazomethane Revisited:â€‰ Steric Demand of the Dipolarophile and the Influence on Product Distribution. Journal of Organic Chemistry, 2007, 72, 650-653.	1.7	28
12	Regioselectivity of Michael Additions to 3-(Pyridin-3-yl or Pyrimidin-2-yl)propenoates and TheirN-Oxides - Experimental and Theoretical Studies. European Journal of Organic Chemistry, 2005, 2005, 3297-3303.	1.2	18
13	Correlation Times and Adiabatic Barriers for Methyl Rotation in SNase. Journal of Biomolecular NMR, 2004, 29, 377-385.	1.6	20
14	Methyl dynamics in crystalline amino acids: MD and NMR. Journal of Computational Chemistry, 2003, 24, 1052-1058.	1.5	10
15	Optimization of quantum mechanical molecular mechanical partitioning schemes: Gaussian delocalization of molecular mechanical charges and the double link atom method. Journal of Chemical Physics, 2002, 117, 10534-10547.	1.2	173
16	Quantized dynamical bottlenecks and transition state control of the reaction of D with H2: Effect of varying the total angular momentum. Journal of Chemical Physics, 2000, 112, 8387-8408.	1.2	38
17	Methyl Motional Parameters in Crystallinel-Alanine:Â Molecular Dynamics Simulation and NMR. Journal of Physical Chemistry B, 2000, 104, 11342-11348.	1.2	27
18	HIV-1 protease cleavage mechanism: A theoretical investigation based on classical MD simulation and reaction path calculations using a hybrid QM/MM potential. Computational and Theoretical Chemistry, 1998, 423, 79-92.	1.5	52

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19	Molecular Dynamics of Staphylococcal Nuclease:Â Comparison of Simulation with15N and13C NMR Relaxation Data. Journal of the American Chemical Society, 1998, 120, 5301-5311.	6.6	121
20	Enzyme mechanisms with hybrid quantum and molecular mechanical potentials. I. Theoretical considerations. International Journal of Quantum Chemistry, 1996, 60, 1189-1200.	1.0	185
21	HIV-1 Protease Cleavage Mechanism Elucidated with Molecular Dynamics Simulation. Journal of the American Chemical Society, 1995, 117, 5561-5572.	6.6	64
22	Preconditioned complex generalized minimal residual algorithm for dense algebraic variational equations in quantum reactive scattering. Journal of Chemical Physics, 1993, 99, 2739-2751.	1.2	12
23	The nature and role of quantized transition states in the accurate quantum dynamics of the reaction O+H2â†'OH+H. Journal of Chemical Physics, 1993, 98, 342-362.	1.2	58
24	Complex generalized minimal residual algorithm for iterative solution of quantumâ€mechanical reactive scattering equations. Journal of Chemical Physics, 1992, 97, 8322-8333.	1.2	14
25	Stateâ€selected chemical reaction dynamics at the S matrix level: Finalâ€state specificities of nearâ€threshold processes at low and high energies. Journal of Chemical Physics, 1992, 96, 4313-4323.	1.2	8
26	Quantum-dynamical characterization of reactive transition states. Faraday Discussions of the Chemical Society, 1991, 91, 289.	2.2	71
27	Global control of suprathreshold reactivity by quantized transition states. Journal of the American Chemical Society, 1991, 113, 486-494.	6.6	95
28	Benchmark calculations of thermal reaction rates. I. Quantal scattering theory. Journal of Chemical Physics, 1991, 94, 2040-2044.	1.2	17
29	Iterative methods for solving the non-sparse equations of quantum mechanical reactive scattering. Computer Physics Communications, 1989, 53, 357-379.	3.0	17