Dan Thomas Major

List of Publications by Year
in descending order

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141 papers	6,749 citations	71004 43 h-index	81351 76 g-index
147 all docs	147 docs citations	147 times ranked	8151 citing authors

#	Article	IF	Citations
1	A cost-effective water-in-salt electrolyte enables highly stable operation of a 2.15-V aqueous lithium-ion battery. Cell Reports Physical Science, 2022, 3, 100688.	2.8	16
2	A Benchmark Study of Quantum Mechanics and Quantum Mechanics-Molecular Mechanics Methods for Carbocation Chemistry. Journal of Chemical Theory and Computation, 2022, 18, 167-178.	2.3	11
3	Concentrationâ€Dependent Selfâ€Assembly of an Unusually Large Hexameric Hydrogenâ€Bonded Molecular Cage. Chemistry - A European Journal, 2021, 27, 4447-4453.	1.7	9
4	Temperature-Dependent Kinetic Isotope Effects in R67 Dihydrofolate Reductase from Path-Integral Simulations. Journal of Physical Chemistry B, 2021, 125, 1369-1377.	1.2	8
5	Benchmarking the Ability of Common Docking Programs to Correctly Reproduce and Score Binding Modes in SARS-CoV-2 Protease Mpro. Journal of Chemical Information and Modeling, 2021, 61, 2957-2966.	2.5	50
6	Electrochemical and Structural Studies of LiNi_{0.85}Co_{0.1}Mn_{0.05}O₂, a Cathode Material for High Energy Density Li-Ion Batteries, Stabilized by Doping with Small Amounts of Tungsten. Journal of the Electrochemical Society, 2021, 168, 060552.	1.3	13
7	Enhancement of Structural, Electrochemical, and Thermal Properties of High-Energy Density Ni-Rich LiNi_{0.85}Co_{0.1}Mn_{0.05}O₂ Cathode Materials for Li-Ion Batteries by Niobium Doping. ACS Applied Materials & Interfaces, 2021, 13, 34145-34156.	4.0	38
8	Molecular Dynamics Simulations of the Apo and Holo States of the Copper Binding Protein CueR Reveal Principal Bending and Twisting Motions. Journal of Physical Chemistry B, 2021, 125, 9417-9425.	1.2	7
9	Can Anions Be Inserted into MXene?. Journal of the American Chemical Society, 2021, 143, 12552-12559.	6.6	63
10	Boron doped Ni-rich LiNi0.85Co0.10Mn0.05O2 cathode materials studied by structural analysis, solid state NMR, computational modeling, and electrochemical performance. Energy Storage Materials, 2021, 42, 594-607.	9.5	42
11	Review of Computational Studies of NCM Cathode Materials for Liâ€ion Batteries. Israel Journal of Chemistry, 2020, 60, 850-862.	1.0	40
12	Layered Cathode Materials for Lithium-Ion Batteries: Review of Computational Studies on LiNi_{1â€“xâ€“y}Co_xMn_yO₂ and LiNi_{1â€“xâ€“y}Co_xAl_yO₂. Chemistry of Materials, 2020, 32, 915-952.	3.2	196
13	Role of Microsolvation and Quantum Effects in the Accurate Prediction of Kinetic Isotope Effects: The Case of Hydrogen Atom Abstraction in Ethanol by Atomic Hydrogen in Aqueous Solution. Journal of Chemical Theory and Computation, 2020, 16, 847-859.	2.3	13
14	Enzymatic control of product distribution in terpene synthases: insights from multiscale simulations. Current Opinion in Biotechnology, 2020, 65, 248-258.	3.3	26
15	Vacancyâ€Driven High Rate Capabilities in Calciumâ€Doped Na_{0.4}MnO₂ Cathodes for Aqueous Sodiumâ€ion Batteries. Advanced Energy Materials, 2020, 10, 2002077.	10.2	37
16	First principles study of electrocatalytic behavior of olivine phosphates with mixed alkali and mixed transition metal atoms. RSC Advances, 2020, 10, 29175-29180.	1.7	0
17	The Impression of a Nonexisting Catalytic Effect: The Role of CotB2 in Guiding the Complex Biosynthesis of Cyclooctat-9-en-7-ol. Journal of the American Chemical Society, 2020, 142, 21562-21574.	6.6	20
18	Thermodynamic and Kinetic Control Determine the Sesquiterpene Reaction Pathways Inside Nanocapsules. ACS Catalysis, 2020, 10, 6843-6853.	5.5	8

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19	Cu(I) Controls Conformational States in Human Atox1 Metallochaperone: An EPR and Multiscale Simulation Study. Journal of Physical Chemistry B, 2020, 124, 4399-4411.	1.2	10
20	Four-Step Access to the Sesquiterpene Natural Product Presilphiperfolan-1Î²-ol and Unnatural Derivatives via Supramolecular Catalysis. Journal of the American Chemical Society, 2020, 142, 5894-5900.	6.6	48
21	Understanding the role of active site residues in CotB2 catalysis using a cluster model. Beilstein Journal of Organic Chemistry, 2020, 16, 50-59.	1.3	11
22	Monte Carlo- and Simulated-Annealing-Based Funneled Approach for the Prediction of Cation Ordering in Mixed Transition-Metal Oxide Materials. Journal of Physical Chemistry C, 2020, 124, 27366-27377.	1.5	9
23	EnzyDock: Proteinâ€“Ligand Docking of Multiple Reactive States along a Reaction Coordinate in Enzymes. Journal of Chemical Theory and Computation, 2019, 15, 5116-5134.	2.3	28
24	Current understanding and biotechnological application of the bacterial diterpene synthase CotB2. Beilstein Journal of Organic Chemistry, 2019, 15, 2355-2368.	1.3	17
25	Oscillatory Active-Site Motions Correlate with Kinetic Isotope Effects in Formate Dehydrogenase. ACS Catalysis, 2019, 9, 11199-11206.	5.5	29
26	Crystal structure of LepI, a multifunctional SAM-dependent enzyme which catalyzes pericyclic reactions in leporin biosynthesis. Organic and Biomolecular Chemistry, 2019, 17, 2070-2076.	1.5	15
27	Computational design of biofuels from terpenes and terpenoids. Sustainable Energy and Fuels, 2019, 3, 457-466.	2.5	23
28	Improving Performance of LiNi_{0.8}Co_{0.1}Mn_{0.1}O₂ Cathode Materials for Lithium-Ion Batteries by Doping with Molybdenum-Ions: Theoretical and Experimental Studies. ACS Applied Energy Materials, 2019, 2, 4521-4534.	2.5	91
29	Discovering Monoterpene Catalysis Inside Nanocapsules with Multiscale Modeling and Experiments. Journal of the American Chemical Society, 2019, 141, 6234-6246.	6.6	42
30	Combined Experimental and Theoretical Study of Cobalt Corroles as Catalysts for Oxygen Reduction Reaction. Journal of Physical Chemistry C, 2019, 123, 30129-30136.	1.5	26
31	Endogenous Dynamic Nuclear Polarization for Natural Abundance ¹⁷O and Lithium NMR in the Bulk of Inorganic Solids. Journal of the American Chemical Society, 2019, 141, 451-462.	6.6	69
32	Rapid Convergence of Energy and Free Energy Profiles with Quantum Mechanical Size in Quantum Mechanicalâ€“Molecular Mechanical Simulations of Proton Transfer in DNA. Journal of Chemical Theory and Computation, 2018, 14, 1695-1705.	2.3	34
33	Q6: A comprehensive toolkit for empirical valence bond and related free energy calculations. SoftwareX, 2018, 7, 388-395.	1.2	47
34	Pushing the limit of layered transition metal oxide cathodes for high-energy density rechargeable Li ion batteries. Energy and Environmental Science, 2018, 11, 1271-1279.	15.6	322
35	Comment on â€œSubstrate Folding Modes in Trichodiene Synthase: A Determinant of Chemo- and Stereoselectivityâ€• ACS Catalysis, 2018, 8, 1371-1375.	5.5	17
36	From Surface ZrO₂ Coating to Bulk Zr Doping by High Temperature Annealing of Nickelâ€Rich Lithiated Oxides and Their Enhanced Electrochemical Performance in Lithium Ion Batteries. Advanced Energy Materials, 2018, 8, 1701682.	10.2	443

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37	Predicting accurate cathode properties of layered oxide materials using the SCAN meta-GGA density functional. Npj Computational Materials, 2018, 4, .	3.5	99
38	Evolutionary Effects on Bound Substrate pK_a in Dihydrofolate Reductase. Journal of the American Chemical Society, 2018, 140, 16650-16660.	6.6	17
39	Towards a comprehensive understanding of the structural dynamics of a bacterial diterpene synthase during catalysis. Nature Communications, 2018, 9, 3971.	5.8	57
40	Slow-Starter Enzymes: Role of Active-Site Architecture in the Catalytic Control of the Biosynthesis of Taxadiene by Taxadiene Synthase. Biochemistry, 2018, 57, 3773-3779.	1.2	31
41	A promising drug candidate for the treatment of glaucoma based on a P2Y6-receptor agonist. Purinergic Signalling, 2018, 14, 271-284.	1.1	14
42	Theoretical Study of the Electrocatalytic Reduction of Oxygen by Metallocorroles. Journal of Physical Chemistry C, 2018, 122, 17686-17694.	1.5	26
43	Effect of Asp122 Mutation on the Hydride Transfer in E. coli DHFR Demonstrates the Goldilocks of Enzyme Flexibility. Journal of Physical Chemistry B, 2018, 122, 8006-8017.	1.2	11
44	Understanding the Role of Minor Molybdenum Doping in LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂ Electrodes: from Structural and Surface Analyses and Theoretical Modeling to Practical Electrochemical Cells. ACS Applied Materials & Interfaces, 2018, 10, 29608-29621.	4.0	97
45	Complex terpenes in one pot. Nature Catalysis, 2018, 1, 567-568.	16.1	8
46	Unraveling the Effects of Al Doping on the Electrochemical Properties of LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂Using First Principles. Journal of the Electrochemical Society, 2017, 164, A6359-A6365.	1.3	118
47	Chemical Control in the Battle against Fidelity in Promiscuous Natural Product Biosynthesis: The Case of Trichodiene Synthase. ACS Catalysis, 2017, 7, 812-818.	5.5	48
48	The role of the Met20 loop in the hydride transfer in Escherichia coli dihydrofolate reductase. Journal of Biological Chemistry, 2017, 292, 14229-14239.	1.6	24
49	Catalytic Control in the Facile Proton Transfer in Taxadiene Synthase. ACS Catalysis, 2017, 7, 7653-7657.	5.5	33
50	Origin of Structural Degradation During Cycling and Low Thermal Stability of Ni-Rich Layered Transition Metal-Based Electrode Materials. Journal of Physical Chemistry C, 2017, 121, 22628-22636.	1.5	199
51	A surprising substituent effect in corroles on the electrochemical activation of oxygen reduction. Chemical Communications, 2017, 53, 12942-12945.	2.2	37
52	Electrostatic Control of Chemistry in Terpene Cyclases. ACS Catalysis, 2017, 7, 5461-5465.	5.5	38
53	Shaping Polyyne Rods by Using an Electric Field. ChemistryOpen, 2017, 6, 733-738.	0.9	4
54	Study of Cathode Materials for Lithium-Ion Batteries: Recent Progress and New Challenges. Inorganics, 2017, 5, 32.	1.2	68

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55	Is it True That the Normal Valenceâ€Length Correlation Is Irrelevant for Metalâ€“Metal Bonds?. Chemistry - A European Journal, 2016, 22, 5269-5276.	1.7	11
56	Electronic Structure and Bonding in Co-Based Single and Mixed Valence Oxides: A Quantum Chemical Perspective. Inorganic Chemistry, 2016, 55, 3307-3315.	1.9	40
57	Nucleoside-2â€²,3â€²/3â€²,5â€²-bis(thio)phosphate antioxidants are also capable of disassembly of amyloid beta₄₂-Zn(<scp>ii</scp>)/Cu(<scp>ii</scp>) aggregates via Zn(<scp>ii</scp>)/Cu(<scp>ii</scp>)-chelation. Organic and Biomolecular Chemistry, 2016, 14, 4640-4653.	1.5	9
58	Structural and Kinetic Studies of Formate Dehydrogenase from Candida boidinii. Biochemistry, 2016, 55, 2760-2771.	1.2	76
59	Improved Sugar Puckering Profiles for Nicotinamide Ribonucleoside for Hybrid QM/MM Simulations. Journal of Chemical Theory and Computation, 2016, 12, 5179-5189.	2.3	5
60	Unique Behavior of Dimethoxyethane (DME)/Mg(N(SO₂CF₃)₂)₂ Solutions. Journal of Physical Chemistry C, 2016, 120, 19586-19594.	1.5	99
61	Electron-Hybridization-Induced Enhancement of Photoactivity in Indium-Doped Co₃O₄. Journal of Physical Chemistry C, 2016, 120, 28983-28991.	1.5	4
62	Stabilizing nickel-rich layered cathode materials by a high-charge cation doping strategy: zirconium-doped LiNi_{0.6}Co_{0.2}Mn_{0.2}O₂. Journal of Materials Chemistry A, 2016, 4, 16073-16084.	5.2	295
63	Practical Aspects of Multiscale Classical and Quantum Simulations of Enzyme Reactions. Methods in Enzymology, 2016, 577, 251-286.	0.4	8
64	First principles model calculations of the biosynthetic pathway in selinadiene synthase. Bioorganic and Medicinal Chemistry, 2016, 24, 4867-4870.	1.4	11
65	Anomalous magnetotransport behavior in Fe-doped MnNiGe alloys. Physical Review B, 2016, 93, .	1.1	24
66	Improving Energy Density and Structural Stability of Manganese Oxide Cathodes for Na-Ion Batteries by Structural Lithium Substitution. Chemistry of Materials, 2016, 28, 9064-9076.	3.2	191
67	A combined computational and experimental investigation of Mg doped Î±-Fe₂O₃. Physical Chemistry Chemical Physics, 2016, 18, 781-791.	1.3	15
68	Hydrogen adsorption in ZIF-7: A DFT and ab-initio molecular dynamics study. Chemical Physics Letters, 2016, 651, 178-182.	1.2	12
69	Thermodynamic and kinetic studies of LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂ as a positive electrode material for Li-ion batteries using first principles. Physical Chemistry Chemical Physics, 2016, 18, 6799-6812.	1.3	126
70	First-principles evaluation of the inherent stabilities of pure Li x MPO 4 (M=Mn, Fe, Co,) and mixed binary Li x Fe y Mâ€² 1-y PO 4 (M'=Mn, Co) olivine phosphates. Materials Chemistry and Physics, 2016, 174, 54-58.	2.0	7
71	Chapter 10. Nuclear Quantum Effects in Enzymatic Reactions. RSC Theoretical and Computational Chemistry Series, 2016, , 340-374.	0.7	1
72	Metallocorroles as Nonpreciousâ€Metal Catalysts for Oxygen Reduction. Angewandte Chemie - International Edition, 2015, 54, 14080-14084.	7.2	128

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73	Acylation or phosphorylation of hydroxyurea unexpectedly takes place on N rather than on O, leading to the formation of amides instead of the expected esters. RSC Advances, 2015, 5, 24038-24043.	1.7	4
74	Nuclear quantum effects in chemical reactions via higher-order path-integral calculations. Chemical Physics, 2015, 450-451, 95-101.	0.9	6
75	Studies of Aluminum-Doped LiNi_{0.5}Co_{0.2}Mn_{0.3}O₂: Electrochemical Behavior, Aging, Structural Transformations, and Thermal Characteristics. Journal of the Electrochemical Society, 2015, 162, A1014-A1027.	1.3	121
76	Nuclear quantum effects and kinetic isotope effects in enzyme reactions. Archives of Biochemistry and Biophysics, 2015, 582, 18-27.	1.4	24
77	Classical and Quantum Modeling of Li and Na Diffusion in FePO₄. Journal of Physical Chemistry C, 2015, 119, 15801-15809.	1.5	29
78	Adenosine/guanosine-3â€²,5â€²-bis-phosphates as biocompatible and selective Zn2+-ion chelators. Characterization and comparison with adenosine/guanosine-5â€²-di-phosphate. Dalton Transactions, 2015, 44, 7305-7317.	1.6	3
79	Magnetism in olivine-type LiCo_{1â^'x}Fe_xPO₄cathode materials: bridging theory and experiment. Physical Chemistry Chemical Physics, 2015, 17, 31202-31215.	1.3	16
80	Identification of Highly Promising Antioxidants/Neuroprotectants Based on Nucleoside 5â€²-Phosphorothioate Scaffold. Synthesis, Activity, and Mechanisms of Action. Journal of Medicinal Chemistry, 2015, 58, 8427-8443.	2.9	13
81	Analysis of the Spectroscopic Aspects of Cationic Dye Basic Orange 21. Journal of Physical Chemistry A, 2015, 119, 9794-9804.	1.1	5
82	Putting DFT to the Test: A First-Principles Study of Electronic, Magnetic, and Optical Properties of Co₃O₄. Journal of Chemical Theory and Computation, 2015, 11, 64-72.	2.3	93
83	Understanding the Reaction Mechanism and Intermediate Stabilization in Mammalian Serine Racemase Using Multiscale Quantum-Classical Simulations. Biochemistry, 2015, 54, 516-527.	1.2	12
84	Free Energy Simulations of Active-Site Mutants of Dihydrofolate Reductase. Journal of Physical Chemistry B, 2015, 119, 906-916.	1.2	20
85	Structural trends in hybrid perovskites [Me₂NH₂]M[HCOO]₃ (M =) Tj ETQq1 1 0.784314 rgBT /O 295-298.	1.3	29
86	Oddâ€“Even Effect in Molecular Electronic Transport via an Aromatic Ring. Langmuir, 2014, 30, 13596-13605.	1.6	33
87	Enzyme structure captures four cysteines aligned for disulfide relay. Protein Science, 2014, 23, 1102-1112.	3.1	11
88	Multiscale Quantumâ€Classical Simulations of Enzymes. Israel Journal of Chemistry, 2014, 54, 1108-1117.	1.0	5
89	Catalytic control in terpenoid cyclases: multiscale modeling of thermodynamic, kinetic, and dynamic effects. Current Opinion in Chemical Biology, 2014, 21, 25-33.	2.8	60
90	How Accurate Are Transition States from Simulations of Enzymatic Reactions?. Journal of Chemical Theory and Computation, 2014, 10, 1863-1871.	2.3	21

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91	Simulations of remote mutants of dihydrofolate reductase reveal the nature of a network of residues coupled to hydride transfer. Journal of Computational Chemistry, 2014, 35, 1411-1417.	1.5	20
92	Challenges in computational studies of enzyme structure, function and dynamics. Journal of Molecular Graphics and Modelling, 2014, 54, 62-79.	1.3	50
93	Phenyl-imidazolo-cytidine Analogues: Structureâ€“Photophysical Activity Relationship and Ability To Detect Single DNA Mismatch. Journal of Organic Chemistry, 2014, 79, 7051-7062.	1.7	11
94	Topotactic elimination of water across a Câ€“C ligand bond in a dense 3-D metalâ€“organic framework. Chemical Communications, 2014, 50, 13292-13295.	2.2	7
95	Controlling dye aggregation, injection energetics and catalytic recombination in organic sensitizer based dye cells using a single electrolyte additive. Energy and Environmental Science, 2013, 6, 3046.	15.6	15
96	Rules for the Design of Highly Fluorescent Nucleoside Probes: 8-(Substituted Cinnamyl)-Adenosine Analogues. Journal of Organic Chemistry, 2013, 78, 11999-12008.	1.7	23
97	Systematic First-Principles Investigation of Mixed Transition Metal Olivine Phosphates LiM_{1-y}Mâ€²_yPO₄ (M/Mâ€² = Mn, Fe, and Co) as Cathode Materials. Journal of Physical Chemistry C, 2013, 117, 17919-17926.	1.5	30
98	Multinuclear Magnetic Resonance Spectroscopy and Density Function Theory Calculations for the Identification of the Equilibrium Species in THF Solutions of Organometallic Complexes Suitable As Electrolyte Solutions for Rechargeable Mg Batteries. Organometallics, 2013, 32, 3165-3173.	1.1	9
99	Quantum and Classical Simulations of Orotidine Monophosphate Decarboxylase: Support for a Direct Decarboxylation Mechanism. Biochemistry, 2013, 52, 4382-4390.	1.2	22
100	Structure of Carboxyl-Acid-Terminated Self-Assembled Monolayers from Molecular Dynamics Simulations and Hybrid Quantum Mechanicsâ€“Molecular Mechanics Vibrational Normal-Mode Analysis. Journal of Physical Chemistry C, 2012, 116, 770-782.	1.5	18
101	Hybrid Quantum and Classical Simulations of the Formate Dehydrogenase Catalyzed Hydride Transfer Reaction on an Accurate Semiempirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2012, 8, 4786-4796.	2.3	25
102	Electrostatically Guided Dynamicsâ€”The Root of Fidelity in a Promiscuous Terpene Synthase?. Journal of the American Chemical Society, 2012, 134, 19454-19462.	6.6	84
103	Collective Reaction Coordinate for Hybrid Quantum and Molecular Mechanics Simulations: A Case Study of the Hydride Transfer in Dihydrofolate Reductase. Journal of Chemical Theory and Computation, 2012, 8, 2484-2496.	2.3	35
104	Studies of Mg2+/Ca2+ complexes of naturally occurring dinucleotides: potentiometric titrations, NMR, and molecular dynamics. Journal of Biological Inorganic Chemistry, 2012, 17, 861-879.	1.1	4
105	Momentum Distribution as a Fingerprint of Quantum Delocalization in Enzymatic Reactions: Open-Chain Path-Integral Simulations of Model Systems and the Hydride Transfer in Dihydrofolate Reductase. Journal of Chemical Theory and Computation, 2012, 8, 1223-1234.	2.3	20
106	Pathâ€integral calculations of heavy atom kinetic isotope effects in condensed phase reactions using higherâ€order trotter factorizations. Journal of Computational Chemistry, 2012, 33, 435-441.	1.5	5
107	Structural Analysis of Electrolyte Solutions for Rechargeable Mg Batteries by Stereoscopic Means and DFT Calculations. Journal of the American Chemical Society, 2011, 133, 6270-6278.	6.6	264
108	Path-Integral Calculations of Nuclear Quantum Effects in Model Systems, Small Molecules, and Enzymes via Gradient-Based Forward Corrector Algorithms. Journal of Chemical Theory and Computation, 2011, 7, 1273-1286.	2.3	31

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109	Hybrid Quantum and Classical Simulations of the Dihydrofolate Reductase Catalyzed Hydride Transfer Reaction on an Accurate Semi-Empirical Potential Energy Surface. Journal of Chemical Theory and Computation, 2011, 7, 3420-3437.	2.3	45
110	Molecular dynamics simulations of the intramolecular proton transfer and carbanion stabilization in the pyridoxal 5â€²-phosphate dependent enzymes l-dopa decarboxylase and alanine racemase. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2011, 1814, 1438-1446.	1.1	25
111	Inhibition of crystallization and growth of celecoxib nanoparticles formed from volatile microemulsions. Journal of Pharmaceutical Sciences, 2011, 100, 4390-4400.	1.6	19
112	Structureâ€“activity relationship studies of 1-(4-chloro-2,5-dimethoxyphenyl)-3-(3-propoxypropyl)thiourea, a non-nucleoside reverse transcriptase inhibitor of human immunodeficiency virus type-1. European Journal of Medicinal Chemistry, 2011, 46, 447-467.	2.6	13
113	What is the conformation of physiologically-active dinucleoside polyphosphates in solution? Conformational analysis of free dinucleoside polyphosphates by NMR and molecular dynamics simulations. Organic and Biomolecular Chemistry, 2010, 8, 4637.	1.5	35
114	Formation of organic nanoparticles from volatile microemulsions. Journal of Colloid and Interface Science, 2010, 342, 283-292.	5.0	32
115	Facile structural elucidation of imidazoles and oxazoles based on NMR spectroscopy and quantum mechanical calculations. Tetrahedron, 2010, 66, 1465-1471.	1.0	12
116	The sonochemical synthesis and characterization of mesoporous chiral titania using a chiral inorganic precursor. Ultrasonics Sonochemistry, 2010, 17, 605-609.	3.8	6
117	Challenges Posed to Bornyl Diphosphate Synthase: Diverging Reaction Mechanisms in Monoterpenes. Journal of the American Chemical Society, 2010, 132, 6349-6360.	6.6	97
118	Understanding Catalytic Specificity in Alanine Racemase from Quantum Mechanical and Molecular Mechanical Simulations of the Arginine 219 Mutant. Biochemistry, 2010, 49, 3957-3964.	1.2	15
119	Differential quantum tunneling contributions in nitroalkane oxidase catalyzed and the uncatalyzed proton transfer reaction. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 20734-20739.	3.3	69
120	Catalyzing Racemizations in the Absence of a Cofactor: The Reaction Mechanism in Proline Racemase. Journal of the American Chemical Society, 2009, 131, 8513-8521.	6.6	42
121	Kinetic Isotope Effects from Hybrid Classical and Quantum Path Integral Computations. RSC Biomolecular Sciences, 2009, , 105-131.	0.4	5
122	Quantum Mechanical Methods for Biomolecular Simulations. Challenges and Advances in Computational Chemistry and Physics, 2009, , 79-101.	0.6	0
123	Combined QM/MM and path integral simulations of kinetic isotope effects in the proton transfer reaction between nitroethane and acetate ion in water. Journal of Computational Chemistry, 2008, 29, 514-522.	1.5	45
124	Polymerâ€“surfactant interactions: Binding mechanism of sodium dodecyl sulfate to poly(diallyldimethylammonium chloride). Journal of Colloid and Interface Science, 2008, 320, 74-81.	5.0	90
125	Hybrid Quantum and Classical Methods for Computing Kinetic Isotope Effects of Chemical Reactions in Solutions and in Enzymes. Methods in Molecular Biology, 2008, 443, 37-62.	0.4	5
126	Î²-Halo-Î±,Î²-unsaturated Î³-Sultones. Journal of Organic Chemistry, 2007, 72, 6824-6831.	1.7	17

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127	An Integrated Path Integral and Free-Energy Perturbationâ˜Umbrella Sampling Method for Computing Kinetic Isotope Effects of Chemical Reactions in Solution and in Enzymes. Journal of Chemical Theory and Computation, 2007, 3, 949-960.	2.3	86
128	Mechanisms and Free Energies of Enzymatic Reactions. Chemical Reviews, 2006, 106, 3188-3209.	23.0	355
129	Path Integral Simulations of Proton Transfer Reactions in Aqueous Solution Using Combined QM/MM Potentials. Journal of Chemical Theory and Computation, 2006, 2, 236-245.	2.3	57
130	A Combined Quantum Mechanical and Molecular Mechanical Study of the Reaction Mechanism and Î±-Amino Acidity in Alanine Racemase. Journal of the American Chemical Society, 2006, 128, 16345-16357.	6.6	125
131	Transition State Stabilization and Î±-Amino Carbon Acidity in Alanine Racemase. Journal of the American Chemical Society, 2006, 128, 8114-8115.	6.6	60
132	Implementation of the bisection sampling method in path integral simulations. Journal of Molecular Graphics and Modelling, 2005, 24, 121-127.	1.3	54
133	Solvent Polarization and Kinetic Isotope Effects in Nitroethane Deprotonation and Implications to the Nitroalkane Oxidase Reaction. Journal of the American Chemical Society, 2005, 127, 16374-16375.	6.6	50
134	Molecular Recognition in Purinergic Receptors. 2. Diastereoselectivity of theh-P2Y1-Receptorâ€. Journal of Medicinal Chemistry, 2004, 47, 4405-4416.	2.9	38
135	Molecular Recognition in Purinergic Receptors. 1. A Comprehensive Computational Study of theh-P2Y1-Receptorâ€. Journal of Medicinal Chemistry, 2004, 47, 4391-4404.	2.9	30
136	Theoretical Study of the pH-Dependent Photophysics Of N1,N6-Ethenoadenine and N3,N4-Ethenocytosine. Journal of Physical Chemistry A, 2003, 107, 8923-8931.	1.1	8
137	Protonation Studies of Modified Adenine and Adenine Nucleotides by Theoretical Calculations and15N NMR. Journal of Organic Chemistry, 2002, 67, 790-802.	1.7	67
138	(15N5)-Labeled Adenine Derivatives:Â Synthesis and Studies of Tautomerism by15N NMR Spectroscopy and Theoretical Calculations. Journal of Organic Chemistry, 2001, 66, 5463-5481.	1.7	119
139	Molecular Recognition of Modified Adenine Nucleotides by the P2Y1-Receptor. 1. A Synthetic, Biochemical, and NMR Approach. Journal of Medicinal Chemistry, 1999, 42, 5325-5337.	2.9	46
140	Molecular Recognition of Modified Adenine Nucleotides by the P2Y1-Receptor. 2. A Computational Approach. Journal of Medicinal Chemistry, 1999, 42, 5338-5347.	2.9	13
141	Characterization of â€œMini-Nucleotidesâ€•as P2X Receptor Agonists in Rat Cardiomyocyte Cultures. An Integrated Synthetic, Biochemical, and Theoretical Study. Journal of Medicinal Chemistry, 1999, 42, 2685-2696.	2.9	20