Ã€ngels GonzÃ¡lez-Lafont

List of Publications by Year
in descending order

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140 papers	3,903 citations	147726 31 h-index	155592 55 g-index
143 all docs	143 docs citations	143 times ranked	3072 citing authors

#	Article	IF	Citations
1	Direct dynamics calculation of the kinetic isotope effect for an organic hydrogen-transfer reaction, including corner-cutting tunneling in 21 dimensions. Journal of the American Chemical Society, 1993, 115, 7806-7817.	6.6	348
2	Interpolated variational transitionâ€state theory: Practical methods for estimating variational transitionâ€state properties and tunneling contributions to chemical reaction rates from electronic structure calculations. Journal of Chemical Physics, 1991, 95, 8875-8894.	1.2	296
3	Direct dynamics calculations with NDDO (neglect of diatomic differential overlap) molecular orbital theory with specific reaction parameters. The Journal of Physical Chemistry, 1991, 95, 4618-4627.	2.9	285
4	Theoretical Study of the Low-Barrier Hydrogen Bond in the Hydrogen Maleate Anion in the Gas Phase. Comparison with Normal Hydrogen Bonds. Journal of the American Chemical Society, 1997, 119, 1081-1086.	6.6	151
5	MORATE: a program for direct dynamics calculations of chemical reaction rates by semiempirical molecular orbital theory. Computer Physics Communications, 1993, 75, 143-159.	3.0	107
6	Tunneling in Green Tea:Â Understanding the Antioxidant Activity of Catechol-Containing Compounds. A Variational Transition-State Theory Study. Journal of the American Chemical Society, 2007, 129, 5846-5854.	6.6	96
7	Temperature dependence of the kinetic isotope effect for a gas-phase SN2 reaction: Cl- + CH3Br. Journal of the American Chemical Society, 1991, 113, 9404-9405.	6.6	88
8	Is an Extremely Low-Field Proton Signal in the NMR Spectrum Conclusive Evidence for a Low-Barrier Hydrogen Bond?. Journal of Physical Chemistry A, 1997, 101, 8727-8733.	1.1	55
9	Evolutionary alteration of ALOX15 specificity optimizes the biosynthesis of antiinflammatory and proresolving lipoxins. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E4266-75.	3.3	54
10	Temperature Dependence of Proton NMR Chemical Shift As a Criterion To Identify Low-Barrier Hydrogen Bonds. Journal of the American Chemical Society, 1998, 120, 10203-10209.	6.6	53
11	Determination of enzymatic reaction pathways using QM/MM methods. International Journal of Quantum Chemistry, 2003, 93, 229-244.	1.0	52
12	A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. Journal of the American Chemical Society, 2006, 128, 16851-16863.	6.6	52
13	Asymmetry of the Hydrogen Bond of Hydrogen Phthalate Anion in Solution. A QM/MM Study. Journal of the American Chemical Society, 1999, 121, 9198-9207.	6.6	51
14	Enzyme Dynamics and Tunneling Enhanced by Compression in the Hydrogen Abstraction Catalyzed by Soybean Lipoxygenase-1. Journal of Physical Chemistry B, 2006, 110, 24708-24719.	1.2	51
15	Understanding the activation energy trends for the C2H4+OHâ†'C2H4OH reaction by using canonical variational transition state theory. Journal of Chemical Physics, 1997, 107, 7266-7274.	1.2	50
16	Variational Transition-State Theory with Optimized Orientation of the Dividing Surface and Semiclassical Tunneling Calculations for Deuterium and Muonium Kinetic Isotope Effects in the Free Radical Association Reaction H + C2H4 â†' C2H5. Journal of Physical Chemistry A, 1999, 103, 5061-5074.	1.1	50
17	On pKaMatching as a Requirement To Form a Low-Barrier Hydrogen Bond. A Theoretical Study in Gas Phase. Journal of Physical Chemistry A, 1997, 101, 3880-3886.	1.1	48
18	Variational Transition State Theory and Tunneling Calculations with Reorientation of the Generalized Transition States for Methyl Cation Transfer. Journal of Physical Chemistry A, 1998, 102, 3420-3428.	1.1	48

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19	Theoretical Modeling of Hydroxyl-Radical-Induced Lipid Peroxidation Reactions. Journal of Physical Chemistry B, 2007, 111, 5684-5693.	1.2	46
20	The reactions CHnD4â^'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics computational methods to determine variational transition-state rate constants. I.. Journal of Chemical Physics, 2001, 114, 2154-2165.	1.2	44
21	Molecular modeling of solvation. Clâ^'(D2O). Journal of Chemical Physics, 1991, 94, 5544-5558.	1.2	42
22	Synthetic Photoswitchable Neurotransmitters Based on Bridged Azobenzenes. Organic Letters, 2019, 21, 3780-3784.	2.4	42
23	Variational Transition-State Theory Rate Constant Calculations with Multidimensional Tunneling Corrections of the Reaction of Acetone with OH. Journal of Physical Chemistry A, 2002, 106, 11760-11770.	1.1	40
24	Variational Transition State Theory as a Tool To Determine Kinetic Selectivity in Reactions Involving a Valley-Ridge Inflection Point. Journal of the American Chemical Society, 2004, 126, 13089-13094.	6.6	40
25	Theoretical Study of the Mechanism of the Hydride Transfer between Ferredoxinâ€"NADP⁺ Reductase and NADP⁺: The Role of Tyr303. Journal of the American Chemical Society, 2012, 134, 20544-20553.	6.6	40
26	Unraveling How Enzymes Can Use Bulky Residues To Drive Site-Selective Câ€"H Activation: The Case of Mammalian Lipoxygenases Catalyzing Arachidonic Acid Oxidation. ACS Catalysis, 2014, 4, 4351-4363.	5.5	39
27	A QM/MM Study of the Racemization of Vinylglycolate Catalyzed by Mandelate Racemase Enzyme. Journal of the American Chemical Society, 2001, 123, 709-721.	6.6	38
28	Testing electronic structure methods for describing intermolecular H Â· Â· Â· H interactions in supramolecular chemistry. Journal of Computational Chemistry, 2004, 25, 99-105.	1.5	35
29	Mechanism of the Gas-Phase HO + H2O â†' H2O + OH Reaction and Several Associated Isotope Exchange Reactions:â€‰ A Canonical Variational Transition State Theory Plus Multidimensional Tunneling Calculation. Journal of Physical Chemistry A, 1999, 103, 1044-1053.	1.1	34
30	The regioselectivity of 4-nitroanisole photosubstitution with primary amines. A mechanistic and theoretical study. Journal of Organic Chemistry, 1990, 55, 3303-3310.	1.7	33
31	On the Ionization State of the Substrate in the Active Site of Glutamate Racemase. A QM/MM Study about the Importance of Being Zwitterionicâ€. Journal of Physical Chemistry A, 2006, 110, 717-725.	1.1	33
32	Searching for Saddle Points by Using the Nudged Elastic Band Method:â€‰ An Implementation for Gas-Phase Systems. Journal of Chemical Theory and Computation, 2006, 2, 895-904.	2.3	33
33	Ligandâ€induced formation of transient dimers of mammalian 12/15â€lipoxygenase: A key to allosteric behavior of this class of enzymes?. Proteins: Structure, Function and Bioinformatics, 2012, 80, 703-712.	1.5	33
34	Understanding the Mechanism of the Hydrogen Abstraction from Arachidonic Acid Catalyzed by the Human Enzyme 15-Lipoxygenase-2. A Quantum Mechanics/Molecular Mechanics Free Energy Simulation. Journal of Chemical Theory and Computation, 2016, 12, 2079-2090.	2.3	33
35	A Monte Carlo simulation of Fe2+ aqueous solvation. Chemical Physics, 1987, 111, 241-247.	0.9	30
36	Entropic Effects on the Dynamical Bottleneck Location and Tunneling Contributions for C2H4 + H â†' C2H5:â€‰ Variable Scaling of External Correlation Energy for Association Reactions. Journal of the American Chemical Society, 1998, 120, 5559-5567.	6.6	30

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37	Variational Transition-State Theory Rate Constant Calculations of the OH + CH3SH Reaction and Several Isotopic Variants. Journal of Physical Chemistry A, 2003, 107, 4490-4496.	1.1	30
38	Insights into the Mechanism of Binding of Arachidonic Acid to Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2010, 114, 7037-7046.	1.2	30
39	The reactions CHnD4â^'n+OHâ†'P and CH4+ODâ†'CH3+HOD as a test of current direct dynamics multicoefficient methods to determine variational transition state rate constants. II. Journal of Chemical Physics, 2001, 115, 4515-4526.	1.2	29
40	A Fast Radical Chain Mechanism in the Polyfluoroalkoxylation of Aromatics through NO2 Group Displacement. Mechanistic and Theoretical Studies. Journal of Organic Chemistry, 2005, 70, 1718-1727.	1.7	29
41	The nucleophilic aromatic photosubstitutions of 4,5-dinitroveratrole with amines. Tetrahedron, 1987, 43, 351-360.	1.0	28
42	Thermodynamics, Kinetics, and Dynamics of the Two Alternative Aniomesolytic Fragmentations of Câ^'O Bonds:â€‰ An Electrochemical and Theoretical Study. Journal of the American Chemical Society, 2002, 124, 4708-4715.	6.6	28
43	Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. Journal of Computational Chemistry, 2005, 26, 569-583.	1.5	27
44	Mechanism of the Hydride Transfer between Anabaena Tyr303Ser FNR_{rd}/FNR_{ox} and NADP⁺/H. A Combined Pre-Steady-State Kinetic/Ensemble-Averaged Transition-State Theory with Multidimensional Tunneling Study. Journal of Physical Chemistry B, 2010, 114, 3368-3379.	1.2	27
45	Geometry optimization and transition state search in enzymes: Different options in the microiterative method. International Journal of Quantum Chemistry, 2004, 98, 367-377.	1.0	26
46	The curvature of the Arrhenius plots predicted by conventional canonical transition-state theory in the absence of tunneling. Theoretical Chemistry Accounts, 2003, 110, 352-357.	0.5	25
47	A QM/MM study of the phosphoryl transfer to the Kemptide substrate catalyzed by protein kinase A. The effect of the phosphorylation state of the protein on the mechanism. Physical Chemistry Chemical Physics, 2011, 13, 530-539.	1.3	25
48	The role of many-body interactions in the stability of hydrated Cu2+ clusters. Chemical Physics, 1990, 141, 379-392.	0.9	23
49	Reaction-Path and Dual-Level Dynamics Calculations of the CH3F + OH Reaction. Journal of Physical Chemistry A, 1998, 102, 10715-10722.	1.1	23
50	Photo-oxidation of lipids by singlet oxygen: a theoretical study. Chemical Physics Letters, 2004, 398, 336-342.	1.2	23
51	Variational Transition-State Theory Study of the Dimethyl Sulfoxide (DMSO) and OH Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 798-808.	1.1	23
52	How the Substrate d-Glutamate Drives the Catalytic Action of Bacillus subtilis Glutamate Racemase. Journal of the American Chemical Society, 2009, 131, 3509-3521.	6.6	23
53	A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. Journal of Chemical Theory and Computation, 2005, 1, 750-761.	2.3	22
54	Computational insight into the catalytic implication of head/tail-first orientation of arachidonic acid in human 5-lipoxygenase: consequences for the positional specificity of oxygenation. Physical Chemistry Chemical Physics, 2016, 18, 23017-23035.	1.3	22

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55	Theoretical study of the role of arginine 127 in the water-promoted mechanism of peptide cleavage by carboxypeptidase A. New Journal of Chemistry, 1998, 22, 319-326.	1.4	21
56	Variational Transition State Calculations of the CH2F2 + OH Hydrogen Abstraction Reaction. Journal of Physical Chemistry A, 2001, 105, 10553-10561.	1.1	21
57	Kinetic isotope effects in chemical and biochemical reactions: physical basis and theoretical methods of calculation. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2016, 6, 584-603.	6.2	21
58	Explanation of Deuterium and Muonium Kinetic Isotope Effects for Hydrogen Atom Addition to an Olefin. Journal of the American Chemical Society, 1998, 120, 12141-12142.	6.6	20
59	Hydrogen Abstraction by Soybean Lipoxygenase-1. Density Functional Theory Study on Active Site Models in Terms of Gibbs Free Energies. Journal of Physical Chemistry B, 2004, 108, 13831-13838.	1.2	20
60	SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. ACS Catalysis, 2015, 5, 4897-4912.	5.5	19
61	Inhibition of Mammalian 15-Lipoxygenase by Three Ebselen-like Drugs. A QM/MM and MM/PBSA Comparative Study. Journal of Physical Chemistry A, 2017, 121, 9752-9763.	1.1	19
62	Variational Transition-State Theory with Multidimensional, Semiclassical, Ground-State Transmission Coefficients. ACS Symposium Series, 1992, , 16-36.	0.5	18
63	On the water-promoted mechanism of peptide cleavage by carboxypeptidase A. A theoretical study. Canadian Journal of Chemistry, 1994, 72, 2077-2083.	0.6	18
64	A QM/MM study of Kemptide phosphorylation catalyzed by protein kinase A. The role of Asp166 as a general acid/base catalyst. Physical Chemistry Chemical Physics, 2015, 17, 3497-3511.	1.3	18
65	How Can Linoleic Acid Be the Preferential Substrate of the Enzyme 15-Lipoxygenase-1? A QM/MM Approach. Journal of Physical Chemistry B, 2016, 120, 1950-1960.	1.2	18
66	Comparing Hydrolysis and Transglycosylation Reactions Catalyzed by Thermus thermophilus Î²-Glycosidase. A Combined MD and QM/MM Study. Frontiers in Chemistry, 2019, 7, 200.	1.8	18
67	Effect of a complex formation on the calculated low-pressure rate constant of a bimolecular gas-phase reaction governed by tunneling. Journal of Computational Chemistry, 1999, 20, 1685-1692.	1.5	17
68	Effective way of modeling chemical catalysis: Empirical valence bond picture of role of solvent and catalyst in alkylation reactions. Journal of Computational Chemistry, 2000, 21, 607-625.	1.5	17
69	An Insight into the Regiospecificity of Linoleic Acid Peroxidation Catalyzed by Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2013, 117, 3747-3754.	1.2	17
70	Role of Arg403 for thermostability and catalytic activity of rabbit 12/15-lipoxygenase. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2013, 1831, 1079-1088.	1.2	17
71	Understanding the Molecular Mechanism of the Ala-versus-Gly Concept Controlling the Product Specificity in Reactions Catalyzed by Lipoxygenases: A Combined Molecular Dynamics and QM/MM Study of Coral 8R-Lipoxygenase. ACS Catalysis, 2017, 7, 4854-4866.	5.5	17
72	The search for stationary points on a quantum mechanical/molecular mechanical potential-energy surface. Theoretical Chemistry Accounts, 2002, 107, 147-153.	0.5	16

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73	Canonical Variational Transition-State Theory Study of the CF3CH2CH3 + OH Reaction. Journal of Physical Chemistry B, 2008, 112, 328-335.	1.2	16
74	Excited states and electronic spectra of monosubstituted benzenes. An AM1 study. Spectrochimica Acta Part A: Molecular Spectroscopy, 1988, 44, 1427-1434.	0.1	15
75	A PM3/d specific reaction parameterization for iron atom in the hydrogen abstraction catalyzed by soybean lipoxygenase-1. Journal of Computational Chemistry, 2007, 28, 997-1005.	1.5	15
76	Substrate binding to mammalian 15-lipoxygenase. Journal of Computer-Aided Molecular Design, 2011, 25, 825-835.	1.3	15
77	Theoretical study of several Fe(H2o)n2+clusters at different temperatures. International Journal of Quantum Chemistry, 1986, 29, 1373-1382.	1.0	14
78	How important is the refinement of transition state structures in enzymatic reactions?. Computational and Theoretical Chemistry, 2003, 632, 297-307.	1.5	14
79	New Insights into the Reaction Mechanism Catalyzed by the Glutamate Racemase Enzyme:Â pH Titration Curves and Classical Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2007, 111, 2385-2397.	1.2	13
80	Mutagenesis of Sequence Determinants of Truncated Porcine ALOX15 Induces Changes in the Reaction Specificity by Altering the Catalytic Mechanism of Initial Hydrogen Abstraction. Chemistry - A European Journal, 2018, 24, 962-973.	1.7	13
81	Mutations of Triad Determinants Changes the Substrate Alignment at the Catalytic Center of Human ALOX5. ACS Chemical Biology, 2019, 14, 2768-2782.	1.6	13
82	Rate constants of gas-phase hydrogen abstraction reactions: a balance between the association and the abstraction dynamical bottlenecks. Computational and Theoretical Chemistry, 2004, 709, 35-43.	1.5	12
83	Rate Constants for the Hydrogen Abstractions in the OH-Initiated Oxidation of Glycolaldehyde. A Variational Transition-state Theory Calculation. Journal of Physical Chemistry A, 2004, 108, 5117-5125.	1.1	12
84	Theoretical Analysis of the Catalytic Mechanism of Helicobacter pylori Glutamate Racemase. Journal of Physical Chemistry B, 2012, 116, 12406-12414.	1.2	12
85	A Monte Carlo simulation of free energy relationships for the electron transfer reaction between Fe+and Fe2+in water. Journal of Computational Chemistry, 1991, 12, 1165-1171.	1.5	11
86	The1H NMR Chemical Shift for the Hydroxy Proton of 4-(Dimethylamino)-2â€˜-hydroxychalcone in Chloroform:â€‰ A Theoretical Approach to Its Inverse Dependence on the Temperature. Organic Letters, 2001, 3, 589-592.	2.4	11
87	Test of variational transition state theory with multidimensional tunneling contributions against experimental kinetic isotope effects for the CH n D 4â^'n + OHâ†'P (n=0, 4) reactions. Theoretical Chemistry Accounts, 2002, 108, 38-40.	0.5	11
88	Kinetic Study on the Reaction of OH Radical with Dimethyl Sulfide in the Absence of Oxygen. ChemPhysChem, 2007, 8, 255-263.	1.0	11
89	On the Regioâ€•and Stereospecificity of Arachidonic Acid Peroxidation Catalyzed by Mammalian 15â€Łypoxygenases: A Combined Molecular Dynamics and QM/MM Study. ChemPhysChem, 2013, 14, 3777-3787.	1.0	11
90	Regioâ€•and Stereospecificity in the Oxygenation of Arachidonic Acid Catalyzed by Leu597 Mutants of Rabbit 15â€Łipoxygenase: A QM/MM Study. ChemPhysChem, 2014, 15, 2303-2310.	1.0	11

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91	A QM/MM study of the associative mechanism for the phosphorylation reaction catalyzed by protein kinase A and its D166A mutant. Journal of Computer-Aided Molecular Design, 2014, 28, 1077-1091.	1.3	11
92	Kinetic Isotope Effects as Tools To Reveal Solvation Changes Accompanying a Proton Transfer. A Canonical Unified Statistical Theory Calculation. The Journal of Physical Chemistry, 1996, 100, 19389-19397.	2.9	10
93	Reaction Mechanism of the Mandelate Anion Racemization Catalyzed by Mandelate Racemase Enzyme:Â A QM/MM Molecular Dynamics Free Energy Study. Journal of Physical Chemistry B, 2005, 109, 21089-21101.	1.2	10
94	A Theoretical Study of the Competitive Homolytic/Heterolytic Aniomesolytic Cleavages of Câˆ’O Alkyl Ether Bonds. Journal of Organic Chemistry, 2005, 70, 540-548.	1.7	10
95	An intermolecular potential function for the Fe(II)-H2O system from ab initio calculations. International Journal of Quantum Chemistry, 1986, 30, 663-670.	1.0	9
96	The Cu+â€“H2O interaction potential and its application to the study of [Cu(H2O)n]+clusters at different temperatures. Journal of the Chemical Society, Faraday Transactions 2, 1988, 84, 693-704.	1.1	9
97	On the interpolation of the frequencies of vibrational modes in variational transition state calculations: an adiabatic or diabatic scheme?. Molecular Physics, 1996, 89, 633-644.	0.8	9
98	On the modulation of the substrate activity for the racemization catalyzed by mandelate racemase enzyme. A QM/MM study. Physical Chemistry Chemical Physics, 2002, 4, 5365-5371.	1.3	9
99	Dependence of the rate constants on the treatment of internal rotation modes: The reaction OH + CH3SH â†’ CH3S + H2O as an example. Journal of Computational Chemistry, 2003, 24, 701-706.	1.5	9
100	A Molecular Dynamics Simulation of the Binding Modes of d-Glutamate and d-Glutamine to Glutamate Racemase. Journal of Chemical Theory and Computation, 2005, 1, 737-749.	2.3	9
101	Methanesulfinic Acid Reaction with OH:â€‰ Mechanism, Rate Constants, and Atmospheric Implications. Journal of Physical Chemistry A, 2007, 111, 7825-7832.	1.1	9
102	Formation pathways of DMSO from DMSâ€OH in the presence of O₂ and NO_x: A theoretical study. Journal of Computational Chemistry, 2009, 30, 173-182.	1.5	9
103	Influence of the enzyme phosphorylation state and the substrate on PKA enzyme dynamics. Biophysical Chemistry, 2012, 161, 17-28.	1.5	9
104	On the evaluation of quasi-thermodynamic magnitudes from rate constant values. Influence of the variational and tunnelling contributions. Chemical Physics Letters, 2002, 353, 154-162.	1.2	8
105	Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: A Master Equation Analysis of the Pressure- and Temperature-Dependent Rate Constants. Chemistry - A European Journal, 2007, 13, 1180-1190.	1.7	8
106	Pressure Dependence in the Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: An Electronic Structure Study. ChemPhysChem, 2005, 6, 1567-1573.	1.0	7
107	Comparative study of the prereactive protein kinase A Michaelis complex with Kemptide substrate. Journal of Computer-Aided Molecular Design, 2007, 21, 603-615.	1.3	7
108	A variational transition state theory description of periselectivity effects on cycloadditions of ketenes with cyclopentadiene. Theoretical Chemistry Accounts, 2011, 128, 569-577.	0.5	7

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109	Introducing Mutations to Modify the C13/C9 Ratio in Linoleic Acid Oxygenations Catalyzed by Rabbit 15â€Lipoxygenase: A QM/MM and MD Study. ChemPhysChem, 2014, 15, 4049-4054.	1.0	7
110	Theoretical study of the unimolecular dissociation of the acetone cation radical. Molecular Physics, 1997, 92, 393-398.	0.8	6
111	Formation pathways of CH3SOH from CH3S(OH)CH3 in the presence of O2: a theoretical study. Theoretical Chemistry Accounts, 2009, 123, 93-103.	0.5	6
112	Understanding how cAMP-dependent protein kinase can catalyze phosphoryl transfer in the presence of Ca2+and Sr2+: a QM/MM study. Physical Chemistry Chemical Physics, 2017, 19, 10377-10394.	1.3	6
113	Unraveling the Molecular Details of the Complete Mechanism That Governs the Synthesis of Prostaglandin G2 Catalyzed by Cyclooxygenase-2. ACS Omega, 2019, 4, 2063-2074.	1.6	6
114	Understanding the Molecular Details of the Mechanism That Governs the Oxidation of Arachidonic Acid Catalyzed by Aspirin-Acetylated Cyclooxygenase-2. ACS Catalysis, 2020, 10, 138-153.	5.5	6
115	A role of Gln596 in fine-tuning mammalian ALOX15 specificity, protein stability and allosteric properties. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2020, 1865, 158680.	1.2	6
116	Formation pathways of DMSO₂ in the addition channel of the OHâ€initiated DMS oxidation: A theoretical study. Journal of Computational Chemistry, 2009, 30, 1477-1489.	1.5	5
117	A theoretical study of the DMSÂ·OH scavenging reaction by OH. Its relevance in DMSO formation. Computational and Theoretical Chemistry, 2011, 965, 249-258.	1.1	5
118	Conformational Heterogeneity and Cooperative Effects of Mammalian ALOX15. International Journal of Molecular Sciences, 2021, 22, 3285.	1.8	5
119	Accounting for the instantaneous disorder in the enzymeâ€“substrate Michaelis complex to calculate the Gibbs free energy barrier of an enzyme reaction. Physical Chemistry Chemical Physics, 2021, 23, 13042-13054.	1.3	5
120	Analytical potential from ab initio calculations for the Fe+-H2O and Feo-H2O systems. International Journal of Quantum Chemistry, 1988, 33, 77-85.	1.0	4
121	Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. Theoretical Chemistry Accounts, 2009, 124, 197-215.	0.5	4
122	Is Regioselectivity in the Enzymeâ€Catalyzed Hydroperoxidation of Arachidonic Acid Necessarily Determined by Hydrogen Abstraction? The Case of Rabbit Leu597Ala/Ile663Ala ALOX15 Mutant. ChemPhysChem, 2016, 17, 3321-3332.	1.0	4
123	Unraveling how the Gly526Ser mutation arrests prostaglandin formation from arachidonic acid catalyzed by cyclooxygenase-2: a combined molecular dynamics and QM/MM study. RSC Advances, 2020, 10, 986-997.	1.7	4
124	N-Substituted 5-(1H-Indol-2-yl)-2-methoxyanilines Are Allosteric Inhibitors of the Linoleate Oxygenase Activity of Selected Mammalian ALOX15 Orthologs: Mechanism of Action. Journal of Medicinal Chemistry, 2022, 65, 1979-1995.	2.9	4
125	Molecular Insights into the Regulation of 3-Phosphoinositide-Dependent Protein Kinase 1: Modeling the Interaction between the Kinase and the Pleckstrin Homology Domains. ACS Omega, 2022, 7, 25186-25199.	1.6	4
126	Hydration of Fe+: A Monte Carlo simulation of water clusters and of a dilute aqueous solution. Journal of Computational Chemistry, 1988, 9, 819-826.	1.5	3

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127	On constraining solvent molecule displacements in electron-transfer reactions: a critical discussion. The Journal of Physical Chemistry, 1989, 93, 4677-4682.	2.9	3
128	Effect of the hydrogen bond network in carbonic anhydrase II zinc binding site. A theoretical study. Canadian Journal of Chemistry, 1998, 76, 1027-1032.	0.6	3
129	The effect of electron-withdrawing groups in the fragmentation of the radical anions of benzyl phenyl ethers. Computational and Theoretical Chemistry, 2009, 913, 228-235.	1.5	3
130	The role of acetylated cyclooxygenase-2 in the biosynthesis of resolvin precursors derived from eicosapentaenoic acid. Organic and Biomolecular Chemistry, 2022, 20, 1260-1274.	1.5	3
131	Theoretical Characterization of the Step-by-Step Mechanism of Conversion of Leukotriene A4 to Leukotriene B4 Catalysed by the Enzyme Leukotriene A4 Hydrolase. International Journal of Molecular Sciences, 2022, 23, 3140.	1.8	3
132	Effect of solvent fluctuations in the electron-transfer process between two Fe+ ions. Journal of the Chemical Society Faraday Transactions I, 1989, 85, 1207.	1.0	2
133	Canonical Variational Transition-State Theory Study of the CF3CHFCH2F + OH Reaction. Journal of Physical Chemistry A, 2010, 114, 2768-2777.	1.1	2
134	Variational transitionâ€state theory study of the rate constant of the DMSÂ·OH scavenging reaction by O₂. Journal of Computational Chemistry, 2011, 32, 2104-2118.	1.5	2
135	A protocol to obtain multidimensional quantum tunneling corrections derived from QM(DFT)/MM calculations for an enzyme reaction. Physical Chemistry Chemical Physics, 2020, 22, 27385-27393.	1.3	2
136	The mechanism of exchange of intramolecularly hydrogen-bonded protons in a diamide. Journal of the Chemical Society Perkin Transactions II, 1992, , 1621-1624.	0.9	1
137	Choice of the reaction coordinate in electron-transfer reactions in solution. Journal of the Chemical Society, Faraday Transactions, 1995, 91, 1451-1455.	1.7	1
138	Enthalpies of formation of isopreneâ€™s major oxidation byproducts. Chemical Physics Letters, 2005, 409, 255-259.	1.2	1
139	Deciphering the Molecular Details of the Lipoxin Formation Mechanism in the 5(S),15(S)-DiHpETE Biosynthetic Pathway Catalyzed by Reticulocyte 15-Lipoxygenase-1. Journal of Physical Chemistry B, 2020, 124, 11406-11418.	1.2	1
140	Monte Carlo Simulations of Chemical Reactions in Solution. , 2002, , 125-177.		0