JosÃ© M Lluch

List of Publications by Year
in descending order

283 papers	6,274 citations	71102 41 h-index	133252 59 g-index
289 all docs	289 docs citations	289 times ranked	4969 citing authors

#	Article	IF	Citations
1	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.	6.4	4
2	The role of acetylated cyclooxygenase-2 in the biosynthesis of resolvin precursors derived from eicosapentaenoic acid. Organic and Biomolecular Chemistry, 2022, 20, 1260-1274.	2.8	3
3	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.	4.1	3
4	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.	3.5	4
5	Conformational Heterogeneity and Cooperative Effects of Mammalian ALOX15. International Journal of Molecular Sciences, 2021, 22, 3285.	4.1	5
6	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.	2.8	5
7	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.	11.2	6
8	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.	2.8	2
9	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.	2.6	1
10	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.	2.4	6
11	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.	3.6	4
12	Deciphering the grounds of the suitability of acylhydrazones as efficient photoswitches. Physical Chemistry Chemical Physics, 2019, 21, 16075-16082.	2.8	5
13	Mutations of Triad Determinants Changes the Substrate Alignment at the Catalytic Center of Human ALOX5. ACS Chemical Biology, 2019, 14, 2768-2782.	3.4	13
14	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.	3.5	6
15	Discovery of processive catalysis by an exo-hydrolase with a pocket-shaped active site. Nature Communications, 2019, 10, 2222.	12.8	20
16	Synthetic Photoswitchable Neurotransmitters Based on Bridged Azobenzenes. Organic Letters, 2019, 21, 3780-3784.	4.6	42
17	Comparing Hydrolysis and Transglycosylation Reactions Catalyzed by Thermus thermophilus Î²-Glycosidase. A Combined MD and QM/MM Study. Frontiers in Chemistry, 2019, 7, 200.	3.6	18
18	Rationally designed azobenzene photoswitches for efficient two-photon neuronal excitation. Nature Communications, 2019, 10, 907.	12.8	86

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19	Ultrafast action chemistry in slow motion: atomistic description of the excitation and fluorescence processes in an archetypal fluorescent protein. Physical Chemistry Chemical Physics, 2018, 20, 11067-11080.	2.8	4
20	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.	3.3	13
21	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.	11.2	17
22	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.	2.8	6
23	Computational insights into active site shaping for substrate specificity and reaction regioselectivity in the EXTL2 retaining glycosyltransferase. Organic and Biomolecular Chemistry, 2017, 15, 9095-9107.	2.8	13
24	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.	2.5	19
25	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.	14.6	21
26	The Quest for Photoswitches Activated by Nearâ€Infrared Light: A Theoretical Study of the Photochemistry of BF₂â€Coordinated Azo Derivatives. ChemPhysChem, 2016, 17, 2824-2838.	2.1	6
27	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.	5.3	33
28	Î±1,4-N-Acetylhexosaminyltransferase EXTL2: The Missing Link for Understanding Glycosidic Bond Biosynthesis with Retention of Configuration. ACS Catalysis, 2016, 6, 2577-2589.	11.2	13
29	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.	2.8	22
30	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.	2.1	4
31	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.	7.1	54
32	Chromophore interactions leading to different absorption spectra in mNeptune1 and mCardinal red fluorescent proteins. Physical Chemistry Chemical Physics, 2016, 18, 16964-16976.	2.8	9
33	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.	2.6	18
34	Theoretical Computerâ€Aided Mutagenic Study on the Triple Green Fluorescent Protein Mutant S65T/H148D/Y145F. ChemPhysChem, 2015, 16, 2134-2139.	2.1	3
35	A Native Ternary Complex Trapped in a Crystal Reveals the Catalytic Mechanism of a Retaining Glycosyltransferase. Angewandte Chemie - International Edition, 2015, 54, 9898-9902.	13.8	35
36	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.	2.8	18

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37	QM/MM Studies Reveal How Substrateâ€“Substrate and Enzymeâ€“Substrate Interactions Modulate Retaining Glycosyltransferases Catalysis and Mechanism. Advances in Protein Chemistry and Structural Biology, 2015, 100, 225-254.	2.3	14
38	SP20 Phosphorylation Reaction Catalyzed by Protein Kinase A: QM/MM Calculations Based on Recently Determined Crystallographic Structures. ACS Catalysis, 2015, 5, 4897-4912.	11.2	19
39	Transient low-barrier hydrogen bond in the photoactive state of green fluorescent protein. Physical Chemistry Chemical Physics, 2015, 17, 30876-30888.	2.8	14
40	Molecular modelling of the pH influence in the geometry and the absorbance spectrum of near-infrared TagRFP675 fluorescent protein. Physical Chemistry Chemical Physics, 2015, 17, 29363-29373.	2.8	2
41	Unveiling How an Archetypal Fluorescent Protein Operates: Theoretical Perspective on the Ultrafast Excited State Dynamics of GFP Variant S65T/H148D. Journal of Physical Chemistry B, 2015, 119, 2274-2291.	2.6	16
42	Regioâ€•and Stereospecificity in the Oxygenation of Arachidonic Acid Catalyzed by Leu597 Mutants of Rabbit 15â€Lipoxygenase: A QM/MM Study. ChemPhysChem, 2014, 15, 2303-2310.	2.1	11
43	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.	11.2	39
44	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.	2.1	7
45	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.	2.9	11
46	New insights into the structureâ€“spectrum relationship in S65T/H148D and E222Q/H148D green fluorescent protein mutants: a theoretical assessment. Organic and Biomolecular Chemistry, 2014, 12, 9845-9852.	2.8	5
47	Are There Really Low-Barrier Hydrogen Bonds in Proteins? The Case of Photoactive Yellow Protein. Journal of the American Chemical Society, 2014, 136, 3542-3552.	13.7	51
48	A computational and experimental study of O-glycosylation. Catalysis by human UDP-GalNAc polypeptide:GalNAc transferase-T2. Organic and Biomolecular Chemistry, 2014, 12, 2645-2655.	2.8	39
49	A time-dependent DFT/molecular dynamics study of the proton-wire responsible for the red fluorescence in the LSSmKate2 protein. Highlights in Theoretical Chemistry, 2014, , 133-141.	0.0	0
50	A time-dependent DFT/molecular dynamics study of the proton-wire responsible for the red fluorescence in the LSSmKate2 protein. Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	10
51	An Insight into the Regiospecificity of Linoleic Acid Peroxidation Catalyzed by Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2013, 117, 3747-3754.	2.6	17
52	On the Regioâ€•and Stereospecificity of Arachidonic Acid Peroxidation Catalyzed by Mammalian 15â€Lypoxygenases: A Combined Molecular Dynamics and QM/MM Study. ChemPhysChem, 2013, 14, 3777-3787.	2.1	11
53	Substrate-Assisted and Nucleophilically Assisted Catalysis in Bovine Î±1,3-Galactosyltransferase. Mechanistic Implications for Retaining Glycosyltransferases. Journal of the American Chemical Society, 2013, 135, 7053-7063.	13.7	42
54	A theoretical study of the photochemistry of indigo in its neutral and dianionic (leucoindigo) forms. Physical Chemistry Chemical Physics, 2013, 15, 20236.	2.8	37

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55	How Does the Environment Affect the Absorption Spectrum of the Fluorescent Protein mKeima?. Journal of Chemical Theory and Computation, 2013, 9, 1731-1742.	5.3	24
56	Retaining Glycosyltransferase Mechanism Studied by QM/MM Methods: Lipopolysaccharyl-Î±-1,4-galactosyltransferase C Transfers Î±-Galactose via an Oxocarbenium Ion-like Transition State. Journal of the American Chemical Society, 2012, 134, 4743-4752.	13.7	89
57	Peek at the Potential Energy Surfaces of the LSSmKate1 and LSSmKate2 Proteins. Journal of Physical Chemistry B, 2012, 116, 14302-14310.	2.6	16
58	Theoretical Analysis of the Catalytic Mechanism of Helicobacter pylori Glutamate Racemase. Journal of Physical Chemistry B, 2012, 116, 12406-12414.	2.6	12
59	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.	13.7	40
60	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.	2.6	33
61	Essential role of glutamate 317 in galactosyl transfer by Î±3GalT: a computational study. Carbohydrate Research, 2012, 356, 204-208.	2.3	17
62	Influence of the enzyme phosphorylation state and the substrate on PKA enzyme dynamics. Biophysical Chemistry, 2012, 161, 17-28.	2.8	9
63	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.	2.8	25
64	Photo-deactivation pathways of a double H-bonded photochromic Schiff base investigated by combined theoretical calculations and experimental time-resolved studies. Physical Chemistry Chemical Physics, 2011, 13, 14960.	2.8	51
65	Substrate binding to mammalian 15-lipoxygenase. Journal of Computer-Aided Molecular Design, 2011, 25, 825-835.	2.9	15
66	A variational transition state theory description of periselectivity effects on cycloadditions of ketenes with cyclopentadiene. Theoretical Chemistry Accounts, 2011, 128, 569-577.	1.4	7
67	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.	3.3	2
68	A theoretical study of the DMSÂ·OH scavenging reaction by OH. Its relevance in DMSO formation. Computational and Theoretical Chemistry, 2011, 965, 249-258.	2.5	5
69	A method to compute probability current in generic coordinates. Journal of Chemical Physics, 2011, 134, 074115.	3.0	0
70	Modulating the Photochemistry of Bipyridylic Compounds by Symmetric Substitutions. ChemPhysChem, 2010, 11, 3696-3703.	2.1	5
71	Bipyridyl Derivatives as Photomemory Devices: A Comparative Electronicâ€Structure Study. Chemistry - A European Journal, 2010, 16, 6693-6703.	3.3	20
72	Insights into the Mechanism of Binding of Arachidonic Acid to Mammalian 15-Lipoxygenases. Journal of Physical Chemistry B, 2010, 114, 7037-7046.	2.6	30

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73	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.	2.6	27
74	Canonical Variational Transition-State Theory Study of the CF3CHFCH2F + OH Reaction. Journal of Physical Chemistry A, 2010, 114, 2768-2777.	2.5	2
75	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.	3.3	9
76	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.	3.3	5
77	The 65th birthday of Professor Santiago Olivella Nello. Theoretical Chemistry Accounts, 2009, 123, 1-2.	1.4	0
78	Formation pathways of CH3SOH from CH3S(OH)CH3 in the presence of O2: a theoretical study. Theoretical Chemistry Accounts, 2009, 123, 93-103.	1.4	6
79	Benchmark calculations on models of the phosphoryl transfer reaction catalyzed by protein kinase A. Theoretical Chemistry Accounts, 2009, 124, 197-215.	1.4	4
80	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
81	A Theoretical Assessment of Factors Causing Different Molecular Volumes in Isotopologues. Journal of Physical Chemistry A, 2009, 113, 14161-14169.	2.5	3
82	How the Substrate d-Glutamate Drives the Catalytic Action of Bacillus subtilis Glutamate Racemase. Journal of the American Chemical Society, 2009, 131, 3509-3521.	13.7	23
83	Study of the Photochemical Properties and Conical Intersections of [2,2â€²â€Bipyridyl]â€3â€amineâ€3â€²â€ol. ChemPhysChem, 2008, 9, 2068-2076.	2.1	10
84	A Potential Energy Function for Heterogeneous Proton-Wires. Ground and Photoactive States of the Proton-Wire in the Green Fluorescent Protein. Journal of Chemical Theory and Computation, 2008, 4, 1138-1150.	5.3	40
85	Operation of the Proton Wire in Green Fluorescent Protein. A Quantum Dynamics Simulation. Journal of Physical Chemistry B, 2008, 112, 5500-5511.	2.6	63
86	Canonical Variational Transition-State Theory Study of the CF3CH2CH3 + OH Reaction. Journal of Physical Chemistry B, 2008, 112, 328-335.	2.6	16
87	Exploring the Effects of Intramolecular Vibrational Energy Redistribution on the Operation of the Proton Wire in Green Fluorescent Protein. Journal of Physical Chemistry B, 2008, 112, 13443-13452.	2.6	16
88	Electronic-structure and quantum dynamical study of the photochromism of the aromatic Schiff base salicylideneaniline. Journal of Chemical Physics, 2008, 129, 214308.	3.0	92
89	Electronic and quantum dynamical insight into the ultrafast proton transfer of 1-hydroxy-2-acetonaphthone. Journal of Chemical Physics, 2007, 127, 084318.	3.0	22
90	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.	13.7	96

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91	Secondary Kinetic Isotope Effect on the Photoenolization of Triplet O-Methylanthrones. A Microcanonical Transition State Theory Calculation. Journal of Physical Chemistry A, 2007, 111, 10090-10097.	2.5	1
92	Methanesulfinic Acid Reaction with OH:â€‰ Mechanism, Rate Constants, and Atmospheric Implications. Journal of Physical Chemistry A, 2007, 111, 7825-7832.	2.5	9
93	Theoretical Modeling of Hydroxyl-Radical-Induced Lipid Peroxidation Reactions. Journal of Physical Chemistry B, 2007, 111, 5684-5693.	2.6	46
94	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.	2.6	13
95	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.	3.3	8
96	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.	3.3	15
97	Kinetic Study on the Reaction of OH Radical with Dimethyl Sulfide in the Absence of Oxygen. ChemPhysChem, 2007, 8, 255-263.	2.1	11
98	A Comparative Study on the Photochemistry of Two Bipyridyl Derivatives: [2,2â€²-Bipyridyl]-3,3â€²-diamine and [2,2â€²-Bipyridyl]-3,3â€²-diol. ChemPhysChem, 2007, 8, 1199-1206.	2.1	15
99	Comparative study of the prereactive protein kinase A Michaelis complex with Kemptide substrate. Journal of Computer-Aided Molecular Design, 2007, 21, 603-615.	2.9	7
100	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.	2.6	51
101	Variational Transition-State Theory Study of the Dimethyl Sulfoxide (DMSO) and OH Reactionâ€. Journal of Physical Chemistry A, 2006, 110, 798-808.	2.5	23
102	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.	2.5	33
103	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.	5.3	33
104	Charge-Transfer Ï€Ï€* Excited State in the 7-Azaindole Dimer. A Hybrid Configuration Interactions Singles/Time-Dependent Density Functional Theory Description. Journal of Physical Chemistry A, 2006, 110, 1145-1151.	2.5	30
105	Potential Energy Landscape of the Photoinduced Multiple Proton-Transfer Process in the Green Fluorescent Protein:Â Classical Molecular Dynamics and Multiconfigurational Electronic Structure Calculations. Journal of the American Chemical Society, 2006, 128, 3564-3574.	13.7	80
106	Theoretical Study on the Excited-State Intramolecular Proton Transfer in the Aromatic Schiff Base Salicylidene Methylamine:Â an Electronic Structure and Quantum Dynamical Approach. Journal of Physical Chemistry A, 2006, 110, 4649-4656.	2.5	57
107	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.	13.7	52
108	Molecular modeling of the kinetic isotope effect on the intramolecular hydrogen atom transfer in triplet 6,9-dimethylbenzosuberone. Chemical Physics, 2006, 328, 410-420.	1.9	3

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109	On the intramolecular proton transfer of 3-hydroxyflavone in the first singlet excited state: A theoretical study. Chemical Physics, 2006, 325, 243-250.	1.9	38
110	Theoretical study of the photoinduced intramolecular proton transfer and rotational processes in 2-(2â€²hydroxyphenyl)-4-methyloxazole in gas phase and embedded in Î²-cyclodextrin. Journal of Photochemistry and Photobiology A: Chemistry, 2005, 173, 365-374.	3.9	17
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112	Enthalpies of formation of isopreneâ€™s major oxidation byproducts. Chemical Physics Letters, 2005, 409, 255-259.	2.6	1
113	Electronic structure study of the initiation routes of the dimethyl sulfide oxidation by OH. Journal of Computational Chemistry, 2005, 26, 569-583.	3.3	27
114	Pressure Dependence in the Methyl Vinyl Ketone+OH and Methacrolein+OH Oxidation Reactions: An Electronic Structure Study. ChemPhysChem, 2005, 6, 1567-1573.	2.1	7
115	Elongated Dihydrogen Versus Compressed Dihydride Complexes: The Temperature Dependence of the H-D Spin-Spin Coupling Constant as a Criterion To Distinguish between Them. Chemistry - A European Journal, 2005, 11, 6315-6325.	3.3	20
116	Determination of the Temperature Dependence of the Hâ‹¯D Spinâ‹¯Spin Coupling Constant and the Isotope Effect on the Proton Chemical Shift for the Compressed Dihydride Complex [Cp*Ir(Pâ‹¯P)H2]2+. Journal of the American Chemical Society, 2005, 127, 5632-5640.	13.7	37
117	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.	5.3	9
118	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.	2.6	10
119	A Theoretical Study of the Competitive Homolytic/Heterolytic Aniomesolytic Cleavages of Câ‹¯O Alkyl Ether Bonds. Journal of Organic Chemistry, 2005, 70, 540-548.	3.2	10
120	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.	3.2	29
121	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.	5.3	22
122	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.	2.6	20
123	Fast hydrogen elimination from the [Ru(PH3)3(CO)(H)2] and [Ru(PH3)4(H)2] complexes in the first singlet excited states: A diabatic quantum dynamics study. Journal of Chemical Physics, 2004, 121, 6258-6267.	3.0	4
124	Geometry optimization and transition state search in enzymes: Different options in the microiterative method. International Journal of Quantum Chemistry, 2004, 98, 367-377.	2.0	26
125	Quantum Dynamics Study of the Excited-State Double-Proton Transfer in 2,2â€²-Bipyridyl-3,3â€²-diol. ChemPhysChem, 2004, 5, 1372-1378.	2.1	37
126	Testing electronic structure methods for describing intermolecular H Â· Â· Â· H interactions in supramolecular chemistry. Journal of Computational Chemistry, 2004, 25, 99-105.	3.3	35

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127	Elongated Dihydrogen Complexes: What Remains of the Hâ€"H Bond?. ChemInform, 2004, 35, no.	0.0	0
128	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
129	Photoinduced proton transfer from the green fluorescent protein chromophore to a water molecule: analysis of the transfer coordinate. Chemical Physics Letters, 2004, 396, 202-207.	2.6	34
130	Photo-oxidation of lipids by singlet oxygen: a theoretical study. Chemical Physics Letters, 2004, 398, 336-342.	2.6	23
131	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.	13.7	40
132	Kinetic Isotope Effect on the Photoenolization ofo-Methylanthrone. A Microcanonical Transition State Theory Calculation. Journal of Physical Chemistry A, 2004, 108, 4536-4541.	2.5	6
133	Molecular Dynamics of Excited State Intramolecular Proton Transfer:â€‰ 2-(2â€˜-Hydroxyphenyl)-4-methyloxazole in Gas Phase, Solution, and Protein Environments. Journal of Physical Chemistry B, 2004, 108, 6616-6623.	2.6	22
134	Synthesis and Properties of Compressed Dihydride Complexes of Iridium:Â Theoretical and Spectroscopic Investigations. Journal of the American Chemical Society, 2004, 126, 8813-8822.	13.7	79
135	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.	2.5	12
136	Ground and Excited State Hydrogen Atom Transfer Reactions and Cyclization of 2-Acetylbenzoic Acid. Journal of Physical Chemistry A, 2004, 108, 9331-9341.	2.5	12
137	Elongated dihydrogen complexes: what remains of the Hâ€"H Bond?. Chemical Society Reviews, 2004, 33, 175-182.	38.1	178
138	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.	1.4	25
139	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.	3.3	9
140	How important is the refinement of transition state structures in enzymatic reactions?. Computational and Theoretical Chemistry, 2003, 632, 297-307.	1.5	14
141	A theoretical study of the ground and first excited singlet state proton transfer reaction in isolated 7-azaindoleâ€"water complexes. Chemical Physics, 2003, 290, 319-336.	1.9	51
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