

Vicent Moliner

List of Publications by Year in descending order

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207
papers

4,997
citations

87723

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155451

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215
all docs

215
docs citations

215
times ranked

3731
citing authors

#	ARTICLE	IF	CITATIONS
1	Theoretical insights in enzyme catalysis. <i>Chemical Society Reviews</i> , 2004, 33, 98-107.	18.7	150
2	Revealing the molecular mechanisms of proteolysis of SARS-CoV-2 M ^{pro} by QM/MM computational methods. <i>Chemical Science</i> , 2020, 11, 10626-10630.	3.7	130
3	Transition-state structural refinement with GRACE and CHARMM: Flexible QM/MM modelling for lactate dehydrogenase. <i>Physical Chemistry Chemical Physics</i> , 1999, 1, 1323-1331.	1.3	126
4	Improving the QM/MM Description of Chemical Processes: A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 1008-1016.	2.3	120
5	Unraveling the role of protein dynamics in dihydrofolate reductase catalysis. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2013, 110, 16344-16349.	3.3	119
6	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. <i>Journal of Physical Chemistry B</i> , 2004, 108, 8427-8433.	1.2	95
7	A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction. <i>Journal of the American Chemical Society</i> , 2001, 123, 1709-1712.	6.6	92
8	Mechanism of inhibition of SARS-CoV-2 M ^{pro} by N3 peptidyl Michael acceptor explained by QM/MM simulations and design of new derivatives with tunable chemical reactivity. <i>Chemical Science</i> , 2021, 12, 1433-1444.	3.7	87
9	Theoretical Modeling of Enzyme Catalytic Power: Analysis of Electrostatic and Electrostatic Factors in Catechol O-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2003, 125, 7726-7737.	6.6	79
10	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of Transition State Structure for the Hydride Transfer Step. <i>Journal of the American Chemical Society</i> , 1999, 121, 12140-12147.	6.6	78
11	Dynamic and Electrostatic Effects on the Reaction Catalyzed by HIV-1 Protease. <i>Journal of the American Chemical Society</i> , 2016, 138, 16283-16298.	6.6	68
12	Dynamic Effects on Reaction Rates in a Michael Addition Catalyzed by Chalcone Isomerase. Beyond the Frozen Environment Approach. <i>Journal of the American Chemical Society</i> , 2008, 130, 7477-7488.	6.6	61
13	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. <i>Journal of the American Chemical Society</i> , 2011, 133, 12050-12062.	6.6	61
14	Temperature Dependence of the Kinetic Isotope Effects in Thymidylate Synthase. A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2011, 133, 6692-6702.	6.6	60
15	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. <i>Chemistry - A European Journal</i> , 2003, 9, 984-991.	1.7	57
16	Coupling between Protein and Reaction Dynamics in Enzymatic Processes: Application of Grote-Hynes Theory to Catechol O-Methyltransferase. <i>Journal of the American Chemical Society</i> , 2006, 128, 6186-6193.	6.6	57
17	Increased Dynamic Effects in a Catalytically Compromised Variant of <i>Escherichia coli</i> Dihydrofolate Reductase. <i>Journal of the American Chemical Society</i> , 2013, 135, 18689-18696.	6.6	56
18	A QM/MM Study of the Conformational Equilibria in the Chorismate Mutase Active Site. The Role of the Enzymatic Deformation Energy Contribution. <i>Journal of Physical Chemistry B</i> , 2000, 104, 11308-11315.	1.2	54

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19	Discovery of SARS-CoV-2 M ^{pro} peptide inhibitors from modelling substrate and ligand binding. <i>Chemical Science</i> , 2021, 12, 13686-13703.	3.7	54
20	A Theoretical Analysis of Rate Constants and Kinetic Isotope Effects Corresponding to Different Reactant Valleys in Lactate Dehydrogenase. <i>Journal of the American Chemical Society</i> , 2006, 128, 16851-16863.	6.6	52
21	QM/MM Study of the Enzymatic Biodegradation Mechanism of Polyethylene Terephthalate. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3041-3051.	2.5	52
22	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. <i>Journal of the American Chemical Society</i> , 1997, 119, 6415-6422.	6.6	51
23	QM/MM Determination of Kinetic Isotope Effects for COMT-Catalyzed Methyl Transfer Does Not Support Compression Hypothesis. <i>Journal of the American Chemical Society</i> , 2004, 126, 8634-8635.	6.6	51
24	Theoretical Study of Phosphodiester Hydrolysis in Nucleotide Pyrophosphatase/Phosphodiesterase. Environmental Effects on the Reaction Mechanism. <i>Journal of the American Chemical Society</i> , 2010, 132, 6955-6963.	6.6	51
25	Studying the role of protein dynamics in an SN2 enzyme reaction using free-energy surfaces and solvent coordinates. <i>Nature Chemistry</i> , 2013, 5, 566-571.	6.6	49
26	Computational strategies for the design of new enzymatic functions. <i>Archives of Biochemistry and Biophysics</i> , 2015, 582, 68-79.	1.4	49
27	Protein Conformational Landscapes and Catalysis. Influence of Active Site Conformations in the Reaction Catalyzed by L-Lactate Dehydrogenase. <i>ACS Catalysis</i> , 2015, 5, 1172-1185.	5.5	48
28	Insights on the Origin of Catalysis on Glycine N-Methyltransferase from Computational Modeling. <i>Journal of the American Chemical Society</i> , 2018, 140, 4327-4334.	6.6	48
29	A Theoretical Study of the Catalytic Mechanism of Formate Dehydrogenase. <i>Journal of Physical Chemistry B</i> , 2008, 112, 10012-10022.	1.2	46
30	A Comparative Study of Claisen and Cope Rearrangements Catalyzed by Chorismate Mutase. An Insight into Enzymatic Efficiency: A Transition State Stabilization or Substrate Preorganization?. <i>Journal of the American Chemical Society</i> , 2004, 126, 311-319.	6.6	45
31	A theoretical study of water adsorption on (10-10) and (0001) ZnO surfaces: molecular cluster, basis set and effective core potential dependence. <i>Computational and Theoretical Chemistry</i> , 1995, 330, 347-351.	1.5	44
32	Theoretical Study of the Elimination Kinetics of Carboxylic Acid Derivatives in the Gas Phase. Decomposition of 2-Chloropropionic Acid. <i>Journal of Physical Chemistry A</i> , 1997, 101, 1859-1865.	1.1	44
33	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. <i>Theoretical Chemistry Accounts</i> , 2001, 105, 207-212.	0.5	44
34	On the Nature of the Transition State in CatecholO-Methyltransferase. A Complementary Study Based on Molecular Dynamics and Potential Energy Surface Explorations. <i>Journal of the American Chemical Society</i> , 2005, 127, 10648-10655.	6.6	43
35	Computational design of biological catalysts. <i>Chemical Society Reviews</i> , 2008, 37, 2634.	18.7	41
36	Theoretical Modeling of the Reaction Mechanism of Phosphate Monoester Hydrolysis in Alkaline Phosphatase. <i>Journal of Physical Chemistry B</i> , 2009, 113, 7816-7824.	1.2	41

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37	Theoretical Exploration of the Oxidative Properties of a [(tren ^{Me}) ₂ Cu ₂] ⁺ Adduct Relevant to Copper Monooxygenase Enzymes: Insights into Competitive Dehydrogenation versus Hydroxylation Reaction Pathways. <i>Chemistry - A European Journal</i> , 2008, 14, 6465-6473.	1.7	40
38	Heavy enzymesâ€”experimental and computational insights in enzyme dynamics. <i>Current Opinion in Chemical Biology</i> , 2014, 21, 11-18.	2.8	39
39	A density functional study of flavonoid compounds with anti-HIV activity. <i>European Journal of Medicinal Chemistry</i> , 2006, 41, 616-623.	2.6	38
40	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ€”Ligand Interaction for Inhibitors of HIV-1 Integrase. <i>Chemistry - A European Journal</i> , 2007, 13, 7715-7724.	1.7	38
41	Computational Study of the Catalytic Mechanism of the Cruzain Cysteine Protease. <i>ACS Catalysis</i> , 2017, 7, 1207-1215.	5.5	38
42	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 12478-12482.	7.2	38
43	Theoretical modelling of tripodal CuN ₃ and CuN ₄ cuprous complexes interacting with O ₂ , CO or CH ₃ CN. <i>Journal of Biological Inorganic Chemistry</i> , 2006, 11, 593-608.	1.1	35
44	A Quantum Mechanics/Molecular Mechanics Study of the Catalytic Mechanism of the Thymidylate Synthaseâ€”. <i>Biochemistry</i> , 2007, 46, 3704-3713.	1.2	35
45	Chemical Ligation and Isotope Labeling to Locate Dynamic Effects during Catalysis by Dihydrofolate Reductase. <i>Angewandte Chemie - International Edition</i> , 2015, 54, 9016-9020.	7.2	35
46	Protein Isotope Effects in Dihydrofolate Reductase From <i>Geobacillus stearothermophilus</i> Show Entropicâ€”Enthalpic Compensatory Effects on the Rate Constant. <i>Journal of the American Chemical Society</i> , 2014, 136, 17317-17323.	6.6	34
47	Peptide Bond Formation Mechanism Catalyzed by Ribosome. <i>Journal of the American Chemical Society</i> , 2015, 137, 12024-12034.	6.6	34
48	Binding Isotope Effects as a Tool for Distinguishing Hydrophobic and Hydrophilic Binding Sites of HIV-1 RT. <i>Journal of Physical Chemistry B</i> , 2015, 119, 917-927.	1.2	34
49	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. <i>Tetrahedron</i> , 1996, 52, 10693-10704.	1.0	33
50	Long Distance Electron-Transfer Mechanism in Peptidylglycine Î±-Hydroxylating Monooxygenase: A Perfect Fitting for a Water Bridge. <i>Journal of the American Chemical Society</i> , 2007, 129, 11700-11707.	6.6	33
51	Theoretical kinetic isotope effects for the hydride-transfer step in lactate dehydrogenase. <i>Journal of the Chemical Society, Faraday Transactions</i> , 1994, 90, 1703-1707.	1.7	32
52	On Transition Structures for Hydride Transfer Step: A Theoretical Study of the Reaction Catalyzed by Dihydrofolate Reductase Enzyme. <i>Bioorganic Chemistry</i> , 1996, 24, 10-18.	2.0	32
53	Activation Free Energy of Catechol O-Methyltransferase. Corrections to the Potential of Mean Forceâ€”. <i>Journal of Physical Chemistry A</i> , 2006, 110, 503-509.	1.1	32
54	Predicting enzymatic reactivity: from theory to design. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2014, 4, 407-421.	6.2	32

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55	Intermolecular hydrogen bonding in NLO. Theoretical analysis of the nitroaniline and HF cases. <i>New Journal of Chemistry</i> , 1998, 22, 387-392.	1.4	31
56	QM/MM Study of Thymidylate Synthase: Enzymatic Motions and the Temperature Dependence of the Rate Limiting Step. <i>Journal of Physical Chemistry A</i> , 2009, 113, 2176-2182.	1.1	31
57	Theoretical Study of Primary Reaction of Pseudozyma antarctica Lipase B as the Starting Point To Understand Its Promiscuity. <i>ACS Catalysis</i> , 2014, 4, 426-434.	5.5	31
58	First Quantum Mechanics/Molecular Mechanics Studies of the Inhibition Mechanism of Cruzain by Peptidyl Halomethyl Ketones. <i>Biochemistry</i> , 2015, 54, 3381-3391.	1.2	31
59	Convergence of Theory and Experiment on the Role of Preorganization, Quantum Tunneling, and Enzyme Motions into Flavoenzyme-Catalyzed Hydride Transfer. <i>ACS Catalysis</i> , 2017, 7, 3190-3198.	5.5	31
60	A QM/MM study of the complexes formed by aluminum and iron with serum transferrin at neutral and acidic pH. <i>Journal of Inorganic Biochemistry</i> , 2011, 105, 1446-1456.	1.5	30
61	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from Trypanosoma cruzi elucidated via the QM/MM approach. <i>Physical Chemistry Chemical Physics</i> , 2013, 15, 3772.	1.3	30
62	Transition state structure invariance to model system size and calculation levels: a QM/MM study of the carboxylation step catalyzed by Rubisco. <i>Theoretical Chemistry Accounts</i> , 1999, 101, 228-233.	0.5	29
63	Influence of Compression upon Kinetic Isotope Effects for SN2 Methyl Transfer: A Computational Reappraisal. <i>Journal of the American Chemical Society</i> , 2000, 122, 10895-10902.	6.6	29
64	Computing Kinetic Isotope Effects for Chorismate Mutase with High Accuracy. A New DFT/MM Strategy. <i>Journal of Physical Chemistry B</i> , 2005, 109, 3707-3710.	1.2	29
65	QM/MM calculations of kinetic isotope effects in the chorismate mutase active site. <i>Organic and Biomolecular Chemistry</i> , 2003, 1, 483-487.	1.5	28
66	Vibrational analysis of the chorismate rearrangement: relaxed force constants, isotope effects and activation entropies calculated for reaction in vacuum, water and the active site of chorismate mutase. <i>Journal of Physical Organic Chemistry</i> , 2004, 17, 592-601.	0.9	28
67	Catalysis in Glycine N-Methyltransferase: Testing the Electrostatic Stabilization and Compression Hypothesis. <i>Biochemistry</i> , 2006, 45, 14917-14925.	1.2	28
68	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. <i>Journal of the American Chemical Society</i> , 2009, 131, 16156-16161.	6.6	28
69	Protein Flexibility and Preorganization in the Design of Enzymes. The Kemp Elimination Catalyzed by HG3.17. <i>ACS Catalysis</i> , 2015, 5, 2587-2595.	5.5	28
70	Revealing the mechanism for covalent inhibition of glycoside hydrolases by carbasugars at an atomic level. <i>Nature Communications</i> , 2018, 9, 3243.	5.8	28
71	A Quantum Mechanics/Molecular Mechanics Study of the Protein-Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. <i>Journal of Physical Chemistry B</i> , 2008, 112, 14260-14266.	1.2	27
72	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. <i>Chemistry - A European Journal</i> , 2012, 18, 9612-9621.	1.7	26

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73	A Theoretical Study of Addition of Organomagnesium Reagents to Chiral $\hat{I}\pm$ -Alkoxy Carbonyl Compounds. <i>Journal of Organic Chemistry</i> , 1996, 61, 3467-3475.	1.7	25
74	Predicting an Improvement of Secondary Catalytic Activity of Promiscuous Isochorismate Pyruvate Lyase by Computational Design. <i>Journal of the American Chemical Society</i> , 2008, 130, 2894-2895.	6.6	25
75	Do Dynamic Effects Play a Significant Role in Enzymatic Catalysis? A Theoretical Analysis of Formate Dehydrogenase. <i>Chemistry - A European Journal</i> , 2010, 16, 11399-11411.	1.7	25
76	Minimization of dynamic effects in the evolution of dihydrofolate reductase. <i>Chemical Science</i> , 2016, 7, 3248-3255.	3.7	25
77	Am1 and pm3 transition structure for the hydride transfer. A model of reaction catalyzed by dihydrofolate reductase. <i>Computational and Theoretical Chemistry</i> , 1995, 330, 411-416.	1.5	24
78	A theoretical study of the molecular mechanism for the oxidation of methanol by PQQ. <i>Journal of the American Chemical Society</i> , 1995, 117, 8807-8815.	6.6	24
79	On Transition Structures for Hydride Transfer Step in Enzyme Catalysis. A Comparative Study on Models of Glutathione Reductase Derived from Semiempirical, HF, and DFT Methods. <i>Journal of Organic Chemistry</i> , 1996, 61, 7777-7783.	1.7	24
80	A Theoretical Study of the Favorskii Rearrangement. Calculation of Gas-Phase Reaction Paths and Solvation Effects on the Molecular Mechanism for the Transposition of the $\hat{I}\pm$ -Chlorocyclobutanone. <i>Journal of the American Chemical Society</i> , 1997, 119, 1941-1947.	6.6	24
81	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of the N5 Protonation Step. <i>Journal of Physical Chemistry B</i> , 2003, 107, 14036-14041.	1.2	24
82	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. <i>Angewandte Chemie - International Edition</i> , 2007, 46, 286-290.	7.2	24
83	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of $\hat{I}\pm$ -GlcNAcase. <i>Journal of Physical Chemistry B</i> , 2011, 115, 6764-6775.	1.2	24
84	Theoretical studies of HIV-1 reverse transcriptase inhibition. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12614.	1.3	24
85	Singlet-triplet gaps in large multireference systems: Spin-flip-driven alternatives for bioinorganic modeling. <i>Journal of Chemical Physics</i> , 2007, 126, 035102.	1.2	23
86	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. <i>Biophysical Journal</i> , 2008, 94, 2443-2451.	0.2	23
87	Role of Solvent on Nonenzymatic Peptide Bond Formation Mechanisms and Kinetic Isotope Effects. <i>Journal of the American Chemical Society</i> , 2013, 135, 8708-8719.	6.6	23
88	A QM/MM Exploration of the Potential Energy Surface of Pyruvate to Lactate Transformation Catalyzed by LDH. Improving the Accuracy of Semiempirical Descriptions. <i>Journal of Chemical Theory and Computation</i> , 2005, 1, 750-761.	2.3	22
89	QM/MM Calculations Suggest a Novel Intermediate Following the Proton Abstraction Catalyzed by Thymidylate Synthase. <i>Biochemistry</i> , 2013, 52, 2348-2358.	1.2	20
90	Reaction Mechanism of Organocatalytic Michael Addition of Nitromethane to Cinnamaldehyde: A Case Study on Catalyst Regeneration and Solvent Effects. <i>Journal of Physical Chemistry A</i> , 2018, 122, 451-459.	1.1	20

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91	Quantum Mechanical/Molecular Mechanical Study on the Favorskii Rearrangement in Aqueous Media. <i>Journal of Physical Chemistry B</i> , 2001, 105, 2453-2460.	1.2	19
92	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. <i>Advances in Protein Chemistry and Structural Biology</i> , 2011, 85, 81-142.	1.0	19
93	Computational Analysis of Human OGA Structure in Complex with PUGNAc and NAG-Thiazoline Derivatives. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 2775-2783.	2.5	19
94	Investigation of the Hydroxylation Mechanism of Noncoupled Copper Oxygenases by Ab Initio Molecular Dynamics Simulations. <i>Chemistry - A European Journal</i> , 2013, 19, 17328-17337.	1.7	19
95	Exploring the Origin of Amidase Substrate Promiscuity in CALB by a Computational Approach. <i>ACS Catalysis</i> , 2020, 10, 1938-1946.	5.5	19
96	Quantum Mechanics/Molecular Mechanics Studies of the Mechanism of Falcipain-2 Inhibition by the Epoxysuccinate E64. <i>Biochemistry</i> , 2014, 53, 3336-3346.	1.2	18
97	Catalytic enantioselective epoxidation of nitroalkenes. <i>Chemical Communications</i> , 2016, 52, 10060-10063.	2.2	18
98	Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study. <i>Chemical Physics</i> , 1996, 206, 57-61.	0.9	17
99	Flexible QM/MM modelling embraces alternative mechanisms for lactate dehydrogenase. <i>Chemical Communications</i> , 2000, , 1843-1844.	2.2	17
100	Dependence of enzyme reaction mechanism on protonation state of titratable residues and QM level description: lactate dehydrogenase. <i>Chemical Communications</i> , 2005, , 5873.	2.2	17
101	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. <i>Bioorganic and Medicinal Chemistry</i> , 2007, 15, 3818-3824.	1.4	17
102	Using GroteâHynes Theory To Quantify Dynamical Effects on the Reaction Rate of Enzymatic Processes. The Case of Methyltransferases. <i>Journal of Physical Chemistry B</i> , 2008, 112, 529-534.	1.2	17
103	Application of GroteâHynes Theory to the Reaction Catalyzed by Thymidylate Synthase. <i>Journal of Physical Chemistry B</i> , 2010, 114, 13593-13600.	1.2	17
104	Benchmarking Quantum Mechanics/Molecular Mechanics (QM/MM) Methods on the Thymidylate Synthase-Catalyzed Hydride Transfer. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 1375-1388.	2.3	17
105	Quantum mechanics/molecular mechanics studies of the mechanism of cysteine protease inhibition by peptidyl-2,3-epoxyketones. <i>Physical Chemistry Chemical Physics</i> , 2017, 19, 12740-12748.	1.3	17
106	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M ^{pro} Explored by QM/MM Simulations. <i>ACS Catalysis</i> , 2022, 12, 698-708.	5.5	17
107	IR Spectroscopic study of hydrogen bonding using a metal carbonyl probe. <i>Journal of the Chemical Society Dalton Transactions</i> , 1999, , 3893-3898.	1.1	16
108	Intrinsically Competitive Photoinduced Polycyclization and Double-Bond Shift through a Boatlike Conical Intersection. <i>Angewandte Chemie - International Edition</i> , 2001, 40, 1466-1468.	7.2	16

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109	Theoretical Modeling on the Reaction Mechanism of p-Nitrophenylmethylphosphate Alkaline Hydrolysis and its Kinetic Isotope Effects. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 439-442.	2.3	16
110	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of <i>CpNagI</i> in Complex with PUGNAc. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7029-7036.	1.2	16
111	Understanding the different activities of highly promiscuous MbtI by computational methods. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 3482.	1.3	16
112	Revealing the Origin of the Efficiency of the De Novo Designed Kemp Eliminase HG3.17 by Comparison with the Former Developed HG3. <i>Chemistry - A European Journal</i> , 2017, 23, 7582-7589.	1.7	16
113	QM/MM Theoretical Studies of a de Novo Retro-Aldolase Design. <i>ACS Catalysis</i> , 2019, 9, 2482-2492.	5.5	16
114	An AM1 theoretical study on the effect of Zn ²⁺ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. <i>Tetrahedron</i> , 2002, 58, 2695-2700.	1.0	15
115	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. <i>Physical Chemistry Chemical Physics</i> , 2010, 12, 11657.	1.3	15
116	The influence of active site conformations on the hydride transfer step of the thymidylate synthase reaction mechanism. <i>Physical Chemistry Chemical Physics</i> , 2015, 17, 30793-30804.	1.3	15
117	Quantum Mechanics/Molecular Mechanics Studies of the Mechanism of Cysteine Proteases Inhibition by Dipeptidyl Nitroalkenes. <i>Chemistry - A European Journal</i> , 2020, 26, 2002-2012.	1.7	15
118	A PM3 Quantum Chemical Study of the Pyruvate Reduction Mechanism Catalyzed by Lactate Dehydrogenase. <i>Bioorganic Chemistry</i> , 1993, 21, 260-274.	2.0	14
119	"Eppur si muove" (yet it moves). <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 15013-15014.	3.3	14
120	Computational Study of the Michaelis Complex Formation and the Effect on the Reaction Mechanism of Cruzain Cysteine Protease. <i>ACS Omega</i> , 2018, 3, 18613-18622.	1.6	14
121	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. <i>Angewandte Chemie</i> , 2018, 130, 12658-12662.	1.6	14
122	Conformational equilibrium of chorismate. A QM/MM theoretical study combining statistical simulations and geometry optimisations in gas phase and in aqueous solution. <i>Computational and Theoretical Chemistry</i> , 2003, 632, 197-206.	1.5	13
123	The effect of MM polarization on the QM/MM transition state stabilization: application to chorismate mutase. <i>Molecular Physics</i> , 2008, 106, 1511-1515.	0.8	13
124	A theoretical study of carbon-carbon bond formation by a Michael-type addition. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 5598.	1.5	13
125	A density functional theory analysis of the gas and solution phase isomerization reactions of MCN, (M) Tj ETQq1 1 0.784314 rgBT /Over	1.5	12
126	Why Are Some Enzymes Dimers? Flexibility and Catalysis in <i>Thermotoga maritima</i> Dihydrofolate Reductase. <i>ACS Catalysis</i> , 2019, 9, 5902-5911.	5.5	12

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127	Theoretical study of the inhibition mechanism of human 20S proteasome by dihydroeponemycin. <i>European Journal of Medicinal Chemistry</i> , 2019, 164, 399-407.	2.6	12
128	Glycoside hydrolase stabilization of transition state charge: new directions for inhibitor design. <i>Chemical Science</i> , 2020, 11, 10488-10495.	3.7	12
129	Electrostatic effects in enzyme catalysis: a quantum mechanics/molecular mechanics study of the nucleophilic substitution reaction in haloalkane dehalogenase. <i>Theoretical Chemistry Accounts</i> , 2004, 112, 327.	0.5	11
130	Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their CuM Coordination Sphere. <i>Inorganic Chemistry</i> , 2009, 48, 7003-7005.	1.9	11
131	Tuning the Phosphoryl Donor Specificity of Dihydroxyacetone Kinase from ATP to Inorganic Polyphosphate. An Insight from Computational Studies. <i>International Journal of Molecular Sciences</i> , 2015, 16, 27835-27849.	1.8	11
132	Transition-state structures for describing the enzyme-catalyzed mechanisms of rubisco. <i>Theoretical Chemistry Accounts</i> , 1999, 101, 234-240.	0.5	10
133	A Novel Strategy to Study Electrostatic Effects in Chemical Reactions: Differences between the Role of Solvent and the Active Site of Chalcone Isomerase in a Michael Addition. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1532-1535.	2.3	10
134	Is Promiscuous CALB a Good Scaffold for Designing New Epoxidases?. <i>Molecules</i> , 2015, 20, 17789-17806.	1.7	10
135	QM/MM study of lactate oxidation by flavocytochrome b ₂ . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 15609-15618.	1.3	10
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