Vicent Moliner

List of Publications by Year
in descending order

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207	4,997	87888	155660
papers	citations	38 h-index	55 g-index

215	215	215	3731
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Theoretical insights in enzyme catalysis. Chemical Society Reviews, 2004, 33, 98-107.	38.1	150
2	Revealing the molecular mechanisms of proteolysis of SARS-CoV-2 M^{pro}by QM/MM computational methods. Chemical Science, 2020, 11, 10626-10630.	7.4	130
3	Transition-state structural refinement with GRACE and CHARMM: Flexible QM/MM modelling for lactate dehydrogenase. Physical Chemistry Chemical Physics, 1999, 1, 1323-1331.	2.8	126
4	Improving the QM/MM Description of Chemical Processes:Â A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. Journal of Chemical Theory and Computation, 2005, 1, 1008-1016.	5.3	120
5	Unraveling the role of protein dynamics in dihydrofolate reductase catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 16344-16349.	7.1	119
6	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. Journal of Physical Chemistry B, 2004, 108, 8427-8433.	2.6	95
7	A Hybrid Potential Reaction Path and Free Energy Study of the Chorismate Mutase Reaction. Journal of the American Chemical Society, 2001, 123, 1709-1712.	13.7	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. Chemical Science, 2021, 12, 1433-1444.	7.4	87
9	Theoretical Modeling of Enzyme Catalytic Power:Â Analysis of â€œCraticâ€•and Electrostatic Factors in CatecholO-Methyltransferase. Journal of the American Chemical Society, 2003, 125, 7726-7737.	13.7	79
10	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of Transition State Structure for the Hydride Transfer Step. Journal of the American Chemical Society, 1999, 121, 12140-12147.	13.7	78
11	Dynamic and Electrostatic Effects on the Reaction Catalyzed by HIV-1 Protease. Journal of the American Chemical Society, 2016, 138, 16283-16298.	13.7	68
12	Dynamic Effects on Reaction Rates in a Michael Addition Catalyzed by Chalcone Isomerase. Beyond the Frozen Environment Approach. Journal of the American Chemical Society, 2008, 130, 7477-7488.	13.7	61
13	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. Journal of the American Chemical Society, 2011, 133, 12050-12062.	13.7	61
14	Temperature Dependence of the Kinetic Isotope Effects in Thymidylate Synthase. A Theoretical Study. Journal of the American Chemical Society, 2011, 133, 6692-6702.	13.7	60
15	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. Chemistry - A European Journal, 2003, 9, 984-991.	3.3	57
16	Coupling between Protein and Reaction Dynamics in Enzymatic Processes:Â Application of Groteâ^'Hynes Theory to CatecholO-Methyltransferase. Journal of the American Chemical Society, 2006, 128, 6186-6193.	13.7	57
17	Increased Dynamic Effects in a Catalytically Compromised Variant of Escherichia coli Dihydrofolate Reductase. Journal of the American Chemical Society, 2013, 135, 18689-18696.	13.7	56
18	A QM/MM Study of the Conformational Equilibria in the Chorismate Mutase Active Site. The Role of the Enzymatic Deformation Energy Contribution. Journal of Physical Chemistry B, 2000, 104, 11308-11315.	2.6	54

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19	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	7.4	54
20	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
21	QM/MM Study of the Enzymatic Biodegradation Mechanism of Polyethylene Terephthalate. Journal of Chemical Information and Modeling, 2021, 61, 3041-3051.	5.4	52
22	Theoretical Study of the Gas Phase Decomposition of Glycolic, Lactic, and 2-Hydroxyisobutyric Acids. Journal of the American Chemical Society, 1997, 119, 6415-6422.	13.7	51
23	QM/MM Determination of Kinetic Isotope Effects for COMT-Catalyzed Methyl Transfer Does Not Support Compression Hypothesis. Journal of the American Chemical Society, 2004, 126, 8634-8635.	13.7	51
24	Theoretical Study of Phosphodiester Hydrolysis in Nucleotide Pyrophosphatase/Phosphodiesterase. Environmental Effects on the Reaction Mechanism. Journal of the American Chemical Society, 2010, 132, 6955-6963.	13.7	51
25	Studying the role of protein dynamics in an SN2 enzyme reaction using free-energy surfaces and solvent coordinates. Nature Chemistry, 2013, 5, 566-571.	13.6	49
26	Computational strategies for the design of new enzymatic functions. Archives of Biochemistry and Biophysics, 2015, 582, 68-79.	3.0	49
27	Protein Conformational Landscapes and Catalysis. Influence of Active Site Conformations in the Reaction Catalyzed by L-Lactate Dehydrogenase. ACS Catalysis, 2015, 5, 1172-1185.	11.2	48
28	Insights on the Origin of Catalysis on Glycine N-Methyltransferase from Computational Modeling. Journal of the American Chemical Society, 2018, 140, 4327-4334.	13.7	48
29	A Theoretical Study of the Catalytic Mechanism of Formate Dehydrogenase. Journal of Physical Chemistry B, 2008, 112, 10012-10022.	2.6	46
30	A Comparative Study of Claisen and Cope Rearrangements Catalyzed by Chorismate Mutase. An Insight into Enzymatic Efficiency:Â Transition State Stabilization or Substrate Preorganization?. Journal of the American Chemical Society, 2004, 126, 311-319.	13.7	45
31	A theoretical study of water adsorption on (10-10) and (0001) ZnO surfaces: molecular cluster, basis set and effective core potential dependence. Computational and Theoretical Chemistry, 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. Journal of Physical Chemistry A, 1997, 101, 1859-1865.	2.5	44
33	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. Theoretical Chemistry Accounts, 2001, 105, 207-212.	1.4	44
34	On the Nature of the Transition State in CatecholO-Methyltransferase. A Complementary Study Based on Molecular Dynamics and Potential Energy Surface Explorations. Journal of the American Chemical Society, 2005, 127, 10648-10655.	13.7	43
35	Computational design of biological catalysts. Chemical Society Reviews, 2008, 37, 2634.	38.1	41
36	Theoretical Modeling of the Reaction Mechanism of Phosphate Monoester Hydrolysis in Alkaline Phosphatase. Journal of Physical Chemistry B, 2009, 113, 7816-7824.	2.6	41

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37	Theoretical Exploration of the Oxidative Properties of a [(tren^{Me1})CuO₂]⁺ Adduct Relevant to Copper Monooxygenase Enzymes: Insights into Competitive Dehydrogenation versus Hydroxylation Reaction Pathways. Chemistry - A European Journal, 2008, 14, 6465-6473.	3.3	40
38	Heavy enzymesâ€"experimental and computational insights in enzyme dynamics. Current Opinion in Chemical Biology, 2014, 21, 11-18.	6.1	39
39	A density functional study ofÂflavonoid compounds with anti-HIV activity. European Journal of Medicinal Chemistry, 2006, 41, 616-623.	5.5	38
40	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ€"Ligand Interaction for Inhibitors of HIV-1 Integrase. Chemistry - A European Journal, 2007, 13, 7715-7724.	3.3	38
41	Computational Study of the Catalytic Mechanism of the Cruzain Cysteine Protease. ACS Catalysis, 2017, 7, 1207-1215.	11.2	38
42	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie - International Edition, 2018, 57, 12478-12482.	13.8	38
43	Theoretical modelling of tripodal CuN3 and CuN4 cuprous complexes interacting with O2, CO or CH3CN. Journal of Biological Inorganic Chemistry, 2006, 11, 593-608.	2.6	35
44	A Quantum Mechanics/Molecular Mechanics Study of the Catalytic Mechanism of the Thymidylate Synthaseâ€. Biochemistry, 2007, 46, 3704-3713.	2.5	35
45	Chemical Ligation and Isotope Labeling to Locate Dynamic Effects during Catalysis by Dihydrofolate Reductase. Angewandte Chemie - International Edition, 2015, 54, 9016-9020.	13.8	35
46	Protein Isotope Effects in Dihydrofolate Reductase From Geobacillus stearothermophilus Show Entropicâ€"Enthalpic Compensatory Effects on the Rate Constant. Journal of the American Chemical Society, 2014, 136, 17317-17323.	13.7	34
47	Peptide Bond Formation Mechanism Catalyzed by Ribosome. Journal of the American Chemical Society, 2015, 137, 12024-12034.	13.7	34
48	Binding Isotope Effects as a Tool for Distinguishing Hydrophobic and Hydrophilic Binding Sites of HIV-1 RT. Journal of Physical Chemistry B, 2015, 119, 917-927.	2.6	34
49	Theoretical study of the solvent effects on the mechanisms of addition of dimethyl acetylenedicarboxylate to 1-methyl-2-vinylpyrrole. Tetrahedron, 1996, 52, 10693-10704.	1.9	33
50	Long Distance Electron-Transfer Mechanism in Peptidylglycine Î±-Hydroxylating Monooxygenase:â€‰ A Perfect Fitting for a Water Bridge. Journal of the American Chemical Society, 2007, 129, 11700-11707.	13.7	33
51	Theoretical kinetic isotope effects for the hydride-transfer step in lactate dehydrogenase. Journal of the Chemical Society, Faraday Transactions, 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. Bioorganic Chemistry, 1996, 24, 10-18.	4.1	32
53	Activation Free Energy of CatecholO-Methyltransferase. Corrections to the Potential of Mean Forceâ€. Journal of Physical Chemistry A, 2006, 110, 503-509.	2.5	32
54	Predicting enzymatic reactivity: from theory to design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 407-421.	14.6	32

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55	Intermolecular hydrogen bonding in NLO. Theoretical analysis of the nitroaniline and HF cases. New Journal of Chemistry, 1998, 22, 387-392.	2.8	31
56	QM/MM Study of Thymidylate Synthase: Enzymatic Motions and the Temperature Dependence of the Rate Limiting Step. Journal of Physical Chemistry A, 2009, 113, 2176-2182.	2.5	31
57	Theoretical Study of Primary Reaction of Pseudozyma antarctica Lipase B as the Starting Point To Understand Its Promiscuity. ACS Catalysis, 2014, 4, 426-434.	11.2	31
58	First Quantum Mechanics/Molecular Mechanics Studies of the Inhibition Mechanism of Cruzain by Peptidyl Halomethyl Ketones. Biochemistry, 2015, 54, 3381-3391.	2.5	31
59	Convergence of Theory and Experiment on the Role of Preorganization, Quantum Tunneling, and Enzyme Motions into Flavoenzyme-Catalyzed Hydride Transfer. ACS Catalysis, 2017, 7, 3190-3198.	11.2	31
60	A QM/MM study of the complexes formed by aluminum and iron with serum transferrin at neutral and acidic pH. Journal of Inorganic Biochemistry, 2011, 105, 1446-1456.	3.5	30
61	The catalytic mechanism of glyceraldehyde 3-phosphate dehydrogenase from Trypanosoma cruzi elucidated via the QM/MM approach. Physical Chemistry Chemical Physics, 2013, 15, 3772.	2.8	30
62	Transition state structure invariance to model system size and calculation levels: a QM/MM study of the carboxylation step catalyzed by Rubisco. Theoretical Chemistry Accounts, 1999, 101, 228-233.	1.4	29
63	Influence of Compression upon Kinetic Isotope Effects for SN2 Methyl Transfer:Â A Computational Reappraisal. Journal of the American Chemical Society, 2000, 122, 10895-10902.	13.7	29
64	Computing Kinetic Isotope Effects for Chorismate Mutase with High Accuracy. A New DFT/MM Strategy. Journal of Physical Chemistry B, 2005, 109, 3707-3710.	2.6	29
65	QM/MM calculations of kinetic isotope effects in the chorismate mutase active site. Organic and Biomolecular Chemistry, 2003, 1, 483-487.	2.8	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. Journal of Physical Organic Chemistry, 2004, 17, 592-601.	1.9	28
67	Catalysis in Glycine N-Methyltransferase:â€‰ Testing the Electrostatic Stabilization and Compression Hypothesis. Biochemistry, 2006, 45, 14917-14925.	2.5	28
68	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. Journal of the American Chemical Society, 2009, 131, 16156-16161.	13.7	28
69	Protein Flexibility and Preorganization in the Design of Enzymes. The Kemp Elimination Catalyzed by HG3.17. ACS Catalysis, 2015, 5, 2587-2595.	11.2	28
70	Revealing the mechanism for covalent inhibition of glycoside hydrolases by carbasugars at an atomic level. Nature Communications, 2018, 9, 3243.	12.8	28
71	A Quantum Mechanics/Molecular Mechanics Study of the Proteinâ^'Ligand Interaction of Two Potent Inhibitors of Human O-GlcNAcase: PUGNAc and NAG-Thiazoline. Journal of Physical Chemistry B, 2008, 112, 14260-14266.	2.6	27
72	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. Chemistry - A European Journal, 2012, 18, 9612-9621.	3.3	26

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73	A Theoretical Study of Addition of Organomagnesium Reagents to Chiral Î±-Alkoxy Carbonyl Compounds. Journal of Organic Chemistry, 1996, 61, 3467-3475.	3.2	25
74	Predicting an Improvement of Secondary Catalytic Activity of Promiscuos Isochorismate Pyruvate Lyase by Computational Design. Journal of the American Chemical Society, 2008, 130, 2894-2895.	13.7	25
75	Do Dynamic Effects Play a Significant Role in Enzymatic Catalysis? A Theoretical Analysis of Formate Dehydrogenase. Chemistry - A European Journal, 2010, 16, 11399-11411.	3.3	25
76	Minimization of dynamic effects in the evolution of dihydrofolate reductase. Chemical Science, 2016, 7, 3248-3255.	7.4	25
77	Am1 and pm3 transition structure for the hydride transfer. A model of reaction catalyzed by dihydrofolate reductase. Computational and Theoretical Chemistry, 1995, 330, 411-416.	1.5	24
78	A theoretical study of the molecular mechanism for the oxidation of methanol by PQQ. Journal of the American Chemical Society, 1995, 117, 8807-8815.	13.7	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. Journal of Organic Chemistry, 1996, 61, 7777-7783.	3.2	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 Î±-Chlorocyclobutanone. Journal of the American Chemical Society, 1997, 119, 1941-1947.	13.7	24
81	Catalytic Mechanism of Dihydrofolate Reductase Enzyme. A Combined Quantum-Mechanical/Molecular-Mechanical Characterization of the N5 Protonation Step. Journal of Physical Chemistry B, 2003, 107, 14036-14041.	2.6	24
82	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. Angewandte Chemie - International Edition, 2007, 46, 286-290.	13.8	24
83	Enzyme Molecular Mechanism as a Starting Point to Design New Inhibitors: A Theoretical Study of O-GlcNAcase. Journal of Physical Chemistry B, 2011, 115, 6764-6775.	2.6	24
84	Theoretical studies of HIV-1 reverse transcriptase inhibition. Physical Chemistry Chemical Physics, 2012, 14, 12614.	2.8	24
85	Singlet-triplet gaps in large multireference systems: Spin-flip-driven alternatives for bioinorganic modeling. Journal of Chemical Physics, 2007, 126, 035102.	3.0	23
86	A Quantum Mechanic/Molecular Mechanic Study of the Wild-Type and N155S Mutant HIV-1 Integrase Complexed with Diketo Acid. Biophysical Journal, 2008, 94, 2443-2451.	0.5	23
87	Role of Solvent on Nonenzymatic Peptide Bond Formation Mechanisms and Kinetic Isotope Effects. Journal of the American Chemical Society, 2013, 135, 8708-8719.	13.7	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. Journal of Chemical Theory and Computation, 2005, 1, 750-761.	5.3	22
89	QM/MM Calculations Suggest a Novel Intermediate Following the Proton Abstraction Catalyzed by Thymidylate Synthase. Biochemistry, 2013, 52, 2348-2358.	2.5	20
90	Reaction Mechanism of Organocatalytic Michael Addition of Nitromethane to Cinnamaldehyde: A Case Study on Catalyst Regeneration and Solvent Effects. Journal of Physical Chemistry A, 2018, 122, 451-459.	2.5	20

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91	Quantum Mechanical/Molecular Mechanical Study on the Favorskii Rearrangement in Aqueous Media. Journal of Physical Chemistry B, 2001, 105, 2453-2460.	2.6	19
92	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. Advances in Protein Chemistry and Structural Biology, 2011, 85, 81-142.	2.3	19
93	Computational Analysis of Human OGA Structure in Complex with PUGNAc and NAG-Thiazoline Derivatives. Journal of Chemical Information and Modeling, 2012, 52, 2775-2783.	5.4	19
94	Investigation of the Hydroxylation Mechanism of Noncoupled Copper Oxygenases by Ab Initio Molecular Dynamics Simulations. Chemistry - A European Journal, 2013, 19, 17328-17337.	3.3	19
95	Exploring the Origin of Amidase Substrate Promiscuity in CALB by a Computational Approach. ACS Catalysis, 2020, 10, 1938-1946.	11.2	19
96	Quantum Mechanics/Molecular Mechanics Studies of the Mechanism of Falcipain-2 Inhibition by the Epoxysuccinate E64. Biochemistry, 2014, 53, 3336-3346.	2.5	18
97	Catalytic enantioselective epoxidation of nitroalkenes. Chemical Communications, 2016, 52, 10060-10063.	4.1	18
98	Rotational constants and dipole moments of interstellar polyynes: a comparative MP2 and density functional (BP86) study. Chemical Physics, 1996, 206, 57-61.	1.9	17
99	Flexible QM/MM modelling embraces alternative mechanisms for lactate dehydrogenase. Chemical Communications, 2000, , 1843-1844.	4.1	17
100	Dependence of enzyme reaction mechanism on protonation state of titratable residues and QM level description: lactate dehydrogenase. Chemical Communications, 2005, , 5873.	4.1	17
101	Calculation of binding energy using BLYP/MM for the HIV-1 integrase complexed with the S-1360 and two analogues. Bioorganic and Medicinal Chemistry, 2007, 15, 3818-3824.	3.0	17
102	Using Groteâ^'Hynes Theory To Quantify Dynamical Effects on the Reaction Rate of Enzymatic Processes. The Case of Methyltransferases. Journal of Physical Chemistry B, 2008, 112, 529-534.	2.6	17
103	Application of Groteâ^'Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. Journal of Physical Chemistry B, 2010, 114, 13593-13600.	2.6	17
104	Benchmarking Quantum Mechanics/Molecular Mechanics (QM/MM) Methods on the Thymidylate Synthase-Catalyzed Hydride Transfer. Journal of Chemical Theory and Computation, 2017, 13, 1375-1388.	5.3	17
105	Quantum mechanics/molecular mechanics studies of the mechanism of cysteine protease inhibition by peptidyl-2,3-epoxyketones. Physical Chemistry Chemical Physics, 2017, 19, 12740-12748.	2.8	17
106	Impact of Warhead Modulations on the Covalent Inhibition of SARS-CoV-2 M^{pro} Explored by QM/MM Simulations. ACS Catalysis, 2022, 12, 698-708.	11.2	17
107	IR Spectroscopic study of hydrogen bonding using a metal carbonyl probe. Journal of the Chemical Society Dalton Transactions, 1999, , 3893-3898.	1.1	16
108	Intrinsically Competitive Photoinduced Polycyclization and Double-Bond Shift through a Boatlike Conical Intersection. Angewandte Chemie - International Edition, 2001, 40, 1466-1468.	13.8	16

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109	Theoretical Modeling on the Reaction Mechanism of p-Nitrophenylmethylphosphate Alkaline Hydrolysis and its Kinetic Isotope Effects. Journal of Chemical Theory and Computation, 2009, 5, 439-442.	5.3	16
110	Quantum Mechanical/Molecular Mechanical Molecular Dynamics Simulation of Wild-Type and Seven Mutants of CpNagJ in Complex with PUGNAc. Journal of Physical Chemistry B, 2010, 114, 7029-7036.	2.6	16
111	Understanding the different activities of highly promiscuous MbtI by computational methods. Physical Chemistry Chemical Physics, 2012, 14, 3482.	2.8	16
112	Revealing the Origin of the Efficiency of the De Novo Designed Kemp Eliminase HGâ€3.17 by Comparison with the Former Developed HGâ€3. Chemistry - A European Journal, 2017, 23, 7582-7589.	3.3	16
113	QM/MM Theoretical Studies of a de Novo Retro-Aldolase Design. ACS Catalysis, 2019, 9, 2482-2492.	11.2	16
114	An AM1 theoretical study on the effect of Zn2+ Lewis acid catalysis on the mechanism of the cycloaddition between 3-phenyl-1-(2-pyridyl)-2-propen-1-one and cyclopentadiene. Tetrahedron, 2002, 58, 2695-2700.	1.9	15
115	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. Physical Chemistry Chemical Physics, 2010, 12, 11657.	2.8	15
116	The influence of active site conformations on the hydride transfer step of the thymidylate synthase reaction mechanism. Physical Chemistry Chemical Physics, 2015, 17, 30793-30804.	2.8	15
117	Quantum Mechanics/Molecular Mechanics Studies of the Mechanism of Cysteine Proteases Inhibition by Dipeptidyl Nitroalkenes. Chemistry - A European Journal, 2020, 26, 2002-2012.	3.3	15
118	A PM3 Quantum Chemical Study of the Pyruvate Reduction Mechanism Catalyzed by Lactate Dehydrogenase. Bioorganic Chemistry, 1993, 21, 260-274.	4.1	14
119	"Eppur si muove" (yet it moves). Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 15013-15014.	7.1	14
120	Computational Study of the Michaelis Complex Formation and the Effect on the Reaction Mechanism of Cruzain Cysteine Protease. ACS Omega, 2018, 3, 18613-18622.	3.5	14
121	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie, 2018, 130, 12658-12662.	2.0	14
122	Conformational equilibrium of chorismate. A QM/MM theoretical study combining statistical simulations and geometry optimisations in gas phase and in aqueous solution. Computational and Theoretical Chemistry, 2003, 632, 197-206.	1.5	13
123	The effect of MM polarization on the QM/MM transition state stabilization: application to chorismate mutase. Molecular Physics, 2008, 106, 1511-1515.	1.7	13
124	A theoretical study of carbonâ€“carbon bond formation by a Michael-type addition. Organic and Biomolecular Chemistry, 2012, 10, 5598.	2.8	13
125	A density functional theory analysis of the gas and solution phase isomerization reactions of MCN, (M) Tj ETQq1 1 0.784314 rgBT /Ov	1.5	12
126	Why Are Some Enzymes Dimers? Flexibility and Catalysis in Thermotoga maritima Dihydrofolate Reductase. ACS Catalysis, 2019, 9, 5902-5911.	11.2	12

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127	Theoretical study of the inhibition mechanism of human 20S proteasome by dihydroeponemycin. European Journal of Medicinal Chemistry, 2019, 164, 399-407.	5.5	12
128	Glycoside hydrolase stabilization of transition state charge: new directions for inhibitor design. Chemical Science, 2020, 11, 10488-10495.	7.4	12
129	Electrostatic effects in enzyme catalysis: a quantum mechanics/molecular mechanics study of the nucleophilic substitution reaction in haloalkane dehalogenase. Theoretical Chemistry Accounts, 2004, 112, 327.	1.4	11
130	Dioxygen Activation by Mononuclear Copper Enzymes: Insights from a Tripodal Ligand Mimicking Their CuM Coordination Sphere. Inorganic Chemistry, 2009, 48, 7003-7005.	4.0	11
131	Tuning the Phosphoryl Donor Specificity of Dihydroxyacetone Kinase from ATP to Inorganic Polyphosphate. An Insight from Computational Studies. International Journal of Molecular Sciences, 2015, 16, 27835-27849.	4.1	11
132	Transition-state structures for describing the enzyme-catalyzed mechanisms of rubisco. Theoretical Chemistry Accounts, 1999, 101, 234-240.	1.4	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. Journal of Chemical Theory and Computation, 2012, 8, 1532-1535.	5.3	10
134	Is Promiscuous CALB a Good Scaffold for Designing New Epoxidases?. Molecules, 2015, 20, 17789-17806.	3.8	10
135	QM/MM study of<scp>l</scp>-lactate oxidation by flavocytochrome b₂. Physical Chemistry Chemical Physics, 2016, 18, 15609-15618.	2.8	10
136	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. Angewandte Chemie - International Edition, 2018, 57, 3128-3131.	13.8	10
137	Transfer hydrogenations catalyzed by streptavidin-hosted secondary amine organocatalysts. Chemical Communications, 2021, 57, 1919-1922.	4.1	10
138	Enzymatic Î”¹-Dehydrogenation of 3-Ketosteroidsâ€”Reconciliation of Kinetic Isotope Effects with the Reaction Mechanism. ACS Catalysis, 2021, 11, 8211-8225.	11.2	10
139	A theoretical study of the unimolecular decomposition of N-chloro-Î±-amino acids in aqueous solution. Chemical Physics, 1998, 229, 125-136.	1.9	9
140	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie - International Edition, 2005, 44, 904-909.	13.8	9
141	Theoretical Study of Catalytic Efficiency of a Dielsâ€“Alderase Catalytic Antibody: An Indirect Effect Produced During the Maturation Process. Chemistry - A European Journal, 2008, 14, 596-602.	3.3	9
142	Selective oxidation of alkyl and aryl glyceryl monoethers catalysed by an engineered and immobilised glycerol dehydrogenase. Chemical Science, 2020, 11, 12009-12020.	7.4	9
143	Nature of Irreversible Inhibition of Human 20S Proteasome by Salinosporamide A. The Critical Role of Lysâ€“Asp Dyad Revealed from Electrostatic Effects Analysis. ACS Catalysis, 2021, 11, 3575-3589.	11.2	9
144	A theoretical study of the effect of basis sets on stationary structures for the addition of carbon dioxide to methylamine: A relation among geometries, energy status, and electronic structures. International Journal of Quantum Chemistry, 1993, 45, 433-444.	2.0	8

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145	Transition structures for hydride transfer reactions in vacuo and their role in enzyme catalysis. Computational and Theoretical Chemistry, 1996, 371, 299-312.	1.5	8
146	Towards an understanding of the molecular mechanism of the unimolecular decomposition of the N-chloro-Î±-amino acids on the ground and excited states surfaces in aqueous medium. Chemical Physics Letters, 1998, 283, 294-300.	2.6	8
147	A theoretical study on the molecular mechanism for the normal Reimerâ€“Tiemann reaction. Chemical Physics Letters, 2000, 318, 270-275.	2.6	8
148	A QM/MM study of the reaction mechanism for the 3â€²-processing step catalyzed by HIV-1 integrase. Computational and Theoretical Chemistry, 2009, 898, 115-120.	1.5	8
149	Theoretical QM/MM studies of enzymatic pericyclic reactions. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 115-131.	3.6	8
150	Isolation, X-ray crystal structure and theoretical calculations of the new compound 8-Epicordatin and identification of others terpenes and steroids from the bark and leaves of Croton palanostigma Klotzsch. Journal of the Brazilian Chemical Society, 2010, 21, 731-739.	0.6	8
151	Molecular mechanism of chorismate mutase activity of promiscuos MbtI. Theoretical Chemistry Accounts, 2011, 128, 601-607.	1.4	8
152	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. Chemical Communications, 2012, 48, 11253.	4.1	8
153	Parallel reaction pathways and noncovalent intermediates in thymidylate synthase revealed by experimental and computational tools. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 10311-10314.	7.1	8
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