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	Computational design of an amidase by combining the best electrostatic features of two promiscuous hydrolases. Chemical Science, 2022, 13, 4779-4787.	7.4	6
2	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
3	Exploring the Catalytic Mechanism of the RNA Cap Modification by nsp16-nsp10 Complex of SARS-CoV-2 through a QM/MM Approach. International Journal of Molecular Sciences, 2022, 23, 300.	4.1	4
4	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
5	A QM/MM study on the origin of retro-aldolase activity of a catalytic antibody. Chemical Communications, 2021, 57, 5306-5309.	4.1	0
6	Transfer hydrogenations catalyzed by streptavidin-hosted secondary amine organocatalysts. Chemical Communications, 2021, 57, 1919-1922.	4.1	10
7	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
8	Caught in Action: X-ray Structure of Thymidylate Synthase with Noncovalent Intermediate Analog. Biochemistry, 2021, 60, 1243-1247.	2.5	1
9	Elucidating the Dual Mode of Action of Dipeptidyl Enoates in the Inhibition of Rhodesain Cysteine Proteases. Chemistry - A European Journal, 2021, 27, 10142-10150.	3.3	6
10	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
11	Combined Theoretical and Experimental Study to Unravel the Differences in Promiscuous Amidase Activity of Two Nonhomologous Enzymes. ACS Catalysis, 2021, 11, 8635-8644.	11.2	6
12	QM/MM Study of the Enzymatic Biodegradation Mechanism of Polyethylene Terephthalate. Journal of Chemical Information and Modeling, 2021, 61, 3041-3051.	5.4	52
13	Computational Studies Suggest Promiscuous Candida antarctica Lipase B as an Environmentally Friendly Alternative for the Production of Epoxides. Journal of Chemical Information and Modeling, 2021, 61, 3604-3614.	5.4	5
14	Fundamental Insight into Glycoside Hydrolase-Catalyzed Hydrolysis of the Universal Koshland Substratesâ€“Glycopyranosyl Fluorides. ACS Catalysis, 2021, 11, 10383-10393.	11.2	3
15	On the Origin of the Different Reversible Characters of Salinosporamide A and Homosalinosporamide A in the Covalent Inhibition of the Human 20S Proteasome. ACS Catalysis, 2021, 11, 11806-11819.	11.2	5
16	Unrevealing the Proteolytic Activity of RgpB Gingipain from Computational Simulations. Journal of Chemical Information and Modeling, 2021, 61, 4582-4593.	5.4	4
17	Discovery of SARS-CoV-2 M^{pro} peptide inhibitors from modelling substrate and ligand binding. Chemical Science, 2021, 12, 13686-13703.	7.4	54
18	The role of streptavidin and its variants in catalysis by biotinylated secondary amines. Organic and Biomolecular Chemistry, 2021, 19, 10424-10431.	2.8	2

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19	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0
20	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
21	Exploring the Origin of Amidase Substrate Promiscuity in CALB by a Computational Approach. ACS Catalysis, 2020, 10, 1938-1946.	11.2	19
22	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
23	Glycoside hydrolase stabilization of transition state charge: new directions for inhibitor design. Chemical Science, 2020, 11, 10488-10495.	7.4	12
24	Are Heme-Dependent Enzymes Always Using a Redox Mechanism? A Theoretical Study of the Kemp Elimination Catalyzed by a Promiscuous Aldoxime Dehydratase. ACS Catalysis, 2020, 10, 11110-11119.	11.2	7
25	Understanding the Directed Evolution of De Novo Retro-Aldolases from QM/MM Studies. ACS Catalysis, 2020, 10, 7871-7883.	11.2	6
26	Electric Field Measurements Reveal the Pivotal Role of Cofactorâ€“Substrate Interaction in Dihydrofolate Reductase Catalysis. ACS Catalysis, 2020, 10, 7907-7914.	11.2	2
27	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
28	Examination of the performance of semiempirical methods in QM/MM studies of the SN2-like reaction of an adenylyl group transfer catalysed by ANT4â€². Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	1
29	Loss of Hyperconjugative Effects Drives Hydride Transfer during Dihydrofolate Reductase Catalysis. ACS Catalysis, 2019, 9, 10343-10349.	11.2	1
30	QM/MM Theoretical Studies of a de Novo Retro-Aldolase Design. ACS Catalysis, 2019, 9, 2482-2492.	11.2	16
31	Why Are Some Enzymes Dimers? Flexibility and Catalysis in Thermotoga maritima Dihydrofolate Reductase. ACS Catalysis, 2019, 9, 5902-5911.	11.2	12
32	Heavy Enzymes and the Rational Redesign of Protein Catalysts. ChemBioChem, 2019, 20, 2807-2812.	2.6	5
33	Editorial: Challenges in Computational Enzymology. Frontiers in Chemistry, 2019, 7, 690.	3.6	3
34	Theoretical study of the inhibition mechanism of human 20S proteasome by dihydroeponemycin. European Journal of Medicinal Chemistry, 2019, 164, 399-407.	5.5	12
35	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
36	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

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37	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
38	Computational study of the phosphoryl donor activity of dihydroxyacetone kinase from ATP to inorganic polyphosphate. International Journal of Quantum Chemistry, 2018, 118, e25520.	2.0	2
39	Origin of Enzymatic Kinetic Isotope Effects in Human Purine Nucleoside Phosphorylase. ACS Catalysis, 2018, 8, 815-827.	11.2	5
40	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
41	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
42	Temperature dependence of dynamic, tunnelling and kinetic isotope effects in formate dehydrogenase. Physical Chemistry Chemical Physics, 2018, 20, 25722-25737.	2.8	2
43	Experimental and Computational Studies Delineate the Role of Asparagine 177 in Hydride Transfer forE. coliThymidylate Synthase. ACS Catalysis, 2018, 8, 10241-10253.	11.2	2
44	Isotope Substitution of Promiscuous Alcohol Dehydrogenase Reveals the Origin of Substrate Preference in the Transition State. Angewandte Chemie, 2018, 130, 3182-3185.	2.0	2
45	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie - International Edition, 2018, 57, 12478-12482.	13.8	38
46	Reactivity and Selectivity of Iminium Organocatalysis Improved by a Protein Host. Angewandte Chemie, 2018, 130, 12658-12662.	2.0	14
47	Revealing the mechanism for covalent inhibition of glycoside hydrolases by carbasugars at an atomic level. Nature Communications, 2018, 9, 3243.	12.8	28
48	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
49	Theoretical estimation of redox potential of biological quinone cofactors. Journal of Computational Chemistry, 2017, 38, 1612-1621.	3.3	6
50	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
51	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
52	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
53	Computational Study of the Catalytic Mechanism of the Cruzain Cysteine Protease. ACS Catalysis, 2017, 7, 1207-1215.	11.2	38
54	Theoretical Study of the Phosphoryl Transfer Reaction from ATP to Dha Catalyzed by DhaK from Escherichia coli. Journal of Physical Chemistry B, 2017, 121, 8878-8892.	2.6	7

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55	Molecular mechanism of the site-specific self-cleavage of the RNA phosphodiester backbone by a twister ribozyme. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6
56	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
57	Catalytic enantioselective epoxidation of nitroalkenes. Chemical Communications, 2016, 52, 10060-10063.	4.1	18
58	QM/MM study of<scp>l</scp>-lactate oxidation by flavocytochrome b₂. Physical Chemistry Chemical Physics, 2016, 18, 15609-15618.	2.8	10
59	Minimization of dynamic effects in the evolution of dihydrofolate reductase. Chemical Science, 2016, 7, 3248-3255.	7.4	25
60	Computational Studies of Candida Antarctica Lipase B to Test Its Capability as a Starting Point To Redesign New Dielsâ€“Alderases. Journal of Physical Chemistry B, 2016, 120, 2053-2070.	2.6	5
61	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
62	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
63	Is Promiscuous CALB a Good Scaffold for Designing New Epoxidases?. Molecules, 2015, 20, 17789-17806.	3.8	10
64	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
65	Theoretical studies of the hydrolysis of antibiotics catalyzed by a metallo-Î²-lactamase. Archives of Biochemistry and Biophysics, 2015, 582, 116-126.	3.0	7
66	Special issue in computational modeling on biological systems. Archives of Biochemistry and Biophysics, 2015, 582, 1-2.	3.0	0
67	First Quantum Mechanics/Molecular Mechanics Studies of the Inhibition Mechanism of Cruzain by Peptidyl Halomethyl Ketones. Biochemistry, 2015, 54, 3381-3391.	2.5	31
68	Computational strategies for the design of new enzymatic functions. Archives of Biochemistry and Biophysics, 2015, 582, 68-79.	3.0	49
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	A computational study of the phosphoryl transfer reaction between ATP and Dha in aqueous solution. Organic and Biomolecular Chemistry, 2015, 13, 10179-10190.	2.8	4
71	Peptide Bond Formation Mechanism Catalyzed by Ribosome. Journal of the American Chemical Society, 2015, 137, 12024-12034.	13.7	34
72	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

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73	Measurement and prediction of quantum coherence effects in biological processes. Physical Chemistry Chemical Physics, 2015, 17, 30772-30774.	2.8	0
74	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
75	Exploring Chemical Reactivity in Enzyme Catalyzed Processes Using QM/MM Methods: An Application to Dihydrofolate Reductase. Challenges and Advances in Computational Chemistry and Physics, 2015, , 383-413.	0.6	1
76	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
77	Quantum Mechanics/Molecular Mechanics Studies of the Mechanism of Falcipain-2 Inhibition by the Epoxysuccinate E64. Biochemistry, 2014, 53, 3336-3346.	2.5	18
78	Electron and Hydrogen Atom Transfers in the Hydride Carrier Protein EmoB. Journal of Chemical Theory and Computation, 2014, 10, 5036-5046.	5.3	6
79	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
80	Predicting enzymatic reactivity: from theory to design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 407-421.	14.6	32
81	Heavy enzymesâ€”experimental and computational insights in enzyme dynamics. Current Opinion in Chemical Biology, 2014, 21, 11-18.	6.1	39
82	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
83	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
84	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
85	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
86	QM/MM Calculations Suggest a Novel Intermediate Following the Proton Abstraction Catalyzed by Thymidylate Synthase. Biochemistry, 2013, 52, 2348-2358.	2.5	20
87	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
88	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
89	A theoretical study of carbonâ€“carbon bond formation by a Michael-type addition. Organic and Biomolecular Chemistry, 2012, 10, 5598.	2.8	13
90	Modeling methods for studying post-translational and transcriptional modifying enzymes. Current Opinion in Chemical Biology, 2012, 16, 465-471.	6.1	5

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91	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. Chemical Communications, 2012, 48, 11253.	4.1	8
92	Understanding the different activities of highly promiscuous MbtI by computational methods. Physical Chemistry Chemical Physics, 2012, 14, 3482.	2.8	16
93	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
94	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
95	Theoretical studies of HIV-1 reverse transcriptase inhibition. Physical Chemistry Chemical Physics, 2012, 14, 12614.	2.8	24
96	Computational study on hydrolysis of cefotaxime in gas phase and in aqueous solution. Journal of Computational Chemistry, 2012, 33, 1948-1959.	3.3	6
97	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. Chemistry - A European Journal, 2012, 18, 9612-9621.	3.3	26
98	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. Advances in Protein Chemistry and Structural Biology, 2011, 85, 81-142.	2.3	19
99	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
100	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. Journal of the American Chemical Society, 2011, 133, 12050-12062.	13.7	61
101	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
102	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
103	Molecular mechanism of chorismate mutase activity of promiscuos MbtI. Theoretical Chemistry Accounts, 2011, 128, 601-607.	1.4	8
104	"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
105	Theoretical QM/MM studies of enzymatic pericyclic reactions. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 115-131.	3.6	8
106	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
107	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
108	Application of Groteâ˜Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. Journal of Physical Chemistry B, 2010, 114, 13593-13600.	2.6	17

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109	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
110	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
111	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. Physical Chemistry Chemical Physics, 2010, 12, 11657.	2.8	15
112	Computational Modeling of Biological Systems: The LDH Story. Challenges and Advances in Computational Chemistry and Physics, 2010, , 355-374.	0.6	0
113	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
114	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
115	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
116	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. Journal of the American Chemical Society, 2009, 131, 16156-16161.	13.7	28
117	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
118	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
119	Coupling of the guanosine glycosidic bond conformation and the ribonucleotide cleavage reaction: Implications for barnase catalysis. Proteins: Structure, Function and Bioinformatics, 2008, 70, 415-428.	2.6	2
120	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
121	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
122	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
123	Theoretical site-directed mutagenesis: Asp168Ala mutant of lactate dehydrogenase. Journal of the Royal Society Interface, 2008, 5, 217-224.	3.4	3
124	Computational design of biological catalysts. Chemical Society Reviews, 2008, 37, 2634.	38.1	41
125	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
126	A Theoretical Study of the Catalytic Mechanism of Formate Dehydrogenase. Journal of Physical Chemistry B, 2008, 112, 10012-10022.	2.6	46

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127	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
128	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
129	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
130	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
131	Singlet-triplet gaps in large multireference systems: Spin-flip-driven alternatives for bioinorganic modeling. Journal of Chemical Physics, 2007, 126, 035102.	3.0	23
132	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
133	A Quantum Mechanics/Molecular Mechanics Study of the Catalytic Mechanism of the Thymidylate Synthaseâ€. Biochemistry, 2007, 46, 3704-3713.	2.5	35
134	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
135	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. Angewandte Chemie - International Edition, 2007, 46, 286-290.	13.8	24
136	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
137	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
138	Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangementâ€. Journal of Physical Chemistry A, 2006, 110, 726-730.	2.5	3
139	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
140	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
141	Catalysis in Glycine N-Methyltransferase:â€‰ Testing the Electrostatic Stabilization and Compression Hypothesis. Biochemistry, 2006, 45, 14917-14925.	2.5	28
142	A density functional study ofÂflavonoid compounds with anti-HIV activity. European Journal of Medicinal Chemistry, 2006, 41, 616-623.	5.5	38
143	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
144	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie - International Edition, 2005, 44, 904-909.	13.8	9

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145	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie, 2005, 117, 926-931.	2.0	3
146	Dependence of enzyme reaction mechanism on protonation state of titratable residues and QM level description: lactate dehydrogenase. Chemical Communications, 2005, , 5873.	4.1	17
147	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
148	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
149	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
150	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
151	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
152	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
153	Theoretical Insights in Enzyme Catalysis. ChemInform, 2004, 35, no.	0.0	0
154	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. Journal of Physical Chemistry B, 2004, 108, 8427-8433.	2.6	95
155	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
156	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
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