IÃ±aki TuÃ±Ã³n

List of Publications by Year
in descending order

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197	6,229	66343	98798
papers	citations	42 h-index	67 g-index

210	210	210	5037
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Testing Affordable Strategies for the Computational Study of Reactivity in Cysteine Proteases: The Case of SARS-CoV-2 3CL Protease Inhibition. Journal of Chemical Theory and Computation, 2022, 18, 4005-4013.	5.3	9
2	Spatial and Temporal Resolution of the Oxygen-Independent Photoinduced DNA Interstrand Cross-Linking by a Nitroimidazole Derivative. Journal of Chemical Information and Modeling, 2022, 62, 3239-3252.	5.4	6
3	How a Second Mg²⁺ Ion Affects the Phosphoryl-Transfer Mechanism in a Protein Kinase: A Computational Study. ACS Catalysis, 2021, 11, 169-183.	11.2	7
4	Computational simulations on the binding and reactivity of a nitrile inhibitor of the SARS-CoV-2 main protease. Chemical Communications, 2021, 57, 9096-9099.	4.1	32
5	Multiscale Simulations of SARS-CoV-2 3CL Protease Inhibition with Aldehyde Derivatives. Role of Protein and Inhibitor Conformational Changes in the Reaction Mechanism. ACS Catalysis, 2021, 11, 4157-4168.	11.2	40
6	Mechanistic study of the biosynthesis of R-phenylcarbinol by acetohydroxyacid synthase enzyme using hybrid quantum mechanics/molecular mechanics simulations. Archives of Biochemistry and Biophysics, 2021, 701, 108807.	3.0	1
7	Targeting the JAK/STAT Pathway: A Combined Ligand- and Target-Based Approach. Journal of Chemical Information and Modeling, 2021, 61, 3091-3108.	5.4	8
8	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. Biomolecules, 2021, 11, 1051.	4.0	3
9	Inhibition Mechanism of SARSâ€CoVâ€2 Main Protease with Ketoneâ€Based Inhibitors Unveiled by Multiscale Simulations: Insights for Improved Designs**. Angewandte Chemie - International Edition, 2021, 60, 25933-25941.	13.8	24
10	A microscopic description of SARS-CoV-2 main protease inhibition with Michael acceptors. Strategies for improving inhibitor design. Chemical Science, 2021, 12, 3489-3496.	7.4	40
11	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0
12	Elucidating the Catalytic Reaction Mechanism of Orotate Phosphoribosyltransferase by Means of X-ray Crystallography and Computational Simulations. ACS Catalysis, 2020, 10, 1871-1885.	11.2	9
13	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
14	Seeking the Source of Catalytic Efficiency of Lindane Dehydrochlorinase, LinA. Journal of Physical Chemistry B, 2020, 124, 10353-10364.	2.6	1
15	On the Nature of the Enzymeâ€“Substrate Complex and the Reaction Mechanism in Human Arginase I. A Combined Molecular Dynamics and QM/MM Study. ACS Catalysis, 2020, 10, 8321-8333.	11.2	9
16	Unraveling the SARS-CoV-2 Main Protease Mechanism Using Multiscale Methods. ACS Catalysis, 2020, 10, 12544-12554.	11.2	107
17	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. Journal of Physical Chemistry Letters, 2019, 10, 6750-6754.	4.6	19
18	The transition state and cognate concepts. Advances in Physical Organic Chemistry, 2019, 53, 29-68.	0.5	8

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19	Mechanistic insights into the phosphoryl transfer reaction in cyclin-dependent kinase 2: A QM/MM study. PLoS ONE, 2019, 14, e0215793.	2.5	8
20	Loss of Hyperconjugative Effects Drives Hydride Transfer during Dihydrofolate Reductase Catalysis. ACS Catalysis, 2019, 9, 10343-10349.	11.2	1
21	Studying the phosphoryl transfer mechanism of theE. coliphosphofructokinase-2: from X-ray structure to quantum mechanics/molecular mechanics simulations. Chemical Science, 2019, 10, 2882-2892.	7.4	15
22	Why Are Some Enzymes Dimers? Flexibility and Catalysis in Thermotoga maritima Dihydrofolate Reductase. ACS Catalysis, 2019, 9, 5902-5911.	11.2	12
23	Heavy Enzymes and the Rational Redesign of Protein Catalysts. ChemBioChem, 2019, 20, 2807-2812.	2.6	5
24	A first peek into sub-picosecond dynamics of spin energy levels in magnetic biomolecules. Physical Chemistry Chemical Physics, 2019, 21, 10908-10913.	2.8	7
25	Modeling caspase-1 inhibition: Implications for catalytic mechanism and drug design. European Journal of Medicinal Chemistry, 2019, 169, 159-167.	5.5	8
26	Translocation of Enzymes into a Mesoporous MOF for Enhanced Catalytic Activity Under Extreme Conditions. Chemical Science, 2019, 10, 4082-4088.	7.4	47
27	A molecular dynamics study on the role of the protonation state in the biosynthesis of R-PAC by AHAS. Chemical Physics Letters, 2019, 716, 247-251.	2.6	4
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	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
30	Origin of Enzymatic Kinetic Isotope Effects in Human Purine Nucleoside Phosphorylase. ACS Catalysis, 2018, 8, 815-827.	11.2	5
31	Dynamics of the excited-state hydrogen transfer in a (dG)Â·(dC) homopolymer: intrinsic photostability of DNA. Chemical Science, 2018, 9, 7902-7911.	7.4	29
32	Catalytic Reaction Mechanism in Native and Mutant Catechol-O-methyltransferase from the Adaptive String Method and Mean Reaction Force Analysis. Journal of Physical Chemistry B, 2018, 122, 8861-8871.	2.6	8
33	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
34	Reaction coordinates and transition states in enzymatic catalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1329.	14.6	27
35	Molecular Mechanism of Inhibition of DNA Methylation by Zebularine. ACS Catalysis, 2017, 7, 1728-1732.	11.2	7
36	Free energy profiles for two ubiquitous damaging agents: methylation and hydroxylation of guanine in B-DNA. Physical Chemistry Chemical Physics, 2017, 19, 14695-14701.	2.8	3

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37	A DFT study on the chiral synthesis of R-phenylacetyl carbinol within the quantum chemical cluster approach. Chemical Physics Letters, 2017, 677, 30-34.	2.6	5
38	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
39	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
40	Regioselectivity of the OH Radical Addition to Uracil in Nucleic Acids. A Theoretical Approach Based on QM/MM Simulations. Journal of Chemical Theory and Computation, 2017, 13, 5089-5096.	5.3	13
41	Adaptive Finite Temperature String Method in Collective Variables. Journal of Physical Chemistry A, 2017, 121, 9764-9772.	2.5	40
42	Quantifying the limits of transition state theory in enzymatic catalysis. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 12390-12395.	7.1	22
43	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
44	Insights into the inhibited form of the redox-sensitive SufE-like sulfur acceptor CsdE. PLoS ONE, 2017, 12, e0186286.	2.5	0
45	Thermal Isomerization Mechanism in Dronpa and Its Mutants. Journal of Physical Chemistry B, 2016, 120, 12820-12825.	2.6	9
46	Unraveling the Reaction Mechanism of Enzymatic C5-Cytosine Methylation of DNA. A Combined Molecular Dynamics and QM/MM Study of Wild Type and Gln119 Variant. ACS Catalysis, 2016, 6, 3262-3276.	11.2	30
47	Mechanism of Sulfur Transfer Across Proteinâ€"Protein Interfaces: The Cysteine Desulfurase Model System. ACS Catalysis, 2016, 6, 3975-3984.	11.2	12
48	Singlet Oxygen Attack on Guanine: Reactivity and Structural Signature within the Bâ€DNA Helix. Chemistry - A European Journal, 2016, 22, 12358-12362.	3.3	34
49	DFT Study on the Interaction of Tris(benzene-1,2-dithiolato)molybdenum Complex with Water. A Hydrolysis Mechanism Involving a Feasible Seven-Coordinate Aquomolybdenum Intermediate. Journal of Physical Chemistry A, 2016, 120, 9636-9646.	2.5	5
50	Minimization of dynamic effects in the evolution of dihydrofolate reductase. Chemical Science, 2016, 7, 3248-3255.	7.4	25
51	Chapter 3. A Transition State Theory Perspective for Enzymatic Reactions: Fundamentals and Applications. RSC Theoretical and Computational Chemistry Series, 2016, , 54-88.	0.7	0
52	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
53	Transition state ensemble optimization for reactions of arbitrary complexity. Journal of Chemical Physics, 2015, 143, 134111.	3.0	5
54	Enzyme Promiscuity in Enolase Superfamily. Theoretical Study of o-Succinylbenzoate Synthase Using QM/MM Methods. Journal of Physical Chemistry B, 2015, 119, 1899-1911.	2.6	6

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55	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
56	Are there dynamical effects in enzyme catalysis? Some thoughts concerning the enzymatic chemical step. Archives of Biochemistry and Biophysics, 2015, 582, 42-55.	3.0	36
57	Computational strategies for the design of new enzymatic functions. Archives of Biochemistry and Biophysics, 2015, 582, 68-79.	3.0	49
58	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
59	Peptide Bond Formation Mechanism Catalyzed by Ribosome. Journal of the American Chemical Society, 2015, 137, 12024-12034.	13.7	34
60	Dehydrochlorination of Hexachlorocyclohexanes Catalyzed by the LinA Dehydrohalogenase. A QM/MM Study. Journal of Physical Chemistry B, 2015, 119, 15100-15109.	2.6	19
61	Linking Electrostatic Effects and Protein Motions in Enzymatic Catalysis. A Theoretical Analysis of Catechol O-Methyltransferase. Journal of Physical Chemistry B, 2015, 119, 873-882.	2.6	14
62	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
63	Exploring chemical reactivity of complex systems with pathâ€based coordinates: Role of the distance metric. Journal of Computational Chemistry, 2014, 35, 1672-1681.	3.3	15
64	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
65	Dynamics and Reactivity in Thermus aquaticus N6-Adenine Methyltransferase. Journal of the American Chemical Society, 2014, 136, 16227-16239.	13.7	22
66	Predicting enzymatic reactivity: from theory to design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 407-421.	14.6	32
67	The Catalytic Mechanism of Carboxylesterases: A Computational Study. Biochemistry, 2014, 53, 5820-5829.	2.5	53
68	Heavy enzymesâ€”experimental and computational insights in enzyme dynamics. Current Opinion in Chemical Biology, 2014, 21, 11-18.	6.1	39
69	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
70	Toward an Automatic Determination of Enzymatic Reaction Mechanisms and Their Activation Free Energies. Journal of Chemical Theory and Computation, 2013, 9, 3740-3749.	5.3	37
71	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
72	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

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73	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
74	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
75	Modeling methods for studying post-translational and transcriptional modifying enzymes. Current Opinion in Chemical Biology, 2012, 16, 465-471.	6.1	5
76	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. Chemical Communications, 2012, 48, 11253.	4.1	8
77	Understanding the different activities of highly promiscuous MbtI by computational methods. Physical Chemistry Chemical Physics, 2012, 14, 3482.	2.8	16
78	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
79	A Collective Coordinate to Obtain Free Energy Profiles for Complex Reactions in Condensed Phases. Journal of Chemical Theory and Computation, 2012, 8, 1795-1801.	5.3	20
80	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	16
81	Substrate promiscuity in DNA methyltransferase M.PvuII. A mechanistic insight. Organic and Biomolecular Chemistry, 2012, 10, 5395.	2.8	8
82	Computational study on hydrolysis of cefotaxime in gas phase and in aqueous solution. Journal of Computational Chemistry, 2012, 33, 1948-1959.	3.3	6
83	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. Chemistry - A European Journal, 2012, 18, 9612-9621.	3.3	26
84	Reversibility and Diffusion in Mandelythiamin Decarboxylation. Searching Dynamical Effects in Decarboxylation Reactions. Journal of the American Chemical Society, 2012, 134, 10509-10514.	13.7	8
85	Tetraethylorthosilicate as molecular precursor to the formation of amorphous silica networks. A DFT-SCRF study of the base catalyzed hydrolysis. Journal of Molecular Modeling, 2012, 18, 3301-3310.	1.8	12
86	Hybrid Schemes Based on Quantum Mechanics/Molecular Mechanics Simulations. Advances in Protein Chemistry and Structural Biology, 2011, 85, 81-142.	2.3	19
87	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
88	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. Journal of the American Chemical Society, 2011, 133, 12050-12062.	13.7	61
89	Molecular mechanism of chorismate mutase activity of promiscuos MbtI. Theoretical Chemistry Accounts, 2011, 128, 601-607.	1.4	8
90	A Simple Model for Barrier Frequencies for Enzymatic Reactions. ChemPhysChem, 2011, 12, 184-190.	2.1	2

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91	Does glycosyl transfer involve an oxacarbenium intermediate? Computational simulation of the lifetime of the methoxymethyl cation in water. Pure and Applied Chemistry, 2011, 83, 1507-1514.	1.9	9
92	Theoretical QM/MM studies of enzymatic pericyclic reactions. Interdisciplinary Sciences, Computational Life Sciences, 2010, 2, 115-131.	3.6	8
93	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
94	Digitalis purpurea P5Î²R2, encoding steroid 5Î²â€reductase, is a novel defenseâ€related gene involved in cardenolide biosynthesis. New Phytologist, 2010, 185, 687-700.	7.3	57
95	Application of Groteâ˜Hynes Theory to the Reaction Catalyzed by Thymidylate Synthase. Journal of Physical Chemistry B, 2010, 114, 13593-13600.	2.6	17
96	Computational Simulation of the Lifetime of the Methoxymethyl Cation in Water. A Simple Model for a Glycosyl Cation: When Is an Intermediate an Intermediate?. Journal of Physical Chemistry B, 2010, 114, 5769-5774.	2.6	11
97	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
98	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
99	Theoretical Study of the Catalytic Mechanism of DNA-(N4-Cytosine)-Methyltransferase from the Bacterium Proteus vulgaris. Journal of Physical Chemistry B, 2010, 114, 8467-8473.	2.6	10
100	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. Physical Chemistry Chemical Physics, 2010, 12, 11657.	2.8	15
101	Computational Modeling of Biological Systems: The LDH Story. Challenges and Advances in Computational Chemistry and Physics, 2010, , 355-374.	0.6	0
102	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
103	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
104	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. Journal of the American Chemical Society, 2009, 131, 16156-16161.	13.7	28
105	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
106	Critical Role of Substrate Conformational Change in the Proton Transfer Process Catalyzed by 4-Oxalocrotonate Tautomerase. Journal of the American Chemical Society, 2009, 131, 2687-2698.	13.7	18
107	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
108	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

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109	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
110	Theoretical site-directed mutagenesis: Asp168Ala mutant of lactate dehydrogenase. Journal of the Royal Society Interface, 2008, 5, 217-224.	3.4	3
111	Computational design of biological catalysts. Chemical Society Reviews, 2008, 37, 2634.	38.1	41
112	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
113	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
114	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
115	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
116	Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. Journal of Biological Chemistry, 2008, 283, 12393-12401.	3.4	24
117	Enzymatic Effects on Reactant and Transition States. The Case of Chalcone Isomerase. Journal of the American Chemical Society, 2007, 129, 9117-9124.	13.7	16
118	A Computational Study of the Protein-Ligand Interactions in CDK2 Inhibitors: Using Quantum Mechanics/Molecular Mechanics Interaction Energy as a Predictor of the Biological Activity. Biophysical Journal, 2007, 92, 430-439.	0.5	49
119	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
120	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. Angewandte Chemie - International Edition, 2007, 46, 286-290.	13.8	24
121	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
122	Improving the QM/MM Description of Chemical Processes:â€‰ A Dual Level Strategy To Explore the Potential Energy Surface in Very Large Systems. [J. Chem. Theory Comput. 1, 1008â^'1016 (2005)]. Journal of Chemical Theory and Computation, 2006, 2, 216-216.	5.3	9
123	Hybrid Quantum Mechanics/Molecular Mechanics Simulations with Two-Dimensional Interpolated Corrections:Â Application to Enzymatic Processes. Journal of Physical Chemistry B, 2006, 110, 17663-17670.	2.6	57
124	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
125	Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangementâ€. Journal of Physical Chemistry A, 2006, 110, 726-730.	2.5	3
126	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

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127	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
128	Comparative Computational Analysis of Different Active Site Conformations and Substrates in a Chalcone Isomerase Catalyzed Reaction. Journal of Physical Chemistry B, 2006, 110, 20686-20692.	2.6	15
129	Catalysis in Glycine N-Methyltransferase:â€‰ Testing the Electrostatic Stabilization and Compression Hypothesis. Biochemistry, 2006, 45, 14917-14925.	2.5	28
130	FT-Raman and QM/MM study of the interaction between histamine and DNA. Chemical Physics, 2006, 324, 579-590.	1.9	26
131	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie - International Edition, 2005, 44, 904-909.	13.8	9
132	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie, 2005, 117, 926-931.	2.0	3
133	The Mechanism of Formamide Hydrolysis in Water from Ab Initio Calculations and Simulations. Chemistry - A European Journal, 2005, 11, 6743-6753.	3.3	90
134	Dependence of enzyme reaction mechanism on protonation state of titratable residues and QM level description: lactate dehydrogenase. Chemical Communications, 2005, , 5873.	4.1	17
135	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
136	Dynamic and Electrostatic Effects in Enzymatic Processes. An Analysis of the Nucleophilic Substitution Reaction in Haloalkane Dehalogenase. Journal of the American Chemical Society, 2005, 127, 1946-1957.	13.7	42
137	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
138	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
139	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
140	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
141	Theoretical Insights in Enzyme Catalysis. ChemInform, 2004, 35, no.	0.0	0
142	Amino acid chemistry in solution: structural properties and vibrational dynamics of serine using density functional theory and a continuum solvent model. Chemical Physics, 2004, 303, 85-96.	1.9	33
143	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. Journal of Physical Chemistry B, 2004, 108, 8427-8433.	2.6	95
144	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

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145	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
146	Theoretical insights in enzyme catalysis. Chemical Society Reviews, 2004, 33, 98-107.	38.1	150
147	Fundamental Principles Governing Solvent Use: Solvent Effects on Chemical Systems. ChemInform, 2003, 34, no.	0.0	0
148	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. Chemistry - A European Journal, 2003, 9, 984-991.	3.3	57
149	A theoretical study of solvent effects on the conformational equilibria of neutral glycine in aqueous solution. Computational and Theoretical Chemistry, 2003, 623, 203-210.	1.5	24
150	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
151	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
152	Internal Rotation of 1,2-Dichloroethane in Haloalkane Dehalogenase. A Test Case for Analyzing Electrostatic Effects in Enzymes. Journal of Physical Chemistry B, 2003, 107, 6234-6238.	2.6	14
153	Structural and Vibrational Study of the Tautomerism of Histamine Free-Base in Solution. Journal of the American Chemical Society, 2003, 125, 2328-2340.	13.7	50
154	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
155	QM/MM calculations of kinetic isotope effects in the chorismate mutase active site. Organic and Biomolecular Chemistry, 2003, 1, 483-487.	2.8	28
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