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	GEPOL: An improved description of molecular surfaces. III. A new algorithm for the computation of a solvent-excluding surface. Journal of Computational Chemistry, 1994, 15, 1127-1138.	3.3	760
2	GEPOL: An improved description of molecular surfaces II. Computing the molecular area and volume. Journal of Computational Chemistry, 1991, 12, 1077-1088.	3.3	237
3	Theoretical insights in enzyme catalysis. Chemical Society Reviews, 2004, 33, 98-107.	38.1	150
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	Unraveling the SARS-CoV-2 Main Protease Mechanism Using Multiscale Methods. ACS Catalysis, 2020, 10, 12544-12554.	11.2	107
7	Hydroxide Ion in Liquid Water: Structure, Energetics, and Proton Transfer Using a Mixed Discrete-Continuum ab Initio Model. The Journal of Physical Chemistry, 1995, 99, 3798-3805.	2.9	95
8	Hybrid QM/MM Potentials of Mean Force with Interpolated Corrections. Journal of Physical Chemistry B, 2004, 108, 8427-8433.	2.6	95
9	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
10	The Mechanism of Formamide Hydrolysis in Water from Ab Initio Calculations and Simulations. Chemistry - A European Journal, 2005, 11, 6743-6753.	3.3	90
11	Aminoacid zwitterions in solution: Geometric, energetic, and vibrational analysis using density functional theory-continuum model calculations. Journal of Chemical Physics, 1998, 109, 592-603.	3.0	87
12	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
13	Neutral and Alkaline Hydrolyses of Model Î²-Lactam Antibiotics. An ab Initio Study of Water Catalysis. Journal of the American Chemical Society, 1998, 120, 2146-2155.	13.7	71
14	Methylamines basicity calculations: in vacuo and in solution comparative analysis. The Journal of Physical Chemistry, 1992, 96, 9043-9048.	2.9	70
15	Intramolecular Proton Transfer of Glycine in Aqueous Solution Using Quantum Mechanicsâ^'Molecular Mechanics Simulations. Journal of Physical Chemistry A, 1998, 102, 8673-8678.	2.5	68
16	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
17	Promiscuity in Alkaline Phosphatase Superfamily. Unraveling Evolution through Molecular Simulations. Journal of the American Chemical Society, 2011, 133, 12050-12062.	13.7	61
18	Proton solvation in liquid water: an ab initio study using the continuum model. The Journal of Physical Chemistry, 1993, 97, 5547-5552.	2.9	59

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19	On the tautomerization process of glycine in aqueous solution. Chemical Physics Letters, 2000, 321, 433-437.	2.6	57
20	Preorganization and Reorganization as Related Factors in Enzyme Catalysis: The Chorismate Mutase Case. Chemistry - A European Journal, 2003, 9, 984-991.	3.3	57
21	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
22	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
23	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
24	Ab Initio Calculations on Neutral and Alkaline Hydrolyses of Î²-Lactam Antibiotics. A Theoretical Study Including Solvent Effects. Journal of Physical Chemistry B, 1997, 101, 3581-3588.	2.6	56
25	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
26	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
27	The Catalytic Mechanism of Carboxylesterases: A Computational Study. Biochemistry, 2014, 53, 5820-5829.	2.5	53
28	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
29	Coupled density functional/molecular mechanics Monte Carlo simulations of ions in water. The bromide ion. Chemical Physics Letters, 1995, 241, 450-456.	2.6	51
30	A Hybrid Density Functional-Classical Molecular Dynamics Simulation of a Water Molecule in Liquid Water. Journal of Molecular Modeling, 1995, 1, 196-201.	1.8	51
31	Computation of hydration free energies using a parameterized continuum model: Study of equilibrium geometries and reactive processes in water solution. Journal of Computational Chemistry, 1996, 17, 148-155.	3.3	51
32	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
33	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
34	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
35	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
36	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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37	Computational strategies for the design of new enzymatic functions. Archives of Biochemistry and Biophysics, 2015, 582, 68-79.	3.0	49
38	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
39	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
40	Theoretical study of the inversion of the alcohol acidity scale in aqueous solution. Toward an interpretation of the acid-base behavior of organic compounds in solution. Journal of the American Chemical Society, 1993, 115, 2226-2230.	13.7	47
41	Translocation of Enzymes into a Mesoporous MOF for Enhanced Catalytic Activity Under Extreme Conditions. Chemical Science, 2019, 10, 4082-4088.	7.4	47
42	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
43	Transition structure selectivity in enzyme catalysis: a QM/MM study of chorismate mutase. Theoretical Chemistry Accounts, 2001, 105, 207-212.	1.4	44
44	Continuum-uniform approach calculations of the solubility of hydrocarbons in water. Chemical Physics Letters, 1993, 203, 289-294.	2.6	43
45	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
46	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
47	Computational design of biological catalysts. Chemical Society Reviews, 2008, 37, 2634.	38.1	41
48	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
49	Adaptive Finite Temperature String Method in Collective Variables. Journal of Physical Chemistry A, 2017, 121, 9764-9772.	2.5	40
50	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
51	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
52	Heavy enzymesâ€"experimental and computational insights in enzyme dynamics. Current Opinion in Chemical Biology, 2014, 21, 11-18.	6.1	39
53	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
54	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

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55	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
56	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
57	Intramolecular proton transfer of serine in aqueous solution. Mechanism and energetics. Theoretical Chemistry Accounts, 2000, 104, 89-95.	1.4	34
58	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
59	Peptide Bond Formation Mechanism Catalyzed by Ribosome. Journal of the American Chemical Society, 2015, 137, 12024-12034.	13.7	34
60	Singlet Oxygen Attack on Guanine: Reactivity and Structural Signature within the Bâ€ÐDNA Helix. Chemistry - A European Journal, 2016, 22, 12358-12362.	3.3	34
61	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
62	Can Hydrophobic Interactions Be Correctly Reproduced by the Continuum Models?. The Journal of Physical Chemistry, 1996, 100, 9955-9959.	2.9	32
63	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
64	Predicting enzymatic reactivity: from theory to design. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2014, 4, 407-421.	14.6	32
65	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
66	Role of Protein Flexibility in Enzymatic Catalysis:â€‰ Quantum Mechanicalâ^'Molecular Mechanical Study of the Deacylation Reaction in Class A Î²-Lactamases. Journal of the American Chemical Society, 2002, 124, 1809-1816.	13.7	31
67	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
68	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
69	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
70	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
71	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
72	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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73	Catalysis in Glycine N-Methyltransferase:â€‰ Testing the Electrostatic Stabilization and Compression Hypothesis. Biochemistry, 2006, 45, 14917-14925.	2.5	28
74	Mechanism and Plasticity of Isochorismate Pyruvate Lyase: A Computational Study. Journal of the American Chemical Society, 2009, 131, 16156-16161.	13.7	28
75	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
76	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
77	Reaction coordinates and transition states in enzymatic catalysis. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2018, 8, e1329.	14.6	27
78	FT-Raman and QM/MM study of the interaction between histamine and DNA. Chemical Physics, 2006, 324, 579-590.	1.9	26
79	Hydrolysis of Phosphotriesters: A Theoretical Analysis of the Enzymatic and Solution Mechanisms. Chemistry - A European Journal, 2012, 18, 9612-9621.	3.3	26
80	Proton transfer between water molecules: a theoretical study of solvent effects using the continuum and the discrete-continuum models. The Journal of Physical Chemistry, 1993, 97, 11087-11091.	2.9	25
81	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
82	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
83	Minimization of dynamic effects in the evolution of dihydrofolate reductase. Chemical Science, 2016, 7, 3248-3255.	7.4	25
84	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
85	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
86	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
87	Computer-Aided Rational Design of Catalytic Antibodies: The 1F7 Case. Angewandte Chemie - International Edition, 2007, 46, 286-290.	13.8	24
88	Analysis of the Decarboxylation Step in Mammalian Histidine Decarboxylase. Journal of Biological Chemistry, 2008, 283, 12393-12401.	3.4	24
89	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
90	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

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91	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
92	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
93	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
94	Dynamics and Reactivity in Thermus aquaticus N6-Adenine Methyltransferase. Journal of the American Chemical Society, 2014, 136, 16227-16239.	13.7	22
95	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
96	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
97	A quantum mechanics/molecular mechanics study of the acylation reaction of TEM1 Î²-lactamase and penicillanate. Perkin Transactions II RSC, 2000, , 761-767.	1.1	19
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	Dehydrochlorination of Hexachlorocyclohexanes Catalyzed by the LinA Dehydrohalogenase. A QM/MM Study. Journal of Physical Chemistry B, 2015, 119, 15100-15109.	2.6	19
100	Hypoxia-Selective Dissociation Mechanism of a Nitroimidazole Nucleoside in a DNA Environment. Journal of Physical Chemistry Letters, 2019, 10, 6750-6754.	4.6	19
101	HCnN: The largest molecules in the interstellar medium. Journal of Chemical Education, 1990, 67, 905.	2.3	18
102	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
103	Transition structures of the Friedelâ€“Crafts reaction in solution. Journal of the Chemical Society, Faraday Transactions, 1994, 90, 1757-1761.	1.7	17
104	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
105	Dependence of enzyme reaction mechanism on protonation state of titratable residues and QM level description: lactate dehydrogenase. Chemical Communications, 2005, , 5873.	4.1	17
106	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
107	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
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	Modeling ?-lactam interactions in aqueous solution through combined quantum mechanics-molecular mechanics methods. Journal of Computational Chemistry, 1999, 20, 1401-1411.	3.3	16
110	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
111	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
112	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
113	Understanding the different activities of highly promiscuous MbtI by computational methods. Physical Chemistry Chemical Physics, 2012, 14, 3482.	2.8	16
114	Enzyme dynamics and catalysis in the mechanism of DNA polymerase. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	16
115	Revealing the Origin of the Efficiency of the De Novo Designed Kemp Eliminase HCâ€3.17 by Comparison with the Former Developed HCâ€3. Chemistry - A European Journal, 2017, 23, 7582-7589.	3.3	16
116	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
117	Theoretical study of the temperature dependence of dynamic effects in thymidylate synthase. Physical Chemistry Chemical Physics, 2010, 12, 11657.	2.8	15
118	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
119	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
120	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
121	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
122	Water-Assisted Alkaline Hydrolysis of Monobactams: A Theoretical Study. Chemistry - A European Journal, 2002, 8, 859-867.	3.3	13
123	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
124	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
125	Solvent Effects on the Thermodynamics and Kinetics of the Proton Transfer between Hydronium Ion and Ammonia. A Theoretical Study Using the Continuum and the Discrete Models. The Journal of Physical Chemistry, 1995, 99, 12525-12528.	2.9	12
126	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

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127	Mechanism of Sulfur Transfer Across Proteinâ€“Protein Interfaces: The Cysteine Desulfurase Model System. ACS Catalysis, 2016, 6, 3975-3984.	11.2	12
128	Why Are Some Enzymes Dimers? Flexibility and Catalysis in Thermotoga maritima Dihydrofolate Reductase. ACS Catalysis, 2019, 9, 5902-5911.	11.2	12
129	Molecular surface calculations on organic compounds. Computational and Theoretical Chemistry, 1992, 254, 369-377.	1.5	11
130	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
131	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
132	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
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	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
135	AB initio rotational constants of the nitriles derived from cyanodiacetylene (HC4CN). Astrophysical Journal, 1994, 437, 532.	4.5	10
136	AB Initio Rotational Constants of Isocyanopolyynes. Astrophysical Journal, 1993, 415, L151.	4.5	10
137	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie - International Edition, 2005, 44, 904-909.	13.8	9
138	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
139	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
140	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
141	Thermal Isomerization Mechanism in Dronpa and Its Mutants. Journal of Physical Chemistry B, 2016, 120, 12820-12825.	2.6	9
142	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
143	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
144	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

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145	Theoretical rotational constants of MeCnN species. Chemical Physics Letters, 1990, 166, 54-56.	2.6	8
146	Molecular dynamics simulation in aqueous solution of N -methylazetidinone as a model of Î² -lactam antibiotics. Theoretical Chemistry Accounts, 1999, 101, 336-342.	1.4	8
147	Analysis of a concerted mechanism in Î²-lactam enzymatic hydrolysis. A quantum mechanics/molecular mechanics study. Journal of the Chemical Society Perkin Transactions II, 1999, , 1351-1356.	0.9	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	Molecular mechanism of chorismate mutase activity of promiscuos MbtI. Theoretical Chemistry Accounts, 2011, 128, 601-607.	1.4	8
151	Do zwitterionic species exist in the non-enzymatic peptide bond formation?. Chemical Communications, 2012, 48, 11253.	4.1	8
152	Substrate promiscuity in DNA methyltransferase M.PvuII. A mechanistic insight. Organic and Biomolecular Chemistry, 2012, 10, 5395.	2.8	8
153	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
154	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
155	The transition state and cognate concepts. Advances in Physical Organic Chemistry, 2019, 53, 29-68.	0.5	8
156	Mechanistic insights into the phosphoryl transfer reaction in cyclin-dependent kinase 2: A QM/MM study. PLoS ONE, 2019, 14, e0215793.	2.5	8
157	Modeling caspase-1 inhibition: Implications for catalytic mechanism and drug design. European Journal of Medicinal Chemistry, 2019, 169, 159-167.	5.5	8
158	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
159	A quantum mechanics-molecular mechanics study of dissociative electron transfer: The methylchloride radical anion in aqueous solution. Journal of Chemical Physics, 2002, 116, 6102-6110.	3.0	7
160	Molecular Mechanism of Inhibition of DNA Methylation by Zebularine. ACS Catalysis, 2017, 7, 1728-1732.	11.2	7
161	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
162	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

#	Article	IF	Citations
163	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
164	Correlation effects in proton transfer reactions in solution. Computational and Theoretical Chemistry, 1996, 371, 117-121.	1.5	6
165	Computational study on hydrolysis of cefotaxime in gas phase and in aqueous solution. Journal of Computational Chemistry, 2012, 33, 1948-1959.	3.3	6
166	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
167	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
168	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
169	The Solvent-Excluding Surface as a descriptor of ionic channels: Gramicidin-A. Computational and Theoretical Chemistry, 1998, 426, 331-338.	1.5	5
170	Modeling methods for studying post-translational and transcriptional modifying enzymes. Current Opinion in Chemical Biology, 2012, 16, 465-471.	6.1	5
171	Transition state ensemble optimization for reactions of arbitrary complexity. Journal of Chemical Physics, 2015, 143, 134111.	3.0	5
172	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
173	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
174	Origin of Enzymatic Kinetic Isotope Effects in Human Purine Nucleoside Phosphorylase. ACS Catalysis, 2018, 8, 815-827.	11.2	5
175	Heavy Enzymes and the Rational Redesign of Protein Catalysts. ChemBioChem, 2019, 20, 2807-2812.	2.6	5
176	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
177	Towards a Rational Design of Antibody Catalysts through Computational Chemistry. Angewandte Chemie, 2005, 117, 926-931.	2.0	3
178	Stereoselectivity Behavior of the AZ28 Antibody Catalyzed Oxy-Cope Rearrangementâ€. Journal of Physical Chemistry A, 2006, 110, 726-730.	2.5	3
179	Theoretical site-directed mutagenesis: Asp168Ala mutant of lactate dehydrogenase. Journal of the Royal Society Interface, 2008, 5, 217-224.	3.4	3
180	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

#	Article	IF	Citations
181	Exploration of the Activation Mechanism of the Epigenetic Regulator MLL3: A QM/MM Study. Biomolecules, 2021, 11, 1051.	4.0	3
182	Theoretical Studies of the Self Cleavage Pistol Ribozyme Mechanism. Topics in Catalysis, 0, , 1.	2.8	3
183	Ab initio rotational constants of interstellar species: Cyanoacetylene hydrogenated derivatives. International Journal of Quantum Chemistry, 1993, 46, 231-238.	2.0	2
184	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
185	A Simple Model for Barrier Frequencies for Enzymatic Reactions. ChemPhysChem, 2011, 12, 184-190.	2.1	2
186	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
187	Loss of Hyperconjugative Effects Drives Hydride Transfer during Dihydrofolate Reductase Catalysis. ACS Catalysis, 2019, 9, 10343-10349.	11.2	1
188	Seeking the Source of Catalytic Efficiency of Lindane Dehydrochlorinase, LinA. Journal of Physical Chemistry B, 2020, 124, 10353-10364.	2.6	1
189	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
190	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
191	Fundamental Principles Governing Solvent Use: Solvent Effects on Chemical Systems. ChemInform, 2003, 34, no.	0.0	0
192	Theoretical Insights in Enzyme Catalysis. ChemInform, 2004, 35, no.	0.0	0
193	Insights into the inhibited form of the redox-sensitive SufE-like sulfur acceptor CsdE. PLoS ONE, 2017, 12, e0186286.	2.5	0
194	Computational Insights Into Enzyme Catalysis. , 2020, , 560-577.		0
195	Inhibition Mechanism of SARSâ€CoVâ€2 Main Protease with Ketoneâ€Based Inhibitors Unveiled by Multiscale Simulations. Insights for Improved Designs. Angewandte Chemie, 0, , .	2.0	0
196	Computational Modeling of Biological Systems: The LDH Story. Challenges and Advances in Computational Chemistry and Physics, 2010, , 355-374.	0.6	0
197	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