

Fahmi Himo

List of Publications by Year in descending order

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53794

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133
all docs

133
docs citations

133
times ranked

8079
citing authors

#	ARTICLE	IF	CITATIONS
1	On the Importance of Considering Multinuclear Metal Sites in Homogeneous Catalysis Modeling. Topics in Catalysis, 2022, 65, 96-104.	2.8	4
2	Computational Study of Mechanism and Enantioselectivity of Imine Reductase from <i>Amycolatopsis orientalis</i> . ChemistryOpen, 2022, 11, e202100250.	1.9	7
3	Solvent Dependency in Stereoselective γ -Lactam Formation of Chiral α -Fluoromalonate Derivatives: Stereodivergent Synthesis of Heterocycles with Fluorine Containing Stereocenters Adjacent to Tertiary Stereocenters. Advanced Synthesis and Catalysis, 2022, 364, 958-965.	4.3	2
4	Status report on the quantum chemical cluster approach for modeling enzyme reactions. Communications Chemistry, 2022, 5, .	4.5	40
5	Binding and Assembly of a Benzotriazole Cavitand in Water. Angewandte Chemie - International Edition, 2022, 61, .	13.8	5
6	Computational and Experimental Study of Turbo-Organomagnesium Amide Reagents: Cubane Aggregates as Reactive Intermediates in Pummerer Coupling. Chemistry - A European Journal, 2021, 27, 2767-2773.	3.3	4
7	Metal Ion Promiscuity and Structure of 2,3-Dihydroxybenzoic Acid Decarboxylase of <i>Aspergillus oryzae</i> . ChemBioChem, 2021, 22, 652-656.	2.6	17
8	Mechanism of the Kinugasa Reaction Revisited. Journal of Organic Chemistry, 2021, 86, 10665-10671.	3.2	11
9	Combined Experimental and Computational Study of Ruthenium <i>N</i> -Hydroxyphthalimidoyl Carbenes in Alkene Cyclopropanation Reactions. ACS Catalysis, 2021, 11, 10950-10963.	11.2	9
10	Enzymatic Stetter Reaction: Computational Study of the Reaction Mechanism of MenD. ACS Catalysis, 2021, 11, 12355-12366.	11.2	6
11	Mechanisms of metal-dependent non-redox decarboxylases from quantum chemical calculations. Computational and Structural Biotechnology Journal, 2021, 19, 3176-3186.	4.1	12
12	Electrophilic Fluorination of Alkenes via Bora-Wagner-Meerwein Rearrangement. Access to α -Difluoroalkyl Boronates. Angewandte Chemie, 2021, 133, 26531.	2.0	4
13	Electrophilic Fluorination of Alkenes via Bora-Wagner-Meerwein Rearrangement. Access to α -Difluoroalkyl Boronates. Angewandte Chemie - International Edition, 2021, 60, 26327-26331.	13.8	31
14	Mechanism of Biocatalytic Friedel-Crafts Acylation by Acyltransferase from <i>Pseudomonas protegens</i> . ACS Catalysis, 2020, 10, 570-577.	11.2	24
15	Mechanisms of Formation and Rearrangement of Benziodoxole-Based CF ₃ and SCF ₃ Transfer Reagents. Journal of Organic Chemistry, 2020, 85, 15577-15585.	3.2	4
16	Computational Study of Pictet-Spenglerase Strictosidine Synthase: Reaction Mechanism and Origins of Enantioselectivity of Natural and Non-Natural Substrates. ACS Catalysis, 2020, 10, 13630-13640.	11.2	20
17	Enantioselective Construction of Tertiary Fluoride Stereocenters by Organocatalytic Fluorocyclization. Journal of the American Chemical Society, 2020, 142, 20048-20057.	13.7	55
18	Unraveling the Mechanism of the Ir ^{III} -Catalyzed Regiospecific Synthesis of α -Chlorocarbonyl Compounds from Allylic Alcohols. Chemistry - A European Journal, 2020, 26, 14978-14986.	3.3	4

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19	Mechanism of 3-Methylglutaconyl CoA Decarboxylase AibA/AibB: Pericyclic Reaction versus Direct Decarboxylation. <i>Angewandte Chemie</i> , 2020, 132, 23173-23177.	2.0	1
20	Esterification of Tertiary Amides: Remarkable Additive Effects of Potassium Alkoxides for Generating Hetero Manganese-Potassium Dinuclear Active Species. <i>Chemistry - A European Journal</i> , 2020, 26, 10647-10647.	3.3	0
21	Mechanism of 3-Methylglutaconyl CoA Decarboxylase AibA/AibB: Pericyclic Reaction versus Direct Decarboxylation. <i>Angewandte Chemie - International Edition</i> , 2020, 59, 22973-22977.	13.8	8
22	Variants of the Acyltransferase from <i>Mycobacterium smegmatis</i> Enable Enantioselective Acyl Transfer in Water. <i>ACS Catalysis</i> , 2020, 10, 10500-10507.	11.2	23
23	Modeling the Reaction of Carboxylic Acids and Isonitriles in a Self-Assembled Capsule. <i>Chemistry - A European Journal</i> , 2020, 26, 10861-10870.	3.3	5
24	Esterification of Tertiary Amides: Remarkable Additive Effects of Potassium Alkoxides for Generating Hetero Manganese-Potassium Dinuclear Active Species. <i>Chemistry - A European Journal</i> , 2020, 26, 10735-10742.	3.3	6
25	Modeling Enzymatic Enantioselectivity using Quantum Chemical Methodology. <i>ACS Catalysis</i> , 2020, 10, 6430-6449.	11.2	71
26	Mechanisms of Metal-Catalyzed Electrophilic F/CF ₃ /SCF ₃ Transfer Reactions from Quantum Chemical Calculations. <i>Topics in Organometallic Chemistry</i> , 2020, , 39-56.	0.7	2
27	Efficient Stereoselective Carbocyclization to <i>cis</i> -1,4-Disubstituted Heterocycles Enabled by Dual Pd/Electron Transfer Mediator (ETM) Catalysis. <i>Journal of the American Chemical Society</i> , 2020, 142, 5751-5759.	13.7	21
28	Origins of Enantioselectivity of <i>Mycobacterium smegmatis</i> Acyl Transferase: A Computational Analysis. <i>Chemistry - A European Journal</i> , 2019, 25, 11945-11954.	3.3	15
29	Computational characterization of enzyme-bound thiamin diphosphate reveals a surprisingly stable tricyclic state: implications for catalysis. <i>Beilstein Journal of Organic Chemistry</i> , 2019, 15, 145-159.	2.2	7
30	Diastereoselective Synthesis of <i>N</i> -Protected 2,3-Dihydropyrroles via Iron-Catalyzed Cycloisomerization of \pm -Allenic Sulfonamides. <i>ACS Catalysis</i> , 2019, 9, 1733-1737.	11.2	26
31	Enzymatic Pictet-Spengler Reaction: Computational Study of the Mechanism and Enantioselectivity of Norcochlorogenic Acid Synthase. <i>Journal of the American Chemical Society</i> , 2019, 141, 11230-11238.	13.7	49
32	Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis. <i>ACS Catalysis</i> , 2019, 9, 6803-6813.	11.2	145
33	Modeling Decomposition of <i>N</i> -Nitrosoamides in a Self-Assembled Capsule. <i>Journal of Organic Chemistry</i> , 2019, 84, 7354-7361.	3.2	5
34	Computational Study of Enantioselective Carbonylation Catalyzed by Benzoylformate Decarboxylase. <i>ACS Catalysis</i> , 2019, 9, 5657-5667.	11.2	13
35	Editorial: Challenges in Computational Enzymology. <i>Frontiers in Chemistry</i> , 2019, 7, 690.	3.6	3
36	Mechanism(s) of thermal decomposition of <i>N</i> -Nitrosoamides: A density functional theory study. <i>Tetrahedron</i> , 2019, 75, 929-935.	1.9	10

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37	Mechanisms of Rh-Catalyzed Oxyfluorination and Oxytrifluoromethylation of Diazocarbonyl Compounds with Hypervalent Fluoroiodine. <i>ACS Catalysis</i> , 2018, 8, 4483-4492.	11.2	35
38	Mechanism and Structure of \hat{I}^3 -Resorcylate Decarboxylase. <i>Biochemistry</i> , 2018, 57, 3167-3175.	2.5	30
39	Mechanistic Insight into Enantioselective Palladium-Catalyzed Oxidative Carbocyclization-Borylation of Enallenes. <i>Chemistry - A European Journal</i> , 2018, 24, 2433-2439.	3.3	11
40	Mechanism and selectivity of rhodium-catalyzed C-H bond arylation of indoles. <i>International Journal of Quantum Chemistry</i> , 2018, 118, e25526.	2.0	7
41	Efficient Formation of 2,3-Dihydrofurans via Iron-Catalyzed Cycloisomerization of \hat{I}^\pm -Allenols. <i>ACS Catalysis</i> , 2018, 8, 12-16.	11.2	42
42	Reaction Mechanism and Substrate Specificity of Iso-orotate Decarboxylase: A Combined Theoretical and Experimental Study. <i>Frontiers in Chemistry</i> , 2018, 6, 608.	3.6	12
43	An Unsymmetric Ligand with a N5 O2 Donor Set and Its Corresponding Dizinc Complex: A Structural and Functional Phosphoesterase Model. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 3986-3986.	2.0	0
44	Highly Selective Palladium-Catalyzed Hydroborylative Carbocyclization of Bisallenenes to Seven-Membered Rings. <i>Journal of the American Chemical Society</i> , 2018, 140, 14324-14333.	13.7	38
45	Computational Study of <i>Mycobacterium smegmatis</i> Acyl Transferase Reaction Mechanism and Specificity. <i>ACS Catalysis</i> , 2018, 8, 10698-10706.	11.2	40
46	Mechanisms of Rh-Catalyzed Oxyaminofluorination and Oxyaminotrifluoromethylthiolation of Diazocarbonyl Compounds with Electrophilic Reagents. <i>Organic Letters</i> , 2018, 20, 6646-6649.	4.6	20
47	Mixed Explicit-Implicit Solvation Approach for Modeling of Alkane Complexation in Water-Soluble Self-Assembled Capsules. <i>Journal of the American Chemical Society</i> , 2018, 140, 12527-12537.	13.7	15
48	An Unsymmetric Ligand with a N ₅ O ₂ Donor Set and Its Corresponding Dizinc Complex: A Structural and Functional Phosphoesterase Model. <i>European Journal of Inorganic Chemistry</i> , 2018, 2018, 4004-4013.	2.0	14
49	A Theoretical Study of the Benzoylformate Decarboxylase Reaction Mechanism. <i>Frontiers in Chemistry</i> , 2018, 6, 205.	3.6	15
50	Mechanistic alternatives for peptide bond formation on the ribosome. <i>Nucleic Acids Research</i> , 2018, 46, 5345-5354.	14.5	12
51	Mechanistic Elucidation of Zirconium-Catalyzed Direct Amidation. <i>Journal of the American Chemical Society</i> , 2017, 139, 2286-2295.	13.7	70
52	Theoretical Study of Enzyme Promiscuity: Mechanisms of Hydration and Carboxylation Activities of Phenolic Acid Decarboxylase. <i>ACS Catalysis</i> , 2017, 7, 1733-1741.	11.2	37
53	Recent Trends in Quantum Chemical Modeling of Enzymatic Reactions. <i>Journal of the American Chemical Society</i> , 2017, 139, 6780-6786.	13.7	199
54	A Combined Experimental-Theoretical Study of the LigW-Catalyzed Decarboxylation of 5-Carboxyvanillate in the Metabolic Pathway for Lignin Degradation. <i>ACS Catalysis</i> , 2017, 7, 4968-4974.	11.2	37

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55	Exploring the Catalytic Promiscuity of Phenolic Acid Decarboxylases: Asymmetric, 1,6-Conjugate Addition of Nucleophiles Across 4-Hydroxystyrene. <i>Advanced Synthesis and Catalysis</i> , 2017, 359, 2066-2075.	4.3	18
56	Quantum Chemical Study of Dual-Substrate Recognition in α -Transaminase. <i>ACS Omega</i> , 2017, 2, 890-898.	3.5	18
57	Metathesis Mechanism of Zinc-Catalyzed Fluorination of Alkenes with Hypervalent Fluoroiodine. <i>ACS Catalysis</i> , 2017, 7, 1093-1100.	11.2	57
58	Quantum Chemical Modeling of Cycloaddition Reaction in a Self-Assembled Capsule. <i>Journal of the American Chemical Society</i> , 2017, 139, 15494-15503.	13.7	35
59	Mechanism and Stereoselectivity of the BINOL-Catalyzed Allylboration of Skatoles. <i>Organic Letters</i> , 2017, 19, 5904-5907.	4.6	21
60	Regioselective <i>para</i> -Carboxylation of Catechols with a Prenylated Flavin Dependent Decarboxylase. <i>Angewandte Chemie - International Edition</i> , 2017, 56, 13893-13897.	13.8	64
61	Quantum chemical study of mechanism and stereoselectivity of secondary alcohol dehydrogenase. <i>Journal of Inorganic Biochemistry</i> , 2017, 175, 259-266.	3.5	23
62	Mechanism and Selectivity of Cooperatively Catalyzed Meyer-Schuster Rearrangement/Tsuji-Trost Allylic Substitution. Evaluation of Synergistic Catalysis by Means of Combined DFT and Kinetics Simulations. <i>Journal of the American Chemical Society</i> , 2017, 139, 10250-10266.	13.7	43
63	Regioselektive <i>para</i> -Carboxylierung von Catecholen mit einer Prenylflavin-abhängigen Decarboxylase. <i>Angewandte Chemie</i> , 2017, 129, 14081-14085.	2.0	6
64	Elucidation of Mechanisms and Selectivities of Metal-Catalyzed Reactions using Quantum Chemical Methodology. <i>Accounts of Chemical Research</i> , 2016, 49, 1006-1018.	15.6	73
65	Peptide Release on the Ribosome Involves Substrate-Assisted Base Catalysis. <i>ACS Catalysis</i> , 2016, 6, 8432-8439.	11.2	15
66	Quantum Chemical Modeling of Enantioconvergency in Soluble Epoxide Hydrolase. <i>ACS Catalysis</i> , 2016, 6, 8145-8155.	11.2	32
67	Origins of Stereoselectivity in Peptide-Catalyzed Kinetic Resolution of Alcohols. <i>ACS Catalysis</i> , 2016, 6, 1165-1171.	11.2	20
68	Nucleophilic Substitution of the Hydroxyl Group in Stereogenic Alcohols with Chirality Transfer. <i>Synlett</i> , 2016, 27, 173-176.	1.8	3
69	Theoretical Study of Phosphodiester Hydrolysis and Transesterification Catalyzed by an Unsymmetric Biomimetic Dizinc Complex. <i>Inorganic Chemistry</i> , 2016, 55, 1872-1882.	4.0	30
70	Enzyme catalysis by entropy without Circe effect. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, 2406-2411.	7.1	50
71	Theoretical study of the reaction mechanism of phenolic acid decarboxylase. <i>FEBS Journal</i> , 2015, 282, 4703-4713.	4.7	47
72	Catalytic Asymmetric Reactions of 4-Substituted Indoles with Nitroethene: A Direct Entry to Ergot Alkaloid Structures. <i>Chemistry - A European Journal</i> , 2015, 21, 17578-17582.	3.3	46

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73	Theoretical Study of Mechanism and Stereoselectivity of Catalytic Kinugasa Reaction. <i>Journal of Organic Chemistry</i> , 2015, 80, 2649-2660.	3.2	48
74	A quantum chemical study of the α -transaminase reaction mechanism. <i>Organic and Biomolecular Chemistry</i> , 2015, 13, 8453-8464.	2.8	70
75	Brønsted Acid-Catalyzed Intramolecular Nucleophilic Substitution of the Hydroxyl Group in Stereogenic Alcohols with Chirality Transfer. <i>Journal of the American Chemical Society</i> , 2015, 137, 4646-4649.	13.7	58
76	Mechanism, reactivity, and selectivity of the iridium-catalyzed C(sp ³)–H borylation of chlorosilanes. <i>Chemical Science</i> , 2015, 6, 1735-1746.	7.4	63
77	A Heterobimetallic Fe ^{III} Mn ^{II} Complex of an Unsymmetrical Dinucleating Ligand: A Structural and Functional Model Complex for the Active Site of Purple Acid Phosphatase of Sweet Potato. <i>European Journal of Inorganic Chemistry</i> , 2014, 2014, 2204-2212.	2.0	35
78	A dinuclear zinc(II) complex of a new unsymmetric ligand with an N5O2 donor set; A structural and functional model for the active site of zinc phosphoesterases. <i>Journal of Inorganic Biochemistry</i> , 2014, 132, 6-17.	3.5	28
79	Quantum Chemical Studies of Mechanisms for Metalloenzymes. <i>Chemical Reviews</i> , 2014, 114, 3601-3658.	47.7	494
80	Theoretical Study of Reaction Mechanism and Stereoselectivity of Arylmalonate Decarboxylase. <i>ACS Catalysis</i> , 2014, 4, 4153-4160.	11.2	44
81	Stereoselective allylboration of imines and indoles under mild conditions. An <i>in situ</i> E/Z isomerization of imines by allylboroxines. <i>Chemical Science</i> , 2014, 5, 2732-2738.	7.4	54
82	Arylation with Unsymmetrical Diaryliodonium Salts: A Chemoselectivity Study. <i>Chemistry - A European Journal</i> , 2013, 19, 10334-10342.	3.3	220
83	Quantum Chemistry as a Tool in Asymmetric Biocatalysis: Limonene Epoxide Hydrolase Test Case. <i>Angewandte Chemie - International Edition</i> , 2013, 52, 4563-4567.	13.8	54
84	Combining Meyer–Schuster Rearrangement with Aldol and Mannich Reactions: Theoretical Study of the Intermediate Interception Strategy. <i>Journal of the American Chemical Society</i> , 2012, 134, 19159-19169.	13.7	26
85	Theoretical Study of Asymmetric Transfer Hydrogenation of Ketones Catalyzed by Amino Acid-Derived Rhodium Complexes. <i>ChemCatChem</i> , 2012, 4, 1095-1104.	3.7	22
86	Luminescence properties of the Cu ₄ I ₆ ²⁺ cluster. <i>CrystEngComm</i> , 2011, 13, 4729.	2.6	22
87	Theoretical Study of the Chemoselectivity of Tungsten-Dependent Acetylene Hydratase. <i>ACS Catalysis</i> , 2011, 1, 937-944.	11.2	31
88	Quantum Chemical Modeling of Enzymatic Reactions: The Case of Decarboxylation. <i>Journal of Chemical Theory and Computation</i> , 2011, 7, 1494-1501.	5.3	66
89	Theoretical Study of Mechanism and Selectivity of Copper-Catalyzed C–H Bond Amidation of Indoles. <i>Journal of Organic Chemistry</i> , 2011, 76, 9246-9252.	3.2	44
90	The quantum chemical cluster approach for modeling enzyme reactions. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , 2011, 1, 323-336.	14.6	232

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91	Quantum chemical modeling of enzymatic reactions: The case of histone lysine methyltransferase. <i>Journal of Computational Chemistry</i> , 2010, 31, 1707-1714.	3.3	63
92	Quantum Chemical Modeling of Enzymatic Reactions – Applications to Epoxide-Transforming Enzymes. , 2010, , 719-747.		11
93	Phosphate Mono- and Diesterase Activities of the Trinuclear Zinc Enzyme Nuclease P1 – Insights from Quantum Chemical Calculations. <i>Inorganic Chemistry</i> , 2010, 49, 6883-6888.	4.0	33
94	Reaction Mechanism of the Trinuclear Zinc Enzyme Phospholipase C: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2533-2540.	2.6	38
95	Origin of Enantioselectivity in the Organocatalytic Reductive Amination of β -Branched Aldehydes. <i>Advanced Synthesis and Catalysis</i> , 2009, 351, 525-529.	4.3	61
96	Theoretical Study of the RNA Hydrolysis Mechanism of the Dinuclear Zinc Enzyme RNase Z. <i>European Journal of Inorganic Chemistry</i> , 2009, 2009, 2967-2972.	2.0	15
97	Recent developments of the quantum chemical cluster approach for modeling enzyme reactions. <i>Journal of Biological Inorganic Chemistry</i> , 2009, 14, 643-651.	2.6	257
98	Technical aspects of quantum chemical modeling of enzymatic reactions: the case of phosphotriesterase. <i>Theoretical Chemistry Accounts</i> , 2008, 120, 515-522.	1.4	67
99	Theoretical Investigation of the Reaction Mechanism of the Dinuclear Zinc Enzyme Dihydroorotase. <i>Chemistry - A European Journal</i> , 2008, 14, 4287-4292.	3.3	47
100	Theoretical Investigation of the Second-Shell Mechanism of Nitrile Hydratase. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 1406-1412.	2.0	24
101	On the Role of Tyrosine as Catalytic Base in Nitrile Hydratase. <i>European Journal of Inorganic Chemistry</i> , 2008, 2008, 3452-3459.	2.0	10
102	Reaction of Carboxylic Acids with Isocyanides: A Mechanistic DFT Study. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 4751-4754.	2.4	12
103	Quantum Chemical Modeling of the Dehalogenation Reaction of Haloalcohol Dehalogenase. <i>Journal of Chemical Theory and Computation</i> , 2008, 4, 1129-1137.	5.3	72
104	Density Functional Theory Study of the Cinchona Thiourea-Catalyzed Henry Reaction: Mechanism and Enantioselectivity. <i>Advanced Synthesis and Catalysis</i> , 2007, 349, 2537-2548.	4.3	99
105	Quantum chemical modeling of enzymatic reactions: The case of 4-oxalocrotonate tautomerase. <i>Bioorganic Chemistry</i> , 2007, 35, 444-457.	4.1	78
106	Insights into the Reaction Mechanism of Soluble Epoxide Hydrolase from Theoretical Active Site Mutants. <i>Journal of Physical Chemistry B</i> , 2006, 110, 21299-21310.	2.6	41
107	Quantum chemical modeling of enzyme active sites and reaction mechanisms. <i>Theoretical Chemistry Accounts</i> , 2006, 116, 232-240.	1.4	180
108	Theoretical Study of the Full Reaction Mechanism of Human Soluble Epoxide Hydrolase. <i>Chemistry - A European Journal</i> , 2006, 12, 6898-6909.	3.3	59

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109	Copper(I)-Catalyzed Synthesis of Azoles. DFT Study Predicts Unprecedented Reactivity and Intermediates. <i>Journal of the American Chemical Society</i> , 2005, 127, 210-216.	13.7	1,497
110	Reaction Mechanism of Deoxyribonucleotidase: A Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2005, 109, 20004-20008.	2.6	18
111	Catalytic Mechanism of Limonene Epoxide Hydrolase, a Theoretical Study. <i>Journal of the American Chemical Society</i> , 2005, 127, 14339-14347.	13.7	78
112	C-C bond formation and cleavage in radical enzymes, a theoretical perspective. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2005, 1707, 24-33.	1.0	53
113	Quantum Chemical Studies of Radical-Containing Enzymes. <i>Chemical Reviews</i> , 2003, 103, 2421-2456.	47.7	266
114	Density Functional Theory Study of the Intramolecular [2 + 3] Cycloaddition of Azide to Nitriles. <i>Journal of Organic Chemistry</i> , 2003, 68, 9076-9080.	3.2	36
115	DNA Repair by Spore Photoproduct Lyase: A Density Functional Theory Study. <i>Journal of Physical Chemistry B</i> , 2003, 107, 11188-11192.	2.6	18
116	Why Is Tetrazole Formation by Addition of Azide to Organic Nitriles Catalyzed by Zinc(II) Salts?. <i>Journal of the American Chemical Society</i> , 2003, 125, 9983-9987.	13.7	333
117	Catalytic Mechanism of Benzylsuccinate Synthase, a Theoretical Study. <i>Journal of Physical Chemistry B</i> , 2002, 106, 7688-7692.	2.6	42
118	Mechanisms of Tetrazole Formation by Addition of Azide to Nitriles. <i>Journal of the American Chemical Society</i> , 2002, 124, 12210-12216.	13.7	303
119	Density Functional Theory Study of the $\dot{\text{I}}^2$ -Carotene Radical Cation. <i>Journal of Physical Chemistry A</i> , 2001, 105, 7933-7937.	2.5	32
120	Catalytic Mechanism of Glyoxalase I: A Theoretical Study. <i>Journal of the American Chemical Society</i> , 2001, 123, 10280-10289.	13.7	50
121	Substituent effects on OH bond strength and hyperfine properties of phenol, as model for modified tyrosyl radicals in proteins. <i>International Journal of Quantum Chemistry</i> , 2000, 76, 714-723.	2.0	68
122	Very Stable Ribonucleotide Substrate Radical Relevant for Class I Ribonucleotide Reductase. <i>Journal of Physical Chemistry B</i> , 2000, 104, 7502-7509.	2.6	37
123	Substituent effects on OH bond strength and hyperfine properties of phenol, as model for modified tyrosyl radicals in proteins. , 2000, 76, 714.		1
124	Catalytic Mechanism of Pyruvate Formate-Lyase (PFL). A Theoretical Study. <i>Journal of the American Chemical Society</i> , 1998, 120, 11449-11455.	13.7	69
125	Effects of Ionizing Radiation on Crystalline Cytosine Monohydrate. <i>Journal of Physical Chemistry B</i> , 1998, 102, 7484-7491.	2.6	68
126	Hydrogen Atom Transfer in Ribonucleotide Reductase (RNR). <i>Journal of Physical Chemistry B</i> , 1998, 102, 10622-10629.	2.6	138

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127	Electronic and Magnetic Properties of Neutral and Charged Quinone and Plastoquinone Radicals. Journal of Physical Chemistry A, 1997, 101, 9496-9504.	2.5	51
128	Theoretical Study of Model Tryptophan Radicals and Radical Cations:Â Comparison with Experimental Data of DNA Photolyase, Cytochrome c Peroxidase, and Ribonucleotide Reductase. Journal of Physical Chemistry B, 1997, 101, 9811-9819.	2.6	46
129	Binding and Assembly of a Benzotriazole Cavitand in Water. Angewandte Chemie, 0, , .	2.0	4