

# Yongjun Liu

## List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

136  
papers

1,320  
citations

19  
h-index

28  
g-index

143  
ext. papers

1,701  
ext. citations

5.4  
avg. IF

5.18  
L-index

#	Paper	IF	Citations
136	Multipoint Costriking Nanodevice Eliminates Primary Tumor Cells and Associated-Circulating Tumor Cells for Enhancing Metastasis Inhibition and Therapeutic Effect on HCC.. <i>Advanced Science</i> , <b>2022</b> , e2101472	13.6	2
135	Amphiphilic small molecular mates match hydrophobic drugs to form nanoassemblies based on drug-mate strategy.. <i>Asian Journal of Pharmaceutical Sciences</i> , <b>2022</b> , 17, 129-138	9	0
134	DT7 peptide-modified lecithin nanoparticles co-loaded with ßsecretase inhibitor and dexamethasone efficiently inhibit T-cell acute lymphoblastic leukemia and reduce gastrointestinal toxicity.. <i>Cancer Letters</i> , <b>2022</b> , 533, 215608	9.9	
133	Artificial Assembled Macrophage Co-Deliver Black Phosphorus Quantum Dot and CDK4/6 Inhibitor for Colorectal Cancer Triple-Therapy.. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2022</b> , 14, 20628-20640	9.5	0
132	Computational Study of the C5-Hydroxylation Mechanism Catalyzed by the Diiron Monooxygenase PtmU3 as Part of the Platensimycin Biosynthesis. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 17783-17796	5.1	2
131	A comparison between exogenous carriers enhanced aerobic granulation under low organic loading in the aspect of sludge characteristics, extracellular polymeric substances and microbial communities.. <i>Bioresource Technology</i> , <b>2021</b> , 346, 126567	11	0
130	Reshaping Antitumor Immunity with Chemo-Photothermal Integrated Nanoplatform to Augment Checkpoint Blockade-Based Cancer Therapy. <i>Advanced Functional Materials</i> , <b>2021</b> , 31, 2100437	15.6	9
129	Formation Mechanism of Cofactor Cys-Tyr in the Cysteine Dioxygenases (CDO and F-CDO) and Its Influence on Catalysis: A QM/MM Study. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 7844-7856	5.1	0
128	Lymph Node Delivery Strategy Enables the Activation of Cytotoxic T Lymphocytes and Natural Killer Cells to Augment Cancer Immunotherapy. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2021</b> , 13, 22213-22224	9.5	4
127	Inactivation Mechanism of Neuronal Nitric Oxide Synthase by ()-2-Amino-5-(2-(methylthio)acetimidamido)pentanoic Acid: Chemical Conversion of the Inactivator in the Active Site. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 9345-9358	5.1	
126	High-Specific Isolation and Instant Observation of Circulating Tumour Cell from HCC Patients via Glypican-3 Immunomagnetic Fluorescent Nanodevice. <i>International Journal of Nanomedicine</i> , <b>2021</b> , 16, 4161-4173	7.3	2
125	Mechanistic Insights into the P450 TleB-Catalyzed Unusual Intramolecular C-N Bond Formation Involved in the Biosynthesis of Indolactam V. <i>Journal of Chemical Information and Modeling</i> , <b>2021</b> , 61, 3638-3648	6.1	3
124	Gas-blasting nanocapsules to accelerate carboplatin lysosome release and nucleus delivery for prostate cancer treatment. <i>Asian Journal of Pharmaceutical Sciences</i> , <b>2021</b> , 16, 192-202	9	0
123	Manipulation of TAMs functions to facilitate the immune therapy effects of immune checkpoint antibodies. <i>Journal of Controlled Release</i> , <b>2021</b> , 336, 621-634	11.7	6
122	Tyrosyl Radical-Mediated Sequential Oxidative Decarboxylation of Coproporphyrinogen III through PCET: Theoretical Insights into the Mechanism of Coproheme Decarboxylase ChdC. <i>Inorganic Chemistry</i> , <b>2021</b> , 60, 13539-13549	5.1	2
121	A Review on Nano-Based Drug Delivery System for Cancer Chemoimmunotherapy. <i>Nano-Micro Letters</i> , <b>2020</b> , 12, 142	19.5	63
120	Engineering Thermo-pH Dual Responsive Hydrogel for Enhanced Tumor Accumulation, Penetration, and Chemo-Protein Combination Therapy. <i>International Journal of Nanomedicine</i> , <b>2020</b> , 15, 4739-4752	7.3	2

119	The Retaining Mechanism of Xylose Transfer Catalyzed by Xyloside H <sub>1</sub> ,3-Xylosyltransferase (XXYLT1): a Quantum Mechanics/Molecular Mechanics Study. <i>Journal of Chemical Information and Modeling</i> , <b>2020</b> , 60, 1585-1594	6.1	5
118	Theoretical Study of Iron Porphyrin Nitrene: Formation Mechanism, Electronic Nature, and Intermolecular C-H Amination. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 1622-1632	5.1	13
117	Mechanistic Investigation of Isonitrile Formation Catalyzed by the Nonheme Iron/ϳKG-Dependent Decarboxylase (ScoE). <i>ACS Catalysis</i> , <b>2020</b> , 10, 2942-2957	13.1	16
116	Mechanical Insights into the Enzymatic Cleavage of Double C-C Bond in Poly(-1,4-isoprene) by the Latex Clearing Protein. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 9627-9637	5.1	5
115	Small Morph Nanoparticles for Deep Tumor Penetration via Caveolae-Mediated Transcytosis. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2020</b> , 12, 38499-38511	9.5	10
114	Imidazoquinoline-Conjugated Degradable Coacervate Conjugate for Local Cancer Immunotherapy. <i>ACS Biomaterials Science and Engineering</i> , <b>2020</b> , 6, 4993-5000	5.5	4
113	Mechanistic Insights into the Oxidative Rearrangement Catalyzed by the Unprecedented Dioxygenase ChaP Involved in Chartreusin Biosynthesis. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 13988-13999	5.1	1
112	Mechanistic Insights into the Oxidative Ring Expansion from Penicillin N to Deacetoxycephalosporin C Catalyzed by a Nonheme Iron(II) and ϳKG-Dependent Oxygenase. <i>Inorganic Chemistry</i> , <b>2020</b> , 59, 12218-12231	5.1	3
111	Nanoparticle-Loaded Polarized-Macrophages for Enhanced Tumor Targeting and Cell-Chemotherapy. <i>Nano-Micro Letters</i> , <b>2020</b> , 13, 6	19.5	8
110	Insights into the Mechanism and Enantioselectivity in the Biosynthesis of Ergot Alkaloid Cycloclavine Catalyzed by Aj_EasH from. <i>Inorganic Chemistry</i> , <b>2019</b> , 58, 13771-13781	5.1	10
109	Mechanical insights into the oxidative cleavage of resveratrol catalyzed by dioxygenase NOV1 from <i>Novosphingobium aromaticivorans</i> : confirmation of dioxygenase mechanism by QM/MM calculations. <i>Catalysis Science and Technology</i> , <b>2019</b> , 9, 444-455	5.5	9
108	Impact of Al-based coagulants on the formation of aerobic granules: Comparison between poly aluminum chloride (PAC) and aluminum sulfate (AS). <i>Science of the Total Environment</i> , <b>2019</b> , 685, 74-84	10.2	13
107	Promoting Early Diagnosis and Precise Therapy of Hepatocellular Carcinoma by Glypican-3-Targeted Synergistic Chemo-Photothermal Theranostics. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2019</b> , 11, 23591-23604	9.5	36
106	Spatial distribution, source identification, and potential risk assessment of toxic contaminants in surface waters from Yulin, China. <i>Environmental Monitoring and Assessment</i> , <b>2019</b> , 191, 293	3.1	4
105	The charge regulation of electronic structure and optical properties of graphitic carbon nitride under strain.. <i>RSC Advances</i> , <b>2019</b> , 9, 7464-7468	3.7	6
104	Conversion mechanism of enoyl thioesters into acyl thioesters catalyzed by 2-enoyl-thioester reductases from <i>Candida Tropicalis</i> . <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 10105-10113	3.6	2
103	Constructing a synthetic pathway for acetyl-coenzyme A from one-carbon through enzyme design. <i>Nature Communications</i> , <b>2019</b> , 10, 1378	17.4	58
102	Co-delivery of sorafenib and VEGF-siRNA via pH-sensitive liposomes for the synergistic treatment of hepatocellular carcinoma. <i>Artificial Cells, Nanomedicine and Biotechnology</i> , <b>2019</b> , 47, 1374-1383	6.1	32

101	Strengthening of aerobic sludge granulation by the endogenous acylated homoserine lactones-secreting strain <i>Aeromonas</i> sp. A-L3. <i>Biochemical Engineering Journal</i> , <b>2019</b> , 151, 107329	4.2	3
100	Preparation and evaluation of etoposide-loaded lipid-based nanosuspensions for high-dose treatment of lymphoma. <i>Nanomedicine</i> , <b>2019</b> , 14, 1403-1427	5.6	3
99	Catalytic mechanism of the PrhA (V150L/A232S) double mutant involved in the fungal meroterpenoid biosynthetic pathway: a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , <b>2019</b> , 21, 25658-25668	3.6	5
98	Mechanism of fatty acid decarboxylation catalyzed by a non-heme iron oxidase (UndA): a QM/MM study. <i>Organic and Biomolecular Chemistry</i> , <b>2019</b> , 17, 9808-9818	3.9	2
97	Mechanism of Uncoupled Carbocyclization and Epimerization Catalyzed by Two Non-Heme Iron/Ketoglutarate Dependent Enzymes. <i>Journal of Chemical Information and Modeling</i> , <b>2019</b> , 59, 5086-5098	6.1	3
96	Synergistic strengthening mechanism of hydraulic selection pressure and poly aluminum chloride (PAC) regulation on the aerobic sludge granulation. <i>Science of the Total Environment</i> , <b>2019</b> , 650, 941-950	10.2	12
95	Computational evidence for the importance of lysine carboxylation in the reaction catalyzed by carboxyl transferase domain of pyruvate carboxylase: a QM/MM study. <i>Theoretical Chemistry Accounts</i> , <b>2019</b> , 138, 1	1.9	1
94	Insights into the dioxygen activation and catalytic mechanism of the nickel-containing quercetinase. <i>Catalysis Science and Technology</i> , <b>2018</b> , 8, 2340-2351	5.5	9
93	A Novel ZnONPs/PVA-Functionalized Biomaterials for Bacterial Cells Immobilization and its Strengthening Effects on Quinoline Biodegradation. <i>Current Microbiology</i> , <b>2018</b> , 75, 316-322	2.4	3
92	Unified D- $\alpha$ -Tocopherol 5-Fu/SAHA bioconjugates self-assemble as complex nanodrug for optimized combination therapy. <i>Nanomedicine</i> , <b>2018</b> , 13, 1285-1301	5.6	3
91	Hormesis of mercuric chloride-human serum albumin adduct on N9 microglial cells via the ERK/MAPKs and JAK/STAT3 signaling pathways. <i>Toxicology</i> , <b>2018</b> , 408, 62-69	4.4	8
90	Oxidative Rearrangement Mechanism of Pentalenolactone F Catalyzed by Cytochrome P450 CYP161C2 (PntM). <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 8933-8941	5.1	8
89	Potential application of a porous graphitic carbon nitride as an organic metal-free photocatalyst for water splitting. <i>Diamond and Related Materials</i> , <b>2018</b> , 87, 50-55	3.5	13
88	Protonation state and fine structure of the active site determine the reactivity of dehydratase: hydration and isomerization of $\beta$ -myrcene catalyzed by linalool dehydratase/isomerase from <i>Castellaniella defragrans</i> . <i>Physical Chemistry Chemical Physics</i> , <b>2018</b> , 20, 17342-17352	3.6	6
87	Insights into the decarboxylative hydroxylation of salicylate catalyzed by the Flavin-dependent monooxygenase salicylate hydroxylase. <i>Theoretical Chemistry Accounts</i> , <b>2018</b> , 137, 1	1.9	7
86	Cascade Cytosol Delivery of Dual-Sensitive Micelle-Tailored Vaccine for Enhancing Cancer Immunotherapy. <i>ACS Applied Materials &amp; Interfaces</i> , <b>2018</b> , 10, 37797-37811	9.5	23
85	Theoretical Insights into the Mechanism and Stereoselectivity of Olefin Cyclopropanation Catalyzed by Two Engineered Cytochrome P450 Enzymes. <i>Inorganic Chemistry</i> , <b>2018</b> , 57, 11738-11745	5.1	16
84	Mechanism of Sulfoxidation and C-B Bond Formation Involved in the Biosynthesis of Ergothioneine Catalyzed by Ergothioneine Synthase (EgtB). <i>ACS Catalysis</i> , <b>2018</b> , 8, 5875-5889	13.1	21

83	Reductive Homocoupling of Organohalides Using Nickel(II) Chloride and Samarium Metal. <i>Chemistry - an Asian Journal</i> , <b>2017</b> , 12, 673-678	4.5	14
82	Insights into the unprecedented epoxidation mechanism of fumitremorgin B endoperoxidase (FtmOx1) from <i>Aspergillus fumigatus</i> by QM/MM calculations. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 7668-7677	3.6	20
81	Cleavage mechanism of the aliphatic C-C bond catalyzed by 2,4-dihydroxyacetophenone dioxygenase from <i>Alcaligenes</i> sp. 4HAP: a QM/MM study. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 911-922	5.5	5
80	Mechanistic insights into the catalytic reaction of ferulic acid decarboxylase from <i>Aspergillus niger</i> : a QM/MM study. <i>Physical Chemistry Chemical Physics</i> , <b>2017</b> , 19, 7733-7742	3.6	20
79	QM/MM studies of the type II isopentenyl diphosphate dimethylallyl diphosphate isomerase demonstrate a novel role for the flavin coenzyme. <i>RSC Advances</i> , <b>2017</b> , 7, 22286-22293	3.7	0
78	Reductive Bis-addition of Aromatic Aldehydes to $\alpha,\beta$ -Unsaturated Esters via the Use of Sm/Cu(I) in Air: A Route to the Construction of Furofuran Lignans. <i>Journal of Organic Chemistry</i> , <b>2017</b> , 82, 5932-5939	4.2	8
77	Theoretical insights into the protonation states of active site cysteine and citrullination mechanism of <i>Porphyromonas gingivalis</i> peptidylarginine deiminase. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2017</b> , 85, 1518-1528	4.2	3
76	Tryptophan lyase (NosL): mechanistic insights into amine dehydrogenation and carboxyl fragment migration by QM/MM calculations. <i>Catalysis Science and Technology</i> , <b>2017</b> , 7, 2846-2856	5.5	11
75	Strengthen effects of dominant strains on aerobic digestion and stabilization of the residual sludge. <i>Bioresource Technology</i> , <b>2017</b> , 235, 202-210	11	10
74	Comparative studies of the catalytic mechanisms of two chorismatases: CH-fkbo and CH-Hyg5. <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2017</b> , 85, 1146-1158	4.2	8
73	Theoretical study of the catalytic mechanism of glyoxylate carbonylase and its mutant V51E. <i>Theoretical Chemistry Accounts</i> , <b>2017</b> , 136, 1	1.9	1
72	Mechanistic insights into the $\beta$ -elimination reaction of L-methionine catalyzed by methionine lyase (MGL). <i>Theoretical Chemistry Accounts</i> , <b>2017</b> , 136, 1	1.9	3
71	Evaluation and quantification of genotoxicity of urban waters by using <i>Vicia faba</i> bioassays. <i>Chemistry and Ecology</i> , <b>2017</b> , 33, 669-683	2.3	2
70	Unsaturated nitrogen-rich polymer poly(L-histidine) gated reversibly switchable mesoporous silica nanoparticles using "graft to" strategy for drug controlled release. <i>Acta Biomaterialia</i> , <b>2017</b> , 63, 150-162	10.8	32
69	A water-assisted nucleophilic mechanism utilized by BphD, the meta-cleavage product hydrolase in biphenyl degradation. <i>Journal of Molecular Graphics and Modelling</i> , <b>2017</b> , 76, 448-455	2.8	2
68	A QM/MM study of the catalytic mechanism of SAM methyltransferase RlmN from <i>Escherichia coli</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2017</b> , 85, 1967-1974	4.2	2
67	Tuning the electronic and optical properties of NDT-based conjugated polymers by adopting fused heterocycles as acceptor units: a theoretical study. <i>Journal of Molecular Modeling</i> , <b>2017</b> , 23, 225	2	2
66	Mechanistic Insights into the Decoupled Desaturation and Epoxidation Catalyzed by Dioxygenase AsqJ Involved in the Biosynthesis of Quinolone Alkaloids. <i>ACS Catalysis</i> , <b>2017</b> , 7, 5534-5543	13.1	39

65	Treatment effects and genotoxicity relevance of the toxic organic pollutants in semi-coking wastewater by combined treatment process. <i>Environmental Pollution</i> , <b>2017</b> , 220, 13-19	9.3	47
64	Catalytic mechanism of acetolactate decarboxylase from <i>Brevibacillus brevis</i> towards both enantiomers of acetolactate. <i>RSC Advances</i> , <b>2016</b> , 6, 80621-80629	3.7	9
63	QM/MM studies on the calcium-assisted elimination mechanism of pectate lyase from <i>Bacillus subtilis</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2016</b> , 84, 1606-1615	4.2	4
62	Mechanism of the Glutathione Persulfide Oxidation Process Catalyzed by Ethylmalonic Encephalopathy Protein 1. <i>ACS Catalysis</i> , <b>2016</b> , 6, 7010-7020	13.1	8
61	Exploring the substrate specificity and catalytic mechanism of imidazolonepropionase (HutI) from <i>Bacillus subtilis</i> . <i>Physical Chemistry Chemical Physics</i> , <b>2016</b> , 18, 27928-27938	3.6	4
60	Theoretical study of the hydrolysis mechanism of dihydrocoumarin catalyzed by serum paraoxonase 1 (PON1): different roles of Glu53 and His115 for catalysis. <i>RSC Advances</i> , <b>2016</b> , 6, 60376-60384	3.7	2
59	Structures and photoelectric properties of five benzotrithiophene isomers-based donor-acceptor copolymers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , <b>2016</b> , 159, 262-8	4.4	4
58	Insights into the catalytic mechanism of N-acetylglucosaminidase glycoside hydrolase from <i>Bacillus subtilis</i> : a QM/MM study. <i>Organic and Biomolecular Chemistry</i> , <b>2016</b> , 14, 3432-42	3.9	8
57	Quantum mechanics and molecular mechanics study of the reaction mechanism of quorum quenching enzyme: N-acyl homoserine lactonase with C6-HSL. <i>RSC Advances</i> , <b>2016</b> , 6, 23396-23402	3.7	2
56	Theoretical study of the hydrolysis mechanism of 2-pyrone-4,6-dicarboxylate (PDC) catalyzed by Lgl. <i>Journal of Molecular Graphics and Modelling</i> , <b>2015</b> , 61, 21-9	2.8	3
55	Quantum Mechanics and Molecular Mechanics Study of the Catalytic Mechanism of Human AMSH-LP Domain Deubiquitinating Enzymes. <i>Biochemistry</i> , <b>2015</b> , 54, 5225-34	3.2	3
54	Catalytic mechanisms of Au <sub>n</sub> and Au <sub>n</sub> Pt <sub>n</sub> (n=1-2) clusters: a DFT investigation on the oxidation of CO by O <sub>2</sub> . <i>Journal of Molecular Modeling</i> , <b>2015</b> , 21, 230	2	10
53	Theoretical identification on the role of Lys15 for <i>Sulfolobus tokodaii</i> hexokinase. <i>RSC Advances</i> , <b>2015</b> , 5, 18622-18632	3.7	2
52	Uncoupled Epimerization and Desaturation by Carbapenem Synthase: Mechanistic Insights from QM/MM Studies. <i>ACS Catalysis</i> , <b>2015</b> , 5, 5556-5566	13.1	27
51	Theoretical studies of traditional and halogen-shared halogen bonds: the doped all-metal aromatic clusters MAI <sub>3</sub> (M = Si, Ge, Sn, Pb) as halogen bond acceptors. <i>Theoretical Chemistry Accounts</i> , <b>2015</b> , 134, 1	1.9	1
50	A QM/MM study of the catalytic mechanism of succinic semialdehyde dehydrogenase from <i>Synechococcus</i> sp. PCC 7002 and <i>Salmonella typhimurium</i> . <i>RSC Advances</i> , <b>2015</b> , 5, 101672-101682	3.7	3
49	Deep-blue electroluminescence from nondoped and doped organic light-emitting diodes (OLEDs) based on a new monoaza[6]helicene. <i>RSC Advances</i> , <b>2015</b> , 5, 75-84	3.7	65
48	Long time molecular dynamic simulation on the agonist binding and activation of the $\beta$ -adrenergic receptor. <i>Molecular Simulation</i> , <b>2015</b> , 41, 564-571	2	1

47	Ring Contraction Catalyzed by the Metal-Dependent Radical SAM Enzyme: 7-Carboxy-7-deazaguanine Synthase from <i>B. multivorans</i> . Theoretical Insights into the Reaction Mechanism and the Influence of Metal Ions. <i>ACS Catalysis</i> , <b>2015</b> , 5, 3953-3965	13.1	19
46	Exploring the substrate-assisted acetylation mechanism by UDP-linked sugar N-acetyltransferase from QM/MM calculations: the role of residue Asn84 and the effects of starting geometries. <i>RSC Advances</i> , <b>2015</b> , 5, 7781-7788	3.7	4
45	A QM/MM study of the reaction mechanism of (R)-hydroxynitrile lyases from <i>Arabidopsis thaliana</i> (AtHNL). <i>Proteins: Structure, Function and Bioinformatics</i> , <b>2015</b> , 83, 66-77	4.2	6
44	QM/MM study on the catalytic mechanism of cyclohexane-1,2-dione hydrolase (CDH). <i>Theoretical Chemistry Accounts</i> , <b>2014</b> , 133, 1	1.9	2
43	Theoretical investigation on the regioselectivity of Ni(COD) <sub>2</sub> -catalyzed [2 + 2 + 2] cycloaddition of unsymmetric diynes and CO <sub>2</sub> . <i>Journal of Organometallic Chemistry</i> , <b>2014</b> , 758, 45-54	2.3	8
42	A QM/MM study of the catalytic mechanism of aspartate ammonia lyase. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 51, 113-9	2.8	7
41	Water promoting electron hole transport between tyrosine and cysteine in proteins via a special mechanism: double proton coupled electron transfer. <i>Journal of the American Chemical Society</i> , <b>2014</b> , 136, 4515-24	16.4	35
40	A QM/MM study of the catalytic mechanism of nicotinamidase. <i>Organic and Biomolecular Chemistry</i> , <b>2014</b> , 12, 1265-77	3.9	10
39	Investigation of the rescue mechanism catalyzed by a nucleophile mutant of rice BGlul. <i>Journal of Molecular Graphics and Modelling</i> , <b>2014</b> , 54, 100-6	2.8	4
38	The structures and properties of halogen bonds involving polyvalent halogen in complexes of FXOn (X = Cl, Br; n = 0B)H <sub>3</sub> CN. <i>New Journal of Chemistry</i> , <b>2014</b> , 38, 1256	3.6	23
37	Insights into the catalytic mechanism of dTDP-glucose 4,6-dehydratase from quantum mechanics/molecular mechanics simulations. <i>RSC Advances</i> , <b>2014</b> , 4, 35449	3.7	6
36	Theoretical investigation on the dissociation of (R)-benzoin catalyzed by benzaldehyde lyase. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 375-382	2.1	5
35	A density functional theory study on the catalytic mechanism of hydroxycinnamoyl-CoA hydratase-lyase. <i>International Journal of Quantum Chemistry</i> , <b>2014</b> , 114, 249-254	2.1	6
34	A theoretical study of the catalytic mechanism of oxalyl-CoA decarboxylase, an enzyme for treating urolithiasis. <i>RSC Advances</i> , <b>2014</b> , 4, 35777	3.7	8
33	QM/MM studies of the mechanism of unusual bifunctional fructose-1,6-bisphosphate aldolase/phosphatase. <i>Physical Chemistry Chemical Physics</i> , <b>2014</b> , 16, 11366-73	3.6	4
32	QM/MM study of the reaction mechanism of the carboxyl transferase domain of pyruvate carboxylase from <i>Staphylococcus aureus</i> . <i>Biochemistry</i> , <b>2014</b> , 53, 4455-66	3.2	7
31	The reaction mechanism of UDP-GlcNAc 5,6-dehydratase: a quantum mechanical/molecular mechanical (QM/MM) study. <i>Theoretical Chemistry Accounts</i> , <b>2014</b> , 133, 1	1.9	0
30	Comparative studies on the discrepant fragmentation mechanisms of the GLy-Asp-Gly-Arg and Arg-Gly-Asp-Gly: evidence for the mobile proton model. <i>European Journal of Mass Spectrometry</i> , <b>2014</b> , 20, 317-25	1.1	1

29	A QM/MM study of the catalytic mechanism of $\beta$ -1,4-glucan lyase from the red seaweed <i>Gracilariopsis lemaneiformis</i> . <i>RSC Advances</i> , <b>2014</b> , 4, 54398-54408	3.7	5
28	Insight into the Predictive Binding Modes of the Influenza A Neuraminidase in Complexes with Avian and Human Receptor Analogues. <i>Avian Biology Research</i> , <b>2014</b> , 7, 172-179	0.8	
27	Theoretical study on the deglycosylation mechanism of rice BGlu1 $\beta$ -glucosidase. <i>International Journal of Quantum Chemistry</i> , <b>2013</b> , 113, 1071-1075	2.1	7
26	QM/MM study of the conversion mechanism of lysine to methylornithine catalyzed by methylornithine synthase (PylB). <i>Theoretical Chemistry Accounts</i> , <b>2013</b> , 132, 1	1.9	6
25	Insight into the mechanism of aminomutase reaction: a case study of phenylalanine aminomutase by computational approach. <i>Journal of Molecular Graphics and Modelling</i> , <b>2013</b> , 46, 65-73	2.8	9
24	X-ray crystallography and QM/MM investigation on the oligosaccharide synthesis mechanism of rice BGlu1 glycosynthases. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , <b>2013</b> , 1834, 536-45	4	8
23	Role of F <sub>1</sub> in the hydrolysis/condensation mechanisms of silicon alkoxide Si(OCH <sub>3</sub> ) <sub>4</sub> : a DFT investigation. <i>New Journal of Chemistry</i> , <b>2013</b> , 37, 1371	3.6	9
22	Theoretical study of the catalytic mechanism of E1 subunit of pyruvate dehydrogenase multienzyme complex from <i>Bacillus stearothermophilus</i> . <i>Biochemistry</i> , <b>2013</b> , 52, 8079-93	3.2	13
21	The reaction mechanism of hydroxyethylphosphonate dioxygenase: a QM/MM study. <i>Organic and Biomolecular Chemistry</i> , <b>2012</b> , 10, 1014-24	3.9	19
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