

Yongjun Liu

List of Publications by Year in descending order

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142
papers

2,117
citations

279487

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329751

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all docs

143
docs citations

143
times ranked

2686
citing authors

#	ARTICLE	IF	CITATIONS
1	A Review on Nano-Based Drug Delivery System for Cancer Chemoimmunotherapy. <i>Nano-Micro Letters</i> , 2020, 12, 142.	14.4	156
2	Constructing a synthetic pathway for acetyl-coenzyme A from one-carbon through enzyme design. <i>Nature Communications</i> , 2019, 10, 1378.	5.8	128
3	Deep-blue electroluminescence from nondoped and doped organic light-emitting diodes (OLEDs) based on a new monoaza[6]helicene. <i>RSC Advances</i> , 2015, 5, 75-84.	1.7	81
4	Treatment effects and genotoxicity relevance of the toxic organic pollutants in semi-coking wastewater by combined treatment process. <i>Environmental Pollution</i> , 2017, 220, 13-19.	3.7	73
5	Pb(ii) metal-organic nanotubes based on cyclodextrins: biphasic synthesis, structures and properties. <i>Chemical Science</i> , 2012, 3, 2282.	3.7	70
6	Promoting Early Diagnosis and Precise Therapy of Hepatocellular Carcinoma by Glypican-3-Targeted Synergistic Chemo-Photothermal Theranostics. <i>ACS Applied Materials & Interfaces</i> , 2019, 11, 23591-23604.	4.0	52
7	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> , 2014, 136, 4515-4524.	6.6	51
8	Mechanisms of Silicon Alkoxide Hydrolysis-Oligomerization Reactions: A DFT Investigation. <i>ChemPhysChem</i> , 2012, 13, 2392-2404.	1.0	47
9	Mechanistic Insights into the Decoupled Desaturation and Epoxidation Catalyzed by Dioxygenase AsqI Involved in the Biosynthesis of Quinolone Alkaloids. <i>ACS Catalysis</i> , 2017, 7, 5534-5543.	5.5	47
10	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> , 2019, 47, 1374-1383.	1.9	45
11	Unsaturated nitrogen-rich polymer poly(L-histidine) gated reversibly switchable mesoporous silica nanoparticles using α -graft to β -strategy for drug controlled release. <i>Acta Biomaterialia</i> , 2017, 63, 150-162.	4.1	41
12	Cascade Cytosol Delivery of Dual-Sensitive Micelle-Tailored Vaccine for Enhancing Cancer Immunotherapy. <i>ACS Applied Materials & Interfaces</i> , 2018, 10, 37797-37811.	4.0	35
13	Mechanism of Sulfoxidation and C-S Bond Formation Involved in the Biosynthesis of Ergothioneine Catalyzed by Ergothioneine Synthase (EgtB). <i>ACS Catalysis</i> , 2018, 8, 5875-5889.	5.5	35
14	Theoretical Insights into the Mechanism and Stereoselectivity of Olefin Cyclopropanation Catalyzed by Two Engineered Cytochrome P450 Enzymes. <i>Inorganic Chemistry</i> , 2018, 57, 11738-11745.	1.9	33
15	Uncoupled Epimerization and Desaturation by Carbapenem Synthase: Mechanistic Insights from QM/MM Studies. <i>ACS Catalysis</i> , 2015, 5, 5556-5566.	5.5	31
16	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> , 2017, 19, 7668-7677.	1.3	29
17	Mechanistic Investigation of Isonitrile Formation Catalyzed by the Nonheme Iron/Fe-KG-Dependent Decarboxylase (ScoE). <i>ACS Catalysis</i> , 2020, 10, 2942-2957.	5.5	29
18	Small Morph Nanoparticles for Deep Tumor Penetration via Caveolae-Mediated Transcytosis. <i>ACS Applied Materials & Interfaces</i> , 2020, 12, 38499-38511.	4.0	28

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19	Reshaping Antitumor Immunity with Chemo-Photothermal Integrated Nanoplatform to Augment Checkpoint Blockade-Based Cancer Therapy. <i>Advanced Functional Materials</i> , 2021, 31, 2100437.	7.8	28
20	Potential application of a porous graphitic carbon nitride as an organic metal-free photocatalyst for water splitting. <i>Diamond and Related Materials</i> , 2018, 87, 50-55.	1.8	27
21	Nanoparticle-Loaded Polarized-Macrophages for Enhanced Tumor Targeting and Cell-Chemotherapy. <i>Nano-Micro Letters</i> , 2021, 13, 6.	14.4	27
22	THEORETICAL STUDIES ON THE MECHANISM OF CYCLIC NUCLEOTIDE MONOPHOSPHATE HYDROLYSIS WITHIN PHOSPHODIESTERASES. <i>Journal of Theoretical and Computational Chemistry</i> , 2012, 11, 573-586.	1.8	26
23	The structures and properties of halogen bonds involving polyvalent halogen in complexes of FXOn (X = Cl, Br; n = 0-3)-CH ₃ CN. <i>New Journal of Chemistry</i> , 2014, 38, 1256.	1.4	26
24	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> , 2019, 650, 941-950.	3.9	25
25	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> , 2019, 685, 74-84.	3.9	24
26	Theoretical Investigations towards the Staudinger Reaction Catalyzed by N-Heterocyclic Carbene: Mechanism and Stereoselectivity. <i>European Journal of Organic Chemistry</i> , 2010, 2010, 6249-6255.	1.2	23
27	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> , 2015, 5, 3953-3965.	5.5	23
28	Reductive Homocoupling of Organohalides Using Nickel(II) Chloride and Samarium Metal. <i>Chemistry - an Asian Journal</i> , 2017, 12, 673-678.	1.7	22
29	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> , 2017, 19, 7733-7742.	1.3	22
30	Theoretical Study of Iron Porphyrin Nitrene: Formation Mechanism, Electronic Nature, and Intermolecular C-H Amination. <i>Inorganic Chemistry</i> , 2020, 59, 1622-1632.	1.9	22
31	The reaction mechanism of hydroxyethylphosphonate dioxygenase: a QM/MM study. <i>Organic and Biomolecular Chemistry</i> , 2012, 10, 1014-1024.	1.5	19
32	The charge regulation of electronic structure and optical properties of graphitic carbon nitride under strain. <i>RSC Advances</i> , 2019, 9, 7464-7468.	1.7	19
33	Lymph Node Delivery Strategy Enables the Activation of Cytotoxic T Lymphocytes and Natural Killer Cells to Augment Cancer Immunotherapy. <i>ACS Applied Materials & Interfaces</i> , 2021, 13, 22213-22224.	4.0	18
34	Manipulation of TAMs functions to facilitate the immune therapy effects of immune checkpoint antibodies. <i>Journal of Controlled Release</i> , 2021, 336, 621-634.	4.8	18
35	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> , 2019, 9, 444-455.	2.1	17
36	An Integrated Nanoaircraft Carrier Modulating Antitumor Immunity to Enhance Immune Checkpoint Blockade Therapy. <i>Advanced Functional Materials</i> , 2021, 31, 2106123.	7.8	17

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37	A simple way of shape-controlled synthesis of ZnSe nanocrystals nanodots, nanoflowers, and nanotubes. <i>CrystEngComm</i> , 2009, 11, 1789.	1.3	15
38	Theoretical Study of the Catalytic Mechanism of E1 Subunit of Pyruvate Dehydrogenase Multienzyme Complex from <i>Bacillus stearothermophilus</i> . <i>Biochemistry</i> , 2013, 52, 8079-8093.	1.2	15
39	Insights into the dioxygen activation and catalytic mechanism of the nickel-containing quercetinase. <i>Catalysis Science and Technology</i> , 2018, 8, 2340-2351.	2.1	15
40	A QM/MM study on the catalytic mechanism of pyruvate decarboxylase. <i>Theoretical Chemistry Accounts</i> , 2012, 131, 1.	0.5	14
41	Strengthen effects of dominant strains on aerobic digestion and stabilization of the residual sludge. <i>Bioresource Technology</i> , 2017, 235, 202-210.	4.8	14
42	Tryptophan lyase (NosL): mechanistic insights into amine dehydrogenation and carboxyl fragment migration by QM/MM calculations. <i>Catalysis Science and Technology</i> , 2017, 7, 2846-2856.	2.1	13
43	Hormesis of mercuric chloride-human serum albumin adduct on N9 microglial cells via the ERK/MAPKs and JAK/STAT3 signaling pathways. <i>Toxicology</i> , 2018, 408, 62-69.	2.0	13
44	Imidazoquinoline-Conjugated Degradable Coacervate Conjugate for Local Cancer Immunotherapy. <i>ACS Biomaterials Science and Engineering</i> , 2020, 6, 4993-5000.	2.6	13
45	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> , 2022, 346, 126567.	4.8	13
46	Catalytic mechanism of acetolactate decarboxylase from <i>Brevibacillus brevis</i> towards both enantiomers of \pm -acetolactate. <i>RSC Advances</i> , 2016, 6, 80621-80629.	1.7	12
47	Oxidative Rearrangement Mechanism of Pentalenolactone F Catalyzed by Cytochrome P450 CYP161C2 (PntM). <i>Inorganic Chemistry</i> , 2018, 57, 8933-8941.	1.9	12
48	Insights into the Mechanism and Enantioselectivity in the Biosynthesis of Ergot Alkaloid Cycloclavine Catalyzed by Aj_EasH from <i>Aspergillus japonicus</i> . <i>Inorganic Chemistry</i> , 2019, 58, 13771-13781.	1.9	12
49	Mechanical Insights into the Enzymatic Cleavage of Double C=C Bond in Poly(<i>cis</i> -1,4-isoprene) by the Latex Clearing Protein. <i>Inorganic Chemistry</i> , 2020, 59, 9627-9637.	1.9	12
50	Theoretical investigation on the regioselectivity of Ni(COD) ₂ -catalyzed [2+2] cycloaddition of unsymmetric diynes and CO ₂ . <i>Journal of Organometallic Chemistry</i> , 2014, 758, 45-54.	0.8	11
51	A QM/MM study of the catalytic mechanism of aspartate ammonia lyase. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 51, 113-119.	1.3	11
52	A QM/MM study of the catalytic mechanism of nicotinamidase. <i>Organic and Biomolecular Chemistry</i> , 2014, 12, 1265.	1.5	11
53	Mechanism of the Glutathione Persulfide Oxidation Process Catalyzed by Ethylmalonic Encephalopathy Protein 1. <i>ACS Catalysis</i> , 2016, 6, 7010-7020.	5.5	11
54	Reductive Bis-addition of Aromatic Aldehydes to \pm -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> , 2017, 82, 5932-5939.	1.7	11

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55	Transformation of <i>gem</i> -Dicyanoethenes by Samarium: Direct Formation of Indenes or Direct Decyanation with in Situ Disilylation. <i>European Journal of Organic Chemistry</i> , 2008, 2008, 5470-5476.	1.2	10
56	Intermolecular Couplization and Cyclization of Chalcones Promoted by Samarium in DMF. <i>Synthetic Communications</i> , 2009, 39, 799-807.	1.1	10
57	Role of F ⁺ in the hydrolysis-condensation mechanisms of silicon alkoxide Si(OCH ₃) ₄ : a DFT investigation. <i>New Journal of Chemistry</i> , 2013, 37, 1371.	1.4	10
58	A theoretical study of the catalytic mechanism of oxalyl-CoA decarboxylase, an enzyme for treating urolithiasis. <i>RSC Advances</i> , 2014, 4, 35777.	1.7	10
59	Catalytic mechanisms of Au ₁₁ and Au ₁₁ -nPt _n (n=1-2) clusters: a DFT investigation on the oxidation of CO by O ₂ . <i>Journal of Molecular Modeling</i> , 2015, 21, 230.	0.8	10
60	Insights into the decarboxylative hydroxylation of salicylate catalyzed by the Flavin-dependent monooxygenase salicylate hydroxylase. <i>Theoretical Chemistry Accounts</i> , 2018, 137, 1.	0.5	10
61	Strengthening of aerobic sludge granulation by the endogenous acylated homoserine lactones-secreting strain <i>Aeromonas</i> sp. A-L3. <i>Biochemical Engineering Journal</i> , 2019, 151, 107329.	1.8	10
62	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> , 2021, 61, 3638-3648.	2.5	10
63	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> , 2022, 9, e2101472.	5.6	10
64	Depleting Tumor Infiltrating B Cells to Boost Antitumor Immunity with Tumor Immune-Microenvironment Reshaped Hybrid Nanocage. <i>ACS Nano</i> , 2022, 16, 4263-4277.	7.3	10
65	Theoretical study on the deglycosylation mechanism of rice BGluc1 β -glucosidase. <i>International Journal of Quantum Chemistry</i> , 2013, 113, 1071-1075.	1.0	9
66	QM/MM study of the conversion mechanism of lysine to methylornithine catalyzed by methylornithine synthase (PylB). <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	9
67	Insight into the mechanism of aminomutase reaction: A case study of phenylalanine aminomutase by computational approach. <i>Journal of Molecular Graphics and Modelling</i> , 2013, 46, 65-73.	1.3	9
68	QM/MM Study of the Reaction Mechanism of the Carboxyl Transferase Domain of Pyruvate Carboxylase from <i>Staphylococcus aureus</i> . <i>Biochemistry</i> , 2014, 53, 4455-4466.	1.2	9
69	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> , 2016, 14, 3432-3442.	1.5	9
70	Comparative studies of the catalytic mechanisms of two chorismatases: CH ₂ Erbo and CH ₂ Hyg5. <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1146-1158.	1.5	9
71	Protonation state and fine structure of the active site determine the reactivity of dehydratase: hydration and isomerization of β -myrcene catalyzed by linalool dehydratase/isomerase from <i>Castellaniella defragrans</i> . <i>Physical Chemistry Chemical Physics</i> , 2018, 20, 17342-17352.	1.3	9
72	Mechanism of fatty acid decarboxylation catalyzed by a non-heme iron oxidase (UndA): a QM/MM study. <i>Organic and Biomolecular Chemistry</i> , 2019, 17, 9808-9818.	1.5	9

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73	<p>Engineering Thermo-pH Dual Responsive Hydrogel for Enhanced Tumor Accumulation, Penetration, and Chemo-Protein Combination Therapy</p>. International Journal of Nanomedicine, 2020, Volume 15, 4739-4752.	3.3	9
74	Title is missing!. Theoretical and Experimental Chemistry, 2000, 36, 303-311.	0.2	8
75	X-ray crystallography and QM/MM investigation on the oligosaccharide synthesis mechanism of rice BGluc1 glycosynthases. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 536-545.	1.1	8
76	Insights into the catalytic mechanism of dTDP-glucose 4,6-dehydratase from quantum mechanics/molecular mechanics simulations. RSC Advances, 2014, 4, 35449.	1.7	8
77	Theoretical investigation on the dissociation of (R)-benzoin catalyzed by benzaldehyde lyase. International Journal of Quantum Chemistry, 2014, 114, 375-382.	1.0	8
78	Spatial distribution, source identification, and potential risk assessment of toxic contaminants in surface waters from Yulin, China. Environmental Monitoring and Assessment, 2019, 191, 293.	1.3	8
79	Conversion mechanism of enoyl thioesters into acyl thioesters catalyzed by 2-enoyl-thioester reductases from <i>Candida Tropicalis</i> . Physical Chemistry Chemical Physics, 2019, 21, 10105-10113.	1.3	8
80	Mechanistic Insights into the Oxidative Ring Expansion from Penicillin N to Deacetoxycephalosporin C Catalyzed by a Nonheme Iron(II) and Î±-KG-Dependent Oxygenase. Inorganic Chemistry, 2020, 59, 12218-12231.	1.9	8
81	The Retaining Mechanism of Xylose Transfer Catalyzed by Xyloside Î±-1,3-Xylosyltransferase (XXYL1): a Quantum Mechanics/Molecular Mechanics Study. Journal of Chemical Information and Modeling, 2020, 60, 1585-1594.	2.5	8
82	High-Specific Isolation and Instant Observation of Circulating Tumour Cell from HCC Patients via Glypican-3 Immunomagnetic Fluorescent Nanodevice. International Journal of Nanomedicine, 2021, Volume 16, 4161-4173.	3.3	8
83	Docking and molecular dynamics studies on the interaction of four imidazoline derivatives with potassium ion channel (Kir6.2). Molecular Simulation, 2010, 36, 166-174.	0.9	7
84	A density functional theory study on the catalytic mechanism of hydroxycinnamoyl-CoA hydratase-lyase. International Journal of Quantum Chemistry, 2014, 114, 249-254.	1.0	7
85	A QM/MM study of the reaction mechanism of (R)-hydroxynitrile lyases from <i>Arabidopsis thaliana</i> (AtHNL). Proteins: Structure, Function and Bioinformatics, 2015, 83, 66-77.	1.5	7
86	Cleavage mechanism of the aliphatic C=C bond catalyzed by 2,4-dihydroxyacetophenone dioxygenase from <i>Alcaligenes</i> sp. 4HAP: a QM/MM study. Catalysis Science and Technology, 2017, 7, 911-922.	2.1	7
87	Tyrosyl Radical-Mediated Sequential Oxidative Decarboxylation of Coproporphyrinogen III through PCET: Theoretical Insights into the Mechanism of Coproheme Decarboxylase ChdC. Inorganic Chemistry, 2021, 60, 13539-13549.	1.9	7
88	Computational Study of the C5-Hydroxylation Mechanism Catalyzed by the Diiron Monooxygenase PtmU3 as Part of the Platensimycin Biosynthesis. Inorganic Chemistry, 2021, 60, 17783-17796.	1.9	7
89	Mechanistic Insights into Pyridine Ring Degradation Catalyzed by 2,5-Dihydroxypyridine Dioxygenase NicX. Inorganic Chemistry, 2022, 61, 2517-2529.	1.9	7
90	Artificial Assembled Macrophage Co-Deliver Black Phosphorus Quantum Dot and CDK4/6 Inhibitor for Colorectal Cancer Triple-Therapy. ACS Applied Materials & Interfaces, 2022, 14, 20628-20640.	4.0	7

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91	STUDY ON THE INTERACTIONS OF Smac MIMETICS WITH XIAP-BIR3 DOMAIN BY DOCKING AND MOLECULAR DYNAMICS SIMULATIONS. <i>Journal of Theoretical and Computational Chemistry</i> , 2010, 09, 797-812.	1.8	6
92	Mechanistic insights into the β -elimination reaction of l-methionine catalyzed by methionine β -lyase (MGL). <i>Theoretical Chemistry Accounts</i> , 2017, 136, 1.	0.5	6
93	A Novel ZnONPs/PVA-Functionalized Biomaterials for Bacterial Cells Immobilization and its Strengthening Effects on Quinoline Biodegradation. <i>Current Microbiology</i> , 2018, 75, 316-322.	1.0	6
94	Preparation and evaluation of etoposide-loaded lipid-based nanosuspensions for high-dose treatment of lymphoma. <i>Nanomedicine</i> , 2019, 14, 1403-1427.	1.7	6
95	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> , 2019, 21, 25658-25668.	1.3	6
96	A QM/MM study of the catalytic mechanism of β -1,4-glucan lyase from the red seaweed <i>Gracilariopsis lemaneiformis</i> . <i>RSC Advances</i> , 2014, 4, 54398-54408.	1.7	5
97	QM/MM studies of the mechanism of unusual bifunctional fructose-1,6-bisphosphate aldolase/phosphatase. <i>Physical Chemistry Chemical Physics</i> , 2014, 16, 11366.	1.3	5
98	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> , 2015, 5, 7781-7788.	1.7	5
99	Evaluation and quantification of genotoxicity of urban waters by using <i>Vicia faba</i> bioassays. <i>Chemistry and Ecology</i> , 2017, 33, 669-683.	0.6	5
100	A QM/MM study of the catalytic mechanism of SAM methyltransferase RlmN from <i>Escherichia coli</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2017, 85, 1967-1974.	1.5	5
101	Mechanism of Uncoupled Carbocyclization and Epimerization Catalyzed by Two Non-Heme Iron/ β -Ketoglutarate Dependent Enzymes. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 5086-5098.	2.5	5
102	Gas-blasting nanocapsules to accelerate carboplatin lysosome release and nucleus delivery for prostate cancer treatment. <i>Asian Journal of Pharmaceutical Sciences</i> , 2021, 16, 192-202.	4.3	5
103	A Hybrid Control Architecture for Connection Management in Translucent WDM Networks. , 2008, , .		4
104	Theoretical studies on the interaction of guanine riboswitch with guanine and its closest analogues. <i>Molecular Simulation</i> , 2010, 36, 929-938.	0.9	4
105	QM/MM investigation on the catalytic mechanism of <i>Bacteroides thetaiotaomicron</i> β -glucosidase BtGH97a. <i>Biochimica Et Biophysica Acta - Proteins and Proteomics</i> , 2012, 1824, 750-758.	1.1	4
106	Investigation of the rescue mechanism catalyzed by a nucleophile mutant of rice BGlul. <i>Journal of Molecular Graphics and Modelling</i> , 2014, 54, 100-106.	1.3	4
107	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> , 2015, 5, 101672-101682.	1.7	4
108	QM/MM studies on the calcium-assisted β -elimination mechanism of pectate lyase from <i>Bacillus subtilis</i> . <i>Proteins: Structure, Function and Bioinformatics</i> , 2016, 84, 1606-1615.	1.5	4

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109	Exploring the substrate specificity and catalytic mechanism of imidazolonepropionase (HutI) from <i>Bacillus subtilis</i> . <i>Physical Chemistry Chemical Physics</i> , 2016, 18, 27928-27938.	1.3	4
110	Structures and photoelectric properties of five benzotrithiophene isomers-based donor-acceptor copolymers. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2016, 159, 262-268.	2.0	4
111	Mechanistic Insights into the Oxidative Rearrangement Catalyzed by the Unprecedented Dioxygenase ChaP Involved in Chartreusin Biosynthesis. <i>Inorganic Chemistry</i> , 2020, 59, 13988-13999.	1.9	4
112	Formation Mechanism of Cofactor Cys-Tyr in the Cysteine Dioxygenases (CDO and) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 50 627 Td (F<...> 7844-7856.	1.9	4
113	Amphiphilic small molecular mates match hydrophobic drugs to form nanoassemblies based on drug-mate strategy. <i>Asian Journal of Pharmaceutical Sciences</i> , 2022, 17, 129-138.	4.3	4
114	QM/MM study on the catalytic mechanism of cyclohexane-1,2-dione hydrolase (CDH). <i>Theoretical Chemistry Accounts</i> , 2014, 133, 1.	0.5	3
115	Theoretical study of the hydrolysis mechanism of 2-pyrone-4,6-dicarboxylate (PDC) catalyzed by LigI. <i>Journal of Molecular Graphics and Modelling</i> , 2015, 61, 21-29.	1.3	3
116	Quantum Mechanics and Molecular Mechanics Study of the Catalytic Mechanism of Human AMSH-LP Domain Deubiquitinating Enzymes. <i>Biochemistry</i> , 2015, 54, 5225-5234.	1.2	3
117	Theoretical studies of traditional and halogen-shared halogen bonds: the doped all-metal aromatic clusters MAI ₃ (M=As, Ge, Sn, Pb) as halogen bond acceptors. <i>Theoretical Chemistry Accounts</i> , 2015, 134, 1.	0.5	3
118	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> , 2016, 6, 23396-23402.	1.7	3
119	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> , 2017, 85, 1518-1528.	1.5	3
120	Unified D- α -Tocopherol 5-Fu/SAHA bioconjugates self-assemble as complex nanodrug for optimized combination therapy. <i>Nanomedicine</i> , 2018, 13, 1285-1301.	1.7	3
121	DT7 peptide-modified lecithin nanoparticles co-loaded with β -secretase inhibitor and dexamethasone efficiently inhibit T-cell acute lymphoblastic leukemia and reduce gastrointestinal toxicity. <i>Cancer Letters</i> , 2022, 533, 215608.	3.2	3
122	Inner-sphere reorganization for redox pairs M(NH ₃) ₆ ²⁺ / ₃₊ (M=Mn, Fe, and Co): Models and calculations. <i>International Journal of Quantum Chemistry</i> , 2002, 86, 468-477.	1.0	2
123	Theoretical Study on the Mechanism for the Addition Reaction of SiH ₃ with Propylene and Acetic Acid. <i>Journal of Physical Chemistry A</i> , 2006, 110, 12439-12442.	1.1	2
124	3D-QSAR Studies on C ₂₄ -Monoalkylated Vitamin D ₃ Lactones and their C ₂ -Modified Derivatives with Inhibitory Activity to Vitamin D Receptor. <i>Molecular Informatics</i> , 2010, 29, 621-632.	1.4	2
125	Theoretical studies on the conformational change of adenosine kinase induced by inhibitors. <i>International Journal of Quantum Chemistry</i> , 2011, 111, 3980-3990.	1.0	2
126	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> , 2014, 20, 317-325.	0.5	2

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127	Theoretical identification on the role of Lys15 for Sulfolobus tokodaii hexokinase. RSC Advances, 2015, 5, 18622-18632.	1.7	2
128	Theoretical study of the hydrolysis mechanism of dihydrocoumarin catalyzed by serum paraoxonase 1 (PON1): different roles of Glu53 and His115 for catalysis. RSC Advances, 2016, 6, 60376-60384.	1.7	2
129	QM/MM studies of the type II isopentenyl diphosphate \rightarrow dimethylallyl diphosphate isomerase demonstrate a novel role for the flavin coenzyme. RSC Advances, 2017, 7, 22286-22293.	1.7	2
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