Yongjun Liu

List of Publications by Year
in descending order

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142	2,117	279798	330143
papers	citations	23 h-index	37 g-index

143	143	143	2686
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Amphiphilic small molecular mates match hydrophobic drugs to form nanoassemblies based on drug-mate strategy. Asian Journal of Pharmaceutical Sciences, 2022, 17, 129-138.	9.1	4
2	A comparison between exogenous carriers enhanced aerobic granulation under low organic loading in the aspect of sludge characteristics, extracellular polymeric substances and microbial communities. Bioresource Technology, 2022, 346, 126567.	9.6	13
3	Mechanistic Insights into Pyridine Ring Degradation Catalyzed by 2,5-Dihydroxypyridine Dioxygenase NicX. Inorganic Chemistry, 2022, 61, 2517-2529.	4.0	7
4	Computational Study of the Peroxygenase Mechanism Catalyzed by Hemoglobin Dehaloperoxidase Involved in the Degradation of Chlorophenols. Inorganic Chemistry, 2022, 61, 2628-2639.	4.0	2
5	Multipoint Costriking Nanodevice Eliminates Primary Tumor Cells and Associatedâ€Circulating Tumor Cells for Enhancing Metastasis Inhibition and Therapeutic Effect on HCC. Advanced Science, 2022, 9, e2101472.	11.2	10
6	Mechanism of Sugar Ring Contraction and Closure Catalyzed by UDP-<scp>d</scp>-apiose/UDP-<scp>d</scp>-xylose Synthase (UAXS). Journal of Chemical Information and Modeling, 2022, 62, 632-646.	5.4	2
7	Depleting Tumor Infiltrating B Cells to Boost Antitumor Immunity with Tumor Immune-Microenvironment Reshaped Hybrid Nanocage. ACS Nano, 2022, 16, 4263-4277.	14.6	10
8	Computational Study of Aromatic Hydroxylation Catalyzed by the Iron-Dependent Hydroxylase PqqB Involved in the Biosynthesis of Redox Cofactor Pyrroloquinoline Quinone. Inorganic Chemistry, 2022, 61, 5943-5956.	4.0	2
9	DT7 peptide-modified lecithin nanoparticles co-loaded with Î³-secretase inhibitor and dexamethasone efficiently inhibit T-cell acute lymphoblastic leukemia and reduce gastrointestinal toxicity. Cancer Letters, 2022, 533, 215608.	7.2	3
10	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.	8.0	7
11	Mechanistic Insights into the Anaerobic Degradation of Globally Abundant Dihydroxypropanesulfonate Catalyzed by the DHPS-Sulfolyase (HpsG). Journal of Chemical Information and Modeling, 2022, 62, 2880-2888.	5.4	1
12	Gas-blasting nanocapsules to accelerate carboplatin lysosome release and nucleus delivery for prostate cancer treatment. Asian Journal of Pharmaceutical Sciences, 2021, 16, 192-202.	9.1	5
13	Nanoparticle-Loaded Polarized-Macrophages for Enhanced Tumor Targeting and Cell-Chemotherapy. Nano-Micro Letters, 2021, 13, 6.	27.0	27
14	Reshaping Antitumor Immunity with Chemoâ€Photothermal Integrated Nanoplatform to Augment Checkpoint Blockadeâ€Based Cancer Therapy. Advanced Functional Materials, 2021, 31, 2100437.	14.9	28
15	Formation Mechanism of Cofactor Cysâ€“Tyr in the Cysteine Dioxygenases (CDO and) Tj ETQq1 1 0.784314 rgBT /Overlock 10 Tf 50 7844-7856.	4.0	4
16	Lymph Node Delivery Strategy Enables the Activation of Cytotoxic T Lymphocytes and Natural Killer Cells to Augment Cancer Immunotherapy. ACS Applied Materials & Interfaces, 2021, 13, 22213-22224.	8.0	18
17	Inactivation Mechanism of Neuronal Nitric Oxide Synthase by (S)-2-Amino-5-(2-(methylthio)acetimidamido)pentanoic Acid: Chemical Conversion of the Inactivator in the Active Site. Inorganic Chemistry, 2021, 60, 9345-9358.	4.0	1
18	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.	6.7	8

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19	Mechanistic Insights into the P450 TleB-Catalyzed Unusual Intramolecular Câ€“N Bond Formation Involved in the Biosynthesis of Indolactam V. Journal of Chemical Information and Modeling, 2021, 61, 3638-3648.	5.4	10
20	Manipulation of TAMs functions to facilitate the immune therapy effects of immune checkpoint antibodies. Journal of Controlled Release, 2021, 336, 621-634.	9.9	18
21	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.	4.0	7
22	An Integrated Nanoaircraft Carrier Modulating Antitumor Immunity to Enhance Immune Checkpoint Blockade Therapy. Advanced Functional Materials, 2021, 31, 2106123.	14.9	17
23	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.	4.0	7
24	Mechanical Insights into the Enzymatic Cleavage of Double Câ€“C Bond in Poly(cis-1,4-isoprene) by the Latex Clearing Protein. Inorganic Chemistry, 2020, 59, 9627-9637.	4.0	12
25	Small Morph Nanoparticles for Deep Tumor Penetration via Caveolae-Mediated Transcytosis. ACS Applied Materials & Interfaces, 2020, 12, 38499-38511.	8.0	28
26	Imidazoquinoline-Conjugated Degradable Coacervate Conjugate for Local Cancer Immunotherapy. ACS Biomaterials Science and Engineering, 2020, 6, 4993-5000.	5.2	13
27	Mechanistic Insights into the Oxidative Rearrangement Catalyzed by the Unprecedented Dioxygenase ChaP Involved in Chartreusin Biosynthesis. Inorganic Chemistry, 2020, 59, 13988-13999.	4.0	4
28	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.	4.0	8
29	A Review on Nano-Based Drug Delivery System for Cancer Chemoimmunotherapy. Nano-Micro Letters, 2020, 12, 142.	27.0	156
30	Engineering Thermo-pH Dual Responsive Hydrogel for Enhanced Tumor Accumulation, Penetration, and Chemo-Protein Combination Therapy . International Journal of Nanomedicine, 2020, Volume 15, 4739-4752.	6.7	9
31	The Retaining Mechanism of Xylose Transfer Catalyzed by Xyloside Î±-1,3-Xylosyltransferase (XXYLT1): a Quantum Mechanics/Molecular Mechanics Study. Journal of Chemical Information and Modeling, 2020, 60, 1585-1594.	5.4	8
32	Theoretical Study of Iron Porphyrin Nitrene: Formation Mechanism, Electronic Nature, and Intermolecular Câ€“H Amination. Inorganic Chemistry, 2020, 59, 1622-1632.	4.0	22
33	Mechanistic Investigation of Isonitrile Formation Catalyzed by the Nonheme Iron/Î±-KG-Dependent Decarboxylase (ScoE). ACS Catalysis, 2020, 10, 2942-2957.	11.2	29
34	Strengthening of aerobic sludge granulation by the endogenous acylated homoserine lactones-secreting strain Aeromonas sp. A-L3. Biochemical Engineering Journal, 2019, 151, 107329.	3.6	10
35	Preparation and evaluation of etoposide-loaded lipid-based nanosuspensions for high-dose treatment of lymphoma. Nanomedicine, 2019, 14, 1403-1427.	3.3	6
36	Insights into the Mechanism and Enantioselectivity in the Biosynthesis of Ergot Alkaloid Cycloclavine Catalyzed by Aj_EasH from Aspergillus japonicus. Inorganic Chemistry, 2019, 58, 13771-13781.	4.0	12

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37	Mechanical insights into the oxidative cleavage of resveratrol catalyzed by dioxygenase NOV1 from Novosphingobium aromaticivorans: confirmation of dioxygenase mechanism by QM/MM calculations. Catalysis Science and Technology, 2019, 9, 444-455.	4.1	17
38	Impact of Al-based coagulants on the formation of aerobic granules: Comparison between poly aluminum chloride (PAC) and aluminum sulfate (AS). Science of the Total Environment, 2019, 685, 74-84.	8.0	24
39	Promoting Early Diagnosis and Precise Therapy of Hepatocellular Carcinoma by Glypican-3-Targeted Synergistic Chemo-Photothermal Theranostics. ACS Applied Materials & Interfaces, 2019, 11, 23591-23604.	8.0	52
40	Spatial distribution, source identification, and potential risk assessment of toxic contaminants in surface waters from Yulin, China. Environmental Monitoring and Assessment, 2019, 191, 293.	2.7	8
41	The charge regulation of electronic structure and optical properties of graphitic carbon nitride under strain. RSC Advances, 2019, 9, 7464-7468.	3.6	19
42	Conversion mechanism of enoyl thioesters into acyl thioesters catalyzed by 2-enoyl-thioester reductases from Candida Tropicalis. Physical Chemistry Chemical Physics, 2019, 21, 10105-10113.	2.8	8
43	Constructing a synthetic pathway for acetyl-coenzyme A from one-carbon through enzyme design. Nature Communications, 2019, 10, 1378.	12.8	128
44	Co-delivery of sorafenib and VEGF-siRNA via pH-sensitive liposomes for the synergistic treatment of hepatocellular carcinoma. Artificial Cells, Nanomedicine and Biotechnology, 2019, 47, 1374-1383.	2.8	45
45	Catalytic mechanism of the PrhA (V150L/A232S) double mutant involved in the fungal meroterpenoid biosynthetic pathway: a QM/MM study. Physical Chemistry Chemical Physics, 2019, 21, 25658-25668.	2.8	6
46	Mechanism of fatty acid decarboxylation catalyzed by a non-heme iron oxidase (UndA): a QM/MM study. Organic and Biomolecular Chemistry, 2019, 17, 9808-9818.	2.8	9
47	Mechanism of Uncoupled Carbocyclization and Epimerization Catalyzed by Two Non-Heme Iron/Î±-Ketoglutarate Dependent Enzymes. Journal of Chemical Information and Modeling, 2019, 59, 5086-5098.	5.4	5
48	Synergistic strengthening mechanism of hydraulic selection pressure and poly aluminum chloride (PAC) regulation on the aerobic sludge granulation. Science of the Total Environment, 2019, 650, 941-950.	8.0	25
49	Computational evidence for the importance of lysine carboxylation in the reaction catalyzed by carboxyl transferase domain of pyruvate carboxylase: a QM/MM study. Theoretical Chemistry Accounts, 2019, 138, 1.	1.4	2
50	Insights into the dioxygen activation and catalytic mechanism of the nickel-containing quercetinase. Catalysis Science and Technology, 2018, 8, 2340-2351.	4.1	15
51	A Novel ZnONPs/PVA-Functionalized Biomaterials for Bacterial Cells Immobilization and its Strengthening Effects on Quinoline Biodegradation. Current Microbiology, 2018, 75, 316-322.	2.2	6
52	Cascade Cytosol Delivery of Dual-Sensitive Micelle-Tailored Vaccine for Enhancing Cancer Immunotherapy. ACS Applied Materials & Interfaces, 2018, 10, 37797-37811.	8.0	35
53	Theoretical Insights into the Mechanism and Stereoselectivity of Olefin Cyclopropanation Catalyzed by Two Engineered Cytochrome P450 Enzymes. Inorganic Chemistry, 2018, 57, 11738-11745.	4.0	33
54	Mechanism of Sulfoxidation and Câ€“S Bond Formation Involved in the Biosynthesis of Ergothioneine Catalyzed by Ergothioneine Synthase (EgtB). ACS Catalysis, 2018, 8, 5875-5889.	11.2	35

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55	Unified D-Î±-Tocopherol 5-Fu/SAHA bioconjugates self-assemble as complex nanodrug for optimized combination therapy. Nanomedicine, 2018, 13, 1285-1301.	3.3	3
56	Hormesis of mercuric chloride-human serum albumin adduct on N9 microglial cells via the ERK/MAPKs and JAK/STAT3 signaling pathways. Toxicology, 2018, 408, 62-69.	4.2	13
57	Oxidative Rearrangement Mechanism of Pentalenolactone F Catalyzed by Cytochrome P450 CYP161C2 (PntM). Inorganic Chemistry, 2018, 57, 8933-8941.	4.0	12
58	Potential application of a porous graphitic carbon nitride as an organic metal-free photocatalyst for water splitting. Diamond and Related Materials, 2018, 87, 50-55.	3.9	27
59	Protonation state and fine structure of the active site determine the reactivity of dehydratase: hydration and isomerization of Î²-myrcene catalyzed by linalool dehydratase/isomerase from Castellaniella defragrans. Physical Chemistry Chemical Physics, 2018, 20, 17342-17352.	2.8	9
60	Insights into the decarboxylative hydroxylation of salicylate catalyzed by the Flavin-dependent monooxygenase salicylate hydroxylase. Theoretical Chemistry Accounts, 2018, 137, 1.	1.4	10
61	Reductive Homocoupling of Organohalides Using Nickel(II) Chloride and Samarium Metal. Chemistry - an Asian Journal, 2017, 12, 673-678.	3.3	22
62	Insights into the unprecedented epoxidation mechanism of fumitremorgin B endoperoxidase (FtmOx1) from Aspergillus fumigatus by QM/MM calculations. Physical Chemistry Chemical Physics, 2017, 19, 7668-7677.	2.8	29
63	Cleavage mechanism of the aliphatic Câ€“C bond catalyzed by 2,4â€²-dihydroxyacetophenone dioxygenase from Alcaligenes sp. 4HAP: a QM/MM study. Catalysis Science and Technology, 2017, 7, 911-922.	4.1	7
64	Mechanistic insights into the catalytic reaction of ferulic acid decarboxylase from Aspergillus niger: a QM/MM study. Physical Chemistry Chemical Physics, 2017, 19, 7733-7742.	2.8	22
65	QM/MM studies of the type II isopentenyl diphosphateâ€“dimethylallyl diphosphate isomerase demonstrate a novel role for the flavin coenzyme. RSC Advances, 2017, 7, 22286-22293.	3.6	2
66	Reductive Bis-addition of Aromatic Aldehydes to Î±,Î²-Unsaturated Esters via the Use of Sm/Cu(I) in Air: A Route to the Construction of Furofuran Lignans. Journal of Organic Chemistry, 2017, 82, 5932-5939.	3.2	11
67	Theoretical insights into the protonation states of active site cysteine and citrullination mechanism of Porphyromonas gingivalis peptidylarginine deiminase. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1518-1528.	2.6	3
68	Tryptophan lyase (NosL): mechanistic insights into amine dehydrogenation and carboxyl fragment migration by QM/MM calculations. Catalysis Science and Technology, 2017, 7, 2846-2856.	4.1	13
69	Strengthen effects of dominant strains on aerobic digestion and stabilization of the residual sludge. Bioresource Technology, 2017, 235, 202-210.	9.6	14
70	Comparative studies of the catalytic mechanisms of two chorismatases: CHâ€frkbo and CHâ€Hyg5. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1146-1158.	2.6	9
71	Theoretical study of the catalytic mechanism of glyoxylate carboligase and its mutant V51E. Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	1
72	Mechanistic insights into the Î³-elimination reaction of l-methionine catalyzed by methionine Î³-lyase (MGL). Theoretical Chemistry Accounts, 2017, 136, 1.	1.4	6

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73	Evaluation and quantification of genotoxicity of urban waters by using Vicia faba bioassays. Chemistry and Ecology, 2017, 33, 669-683.	1.6	5
74	Unsaturated nitrogen-rich polymer poly(l-histidine) gated reversibly switchable mesoporous silica nanoparticles using â€œgraft toâ€•strategy for drug controlled release. Acta Biomaterialia, 2017, 63, 150-162.	8.3	41
75	A water-assisted nucleophilic mechanism utilized by BphD, the meta-cleavage product hydrolase in biphenyl degradation. Journal of Molecular Graphics and Modelling, 2017, 76, 448-455.	2.4	2
76	A QM/MM study of the catalytic mechanism of SAM methyltransferase RlmN from Escherichia coli. Proteins: Structure, Function and Bioinformatics, 2017, 85, 1967-1974.	2.6	5
77	Tuning the electronic and optical properties of NDT-based conjugated polymers by adopting fused heterocycles as acceptor units: a theoretical study. Journal of Molecular Modeling, 2017, 23, 225.	1.8	2
78	Mechanistic Insights into the Decoupled Desaturation and Epoxidation Catalyzed by Dioxygenase AsqJ Involved in the Biosynthesis of Quinolone Alkaloids. ACS Catalysis, 2017, 7, 5534-5543.	11.2	47
79	Treatment effects and genotoxicity relevance of the toxic organic pollutants in semi-coking wastewater by combined treatment process. Environmental Pollution, 2017, 220, 13-19.	7.5	73
80	Quantum mechanics and molecular mechanics study of the reaction mechanism of quorum quenching enzyme: N-acyl homoserine lactonase with C6-HSL. RSC Advances, 2016, 6, 23396-23402.	3.6	3
81	Catalytic mechanism of acetolactate decarboxylase from Brevibacillus brevis towards both enantiomers of Î±-acetolactate. RSC Advances, 2016, 6, 80621-80629.	3.6	12
82	QM/MM studies on the calciumâ€assisted Î²â€elimination mechanism of pectate lyase from bacillus subtilis. Proteins: Structure, Function and Bioinformatics, 2016, 84, 1606-1615.	2.6	4
83	Mechanism of the Glutathione Persulfide Oxidation Process Catalyzed by Ethylmalonic Encephalopathy Protein 1. ACS Catalysis, 2016, 6, 7010-7020.	11.2	11
84	Exploring the substrate specificity and catalytic mechanism of imidazolonepropionase (HutI) from Bacillus subtilis. Physical Chemistry Chemical Physics, 2016, 18, 27928-27938.	2.8	4
85	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.	3.6	2
86	Structures and photoelectric properties of five benzotrithiophene isomers-based donorâ€“acceptor copolymers. Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy, 2016, 159, 262-268.	3.9	4
87	Insights into the catalytic mechanism of N-acetylglucosaminidase glycoside hydrolase from Bacillus subtilis: a QM/MM study. Organic and Biomolecular Chemistry, 2016, 14, 3432-3442.	2.8	9
88	Long time molecular dynamic simulation on the agonist binding and activation of the Î²₂-adrenergic receptor. Molecular Simulation, 2015, 41, 564-571.	2.0	1
89	Ring Contraction Catalyzed by the Metal-Dependent Radical SAM Enzyme: 7-Carboxy-7-deazaguanine Synthase from B. multivorans. Theoretical Insights into the Reaction Mechanism and the Influence of Metal Ions. ACS Catalysis, 2015, 5, 3953-3965.	11.2	23
90	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. RSC Advances, 2015, 5, 7781-7788.	3.6	5

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91	A QM/MM study of the reaction mechanism of (R)â€hydroxynitrile lyases from Arabidopsis thaliana (AtHNL). Proteins: Structure, Function and Bioinformatics, 2015, 83, 66-77.	2.6	7
92	Theoretical study of the hydrolysis mechanism of 2-pyrone-4,6-dicarboxylate (PDC) catalyzed by LigI. Journal of Molecular Graphics and Modelling, 2015, 61, 21-29.	2.4	3
93	Quantum Mechanics and Molecular Mechanics Study of the Catalytic Mechanism of Human AMSH-LP Domain Deubiquitinating Enzymes. Biochemistry, 2015, 54, 5225-5234.	2.5	3
94	Catalytic mechanisms of Au11 and Au11-nPtn (n=1â€“2) clusters: a DFT investigation on the oxidation of CO by O2. Journal of Molecular Modeling, 2015, 21, 230.	1.8	10
95	Theoretical identification on the role of Lys15 for Sulfolobus tokodaii hexokinase. RSC Advances, 2015, 5, 18622-18632.	3.6	2
96	Uncoupled Epimerization and Desaturation by Carbapenem Synthase: Mechanistic Insights from QM/MM Studies. ACS Catalysis, 2015, 5, 5556-5566.	11.2	31
97	Theoretical studies of traditional and halogen-shared halogen bonds: the doped all-metal aromatic clusters MAl3 â^' (MÂ=ÂSi, Ge, Sn, Pb) as halogen bond acceptors. Theoretical Chemistry Accounts, 2015, 134, 1.	1.4	3
98	A QM/MM study of the catalytic mechanism of succinic semialdehyde dehydrogenase from Synechococcus sp. PCC 7002 and Salmonella typhimurium. RSC Advances, 2015, 5, 101672-101682.	3.6	4
99	Deep-blue electroluminescence from nondoped and doped organic light-emitting diodes (OLEDs) based on a new monoaza[6]helicene. RSC Advances, 2015, 5, 75-84.	3.6	81
100	A QM/MM study of the catalytic mechanism of Î±-1,4-glucan lyase from the red seaweed Gracilariopsis lemaneiformis. RSC Advances, 2014, 4, 54398-54408.	3.6	5
101	Insight into the Predictive Binding Modes of the Influenza a Neuraminidase in Complexes with Avian and Human Receptor Analogues. Avian Biology Research, 2014, 7, 172-179.	0.9	0
102	QM/MM study on the catalytic mechanism of cyclohexane-1,2-dione hydrolase (CDH). Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	3
103	Theoretical investigation on the regioselectivity of Ni(COD)2-catalyzed [2Â+Â2Â+Â2] cycloaddition of unsymmetric diynes and CO2. Journal of Organometallic Chemistry, 2014, 758, 45-54.	1.8	11
104	A QM/MM study of the catalytic mechanism of aspartate ammonia lyase. Journal of Molecular Graphics and Modelling, 2014, 51, 113-119.	2.4	11
105	Water Promoting Electron Hole Transport between Tyrosine and Cysteine in Proteins via a Special Mechanism: Double Proton Coupled Electron Transfer. Journal of the American Chemical Society, 2014, 136, 4515-4524.	13.7	51
106	A QM/MM study of the catalytic mechanism of nicotinamidase. Organic and Biomolecular Chemistry, 2014, 12, 1265.	2.8	11
107	Investigation of the rescue mechanism catalyzed by a nucleophile mutant of rice BGlu1. Journal of Molecular Graphics and Modelling, 2014, 54, 100-106.	2.4	4
108	The structures and properties of halogen bonds involving polyvalent halogen in complexes of FXOn (X = Cl, Br; n = 0â€“3)â€“CH3CN. New Journal of Chemistry, 2014, 38, 1256.	2.8	26

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109	Insights into the catalytic mechanism of dTDP-glucose 4,6-dehydratase from quantum mechanics/molecular mechanics simulations. RSC Advances, 2014, 4, 35449.	3.6	8
110	Theoretical investigation on the dissociation of (R)-benzoin catalyzed by benzaldehyde lyase. International Journal of Quantum Chemistry, 2014, 114, 375-382.	2.0	8
111	A density functional theory study on the catalytic mechanism of hydroxycinnamoyl-CoA hydratase-lyase. International Journal of Quantum Chemistry, 2014, 114, 249-254.	2.0	7
112	A theoretical study of the catalytic mechanism of oxalyl-CoA decarboxylase, an enzyme for treating urolithiasis. RSC Advances, 2014, 4, 35777.	3.6	10
113	QM/MM studies of the mechanism of unusual bifunctional fructose-1,6-bisphosphate aldolase/phosphatase. Physical Chemistry Chemical Physics, 2014, 16, 11366.	2.8	5
114	QM/MM Study of the Reaction Mechanism of the Carboxyl Transferase Domain of Pyruvate Carboxylase from Staphylococcus aureus. Biochemistry, 2014, 53, 4455-4466.	2.5	9
115	The reaction mechanism of UDP-GlcNAc 5,6-dehydratase: a quantum mechanical/molecular mechanical (QM/MM) study. Theoretical Chemistry Accounts, 2014, 133, 1.	1.4	1
116	Comparative Studies on the Discrepant Fragmentation Mechanisms of the Gly-Asp-Gly-Arg and Arg-Gly-Asp-Gly: Evidence for the Mobile Proton Model. European Journal of Mass Spectrometry, 2014, 20, 317-325.	1.0	2
117	Theoretical study on the deglycosylation mechanism of rice BGlu1 Î²â€glucosidase. International Journal of Quantum Chemistry, 2013, 113, 1071-1075.	2.0	9
118	QM/MM study of the conversion mechanism of lysine to methylornithine catalyzed by methylornithine synthase (PylB). Theoretical Chemistry Accounts, 2013, 132, 1.	1.4	9
119	Insight into the mechanism of aminomutase reaction: A case study of phenylalanine aminomutase by computational approach. Journal of Molecular Graphics and Modelling, 2013, 46, 65-73.	2.4	9
120	X-ray crystallography and QM/MM investigation on the oligosaccharide synthesis mechanism of rice BGlu1 glycosynthases. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2013, 1834, 536-545.	2.3	8
121	Role of Fâ˜ in the hydrolysisâ€“condensation mechanisms of silicon alkoxide Si(OCH3)4: a DFT investigation. New Journal of Chemistry, 2013, 37, 1371.	2.8	10
122	Theoretical Study of the Catalytic Mechanism of E1 Subunit of Pyruvate Dehydrogenase Multienzyme Complex from Bacillus stearothermophilus. Biochemistry, 2013, 52, 8079-8093.	2.5	15
123	THEORETICAL STUDIES ON THE MECHANISM OF CYCLIC NUCLEOTIDE MONOPHOSPHATE HYDROLYSIS WITHIN PHOSPHODIESTERASES. Journal of Theoretical and Computational Chemistry, 2012, 11, 573-586.	1.8	26
124	The reaction mechanism of hydroxyethylphosphonate dioxygenase: a QM/MM study. Organic and Biomolecular Chemistry, 2012, 10, 1014-1024.	2.8	19
125	QM/MM investigation on the catalytic mechanism of Bacteroides thetaiotaomicron Î±-glucosidase BtGH97a. Biochimica Et Biophysica Acta - Proteins and Proteomics, 2012, 1824, 750-758.	2.3	4
126	A QM/MM study on the catalytic mechanism of pyruvate decarboxylase. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	14

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127	Pb(ii) metalâ€“organic nanotubes based on cyclodextrins: biphasic synthesis, structures and properties. Chemical Science, 2012, 3, 2282.	7.4	70
128	Mechanisms of Silicon Alkoxide Hydrolysisâ€“Oligomerization Reactions: A DFT Investigation. ChemPhysChem, 2012, 13, 2392-2404.	2.1	47
129	Theoretical studies on the conformational change of adenosine kinase induced by inhibitors. International Journal of Quantum Chemistry, 2011, 111, 3980-3990.	2.0	2
130	Theoretical studies on the structural rearrangement of ligand binding pocket in human vitamin D receptor. International Journal of Quantum Chemistry, 2011, 111, 3928-3937.	2.0	0
131	Theoretical Investigations towards the Staudinger Reaction Catalyzed by Nâ€Heterocyclic Carbene: Mechanism and Stereoselectivity. European Journal of Organic Chemistry, 2010, 2010, 6249-6255.	2.4	23
132	3Dâ€QSAR Studies on C24â€Monoalkylated Vitamin D₃ 26,23â€Lactones and their C2Î±â€Modified Derivatives with Inhibitory Activity to Vitamin D Receptor. Molecular Informatics, 2010, 29, 621-632.	2.5	2
133	Theoretical studies on the interaction of guanine riboswitch with guanine and its closest analogues. Molecular Simulation, 2010, 36, 929-938.	2.0	4
134	STUDY ON THE INTERACTIONS OF Smac MIMETICS WITH XIAP-BIR3 DOMAIN BY DOCKING AND MOLECULAR DYNAMICS SIMULATIONS. Journal of Theoretical and Computational Chemistry, 2010, 09, 797-812.	1.8	6
135	Docking and molecular dynamics studies on the interaction of four imidazoline derivatives with potassium ion channel (Kir6.2). Molecular Simulation, 2010, 36, 166-174.	2.0	7
136	Intermolecular Couplization and Cyclization of Chalcones Promoted by Samarium in DMF. Synthetic Communications, 2009, 39, 799-807.	2.1	10
137	A simple way of shape-controlled synthesis of ZnSe nanocrystalsâ€‰:â€‰ nanodots, nanoflowers, and nanotubes. CrystEngComm, 2009, 11, 1789.	2.6	15
138	Transformation of gemâ€Dicyanoethenes by Samarium: Direct Formation of Indenes or Direct Decyanation with in Situ Disilylation. European Journal of Organic Chemistry, 2008, 2008, 5470-5476.	2.4	10
139	A Hybrid Control Architecture for Connection Management in Translucent WDM Networks. , 2008, , .		4
140	Theoretical Study on the Mechanism for the Addition Reaction of SiH3with Propylene and Acetic Acid. Journal of Physical Chemistry A, 2006, 110, 12439-12442.	2.5	2
141	Inner-sphere reorganization for redox pairs M(NH3)62+/3+ (M=Mn, Fe, and Co): Models and calculations. International Journal of Quantum Chemistry, 2002, 86, 468-477.	2.0	2
142	Title is missing!. Theoretical and Experimental Chemistry, 2000, 36, 303-311.	0.8	8