

Haiyang Zhang

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.

52
papers

1,003
citations

18
h-index

30
g-index

56
ext. papers

1,198
ext. citations

4.9
avg, IF

4.59
L-index

#	Paper	IF	Citations
52	Computational Investigation of Structural Basis for Enhanced Binding of Isoflavone Analogues with Mitochondrial Aldehyde Dehydrogenase.. <i>ACS Omega</i> , 2022 , 7, 8115-8127	3.9	1
51	Genomic Analysis of <i>Sphingopyxis</i> sp. USTB-05 for Biodegrading Cyanobacterial Hepatotoxins. <i>Toxins</i> , 2022 , 14, 333	4.9	1
50	Characterization and genomic analysis of an efficient dibutyl phthalate degrading bacterium <i>Microbacterium</i> sp. USTB-Y. <i>World Journal of Microbiology and Biotechnology</i> , 2021 , 37, 212	4.4	
49	Carboxylesterases from bacterial enrichment culture degrade strobilurin fungicides.. <i>Science of the Total Environment</i> , 2021 , 814, 152751	10.2	2
48	Pathway for biodegrading coumarin by a newly isolated <i>Pseudomonas</i> sp. USTB-Z. <i>World Journal of Microbiology and Biotechnology</i> , 2021 , 37, 89	4.4	2
47	Force Field Benchmark of Amino Acids. 3. Hydration with Scaled Lennard-Jones Interactions. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 3571-3582	6.1	3
46	Developing and Assessing Nonbonded Dummy Models of Magnesium Ion with Different Hydration Free Energy References. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 2981-2997	6.1	2
45	Rational Design of Nonbonded Point Charge Models for Divalent Metal Cations with Lennard-Jones 12-6 Potential. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 4031-4044	6.1	2
44	Cyclodextrin inclusion complexes with vitamin A and its esters: A comparative experimental and molecular modeling study. <i>Journal of Molecular Structure</i> , 2021 , 1223, 129001	3.4	8
43	Rational Design of Nonbonded Point Charge Models for Highly Charged Metal Cations with Lennard-Jones 12-6 Potential. <i>Journal of Chemical Information and Modeling</i> , 2021 , 61, 4613-4629	6.1	1
42	Boosted activity by engineering the enzyme microenvironment in cascade reaction: A molecular understanding. <i>Synthetic and Systems Biotechnology</i> , 2021 , 6, 163-172	4.2	3
41	Purification and activity of the first recombinant enzyme for biodegrading hepatotoxin by <i>Sphingopyxis</i> sp. USTB-05. <i>Algal Research</i> , 2020 , 47, 101863	5	3
40	Glycerol induced stability enhancement and conformational changes of β -lactoglobulin. <i>Food Chemistry</i> , 2020 , 308, 125596	8.5	5
39	Cloning and Expression of Genes for Biodegrading Nodularin by sp. USTB-05. <i>Toxins</i> , 2019 , 11,	4.9	5
38	Prediction of Partition Coefficients of Environmental Toxins Using Computational Chemistry Methods. <i>ACS Omega</i> , 2019 , 4, 13772-13781	3.9	15
37	Structural basis of microcystinase activity for biodegrading microcystin-LR. <i>Chemosphere</i> , 2019 , 236, 124281	8.4	9
36	Role of Host-Guest Charge Transfer in Cyclodextrin Complexation: A Computational Study. <i>Journal of Physical Chemistry C</i> , 2019 , 123, 17745-17756	3.8	1

35	Rotational and Translational Diffusion of Proteins as a Function of Concentration. <i>ACS Omega</i> , 2019 , 4, 20654-20664	3.9	7
34	Force Field Benchmark of Amino Acids: I. Hydration and Diffusion in Different Water Models. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1037-1052	6.1	56
33	Force Field Benchmark of Amino Acids. 2. Partition Coefficients between Water and Organic Solvents. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1669-1681	6.1	28
32	Effective Biodegradation of Aflatoxin B1 Using the (BL010) Strain. <i>Toxins</i> , 2018 , 10,	4.9	16
31	Comparison of Implicit and Explicit Solvent Models for the Calculation of Solvation Free Energy in Organic Solvents. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 1034-1043	6.4	96
30	Modeling Coordination-Directed Self-Assembly of ML Nanocapsule Featuring Competitive Guest Encapsulation. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2082-2086	6.4	7
29	Free-Energy Calculations of Ionic Hydration Consistent with the Experimental Hydration Free Energy of the Proton. <i>Journal of Physical Chemistry Letters</i> , 2017 , 8, 2705-2712	6.4	30
28	Enhancement of methanol resistance of <i>Yarrowia lipolytica</i> lipase 2 using β -cyclodextrin as an additive: Insights from experiments and molecular dynamics simulation. <i>Enzyme and Microbial Technology</i> , 2017 , 96, 157-162	3.8	6
27	Comparative Assessment of Computational Methods for Free Energy Calculations of Ionic Hydration. <i>Journal of Chemical Information and Modeling</i> , 2017 , 57, 2763-2775	6.1	16
26	Evaluation of Generalized Born Models for Large Scale Affinity Prediction of Cyclodextrin Host-Guest Complexes. <i>Journal of Chemical Information and Modeling</i> , 2016 , 56, 2080-2092	6.1	18
25	Helical Polymers Showing Inverse Helicity and Synergistic Effect in Chiral Catalysis: Catalytic Functionality Determining Enantiocconfiguration and Helical Frameworks Providing Asymmetric Microenvironment. <i>Macromolecular Chemistry and Physics</i> , 2016 , 217, 880-888	2.6	5
24	Rational Design of Methodology-Independent Metal Parameters Using a Nonbonded Dummy Model. <i>Journal of Chemical Theory and Computation</i> , 2016 , 12, 3250-60	6.4	30
23	Atomistic Simulation of Protein Encapsulation in Metal-Organic Frameworks. <i>Journal of Physical Chemistry B</i> , 2016 , 120, 477-84	3.4	25
22	Pathway for Biodegrading Nodularin (NOD) by <i>Sphingopyxis</i> sp. USTB-05. <i>Toxins</i> , 2016 , 8,	4.9	11
21	NMR Study on the Inclusion Complexes of β -Cyclodextrin with Isoflavones. <i>Molecules</i> , 2016 , 21, 372	4.8	41
20	Generalized Born and Explicit Solvent Models for Free Energy Calculations in Organic Solvents: Cyclodextrin Dimerization. <i>Journal of Chemical Theory and Computation</i> , 2015 , 11, 5103-13	6.4	25
19	Optically active helical polymers with pendent thiourea groups: Chiral organocatalyst for asymmetric michael addition reaction. <i>Journal of Polymer Science Part A</i> , 2015 , 53, 1816-1823	2.5	17
18	Refined Dummy Atom Model of Mg(2+) by Simple Parameter Screening Strategy with Revised Experimental Solvation Free Energy. <i>Journal of Chemical Information and Modeling</i> , 2015 , 55, 2575-86	6.1	22

17	Cooperative Binding of Cyclodextrin Dimers to Isoflavone Analogues Elucidated by Free Energy Calculations. <i>Journal of Physical Chemistry C</i> , 2014 , 118, 7163-7173	3.8	26
16	The first suspension polymerization for preparing optically active microparticles purely constructed from chirally helical substituted polyacetylenes. <i>Macromolecular Rapid Communications</i> , 2014 , 35, 1216-23	4.8	28
15	Theoretical and experimental studies on activity of <i>Yarrowia lipolytica</i> lipase in methanol/water mixtures. <i>Journal of Physical Chemistry B</i> , 2014 , 118, 1976-83	3.4	15
14	Lid closure mechanism of <i>Yarrowia lipolytica</i> lipase in methanol investigated by molecular dynamics simulation. <i>Journal of Chemical Information and Modeling</i> , 2014 , 54, 2033-41	6.1	15
13	Sodium hexadecyl sulfate as an interfacial substance adjusting the adsorption of a protein on carbon nanotubes. <i>ACS Applied Materials & Interfaces</i> , 2014 , 6, 15132-9	9.5	11
12	Polymer monoliths with chelating functionalities for solid phase extraction of metal ions from water. <i>Journal of Chromatography A</i> , 2014 , 1343, 128-34	4.5	37
11	Photoswitchable molecular switches featuring both axial and tetrahedral chirality. <i>Journal of Materials Chemistry C</i> , 2013 , 1, 7346	7.1	31
10	Quantification of Solvent Contribution to the Stability of Noncovalent Complexes. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 4542-51	6.4	33
9	A model for the shuttle motions of puerarin and daidzin inside the cavity of β -cyclodextrin in aqueous acetic acid: insights from molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2012 , 18, 221-7	2	4
8	Insight into the structural deformations of beta-cyclodextrin caused by alcohol cosolvents and guest molecules. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 3880-9	3.4	31
7	Molecular recognition in different environments: β -cyclodextrin dimer formation in organic solvents. <i>Journal of Physical Chemistry B</i> , 2012 , 116, 12684-93	3.4	46
6	Optically active core/shell nanoparticles prepared using self-assembled polymer micelle as reactive nanoreactor. <i>Journal of Polymer Science Part A</i> , 2012 , 50, 4415-4422	2.5	6
5	Analysis of the conformational stability and activity of <i>Candida antarctica</i> lipase B in organic solvents: insight from molecular dynamics and quantum mechanics/simulations. <i>Journal of Biological Chemistry</i> , 2010 , 285, 28434-41	5.4	120
4	Investigation of the inclusions of puerarin and daidzin with beta-cyclodextrin by molecular dynamics simulation. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 4876-83	3.4	54
3	A Novel Medium Poly(vinyl acetate-triallyl isocyanurate-divinylbenzene) Coupled with Oligo- β -Cyclodextrin for the Isolation of Puerarin from Pueraria Flavones. <i>Chromatographia</i> , 2010 , 72, 47-54	2.1	9
2	Thermodynamic and NMR investigations on the adsorption mechanism of puerarin with oligo- β -cyclodextrin-coupled polystyrene-based matrix. <i>Journal of Chemical Technology and Biotechnology</i> , 2009 , 84, 611-617	3.5	12
1	Quantitative predictions from molecular simulations using explicit or implicit interactions. <i>Wiley Interdisciplinary Reviews: Computational Molecular Science</i> , e1560	7.9	4