

Peng Tao

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.

56
papers

885
citations

17
h-index

27
g-index

63
ext. papers

1,102
ext. citations

4.5
avg, IF

4.68
L-index

#	Paper	IF	Citations
56	Dynamics of hydrogen bonds in the secondary structures of allosteric protein phototropin 1.. <i>Computational and Structural Biotechnology Journal</i> , 2022 , 20, 50-64	6.8	0
55	Explore Protein Conformational Space With Variational Autoencoder. <i>Frontiers in Molecular Biosciences</i> , 2021 , 8, 781635	5.6	4
54	QM/MM modeling of class A β -lactamases reveals distinct acylation pathways for ampicillin and cefalexin. <i>Organic and Biomolecular Chemistry</i> , 2021 , 19, 9182-9189	3.9	1
53	Deciphering the protein motion of S1 subunit in SARS-CoV-2 spike glycoprotein through integrated computational methods. <i>Journal of Biomolecular Structure and Dynamics</i> , 2021 , 39, 6705-6712	3.6	7
52	PASSer: Prediction of Allosteric Sites Server. <i>Machine Learning: Science and Technology</i> , 2021 , 2,	5.1	6
51	UMAP as a Dimensionality Reduction Tool for Molecular Dynamics Simulations of Biomacromolecules: A Comparison Study. <i>Journal of Physical Chemistry B</i> , 2021 , 125, 5022-5034	3.4	8
50	Predicting Potential SARS-COV-2 Drugs-In Depth Drug Database Screening Using Deep Neural Network Framework SSnet, Classical Virtual Screening and Docking. <i>International Journal of Molecular Sciences</i> , 2021 , 22,	6.3	12
49	Dimeric allostery mechanism of the plant circadian clock photoreceptor ZEITLUPE. <i>PLoS Computational Biology</i> , 2021 , 17, e1009168	5	2
48	Mechanistic Basis of OXA-48-like β -lactamasesSHydrolysis of Carbapenems. <i>ACS Infectious Diseases</i> , 2021 , 7, 445-460	5.5	5
47	Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. <i>Communications Chemistry</i> , 2020 , 3,	6.3	6
46	Deciphering the Allosteric Process of the Aureochrome 1a LOV Domain. <i>Journal of Physical Chemistry B</i> , 2020 , 124, 8960-8972	3.4	11
45	Allosteric Regulation at the Crossroads of New Technologies: Multiscale Modeling, Networks, and Machine Learning. <i>Frontiers in Molecular Biosciences</i> , 2020 , 7, 136	5.6	18
44	ivis Dimensionality Reduction Framework for Biomacromolecular Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020 , 60, 4569-4581	6.1	6
43	Machine Learning Classification Model for Functional Binding Modes of TEM-1 β -lactamase. <i>Frontiers in Molecular Biosciences</i> , 2019 , 6, 47	5.6	12
42	Probing Protein Allostery as a Residue-Specific Concept via Residue Response Maps. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 4691-4705	6.1	9
41	Directed kinetic transition network model. <i>Journal of Chemical Physics</i> , 2019 , 151, 144112	3.9	7
40	Exploring free energy profile of petroleum thermal cracking mechanisms. <i>Journal of Molecular Modeling</i> , 2019 , 26, 15	2	4

39	Allosteric mechanism of the circadian protein Vivid resolved through Markov state model and machine learning analysis. <i>PLoS Computational Biology</i> , 2019 , 15, e1006801	5	15
38	Dynamical Behavior of β -Lactamases and Penicillin-Binding Proteins in Different Functional States and Its Potential Role in Evolution. <i>Entropy</i> , 2019 , 21, 1130	2.8	4
37	REDAN: Relative Entropy-Based Dynamical Allosteric Network Model. <i>Molecular Physics</i> , 2019 , 117, 1334-1343	4.1	5
36	Recognition of protein allosteric states and residues: Machine learning approaches. <i>Journal of Computational Chemistry</i> , 2018 , 39, 1481-1490	3.5	16
35	Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer. <i>Angewandte Chemie</i> , 2018 , 130, 5462-5466	3.6	6
34	Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer. <i>Angewandte Chemie - International Edition</i> , 2018 , 57, 5364-5368	16.4	13
33	Insights into Key Interactions between Vancomycin and Bacterial Cell Wall Structures. <i>ACS Omega</i> , 2018 , 3, 37-45	3.9	31
32	Innenrücktitelbild: Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer (Angew. Chem. 19/2018). <i>Angewandte Chemie</i> , 2018 , 130, 5655-5655	3.6	
31	Combining protein sequence, structure, and dynamics: A novel approach for functional evolution analysis of PAS domain superfamily. <i>Protein Science</i> , 2018 , 27, 421-430	6.3	6
30	Dynamics Sampling in Transition Pathway Space. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 14-29	6.4	5
29	t-Distributed Stochastic Neighbor Embedding Method with the Least Information Loss for Macromolecular Simulations. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 5499-5510	6.4	33
28	An Orbital-Overlap Complement to Ligand and Binding Site Electrostatic Potential Maps. <i>Journal of Chemical Information and Modeling</i> , 2018 , 58, 1836-1846	6.1	14
27	Revealing Hidden Conformational Space of LOV Protein VIVID Through Rigid Residue Scan Simulations. <i>Scientific Reports</i> , 2017 , 7, 46626	4.9	8
26	The Carboxyl Terminus of Eremomycin Facilitates Binding to the Non-d-Ala-d-Ala Segment of the Peptidoglycan Pentapeptide Stem. <i>Biochemistry</i> , 2016 , 55, 3383-91	3.2	5
25	Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery. <i>PLoS Computational Biology</i> , 2016 , 12, e1004893	5	22
24	Identifying key residues for protein allostery through rigid residue scan. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1689-700	2.8	20
23	Multiple environment single system quantum mechanical/molecular mechanical (MESS-QM/MM) calculations. 1. Estimation of polarization energies. <i>Journal of Physical Chemistry A</i> , 2015 , 119, 1511-23	2.8	21
22	Chemiluminescent Probes for Imaging HS in Living Animals. <i>Chemical Science</i> , 2015 , 6, 1979-1985	9.4	106

21	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. <i>Journal of Chemical Theory and Computation</i> , 2014 , 10, 4198-4207	6.4	13
20	Right- and Left-Handed Helices, What is in between? Interconversion of Helical Structures of Alternating Pyridinedicarboxamide/m-(phenylazo)azobenzene Oligomers. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 5137-49	6.4	8
19	Comparison of Three Chain-of-States Methods: Nudged Elastic Band and Replica Path with Restraints or Constraints. <i>Journal of Chemical Theory and Computation</i> , 2012 , 8, 5035-5051	6.4	20
18	Maintain rigid structures in Verlet based cartesian molecular dynamics simulations. <i>Journal of Chemical Physics</i> , 2012 , 137, 134110	3.9	14
17	A Quantum Chemical Study of the Ground and Excited State Electronic Structures of Carbazole Oligomers with and without Triarylborane Substitutes. <i>Journal of Physical Chemistry C</i> , 2012 , 116, 12434-12442 ¹⁷	3.8	17
16	Reaction Path Optimization and Sampling Methods and Their Applications for Rare Events 2012 ,		1
15	Spin trapping of hydroperoxyl radical by a cyclic nitron conjugated to -cyclodextrin: a computational study. <i>Theoretical Chemistry Accounts</i> , 2012 , 131, 1	1.9	2
14	Matrix metalloproteinase 2 (MMP2) inhibition: DFT and QM/MM studies of the deprotonation-initialized ring-opening reaction of the sulfoxide analogue of SB-3CT. <i>Journal of Physical Chemistry B</i> , 2010 , 114, 1030-7	3.4	19
13	Ab initio classical trajectory study of the fragmentation of C ₃ H ₄ dications on the singlet and triplet surfaces. <i>Journal of Physical Chemistry A</i> , 2010 , 114, 7653-60	2.8	13
12	QM/MM Studies of the Matrix Metalloproteinase 2 (MMP2) Inhibition Mechanism of (S)-SB-3CT and its Oxirane Analogue. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 3580-3587	6.4	21
11	A toolkit to assist ONIOM calculations. <i>Journal of Computational Chemistry</i> , 2010 , 31, 2363-9	3.5	42
10	Common basis for the mechanism of metallo and non-metallo KDO8P synthases. <i>Journal of Inorganic Biochemistry</i> , 2010 , 104, 1267-75	4.2	5
9	Computational Modeling of Human Paraoxonase 1: Preparation of Protein Models, Binding Studies, and Mechanistic Insights. <i>Journal of Physical Organic Chemistry</i> , 2010 , 23, 357-369	2.1	17
8	Electronic structure of the metal center in the Cd(2+), Zn(2+), and Cu(2+) substituted forms of KDO8P synthase: implications for catalysis. <i>Biochemistry</i> , 2009 , 48, 3610-30	3.2	13
7	The energy landscape of 3-deoxy-D-manno-octulosonate 8-phosphate synthase. <i>Biochemistry</i> , 2009 , 48, 11706-14	3.2	13
6	Matrix metalloproteinase 2 inhibition: combined quantum mechanics and molecular mechanics studies of the inhibition mechanism of (4-phenoxyphenylsulfonyl)methylthiirane and its oxirane analogue. <i>Biochemistry</i> , 2009 , 48, 9839-47	3.2	53
5	DFT studies of the ring-opening mechanism of SB-3CT, a potent inhibitor of matrix metalloproteinase 2. <i>Organic Letters</i> , 2009 , 11, 2559-62	6.2	22
4	Photomodulated chiral induction in helical azobenzene oligomers. <i>Organic Letters</i> , 2008 , 10, 1671-4	6.2	48

3	Synthesis of L-daunosamine and L-ristosamine glycosides via photoinduced aziridination. Conversion to thioglycosides for use in glycosylation reactions. <i>Journal of Organic Chemistry</i> , 2006 , 71, 8059-70	4.2	40
2	Protein ligand docking based on empirical method for binding affinity estimation. <i>Journal of Computer-Aided Molecular Design</i> , 2001 , 15, 429-46	4.2	24
1	Calculating Partition Coefficients of Peptides by the Addition Method. <i>Journal of Molecular Modeling</i> , 1999 , 5, 189-195	2	32