Peng Tao

List of Publications by Citations

56	885	17	27
papers	citations	h-index	g-index
63	1,102	4.5	4.68
ext. papers	ext. citations	avg, IF	L-index

#	Paper	IF	Citations
56	Chemiluminescent Probes for Imaging HS in Living Animals. *Chemical Science*, **2015**, 6, 1979-1985	9.4	106
55	Matrix metalloproteinase 2 inhibition: combined quantum mechanics and molecular mechanics studies of the inhibition mechanism of (4-phenoxyphenylsulfonyl)methylthiirane and its oxirane analogue. *Biochemistry*, **2009**, 48, 9839-47	3.2	53
54	Photomodulated chiral induction in helical azobenzene oligomers. *Organic Letters*, **2008**, 10, 1671-4	6.2	48
53	A toolkit to assist ONIOM calculations. *Journal of Computational Chemistry*, **2010**, 31, 2363-9	3.5	42
52	Synthesis of L-daunosamine and L-ristosamine glycosides via photoinduced aziridination. Conversion to thioglycosides for use in glycosylation reactions. *Journal of Organic Chemistry*, **2006**, 71, 8059-70	4.2	40
51	t-Distributed Stochastic Neighbor Embedding Method with the Least Information Loss for Macromolecular Simulations. *Journal of Chemical Theory and Computation*, **2018**, 14, 5499-5510	6.4	33
50	Calculating Partition Coefficients of Peptides by the Addition Method. *Journal of Molecular Modeling*, **1999**, 5, 189-195	2	32
49	Insights into Key Interactions between Vancomycin and Bacterial Cell Wall Structures. *ACS Omega*, **2018**, 3, 37-45	3.9	31
48	Protein ligand docking based on empirical method for binding affinity estimation. *Journal of Computer-Aided Molecular Design*, **2001**, 15, 429-46	4.2	24
47	DFT studies of the ring-opening mechanism of SB-3CT, a potent inhibitor of matrix metalloproteinase 2. *Organic Letters*, **2009**, 11, 2559-62	6.2	22
46	Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery. *PLoS Computational Biology*, **2016**, 12, e1004893	5	22
45	Multiple environment single system quantum mechanical/molecular mechanical (MESS-QM/MM) calculations. 1. Estimation of polarization energies. *Journal of Physical Chemistry A*, **2015**, 119, 1511-23	2.8	21
44	QM/MM Studies of the Matrix Metalloproteinase 2 (MMP2) Inhibition Mechanism of (S)-SB-3CT and its Oxirane Analogue. *Journal of Chemical Theory and Computation*, **2010**, 6, 3580-3587	6.4	21
43	Identifying key residues for protein allostery through rigid residue scan. *Journal of Physical Chemistry A*, **2015**, 119, 1689-700	2.8	20
42	Comparison of Three Chain-of-States Methods: Nudged Elastic Band and Replica Path with Restraints or Constraints. *Journal of Chemical Theory and Computation*, **2012**, 8, 5035-5051	6.4	20
41	Matrix metalloproteinase 2 (MMP2) inhibition: DFT and QM/MM studies of the deprotonation-initialized ring-opening reaction of the sulfoxide analogue of SB-3CT. *Journal of Physical Chemistry B*, **2010**, 114, 1030-7	3.4	19
40	Allosteric Regulation at the Crossroads of New Technologies: Multiscale Modeling, Networks, and Machine Learning. *Frontiers in Molecular Biosciences*, **2020**, 7, 136	5.6	18

39	A Quantum Chemical Study of the Ground and Excited State Electronic Structures of Carbazole Oligomers with and without Triarylborane Substitutes. *Journal of Physical Chemistry C*, **2012**, 116, 12434-12442	3.8	17
38	Computational Modeling of Human Paraoxonase 1: Preparation of Protein Models, Binding Studies, and Mechanistic Insights. *Journal of Physical Organic Chemistry*, **2010**, 23, 357-369	2.1	17
37	Recognition of protein allosteric states and residues: Machine learning approaches. *Journal of Computational Chemistry*, **2018**, 39, 1481-1490	3.5	16
36	Allosteric mechanism of the circadian protein Vivid resolved through Markov state model and machine learning analysis. *PLoS Computational Biology*, **2019**, 15, e1006801	5	15
35	Maintain rigid structures in Verlet based cartesian molecular dynamics simulations. *Journal of Chemical Physics*, **2012**, 137, 134110	3.9	14
34	An Orbital-Overlap Complement to Ligand and Binding Site Electrostatic Potential Maps. *Journal of Chemical Information and Modeling*, **2018**, 58, 1836-1846	6.1	14
33	Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer. *Angewandte Chemie - International Edition*, **2018**, 57, 5364-5368	16.4	13
32	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. *Journal of Chemical Theory and Computation*, **2014**, 10, 4198-4207	6.4	13
31	Ab initio classical trajectory study of the fragmentation of C3H4 dications on the singlet and triplet surfaces. *Journal of Physical Chemistry A*, **2010**, 114, 7653-60	2.8	13
30	Electronic structure of the metal center in the Cd(2+), Zn(2+), and Cu(2+) substituted forms of KDO8P synthase: implications for catalysis. *Biochemistry*, **2009**, 48, 3610-30	3.2	13
29	The energy landscape of 3-deoxy-D-manno-octulosonate 8-phosphate synthase. *Biochemistry*, **2009**, 48, 11706-14	3.2	13
28	Machine Learning Classification Model for Functional Binding Modes of TEM-1 β-Lactamase. *Frontiers in Molecular Biosciences*, **2019**, 6, 47	5.6	12
27	Predicting Potential SARS-COV-2 Drugs-In Depth Drug Database Screening Using Deep Neural Network Framework SSnet, Classical Virtual Screening and Docking. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	12
26	Deciphering the Allosteric Process of the Aureochrome 1a LOV Domain. *Journal of Physical Chemistry B*, **2020**, 124, 8960-8972	3.4	11
25	Probing Protein Allostery as a Residue-Specific Concept via Residue Response Maps. *Journal of Chemical Information and Modeling*, **2019**, 59, 4691-4705	6.1	9
24	Revealing Hidden Conformational Space of LOV Protein VIVID Through Rigid Residue Scan Simulations. *Scientific Reports*, **2017**, 7, 46626	4.9	8
23	Right- and Left-Handed Helices, What is in between? Interconversion of Helical Structures of Alternating Pyridinedicarboxamide/m-(phenylazo)azobenzene Oligomers. *Journal of Chemical Theory and Computation*, **2012**, 8, 5137-49	6.4	8
22	UMAP as a Dimensionality Reduction Tool for Molecular Dynamics Simulations of Biomacromolecules: A Comparison Study. *Journal of Physical Chemistry B*, **2021**, 125, 5022-5034	3.4	8

21	Directed kinetic transition network model. *Journal of Chemical Physics*, **2019**, 151, 144112	3.9	7
20	Deciphering the protein motion of S1 subunit in SARS-CoV-2 spike glycoprotein through integrated computational methods. *Journal of Biomolecular Structure and Dynamics*, **2021**, 39, 6705-6712	3.6	7
19	Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer. *Angewandte Chemie* , **2018**, 130, 5462-5466	3.6	6
18	Combining protein sequence, structure, and dynamics: A novel approach for functional evolution analysis of PAS domain superfamily. *Protein Science*, **2018**, 27, 421-430	6.3	6
17	Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. *Communications Chemistry*, **2020**, 3,	6.3	6
16	ivis Dimensionality Reduction Framework for Biomacromolecular Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 4569-4581	6.1	6
15	PASSer: Prediction of Allosteric Sites Server. *Machine Learning: Science and Technology*, **2021**, 2,	5.1	6
14	The Carboxyl Terminus of Eremomycin Facilitates Binding to the Non-d-Ala-d-Ala Segment of the Peptidoglycan Pentapeptide Stem. *Biochemistry*, **2016**, 55, 3383-91	3.2	5
13	Common basis for the mechanism of metallo and non-metallo KDO8P synthases. *Journal of Inorganic Biochemistry*, **2010**, 104, 1267-75	4.2	5
12	REDAN: Relative Entropy-Based Dynamical Allosteric Network Model. *Molecular Physics*, **2019**, 117, 1334-1343	1.7	5
11	Dynamics Sampling in Transition Pathway Space. *Journal of Chemical Theory and Computation*, **2018**, 14, 14-29	6.4	5
10	Mechanistic Basis of OXA-48-like LactamasesSHydrolysis of Carbapenems. *ACS Infectious Diseases*, **2021**, 7, 445-460	5.5	5
9	Explore Protein Conformational Space With Variational Autoencoder. *Frontiers in Molecular Biosciences*, **2021**, 8, 781635	5.6	4
8	Exploring free energy profile of petroleum thermal cracking mechanisms. *Journal of Molecular Modeling*, **2019**, 26, 15	2	4
7	Dynamical Behavior of Lactamases and Penicillin- Binding Proteins in Different Functional States and Its Potential Role in Evolution. *Entropy*, **2019**, 21, 1130	2.8	4
6	Spin trapping of hydroperoxyl radical by a cyclic nitrone conjugated to -cyclodextrin: a computational study. *Theoretical Chemistry Accounts*, **2012**, 131, 1	1.9	2
5	Dimeric allostery mechanism of the plant circadian clock photoreceptor ZEITLUPE. *PLoS Computational Biology*, **2021**, 17, e1009168	5	2
4	Reaction Path Optimization and Sampling Methods and Their Applications for Rare Events **2012**,		1

List of Publications

3	QM/MM modeling of class A β-lactamases reveals distinct acylation pathways for ampicillin and cefalexin. *Organic and Biomolecular Chemistry*, **2021**, 19, 9182-9189	3.9	1
2	Dynamics of hydrogen bonds in the secondary structures of allosteric protein phototropin 1.. *Computational and Structural Biotechnology Journal*, **2022**, 20, 50-64	6.8	0
1	Innenrücktitelbild: Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer (Angew. Chem. 19/2018). *Angewandte Chemie*, **2018**, 130, 5655-5655	3.6	