Peng Tao

List of Publications by Year
in descending order

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61 papers	1,318 citations	361388 20 h-index	414395 32 g-index
63 all docs	63 docs citations	63 times ranked	1715 citing authors

#	Article	IF	Citations
1	Dynamics of hydrogen bonds in the secondary structures of allosteric protein Avena Sativa phototropin 1. Computational and Structural Biotechnology Journal, 2022, 20, 50-64.	4.1	10
2	Allosteric control of ACE2 peptidase domain dynamics. Organic and Biomolecular Chemistry, 2022, 20, 3605-3618.	2.8	3
3	Mechanistic Insights into Enzyme Catalysis from Explaining Machine-Learned Quantum Mechanical and Molecular Mechanical Minimum Energy Pathways. ACS Physical Chemistry Au, 2022, 2, 316-330.	4.0	5
4	Sparse group selection and analysis of <scp>functionâ€related</scp> residue for <scp>proteinâ€state</scp> recognition. Journal of Computational Chemistry, 2022, 43, 1342-1354.	3.3	0
5	Graph-learning guided mechanistic insights into imipenem hydrolysis in GES carbapenemases. Electronic Structure, 2022, 4, 034001.	2.8	2
6	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.	3.5	10
7	Predicting Potential SARS-COV-2 Drugsâ€"In Depth Drug Database Screening Using Deep Neural Network Framework SSnet, Classical Virtual Screening and Docking. International Journal of Molecular Sciences, 2021, 22, 1573.	4.1	27
8	PASSer: prediction of allosteric sites server. Machine Learning: Science and Technology, 2021, 2, 035015.	5.0	37
9	UMAP as a Dimensionality Reduction Tool for Molecular Dynamics Simulations of Biomacromolecules: A Comparison Study. Journal of Physical Chemistry B, 2021, 125, 5022-5034.	2.6	39
10	Dimeric allostery mechanism of the plant circadian clock photoreceptor ZEITLUPE. PLoS Computational Biology, 2021, 17, e1009168.	3.2	3
11	Mechanistic Basis of OXA-48-like Î²-Lactamasesâ€™ Hydrolysis of Carbapenems. ACS Infectious Diseases, 2021, 7, 445-460.	3.8	18
12	QM/MM modeling of class A Î²-lactamases reveals distinct acylation pathways for ampicillin and cefalexin. Organic and Biomolecular Chemistry, 2021, 19, 9182-9189.	2.8	7
13	Explore Protein Conformational Space With Variational Autoencoder. Frontiers in Molecular Biosciences, 2021, 8, 781635.	3.5	24
14	Exploring free energy profile of petroleum thermal cracking mechanisms. Journal of Molecular Modeling, 2020, 26, 15.	1.8	5
15	Unraveling the energetic significance of chemical events in enzyme catalysis via machine-learning based regression approach. Communications Chemistry, 2020, 3, .	4.5	16
16	Deciphering the Allosteric Process of the Phaeodactylum tricornutum Aureochrome 1a LOV Domain. Journal of Physical Chemistry B, 2020, 124, 8960-8972.	2.6	22
17	Allosteric Regulation at the Crossroads of New Technologies: Multiscale Modeling, Networks, and Machine Learning. Frontiers in Molecular Biosciences, 2020, 7, 136.	3.5	44
18	ivis Dimensionality Reduction Framework for Biomacromolecular Simulations. Journal of Chemical Information and Modeling, 2020, 60, 4569-4581.	5.4	10

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19	Machine Learning Classification Model for Functional Binding Modes of TEM-1 Î²-Lactamase. Frontiers in Molecular Biosciences, 2019, 6, 47.	3.5	13
20	Probing Protein Allostery as a Residue-Specific Concept via Residue Response Maps. Journal of Chemical Information and Modeling, 2019, 59, 4691-4705.	5.4	17
21	Directed kinetic transition network model. Journal of Chemical Physics, 2019, 151, 144112.	3.0	8
22	Allosteric mechanism of the circadian protein Vivid resolved through Markov state model and machine learning analysis. PLoS Computational Biology, 2019, 15, e1006801.	3.2	19
23	Dynamical Behavior of Î²-Lactamases and Penicillin- Binding Proteins in Different Functional States and Its Potential Role in Evolution. Entropy, 2019, 21, 1130.	2.2	7
24	REDAN: relative entropy-based dynamical allosteric network model. Molecular Physics, 2019, 117, 1334-1343.	1.7	10
25	Recognition of protein allosteric states and residues: Machine learning approaches. Journal of Computational Chemistry, 2018, 39, 1481-1490.	3.3	25
26	Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer. Angewandte Chemie, 2018, 130, 5462-5466.	2.0	6
27	Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer. Angewandte Chemie - International Edition, 2018, 57, 5364-5368.	13.8	18
28	Insights into Key Interactions between Vancomycin and Bacterial Cell Wall Structures. ACS Omega, 2018, 3, 37-45.	3.5	56
29	InnenrÃ¼cktitelbild: Direct Measurement of Charge Regulation in Metalloprotein Electron Transfer (Angew. Chem. 19/2018). Angewandte Chemie, 2018, 130, 5655-5655.	2.0	0
30	Combining protein sequence, structure, and dynamics: A novel approach for functional evolution analysis of PAS domain superfamily. Protein Science, 2018, 27, 421-430.	7.6	12
31	Dynamics Sampling in Transition Pathway Space. Journal of Chemical Theory and Computation, 2018, 14, 14-29.	5.3	5
32	t-Distributed Stochastic Neighbor Embedding Method with the Least Information Loss for Macromolecular Simulations. Journal of Chemical Theory and Computation, 2018, 14, 5499-5510.	5.3	74
33	An Orbital-Overlap Complement to Ligand and Binding Site Electrostatic Potential Maps. Journal of Chemical Information and Modeling, 2018, 58, 1836-1846.	5.4	22
34	Revealing Hidden Conformational Space of LOV Protein VIVID Through Rigid Residue Scan Simulations. Scientific Reports, 2017, 7, 46626.	3.3	11
35	The Carboxyl Terminus of Eremomycin Facilitates Binding to the Non-<scp>d</scp>-Ala-<scp>d</scp>-Ala Segment of the Peptidoglycan Pentapeptide Stem. Biochemistry, 2016, 55, 3383-3391.	2.5	8
36	Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery. PLoS Computational Biology, 2016, 12, e1004893.	3.2	32

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37	Identifying Key Residues for Protein Allostery through Rigid Residue Scan. Journal of Physical Chemistry A, 2015, 119, 1689-1700.	2.5	27
38	Multiple Environment Single System Quantum Mechanical/Molecular Mechanical (MESS-QM/MM) Calculations. 1. Estimation of Polarization Energies. Journal of Physical Chemistry A, 2015, 119, 1511-1523.	2.5	23
39	Chemiluminescent probes for imaging H₂S in living animals. Chemical Science, 2015, 6, 1979-1985.	7.4	139
40	Computing the Free Energy along a Reaction Coordinate Using Rigid Body Dynamics. Journal of Chemical Theory and Computation, 2014, 10, 4198-4207.	5.3	14
41	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, 5137-5149.	5.3	8
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.	5.3	23
43	Maintain rigid structures in Verlet based Cartesian molecular dynamics simulations. Journal of Chemical Physics, 2012, 137, 134110.	3.0	17
44	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.	3.1	18
45	Spin trapping of hydroperoxyl radical by a cyclic nitrone conjugated to Î²-cyclodextrin: a computational study. Theoretical Chemistry Accounts, 2012, 131, 1.	1.4	2
46	A toolkit to assist ONIOM calculations. Journal of Computational Chemistry, 2010, 31, 2363-2369.	3.3	51
47	Common basis for the mechanism of metallo and non-metallo KDO8P synthases. Journal of Inorganic Biochemistry, 2010, 104, 1267-1275.	3.5	5
48	Computational modeling of human paraoxonase 1: preparation of protein models, binding studies, and mechanistic insights. Journal of Physical Organic Chemistry, 2010, 23, 357-369.	1.9	19
49	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, 1030-1037.	2.6	20
50	Ab Initio Classical Trajectory Study of the Fragmentation of C3H4Dications on the Singlet and Triplet Surfaces. Journal of Physical Chemistry A, 2010, 114, 7653-7660.	2.5	13
51	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.	5.3	23
52	Electronic Structure of the Metal Center in the Cd²⁺, Zn²⁺, and Cu²⁺ Substituted Forms of KDO8P Synthase: Implications for Catalysis. Biochemistry, 2009, 48, 3610-3630.	2.5	13
53	The Energy Landscape of 3-Deoxy-<scp>d</scp>-manno-octulosonate 8-Phosphate Synthase. Biochemistry, 2009, 48, 11706-11714.	2.5	13
54	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, 9839-9847.	2.5	62

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55	DFT Studies of the Ring-Opening Mechanism of SB-3CT, a Potent Inhibitor of Matrix Metalloproteinase 2. Organic Letters, 2009, 11, 2559-2562.	4.6	23
56	Photomodulated Chiral Induction in Helical Azobenzene Oligomers. Organic Letters, 2008, 10, 1671-1674.	4.6	51
57	Synthesis ofl-Daunosamine andl-Ristosamine Glycosides via Photoinduced Aziridination. Conversion to Thioglycosides for Use in Glycosylation Reactions. Journal of Organic Chemistry, 2006, 71, 8059-8070.	3.2	43
58	Protein ligand docking based on empirical method for binding affinity estimation. , 2001, 15, 429-446.		27
59	Calculating Partition Coefficients of Peptides by the Addition Method. Journal of Molecular Modeling, 1999, 5, 189-195.	1.8	38
60	Reaction Path Optimization and Sampling Methods and Their Applications for Rare Events. , 0, , .		1
61	PASSer2.0: Accurate Prediction of Protein Allosteric Sites Through Automated Machine Learning. Frontiers in Molecular Biosciences, 0, 9, .	3.5	20