Qinghua Liao

List of Publications by Year
in descending order

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20	708	623699 14	752679 20
papers	citations	h-index	g-index

20	20	20	1098
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The N-terminal Helix-Turn-Helix Motif of Transcription Factors MarA and Rob Drives DNA Recognition. Journal of Physical Chemistry B, 2021, 125, 6791-6806.	2.6	6
2	Enzyme Evolution: An Epistatic Ratchet versus a Smooth Reversible Transition. Molecular Biology and Evolution, 2020, 37, 1133-1147.	8.9	26
3	Enhanced sampling and free energy calculations for protein simulations. Progress in Molecular Biology and Translational Science, 2020, 170, 177-213.	1.7	19
4	Long Time-Scale Atomistic Simulations of the Structure and Dynamics of Transcription Factor-DNA Recognition. Journal of Physical Chemistry B, 2019, 123, 3576-3590.	2.6	21
5	Role of Ligand-Driven Conformational Changes in Enzyme Catalysis: Modeling the Reactivity of the Catalytic Cage of Triosephosphate Isomerase. Journal of the American Chemical Society, 2018, 140, 3854-3857.	13.7	27
6	Computer simulations of the catalytic mechanism of wild-type and mutant Î²-phosphoglucomutase. Organic and Biomolecular Chemistry, 2018, 16, 2060-2073.	2.8	11
7	Amyloid-Î² Peptide Interactions with Amphiphilic Surfactants: Electrostatic and Hydrophobic Effects. ACS Chemical Neuroscience, 2018, 9, 1680-1692.	3.5	51
8	Pathways of Amyloid-Î² Aggregation Depend on Oligomer Shape. Journal of the American Chemical Society, 2018, 140, 319-327.	13.7	120
9	Loop Motion in Triosephosphate Isomerase Is Not a Simple Open and Shut Case. Journal of the American Chemical Society, 2018, 140, 15889-15903.	13.7	63
10	AÎ² under stress: the effects of acidosis, Cu²⁺-binding, and oxidation on amyloid Î²-peptide dimers. Chemical Communications, 2018, 54, 7766-7769.	4.1	41
11	Conformational Transitions of the Amyloidâ€Î² Peptide Upon Copper(II) Binding and pH Changes. Israel Journal of Chemistry, 2017, 57, 771-784.	2.3	20
12	Extending the Nonbonded Cationic Dummy Model to Account for Ion-Induced Dipole Interactions. Journal of Physical Chemistry Letters, 2017, 8, 5408-5414.	4.6	33
13	Enzyme Architecture: Modeling the Operation of a Hydrophobic Clamp in Catalysis by Triosephosphate Isomerase. Journal of the American Chemical Society, 2017, 139, 10514-10525.	13.7	38
14	Characterization of Mn(II) ion binding to the amyloid-Î² peptide in Alzheimerâ¿¿s disease. Journal of Trace Elements in Medicine and Biology, 2016, 38, 183-193.	3.0	60
15	Development and Application of a Nonbonded Cu²⁺ Model That Includes the Jahnâ€“Teller Effect. Journal of Physical Chemistry Letters, 2015, 6, 2657-2662.	4.6	64
16	Molecular modeling, dynamics, and an insight into the structural inhibition of cofactor independent phosphoglycerate mutase isoform 1 fromWuchereria bancroftiusing cheminformatics and mutational studies. Journal of Biomolecular Structure and Dynamics, 2013, 31, 765-778.	3.5	12
17	Identification of ligand binding site on RXRÎ³ using molecular docking and dynamics methods. Journal of Molecular Modeling, 2011, 17, 1259-1265.	1.8	3
18	Docking and molecular dynamics study on the inhibitory activity of N, N-disubstituted-trifluoro-3-amino-2-propanols-based inhibitors of cholesteryl ester transfer protein. Journal of Molecular Modeling, 2011, 17, 1727-1734.	1.8	12

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19	Docking and Molecular Dynamics Study on the Inhibitory Activity of Novel Inhibitors on Epidermal Growth Factor Receptor (EGFR). Medicinal Chemistry, 2011, 7, 24-31.	1.5	71
20	3D-QSAR study of corticotropin-releasing factor 1 antagonists and pharmacophore-based drug design. Neurochemistry International, 2010, 56, 107-117.	3.8	10