Ji-Long Zhang

List of Publications by Year in descending order

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#	Article	IF	CITATIONS
1	Molecular Dynamics Simulations Suggest Ligand's Binding to Nicotinamidase/Pyrazinamidase. PLoS ONE, 2012, 7, e39546.	2.5	28
2	Unbinding of glucose from human pulmonary surfactant protein D studied by steered molecular dynamics simulations. Chemical Physics Letters, 2010, 484, 338-343.	2.6	27
3	Structural features and dynamic investigations of the membrane-bound cytochrome P450 17A1. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 2013-2021.	2.6	20
4	MD Simulation Investigation on the Binding Process of Smoke-Derived Germination Stimulants to Its Receptor. Journal of Chemical Information and Modeling, 2019, 59, 1554-1562.	5.4	17
5	Insight into the Dynamic Interaction of Different Carbohydrates with Human Surfactant Protein D: Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2010, 114, 7383-7390.	2.6	12
6	How Does (E)-2-(Acetamidomethylene)succinate Bind to Its Hydrolase? From the Binding Process to the Final Result. PLoS ONE, 2013, 8, e53811.	2.5	12
7	Exploring the interaction between human focal adhesion kinase and inhibitors: a molecular dynamic simulation and free energy calculations. Journal of Biomolecular Structure and Dynamics, 2016, 34, 2351-2366.	3.5	11
8	Drug Design Benefits from Molecular Dynamics: Some Examples. Current Computer-Aided Drug Design, 2013, 9, 532-546.	1.2	11
9	Insights into the epimerization activities of RaCE and pAGE: the quantum mechanics/molecular mechanics simulations. RSC Advances, 2015, 5, 102284-102293.	3.6	10
10	Theoretical improvement of the specific inhibitor of human carbonic anhydrase VII. Computational Biology and Chemistry, 2011, 35, 50-56.	2.3	9
11	Interaction Mechanism of the Germination Stimulants Karrikins and Their Receptor ShKAI2iB. Journal of Physical Chemistry B, 2020, 124, 9812-9819.	2.6	8
12	Mutation and low pH effect on the stability as well as unfolding kinetics of transthyretin dimer. Biophysical Chemistry, 2014, 189, 8-15.	2.8	7
13	Molecular Dynamics Simulation Investigation of the Binding and Interaction of the EphA6–Odin Protein Complex. Journal of Physical Chemistry B, 2022, 126, 4914-4924.	2.6	7
14	How mutations affecting the ligand-receptor interactions: a combined MD and QM/MM calculation on CYP2E1 and its two mutants. Chemical Research in Chinese Universities, 2015, 31, 1029-1038.	2.6	6
15	Molecular dynamics investigation on the interaction of human angiotensin-converting enzyme with tetrapeptide inhibitors. Physical Chemistry Chemical Physics, 2021, 23, 6685-6694.	2.8	6
16	Molecular dynamics (MD) simulations and binding free energy calculation studies between inhibitors and type II dehydroquinase (DHQ2). Molecular Simulation, 2013, 39, 137-144.	2.0	5
17	Effect of External Electric Field on Substrate Transport of a Secondary Active Transporter. Journal of Chemical Information and Modeling, 2016, 56, 1539-1546.	5.4	5
18	<i>In Silico</i> Investigation on KAR Signaling Reveals the Significant Dynamic Change of Its Receptor's Structure. Journal of Chemical Information and Modeling, 2022, 62, 1933-1941.	5.4	4

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19	Theoretical investigation on binding process of allophanate to allophanate hydrolase. Chemical Research in Chinese Universities, 2015, 31, 1023-1028.	2.6	2
20	Theoretical evaluation and improvement on the potency of the rhodanine-based inhibitors for human serotoninN-acetyltransferase. Molecular Simulation, 2014, 40, 1201-1208.	2.0	1
21	Molecular simulation investigation on the interaction between barrier-to-autointegration factor dimer or its Gly25Clu mutant and LEM domain of emerin. Computational Biology and Chemistry, 2014, 53, 184-190.	2.3	1
22	Dearomatization of Benzenoid Arenes Triggered by Triplet Excited State Intramolecular Proton Transfer. Journal of Physical Chemistry A, 2022, 126, 4424-4431.	2.5	1
23	Lacking of ESIPT Band of Aromatic ortho-Aminoaldehyde Derivatives Triggered by the N-H Vibration. Physical Chemistry Chemical Physics, 2022, , .	2.8	0