Xiao Zhu

List of Publications by Year
in descending order

54 papers	5,049 citations	393982 19 h-index	243296 44 g-index
55 all docs	55 docs citations	55 times ranked	8477 citing authors

#	Article	IF	Citations
1	Optimization of the Additive CHARMM All-Atom Protein Force Field Targeting Improved Sampling of the Backbone Ï•, Ï^ and Side-Chain Ï‡₁ and Ï‡₂ Dihedral Angles. Journal of Chemical Theory and Computation, 2012, 8, 3257-3273.	2.3	3,696
2	A Small-Molecule Inhibitor of BCL6 Kills DLBCL Cells In Vitro and In Vivo. Cancer Cell, 2010, 17, 400-411.	7.7	263
3	The biosynthesis of methanobactin. Science, 2018, 359, 1411-1416.	6.0	101
4	Fast and accurate computation schemes for evaluating vibrational entropy of proteins. Journal of Computational Chemistry, 2011, 32, 3188-3193.	1.5	79
5	Temperature-Activated Nucleic Acid Nanostructures. Journal of the American Chemical Society, 2013, 135, 14102-14105.	6.6	68
6	A molecular dynamics simulation study on the conformational stability of amylose-linoleic acid complex in water. Carbohydrate Polymers, 2018, 196, 56-65.	5.1	67
7	Characterization of Interactions between Curcumin and Different Types of Lipid Bilayers by Molecular Dynamics Simulation. Journal of Physical Chemistry B, 2018, 122, 2341-2354.	1.2	45
8	Emulsion-based delivery systems for curcumin: Encapsulation and interaction mechanism between debranched starch and curcumin. International Journal of Biological Macromolecules, 2020, 161, 746-754.	3.6	45
9	Potential of mean force for insertion of antimicrobial peptide melittin into a pore in mixed DOPC/DOPG lipid bilayer by molecular dynamics simulation. Journal of Chemical Physics, 2017, 146, 155101.	1.2	43
10	Complexation process of amylose under different concentrations of linoleic acid using molecular dynamics simulation. Carbohydrate Polymers, 2019, 216, 157-166.	5.1	35
11	An Implicit Solvent Model for SCC-DFTB with Charge-Dependent Radii. Journal of Chemical Theory and Computation, 2010, 6, 2303-2314.	2.3	34
12	Establishing Effective Simulation Protocols for Î²- and Î±/Î²-Mixed Peptides. I. QM and QM/MM Models. Journal of Chemical Theory and Computation, 2007, 3, 1538-1549.	2.3	33
13	Sequence-Dependent Interaction of Î²-Peptides with Membranes. Journal of Physical Chemistry B, 2010, 114, 13585-13592.	1.2	31
14	A Modified QM/MM Hamiltonian with the Self-Consistent-Charge Density-Functional-Tight-Binding Theory for Highly Charged QM Regions. Journal of Chemical Theory and Computation, 2012, 8, 4293-4304.	2.3	30
15	Selective 5-hydroxymethylfurfural production from cellulose formate in DMSO-H2O media. Applied Catalysis B: Environmental, 2021, 285, 119799.	10.8	30
16	Molecular Dynamics Study of Pore Formation by Melittin in a 1,2-Dioleoyl-sn-glycero-3-phosphocholine and 1,2-Di(9Z-octadecenoyl)-sn-glycero-3-phospho-(1â€²-rac-glycerol) Mixed Lipid Bilayer. Industrial & Engineering Chemistry Research, 2015, 54, 10275-10283.	1.8	29
17	Establishing Effective Simulation Protocols for Î²- and Î±/Î²-Peptides. II. Molecular Mechanical (MM) Model for a Cyclic Î²-Residue. Journal of Physical Chemistry B, 2008, 112, 5439-5448.	1.2	27
18	Investigation of the interaction of amyloid Î² peptide (11â€“42) oligomers with a 1-palmitoyl-2-oleoyl-sn-glycero-3-phosphocholine (POPC) membrane using molecular dynamics simulation. Physical Chemistry Chemical Physics, 2018, 20, 6817-6829.	1.3	27

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19	Atomistic Simulations of Dilute Polyelectrolyte Solutions. Journal of Physical Chemistry B, 2012, 116, 4319-4327.	1.2	25
20	Effect of physicochemical properties of peptides from soy protein on their antimicrobial activity. Peptides, 2017, 94, 10-18.	1.2	21
21	Dichlorophenylacrylonitriles as AhR Ligands That Display Selective Breast Cancer Cytotoxicity in vitro. ChemMedChem, 2018, 13, 1447-1458.	1.6	20
22	Local DNA dynamics shape mutational patterns of mononucleotide repeats in human genomes. Nucleic Acids Research, 2015, 43, 5065-5080.	6.5	18
23	Establishing effective simulation protocols for Î²â€•and Î±/Î²â€peptides. III. Molecular mechanical model for acyclic Î²â€amino acids. Journal of Computational Chemistry, 2010, 31, 2063-2077.	1.5	17
24	Molecular Dynamics Study of the Role of the Spine of Hydration in DNA A-Tracts in Determining Nucleosome Occupancy. Journal of Physical Chemistry B, 2012, 116, 13672-13681.	1.2	17
25	Rheological properties, thermal stability and conformational changes of collagen from sea cucumber (Apostichopus japonicas). Food Chemistry, 2022, 389, 133033.	4.2	17
26	Discovery of Non-Nucleotide Small-Molecule STING Agonists via Chemotype Hybridization. Journal of Medicinal Chemistry, 2022, 65, 3518-3538.	2.9	16
27	Molecular modeling tools to characterize the structure and complexation behavior of carbohydrates. Current Opinion in Food Science, 2016, 9, 62-69.	4.1	15
28	Molecular Dynamics Simulations and Experimental Verification to Determine Mechanism of Cosolvents on Increased 5-Hydroxymethylfurfural Yield from Glucose. ACS Sustainable Chemistry and Engineering, 2019, 7, 12997-13003.	3.2	15
29	Quantitative Assessment of the Conformational Heterogeneity in Amylose across Force Fields. Journal of Chemical Theory and Computation, 2019, 15, 6203-6212.	2.3	15
30	Discovery and Preclinical Evaluation of BMS-986242, a Potent, Selective Inhibitor of Indoleamine-2,3-dioxygenase 1. ACS Medicinal Chemistry Letters, 2021, 12, 288-294.	1.3	15
31	Modeling DNA-Bending in the Nucleosome: Role of AA Periodicity. Journal of Physical Chemistry B, 2011, 115, 8638-8644.	1.2	14
32	Enhanced solubility and antimicrobial activity of alamethicin in aqueous solution by complexation with Î³-cyclodextrin. Journal of Functional Foods, 2018, 40, 700-706.	1.6	14
33	Understanding the antimicrobial activity of water soluble Î³-cyclodextrin/alamethicin complex. Colloids and Surfaces B: Biointerfaces, 2018, 172, 451-458.	2.5	14
34	Effect of egg yolk lipids on structure and properties of wheat starch in steamed bread. Journal of Cereal Science, 2019, 86, 77-85.	1.8	14
35	Conformer-Specific and Diastereomer-Specific Spectroscopy of Î±Î²Î± Synthetic Foldamers: Acâ€“Alaâ€Î²_{ACHC}â€“Alaâ€“NHBn. Journal of Physical Chemistry A, 2018, 122, 3697-3710.	1.1	13
36	Self-Assembly of Î²-Peptides: Insight from the Pair and Many-Body Free Energy of Association. Journal of Physical Chemistry C, 2010, 114, 13551-13556.	1.5	11

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37	Modelling and Phenotypic Screening of NAPâ€6 and 10â€Clâ€BBQ, AhR Ligands Displaying Selective Breast Cancer Cytotoxicity in Vitro. ChemMedChem, 2021, 16, 1499-1512.	1.6	11
38	Discovery of Imidazopyridines as Potent Inhibitors of Indoleamine 2,3-Dioxygenase 1 for Cancer Immunotherapy. ACS Medicinal Chemistry Letters, 2021, 12, 494-501.	1.3	10
39	Toward molecular models of proton pumping: Challenges, methods and relevant applications. Science China Chemistry, 2012, 55, 3-18.	4.2	8
40	The antioxidant and tyrosinase inhibition properties of essential oil from the peel of Chinese Torreya grandis Fort.. RSC Advances, 2019, 9, 42360-42366.	1.7	7
41	Scholar: A Campus HPC Resource to Enable Computational Literacy. , 2016, , .		6
42	Community Clusters or the Cloud. , 2019, , .		5
43	Sequence-Dependent pK_aShift Induced by Molecular Self-Assembly: Insights from Computer Simulation. Journal of Physical Chemistry B, 2012, 116, 491-495.	1.2	4
44	Binding of Chlorinated Phenylacrylonitriles to the Aryl Hydrocarbon Receptor: Computational Docking and Molecular Dynamics Simulations. , 0, , .		4
45	Anvil - System Architecture and Experiences from Deployment and Early User Operations. , 2022, , .		4
46	PULSAR. , 2019, , .		3
47	Conformational-Analysis-Guided Discovery of 2,3-Disubstituted Pyridine IDO1 Inhibitors. ACS Medicinal Chemistry Letters, 2021, 12, 1143-1150.	1.3	3
48	Performance examinations of multiple time-stepping algorithms on stampede supercomputer. , 2015, , .		2
49	Mentoring Undergraduates into Cyber-Facilitator Roles. , 2018, , .		2
50	Preparation and evaluation of mushroom (Lentinus edodes) and mealworm (Tenebrio molitor) as dog food attractant. Heliyon, 2020, 6, e05302.	1.4	2
51	Complexation of 26-Mer Amylose with Egg Yolk Lipids with Different Numbers of Tails Using a Molecular Dynamics Simulation. Foods, 2021, 10, 2355.	1.9	2
52	Research Computing Desktops. , 2019, , .		1
53	Electrostatic screening effects on a model system for molecular electronics. , 2012, , .		0
54	Introducing Novices to Scientific Parallel Computing. Journal of Computational Science Education, 2020, 11, 88-92.	0.3	0