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	Discovery of Non-Nucleotide Small-Molecule STING Agonists via Chemotype Hybridization. Journal of Medicinal Chemistry, 2022, 65, 3518-3538.	2.9	16
2	Rheological properties, thermal stability and conformational changes of collagen from sea cucumber (Apostichopus japonicas). Food Chemistry, 2022, 389, 133033.	4.2	17
3	Anvil - System Architecture and Experiences from Deployment and Early User Operations. , 2022, , .		4
4	Selective 5-hydroxymethylfurfural production from cellulose formate in DMSO-H2O media. Applied Catalysis B: Environmental, 2021, 285, 119799.	10.8	30
5	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
6	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
7	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
8	Conformational-Analysis-Guided Discovery of 2,3-Disubstituted Pyridine IDO1 Inhibitors. ACS Medicinal Chemistry Letters, 2021, 12, 1143-1150.	1.3	3
9	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
10	Preparation and evaluation of mushroom (Lentinus edodes) and mealworm (Tenebrio molitor) as dog food attractant. Heliyon, 2020, 6, e05302.	1.4	2
11	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
12	Introducing Novices to Scientific Parallel Computing. Journal of Computational Science Education, 2020, 11, 88-92.	0.3	0
13	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
14	PULSAR. , 2019, , .		3
15	Community Clusters or the Cloud. , 2019, , .		5
16	Research Computing Desktops. , 2019, , .		1
17	Quantitative Assessment of the Conformational Heterogeneity in Amylose across Force Fields. Journal of Chemical Theory and Computation, 2019, 15, 6203-6212.	2.3	15
18	Complexation process of amylose under different concentrations of linoleic acid using molecular dynamics simulation. Carbohydrate Polymers, 2019, 216, 157-166.	5.1	35

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19	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
20	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
21	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
22	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
23	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
24	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
25	The biosynthesis of methanobactin. Science, 2018, 359, 1411-1416.	6.0	101
26	Understanding the antimicrobial activity of water soluble Î³-cyclodextrin/alamethicin complex. Colloids and Surfaces B: Biointerfaces, 2018, 172, 451-458.	2.5	14
27	Dichlorophenylacrylonitriles as AhR Ligands That Display Selective Breast Cancer Cytotoxicity in vitro. ChemMedChem, 2018, 13, 1447-1458.	1.6	20
28	Mentoring Undergraduates into Cyber-Facilitator Roles. , 2018, , .		2
29	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
30	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
31	Effect of physicochemical properties of peptides from soy protein on their antimicrobial activity. Peptides, 2017, 94, 10-18.	1.2	21
32	Scholar: A Campus HPC Resource to Enable Computational Literacy. , 2016, , .		6
33	Molecular modeling tools to characterize the structure and complexation behavior of carbohydrates. Current Opinion in Food Science, 2016, 9, 62-69.	4.1	15
34	Performance examinations of multiple time-stepping algorithms on stampede supercomputer. , 2015, , .		2
35	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
36	Local DNA dynamics shape mutational patterns of mononucleotide repeats in human genomes. Nucleic Acids Research, 2015, 43, 5065-5080.	6.5	18

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37	Temperature-Activated Nucleic Acid Nanostructures. Journal of the American Chemical Society, 2013, 135, 14102-14105.	6.6	68
38	Electrostatic screening effects on a model system for molecular electronics. , 2012, , .		0
39	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
40	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
41	Atomistic Simulations of Dilute Polyelectrolyte Solutions. Journal of Physical Chemistry B, 2012, 116, 4319-4327.	1.2	25
42	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
43	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
44	Toward molecular models of proton pumping: Challenges, methods and relevant applications. Science China Chemistry, 2012, 55, 3-18.	4.2	8
45	Modeling DNA-Bending in the Nucleosome: Role of AA Periodicity. Journal of Physical Chemistry B, 2011, 115, 8638-8644.	1.2	14
46	Fast and accurate computation schemes for evaluating vibrational entropy of proteins. Journal of Computational Chemistry, 2011, 32, 3188-3193.	1.5	79
47	A Small-Molecule Inhibitor of BCL6 Kills DLBCL Cells In Vitro and In Vivo. Cancer Cell, 2010, 17, 400-411.	7.7	263
48	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
49	An Implicit Solvent Model for SCC-DFTB with Charge-Dependent Radii. Journal of Chemical Theory and Computation, 2010, 6, 2303-2314.	2.3	34
50	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
51	Sequence-Dependent Interaction of Î²-Peptides with Membranes. Journal of Physical Chemistry B, 2010, 114, 13585-13592.	1.2	31
52	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
53	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
54	Binding of Chlorinated Phenylacrylonitriles to the Aryl Hydrocarbon Receptor: Computational Docking and Molecular Dynamics Simulations. , 0, , .		4