

Jingjing Guo

List of Publications by Year in descending order

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51
papers

1,443
citations

394421

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345221

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52
docs citations

52
times ranked

2102
citing authors

#	ARTICLE	IF	CITATIONS
1	Molecular Mechanism of Ca ²⁺ in the Allosteric Regulation of Human Parathyroid Hormone Receptor-1. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 5110-5119.	5.4	14
2	Insights into the negative regulation of EGFR upon the binding of an allosteric inhibitor. <i>Chemical Biology and Drug Design</i> , 2022, 99, 650-661.	3.2	3
3	Critical Extracellular Ca ²⁺ Dependence of the Binding between PTH1R and a G-Protein Peptide Revealed by MD Simulations. <i>ACS Chemical Neuroscience</i> , 2022, 13, 1666-1674.	3.5	7
4	Uncovering the Molecular Basis for the Better Gefitinib Sensitivity of EGFR with Complex Mutations over Single Rare Mutation: Insights from Molecular Simulations. <i>Molecules</i> , 2022, 27, 3844.	3.8	4
5	Investigating the Permeation Mechanism of Typical Phthalic Acid Esters (PAEs) and Membrane Response Using Molecular Dynamics Simulations. <i>Membranes</i> , 2022, 12, 596.	3.0	1
6	Deciphering the T790M/L858R-Selective Inhibition Mechanism of an Allosteric Inhibitor of EGFR: Insights from Molecular Simulations. <i>ACS Chemical Neuroscience</i> , 2021, 12, 462-472.	3.5	7
7	Conformational dynamics is critical for the allosteric inhibition of cGAS upon acetyl-mimic mutations. <i>Physical Chemistry Chemical Physics</i> , 2021, 23, 2154-2165.	2.8	4
8	Potential of esterase Dmth in transforming plastic additive dimethyl terephthalate to less toxic mono-methyl terephthalate. <i>Ecotoxicology and Environmental Safety</i> , 2020, 187, 109848.	6.0	41
9	Study on the stereoselective binding of cytosine nucleoside enantiomers to human serum albumin. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2020, 224, 117452.	3.9	7
10	Bacterial lipopolysaccharide core structures mediate effects of butanol ingress. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183150.	2.6	9
11	Pyruvate kinase from <i>Plasmodium falciparum</i> : Structural and kinetic insights into the allosteric mechanism. <i>Biochemical and Biophysical Research Communications</i> , 2020, 532, 370-376.	2.1	7
12	A Safe Polyzwitterionic Hydrogel Electrolyte for Long-Life Quasi-Solid State Zinc Metal Batteries. <i>Advanced Functional Materials</i> , 2020, 30, 2001317.	14.9	188
13	Pyruvate Kinase Regulates the Pentose-Phosphate Pathway in Response to Hypoxia in <i>Mycobacterium tuberculosis</i> . <i>Journal of Molecular Biology</i> , 2019, 431, 3690-3705.	4.2	6
14	A Short Peptide Hydrogel with High Stiffness Induced by 3 × 10 ⁶ Helices to β-Sheet Transition in Water. <i>Advanced Science</i> , 2019, 6, 1901173.	11.2	36
15	Probing the Binding of Bicyclol and Human Serum Albumin by Multispectral Technologies and Molecular Docking Method. <i>Journal of Solution Chemistry</i> , 2019, 48, 1519-1534.	1.2	1
16	Artificial K ⁺ Channels Formed by Pillararene-β-Cyclodextrin Hybrid Molecules: Tuning Cation Selectivity and Generating Membrane Potential. <i>Angewandte Chemie</i> , 2019, 131, 2805-2810.	2.0	19
17	Response of microbial membranes to butanol: interdigitation vs. disorder. <i>Physical Chemistry Chemical Physics</i> , 2019, 21, 11903-11915.	2.8	19
18	Distinct Dynamic and Conformational Features of Human STING in Response to 2,3-dGAMP and c-di-GMP. <i>ChemBioChem</i> , 2019, 20, 1838-1847.	2.6	10

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19	A novel highly selective near-infrared and naked-eye fluorescence probe for imaging peroxynitrite. <i>Analytical Methods</i> , 2019, 11, 1522-1529.	2.7	17
20	How graphene affects the misfolding of human prion protein: A combined experimental and molecular dynamics simulation study. <i>Environmental Research</i> , 2019, 171, 1-10.	7.5	7
21	The molecular mechanism of pH-regulating C3d-CR2 interactions: Insights from molecular dynamics simulation. <i>Chemical Biology and Drug Design</i> , 2019, 93, 628-637.	3.2	0
22	Artificial K ⁺ Channels Formed by Pillararene-Cyclodextrin Hybrid Molecules: Tuning Cation Selectivity and Generating Membrane Potential. <i>Angewandte Chemie - International Edition</i> , 2019, 58, 2779-2784.	13.8	58
23	The molecular mechanism of two coreceptor binding site antibodies X5 and 17b neutralizing HIV-1: Insights from molecular dynamics simulation. <i>Chemical Biology and Drug Design</i> , 2018, 92, 1357-1365.	3.2	2
24	Hinge-Shift Mechanism Modulates Allosteric Regulations in Human Pin1. <i>Journal of Physical Chemistry B</i> , 2018, 122, 5623-5629.	2.6	30
25	Divergent Total Syntheses of (âˆ“)â€Daphnilongeraninâ€B and (âˆ“)â€Daphenylline. <i>Angewandte Chemie - International Edition</i> , 2018, 57, 947-951.	13.8	84
26	Divergent Total Syntheses of (âˆ“)â€Daphnilongeraninâ€B and (âˆ“)â€Daphenylline. <i>Angewandte Chemie</i> , 2018, 130, 959-963.	2.0	16
27	One-pot formation of hydrazide macrocycles with modified cavities: an example of pH-sensitive unimolecular cation channels. <i>Chemical Communications</i> , 2017, 53, 5322-5325.	4.1	8
28	Kinetic Insights into Zn ²⁺ -Induced Amyloid Î²-Protein Aggregation Revealed by Stopped-Flow Fluorescence Spectroscopy. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3909-3917.	2.6	20
29	A unimolecular channel formed by dual helical peptide modified pillar[5]arene: correlating transmembrane transport properties with antimicrobial activity and haemolytic toxicity. <i>Chemical Communications</i> , 2017, 53, 11492-11495.	4.1	20
30	Brazilin inhibits the Zn ²⁺ -mediated aggregation of amyloid Î²-protein and alleviates cytotoxicity. <i>Journal of Inorganic Biochemistry</i> , 2017, 177, 183-189.	3.5	26
31	Brazilin inhibits fibrillogenesis of human islet amyloid polypeptide, disassembles mature fibrils, and alleviates cytotoxicity. <i>RSC Advances</i> , 2017, 7, 43491-43501.	3.6	33
32	The solvent at antigen-binding site regulated C3d-CR2 interactions through the C-terminal tail of C3d at different ion strengths: insights from molecular dynamics simulation. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2016, 1860, 2220-2231.	2.4	5
33	Protein Allostery and Conformational Dynamics. <i>Chemical Reviews</i> , 2016, 116, 6503-6515.	47.7	306
34	Allosteric activation of SENP1 by SUMO1 Î²-grasp domain involves a dock-and-coalesce mechanism. <i>ELife</i> , 2016, 5, .	6.0	15
35	Two Pathways Mediate Interdomain Allosteric Regulation in Pin1. <i>Structure</i> , 2015, 23, 237-247.	3.3	70
36	Dynamically Driven Protein Allostery Exhibits Disparate Responses for Fast and Slow Motions. <i>Biophysical Journal</i> , 2015, 108, 2771-2774.	0.5	25

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37	Two Pathways Mediate Inter-Domain Allosteric Regulation in Pin1. <i>Biophysical Journal</i> , 2015, 108, 528a.	0.5	1
38	Structural Diversity and Initial Oligomerization of PrP106â€“126 Studied by Replica-Exchange and Conventional Molecular Dynamics Simulations. <i>PLoS ONE</i> , 2014, 9, e87266.	2.5	13
39	Exploring the Influence of EGCG on the β -Sheet-Rich Oligomers of Human Islet Amyloid Polypeptide (hIAPP1â€“37) and Identifying Its Possible Binding Sites from Molecular Dynamics Simulation. <i>PLoS ONE</i> , 2014, 9, e94796.	2.5	40
40	Stabilities and structures of islet amyloid polypeptide (IAPP22â€“28) oligomers: From dimer to 16-mer. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2014, 1840, 357-366.	2.4	24
41	The role of Cys179â€“Cys214 disulfide bond in the stability and folding of prion protein: insights from molecular dynamics simulations. <i>Journal of Molecular Modeling</i> , 2014, 20, 2106.	1.8	19
42	The adsorption mechanism and induced conformational changes of three typical proteins with different secondary structural features on graphene. <i>RSC Advances</i> , 2014, 4, 9953.	3.6	54
43	Exploring the Influence of Carbon Nanoparticles on the Formation of β -Sheet-Rich Oligomers of IAPP22â€“28 Peptide by Molecular Dynamics Simulation. <i>PLoS ONE</i> , 2013, 8, e65579.	2.5	48
44	Exploring structural and thermodynamic stabilities of human prion protein pathogenic mutants D202N, E211Q and Q217R. <i>Journal of Structural Biology</i> , 2012, 178, 225-232.	2.8	24
45	Influence of the pathogenic mutations T188K/R/A on the structural stability and misfolding of human prion protein: Insight from molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - General Subjects</i> , 2012, 1820, 116-123.	2.4	32
46	Molecular mechanism of the enhanced virulence of 2009 pandemic Influenza A (H1N1) virus from D222G mutation in the hemagglutinin: a molecular modeling study. <i>Journal of Molecular Modeling</i> , 2012, 18, 4355-4366.	1.8	16
47	The molecular basis of IGF-II/IGF2R recognition: a combined molecular dynamics simulation, free-energy calculation and computational alanine scanning study. <i>Journal of Molecular Modeling</i> , 2012, 18, 1421-1430.	1.8	21
48	The Evolution of HLAâ€“B*3501 Binding Affinity to Variable Immunodominant NP_{418â€“426} Peptides from 1918 to 2009 Pandemic Influenza A Virus: A Molecular Dynamics Simulation and Free Energy Calculation Study. <i>Chemical Biology and Drug Design</i> , 2012, 79, 1025-1032.	3.2	1
49	Investigation on a hostâ€“guest inclusion system by β -cyclodextrin derivative and its analytical application. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2011, 21, 1113-1117.	2.2	8
50	Fluorimetric investigation of supramolecular system by modified β -cyclodextrin and its analytical application. <i>Spectrochimica Acta - Part A: Molecular and Biomolecular Spectroscopy</i> , 2011, 78, 1553-1559.	3.9	11
51	Fabrication of a fiberglass-packed channel in a microchip for flow injection analysis. <i>Mikrochimica Acta</i> , 2007, 159, 191-199.	5.0	6