

Jin Liu

List of Publications by Year in descending order

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44
papers

1,396
citations

331670

21
h-index

345221

36
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46
all docs

46
docs citations

46
times ranked

2010
citing authors

#	ARTICLE	IF	CITATIONS
1	Allostery: An Overview of Its History, Concepts, Methods, and Applications. <i>PLoS Computational Biology</i> , 2016, 12, e1004966.	3.2	194
2	Dynamic binding mode of a Synaptotagmin-1â€“SNARE complex in solution. <i>Nature Structural and Molecular Biology</i> , 2015, 22, 555-564.	8.2	129
3	Principles of Allosteric Interactions in Cell Signaling. <i>Journal of the American Chemical Society</i> , 2014, 136, 17692-17701.	13.7	127
4	Cas9-catalyzed DNA Cleavage Generates Staggered Ends: Evidence from Molecular Dynamics Simulations. <i>Scientific Reports</i> , 2016, 6, 37584.	3.3	105
5	A Comparison of Acetyl- and Methoxycarbonylnitrenes by Computational Methods and a Laser Flash Photolysis Study of Benzoylnitrene. <i>Journal of Organic Chemistry</i> , 2004, 69, 8583-8593.	3.2	84
6	Surface complexes of phthalic acid at the hematite/water interface. <i>Journal of Colloid and Interface Science</i> , 2007, 307, 124-134.	9.4	63
7	The Mechanism of Ubiquitination in the Cullin-RING E3 Ligase Machinery: Conformational Control of Substrate Orientation. <i>PLoS Computational Biology</i> , 2009, 5, e1000527.	3.2	52
8	Flexible Cullins in Cullin-RING E3 Ligases Allosterically Regulate Ubiquitination. <i>Journal of Biological Chemistry</i> , 2011, 286, 40934-40942.	3.4	47
9	Structure and Dynamics of Cas9 HNH Domain Catalytic State. <i>Scientific Reports</i> , 2017, 7, 17271.	3.3	45
10	Energetic redistribution in allostery to execute protein function. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, 7480-7482.	7.1	41
11	The Reaction of Triplet Nitrenes with Oxygen:â€“ A Computational Study. <i>Organic Letters</i> , 2005, 7, 549-552.	4.6	38
12	Molecular Dynamics Reveal the Essential Role of Linker Motions in the Function of Cullinâ€“RING E3 Ligases. <i>Journal of Molecular Biology</i> , 2010, 396, 1508-1523.	4.2	36
13	Rigid Residue Scan Simulations Systematically Reveal Residue Entropic Roles in Protein Allostery. <i>PLoS Computational Biology</i> , 2016, 12, e1004893.	3.2	32
14	2D SMARTCyp Reactivity-Based Site of Metabolism Prediction for Major Drug-Metabolizing Cytochrome P450 Enzymes. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1698-1712.	5.4	30
15	The role of allostery in the ubiquitinâ€“proteasome system. <i>Critical Reviews in Biochemistry and Molecular Biology</i> , 2013, 48, 89-97.	5.2	28
16	Rbx1 Flexible Linker Facilitates Cullin-RING Ligase Function Before Neddylolation and After Deneddylolation. <i>Biophysical Journal</i> , 2010, 99, 736-744.	0.5	27
17	Identifying Cytochrome P450 Functional Networks and Their Allosteric Regulatory Elements. <i>PLoS ONE</i> , 2013, 8, e81980.	2.5	27
18	Identifying Key Residues for Protein Allostery through Rigid Residue Scan. <i>Journal of Physical Chemistry A</i> , 2015, 119, 1689-1700.	2.5	27

#	ARTICLE	IF	CITATIONS
19	Structural and functional insights into the bona fide catalytic state of <i>Streptococcus pyogenes</i> Cas9 HNH nuclease domain. <i>ELife</i> , 2019, 8, .	6.0	25
20	Identification of a unique Ca ²⁺ -binding site in rat acid-sensing ion channel 3. <i>Nature Communications</i> , 2018, 9, 2082.	12.8	24
21	Allosteric regulation of CRISPR-Cas9 for DNA-targeting and cleavage. <i>Current Opinion in Structural Biology</i> , 2020, 62, 166-174.	5.7	24
22	Analogues of Arylamide Phenylpiperazine Ligands To Investigate the Factors Influencing D3 Dopamine Receptor Bitropic Binding and Receptor Subtype Selectivity. <i>ACS Chemical Neuroscience</i> , 2018, 9, 2972-2983.	3.5	23
23	A positive, growth-based PAM screen identifies noncanonical motifs recognized by the <i>S. pyogenes</i> Cas9. <i>Science Advances</i> , 2020, 6, eabb4054.	10.3	21
24	Study of Singlet and Triplet 2,6-Difluorophenyl nitrene by Time-Resolved Infrared Spectroscopy. <i>Journal of Physical Chemistry A</i> , 2005, 109, 2816-2821.	2.5	17
25	Stress and interferon signalling-mediated apoptosis contributes to pleiotropic anticancer responses induced by targeting NGLY1. <i>British Journal of Cancer</i> , 2018, 119, 1538-1551.	6.4	17
26	Design, synthesis, and evaluation of N-(4-(4-phenyl piperazin-1-yl)butyl)-4-(thiophen-3-yl)benzamides as selective dopamine D3 receptor ligands. <i>Bioorganic and Medicinal Chemistry Letters</i> , 2019, 29, 2690-2694.	2.2	17
27	Probing Protein Allostery as a Residue-Specific Concept via Residue Response Maps. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 4691-4705.	5.4	17
28	“Similarity Trap” in Protein-Protein Interactions Could Be Carcinogenic: Simulations of p53 Core Domain Complexed with 53BP1 and BRCA1 BRCT Domains. <i>Structure</i> , 2006, 14, 1811-1821.	3.3	16
29	Quantitative Predictions of Binding Free Energy Changes in Drug-Resistant Influenza Neuraminidase. <i>PLoS Computational Biology</i> , 2012, 8, e1002665.	3.2	16
30	Coordinated Actions of Cas9 HNH and RuvC Nuclease Domains Are Regulated by the Bridge Helix and the Target DNA Sequence. <i>Biochemistry</i> , 2021, , .	2.5	11
31	Assessing the Performance of the Nonbonded Mg ²⁺ Models in a Two-Metal-Dependent Ribonuclease. <i>Journal of Chemical Information and Modeling</i> , 2019, 59, 399-408.	5.4	10
32	Rational Engineering of CRISPR-Cas9 Nuclease to Attenuate Position-Dependent Off-Target Effects. <i>CRISPR Journal</i> , 2022, 5, 329-340.	2.9	9
33	Cullin neddylation may allosterically tune polyubiquitin chain length and topology. <i>Biochemical Journal</i> , 2017, 474, 781-795.	3.7	8
34	Allosteric Modulation of Small Molecule Drugs on ACE2 Conformational Change upon Binding to SARS-CoV-2 Spike Protein. , 2021, , .		5
35	Factors Governing Selectivity of Dopamine Receptor Binding Compounds for D2R and D3R Subtypes. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 2829-2843.	5.4	2
36	Filtering out Low-Affinity Bitropic Ligands for Dopamine Receptors Based on Ligand Conformation. <i>ACS Chemical Neuroscience</i> , 2020, 11, 2523-2527.	3.5	1

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37	Novel Use of Hypoxia-Inducible Polymerizable Protein to Augment Chemotherapy for Pancreatic Cancer. <i>Pharmaceutics</i> , 2022, 14, 128.	4.5	1
38	Searching For the Hinge of E3 Ubiquitin Ligase Machinery with MD Simulations. <i>Biophysical Journal</i> , 2009, 96, 365a.	0.5	0
39	Conformational Control of Ubiquitination in the Cullin-Ring E3 Ligase Machinery. <i>Biophysical Journal</i> , 2010, 98, 26a-27a.	0.5	0
40	Molecular Dynamics Simulations Reveal Distinct Conformational Changes of Three Cullins in Cullin-Ring E3 Ubiquitin Ligases. <i>Biophysical Journal</i> , 2011, 100, 310a.	0.5	0
41	Does Cas9-Catalyzed DNA Cleavage Generate Blunt Ends or Staggered Ends? Insight from Molecular Dynamic Simulations. <i>Biophysical Journal</i> , 2017, 112, 48a.	0.5	0
42	Editorial overview: Allosteric assemblies. <i>Current Opinion in Structural Biology</i> , 2020, 62, vi-vii.	5.7	0
43	Tribute to Ruth Nussinov. <i>Journal of Physical Chemistry B</i> , 2021, 125, 6733-6734.	2.6	0
44	Sparse group selection and analysis of <sc>functionâ€related</sc> residue for <sc>proteinâ€state</sc> recognition. <i>Journal of Computational Chemistry</i> , 2022, 43, 1342-1354.	3.3	0