Jianing Li

List of Publications by Year in descending order

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Version: 2024-02-01

56	2,177	394421	243625
papers	citations	19 h-index	44 g-index

66	66	66	3700
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Outcome-Based Redesign of Physical Chemistry Laboratories During the COVID-19 Pandemic. Journal of Chemical Education, 2022, 99, 639-645.	2.3	1
2	Concerted Rolling and Penetration of Peptides during Membrane Binding. Journal of Chemical Theory and Computation, 2022, 18, 3921-3929.	5.3	0
3	GPCR Intracellular Loop Regulation of Beta-Arrestin-Mediated Endosomal Signaling Dynamics. Journal of Molecular Neuroscience, 2022, 72, 1358-1373.	2.3	4
4	Molecular basis for the adaptive evolution of environment-sensing by H-NS proteins. ELife, 2021, 10, .	6.0	9
5	AMPGAN v2: Machine Learning-Guided Design of Antimicrobial Peptides. Journal of Chemical Information and Modeling, 2021, 61, 2198-2207.	5.4	37
6	Molecular Basis of Class B GPCR Selectivity for the Neuropeptides PACAP and VIP. Frontiers in Molecular Biosciences, 2021, 8, 644644.	3.5	15
7	Iterative Exponential Growth of Oxygen-Linked Aromatic Polymers Driven by Nucleophilic Aromatic Substitution Reactions. Frontiers in Chemistry, 2021, 9, 620017.	3.6	1
8	Carbonyl-to-Alkyne Electron Donation Effects in up to 10-nm-Long, Unimolecular Oligo(p-phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf 5	2.0	0
9	Enhanced sampling protocol to elucidate fusion peptide opening of SARS-CoV-2 spike protein. Biophysical Journal, 2021, 120, 2848-2858.	0.5	7
10	A computational study of cooperative binding to multiple SARS-CoV-2 proteins. Scientific Reports, 2021, 11, 16307.	3.3	7
11	Molecular Basis for Environment Sensing by a Nucleoid-Structuring Bacterial Protein Filament. Journal of Physical Chemistry Letters, 2021, 12, 7878-7884.	4.6	4
12	Thermosetting supramolecular polymerization of compartmentalized DNA fibers with stereo sequence and length control. CheM, 2021, 7, 2395-2414.	11.7	16
13	Glutathione-S-transferase P promotes glycolysis in asthma in association with oxidation of pyruvate kinase M2. Redox Biology, 2021, 47, 102160.	9.0	23
14	Selective Monofunctionalization Enabled by Reactionâ€Historyâ€Dependent Communication in Catalytic Rotaxanes. Angewandte Chemie, 2020, 132, 16811-16817.	2.0	3
15	Aggregation State of Synergistic Antimicrobial Peptides. Journal of Physical Chemistry Letters, 2020, 11, 9501-9506.	4.6	13
16	Selective Monofunctionalization Enabled by Reactionâ€Historyâ€Dependent Communication in Catalytic Rotaxanes. Angewandte Chemie - International Edition, 2020, 59, 16668-16674.	13.8	10
17	Size-Selective Catalytic Polymer Acylation with a Molecular Tetrahedron. CheM, 2020, 6, 1469-1494.	11.7	16
18	Selective USP7 inhibition elicits cancer cell killing through a p53-dependent mechanism. Scientific Reports, 2020, 10, 5324.	3.3	69

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19	Machine Learning in a Molecular Modeling Course for Chemistry, Biochemistry, and Biophysics Students. The Biophysicist, 2020, 1, .	0.3	2
20	PAC1 Receptors: Shapeshifters in Motion. Journal of Molecular Neuroscience, 2019, 68, 331-339.	2.3	18
21	Targeting the PAC1 Receptor for Neurological and Metabolic Disorders. Current Topics in Medicinal Chemistry, 2019, 19, 1399-1417.	2.1	43
22	Chemical Exploration with Virtual Reality in Organic Teaching Laboratories. Journal of Chemical Education, 2019, 96, 1961-1966.	2.3	75
23	Top-down Multiscale Approach To Simulate Peptide Self-Assembly from Monomers. Journal of Chemical Theory and Computation, 2019, 15, 1514-1522.	5.3	10
24	InnenrÃ¼cktitelbild: Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach (Angew. Chem. 4/2019). Angewandte Chemie, 2019, 131, 1231-1231.	2.0	0
25	Assessment of Conformational State Transitions of Class B GPCRs Using Molecular Dynamics. Methods in Molecular Biology, 2019, 1947, 3-19.	0.9	3
26	Spatial Presentation of Cholesterol Units on a DNA Cube as a Determinant of Membrane Protein-Mimicking Functions. Journal of the American Chemical Society, 2019, 141, 1100-1108.	13.7	98
27	H-NS uses an autoinhibitory conformational switch for environment-controlled gene silencing. Nucleic Acids Research, 2019, 47, 2666-2680.	14.5	45
28	Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach. Angewandte Chemie - International Edition, 2019, 58, 1035-1040.	13.8	19
29	Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach. Angewandte Chemie, 2019, 131, 1047-1052.	2.0	8
30	â€œPrintingâ€•DNA Strand Patterns on Small Molecules with Control of Valency, Directionality, and Sequence. Angewandte Chemie, 2019, 131, 3074-3079.	2.0	3
31	â€œPrintingâ€•DNA Strand Patterns on Small Molecules with Control of Valency, Directionality, and Sequence. Angewandte Chemie - International Edition, 2019, 58, 3042-3047.	13.8	14
32	Cysteine perthiosulfenic acid (Cys-SSOH): A novel intermediate in thiol-based redox signaling?. Redox Biology, 2018, 14, 379-385.	9.0	56
33	DNA-imprinted polymer nanoparticles with monodispersity and prescribed DNA-strand patterns. Nature Chemistry, 2018, 10, 184-192.	13.6	80
34	Direct cysteine sulfenylation drives activation of the Src kinase. Nature Communications, 2018, 9, 4522.	12.8	87
35	Highly Coarse-Grained Representations of Transmembrane Proteins. Journal of Chemical Theory and Computation, 2017, 13, 935-944.	5.3	17
36	Capturing the multiscale dynamics of membrane protein complexes with all-atom, mixed-resolution, and coarse-grained models. Physical Chemistry Chemical Physics, 2017, 19, 9181-9188.	2.8	13

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37	Crystalâ€Packingâ€Driven Enrichment of Atropoisomers. Angewandte Chemie - International Edition, 2017, 56, 7097-7101.	13.8	11
38	A New Mixed All-Atom/Coarse-Grained Model: Application to Melittin Aggregation in Aqueous Solution. Journal of Chemical Theory and Computation, 2017, 13, 3881-3897.	5.3	16
39	Crystalâ€Packingâ€Driven Enrichment of Atropoisomers. Angewandte Chemie, 2017, 129, 7203-7207.	2.0	4
40	Precise through-space control of an abiotic electrophilic aromatic substitution reaction. Nature Communications, 2017, 8, 14840.	12.8	13
41	Designing Safer Analgesics via Î¼-Opioid Receptor Pathways. Trends in Pharmacological Sciences, 2017, 38, 1016-1037.	8.7	53
42	Conformational Transitions of the Pituitary Adenylate Cyclase-Activating Polypeptide Receptor, a Human Class B GPCR. Scientific Reports, 2017, 7, 5427.	3.3	19
43	Targeting the apoptotic Mcl-1-PUMA interface with a dual-acting compound. Oncotarget, 2017, 8, 54236-54242.	1.8	16
44	Conformational Heterogeneity of Bax Helix 9 Dimer for Apoptotic Pore Formation. Scientific Reports, 2016, 6, 29502.	3.3	18
45	<scp>BH</scp> 3â€inâ€groove dimerization initiates and helix 9 dimerization expands Bax pore assembly in membranes. EMBO Journal, 2016, 35, 208-236.	7.8	81
46	Controlled Self-Assembly inside C-Shaped Polyaromatic Strips. Synlett, 2016, 27, 2145-2149.	1.8	8
47	Innentitelbild: Regulating Molecular Recognition with C-Shaped Strips Attained by Chirality-Assisted Synthesis (Angew. Chem. 43/2015). Angewandte Chemie, 2015, 127, 12700-12700.	2.0	0
48	Regulating Molecular Recognition with Câ€Shaped Strips Attained by Chiralityâ€Assisted Synthesis. Angewandte Chemie - International Edition, 2015, 54, 12772-12776.	13.8	41
49	Melittin Aggregation in Aqueous Solutions: Insight from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 10390-10398.	2.6	38
50	Interactions of Protein Kinase C-Î± C1A and C1B Domains with Membranes: A Combined Computational and Experimental Study. Journal of the American Chemical Society, 2014, 136, 11757-11766.	13.7	31
51	Ligand-Dependent Activation and Deactivation of the Human Adenosine A2A Receptor. Journal of the American Chemical Society, 2013, 135, 8749-8759.	13.7	99
52	IDSite: An Accurate Approach to Predict P450-Mediated Drug Metabolism. Journal of Chemical Theory and Computation, 2011, 7, 3829-3845.	5.3	44
53	The VSGB 2.0 model: A next generation energy model for high resolution protein structure modeling. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2794-2812.	2.6	773
54	Progress in super long loop prediction. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2920-2935.	2.6	40

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55	Nuclear Magnetic Resonance-Based Quality Assessment of Vermont-Grown Saffron (Crocus sativus) Tj ETQq1 1 0.784314 rgBT /Overlo	2.7	0
56	Essential Dynamics Ensemble Docking for Structure-Based GPCR Drug Discovery. Frontiers in Molecular Biosciences, 0, 9, .	3.5	2