Jianing Li

List of Publications by Year in descending order

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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	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
2	Ligand-Dependent Activation and Deactivation of the Human Adenosine A2A Receptor. Journal of the American Chemical Society, 2013, 135, 8749-8759.	13.7	99
3	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
4	Direct cysteine sulfenylation drives activation of the Src kinase. Nature Communications, 2018, 9, 4522.	12.8	87
5	‹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
6	DNA-imprinted polymer nanoparticles with monodispersity and prescribed DNA-strand patterns. Nature Chemistry, 2018, 10, 184-192.	13.6	80
7	Chemical Exploration with Virtual Reality in Organic Teaching Laboratories. Journal of Chemical Education, 2019, 96, 1961-1966.	2.3	75
8	Selective USP7 inhibition elicits cancer cell killing through a p53-dependent mechanism. Scientific Reports, 2020, 10, 5324.	3.3	69
9	Cysteine perthiosulfenic acid (Cys-SSOH): A novel intermediate in thiol-based redox signaling?. Redox Biology, 2018, 14, 379-385.	9.0	56
10	Designing Safer Analgesics via Î¼-Opioid Receptor Pathways. Trends in Pharmacological Sciences, 2017, 38, 1016-1037.	8.7	53
11	H-NS uses an autoinhibitory conformational switch for environment-controlled gene silencing. Nucleic Acids Research, 2019, 47, 2666-2680.	14.5	45
12	IDSite: An Accurate Approach to Predict P450-Mediated Drug Metabolism. Journal of Chemical Theory and Computation, 2011, 7, 3829-3845.	5.3	44
13	Targeting the PAC1 Receptor for Neurological and Metabolic Disorders. Current Topics in Medicinal Chemistry, 2019, 19, 1399-1417.	2.1	43
14	Regulating Molecular Recognition with Câ€Shaped Strips Attained by Chiralityâ€Assisted Synthesis. Angewandte Chemie - International Edition, 2015, 54, 12772-12776.	13.8	41
15	Progress in super long loop prediction. Proteins: Structure, Function and Bioinformatics, 2011, 79, 2920-2935.	2.6	40
16	Melittin Aggregation in Aqueous Solutions: Insight from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2015, 119, 10390-10398.	2.6	38
17	AMPGAN v2: Machine Learning-Guided Design of Antimicrobial Peptides. Journal of Chemical Information and Modeling, 2021, 61, 2198-2207.	5.4	37
18	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

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19	Glutathione-S-transferase P promotes glycolysis in asthma in association with oxidation of pyruvate kinase M2. Redox Biology, 2021, 47, 102160.	9.0	23
20	Conformational Transitions of the Pituitary Adenylate Cyclase-Activating Polypeptide Receptor, a Human Class B GPCR. Scientific Reports, 2017, 7, 5427.	3.3	19
21	Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach. Angewandte Chemie - International Edition, 2019, 58, 1035-1040.	13.8	19
22	Conformational Heterogeneity of Bax Helix 9 Dimer for Apoptotic Pore Formation. Scientific Reports, 2016, 6, 29502.	3.3	18
23	PAC1 Receptors: Shapeshifters in Motion. Journal of Molecular Neuroscience, 2019, 68, 331-339.	2.3	18
24	Highly Coarse-Grained Representations of Transmembrane Proteins. Journal of Chemical Theory and Computation, 2017, 13, 935-944.	5.3	17
25	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
26	Targeting the apoptotic Mcl-1-PUMA interface with a dual-acting compound. Oncotarget, 2017, 8, 54236-54242.	1.8	16
27	Size-Selective Catalytic Polymer Acylation with a Molecular Tetrahedron. CheM, 2020, 6, 1469-1494.	11.7	16
28	Thermosetting supramolecular polymerization of compartmentalized DNA fibers with stereo sequence and length control. CheM, 2021, 7, 2395-2414.	11.7	16
29	Molecular Basis of Class B GPCR Selectivity for the Neuropeptides PACAP and VIP. Frontiers in Molecular Biosciences, 2021, 8, 644644.	3.5	15
30	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
31	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
32	Precise through-space control of an abiotic electrophilic aromatic substitution reaction. Nature Communications, 2017, 8, 14840.	12.8	13
33	Aggregation State of Synergistic Antimicrobial Peptides. Journal of Physical Chemistry Letters, 2020, 11, 9501-9506.	4.6	13
34	Crystalâ€Packingâ€Driven Enrichment of Atropoisomers. Angewandte Chemie - International Edition, 2017, 56, 7097-7101.	13.8	11
35	Top-down Multiscale Approach To Simulate Peptide Self-Assembly from Monomers. Journal of Chemical Theory and Computation, 2019, 15, 1514-1522.	5.3	10
36	Selective Monofunctionalization Enabled by Reactionâ€Historyâ€Dependent Communication in Catalytic Rotaxanes. Angewandte Chemie - International Edition, 2020, 59, 16668-16674.	13.8	10

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37	Molecular basis for the adaptive evolution of environment-sensing by H-NS proteins. ELife, 2021, 10, .	6.0	9
38	Controlled Self-Assembly inside C-Shaped Polyaromatic Strips. Synlett, 2016, 27, 2145-2149.	1.8	8
39	Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach. Angewandte Chemie, 2019, 131, 1047-1052.	2.0	8
40	Enhanced sampling protocol to elucidate fusion peptide opening of SARS-CoV-2 spike protein. Biophysical Journal, 2021, 120, 2848-2858.	0.5	7
41	A computational study of cooperative binding to multiple SARS-CoV-2 proteins. Scientific Reports, 2021, 11, 16307.	3.3	7
42	Crystalâ€Packingâ€Driven Enrichment of Atropoisomers. Angewandte Chemie, 2017, 129, 7203-7207.	2.0	4
43	Molecular Basis for Environment Sensing by a Nucleoid-Structuring Bacterial Protein Filament. Journal of Physical Chemistry Letters, 2021, 12, 7878-7884.	4.6	4
44	GPCR Intracellular Loop Regulation of Beta-Arrestin-Mediated Endosomal Signaling Dynamics. Journal of Molecular Neuroscience, 2022, 72, 1358-1373.	2.3	4
45	Assessment of Conformational State Transitions of Class B GPCRs Using Molecular Dynamics. Methods in Molecular Biology, 2019, 1947, 3-19.	0.9	3
46	â€œPrintingâ€•DNA Strand Patterns on Small Molecules with Control of Valency, Directionality, and Sequence. Angewandte Chemie, 2019, 131, 3074-3079.	2.0	3
47	Selective Monofunctionalization Enabled by Reactionâ€Historyâ€Dependent Communication in Catalytic Rotaxanes. Angewandte Chemie, 2020, 132, 16811-16817.	2.0	3
48	Machine Learning in a Molecular Modeling Course for Chemistry, Biochemistry, and Biophysics Students. The Biophysicist, 2020, 1, .	0.3	2
49	Essential Dynamics Ensemble Docking for Structure-Based GPCR Drug Discovery. Frontiers in Molecular Biosciences, 0, 9, .	3.5	2
50	Iterative Exponential Growth of Oxygen-Linked Aromatic Polymers Driven by Nucleophilic Aromatic Substitution Reactions. Frontiers in Chemistry, 2021, 9, 620017.	3.6	1
51	Outcome-Based Redesign of Physical Chemistry Laboratories During the COVID-19 Pandemic. Journal of Chemical Education, 2022, 99, 639-645.	2.3	1
52	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
53	InnenrÃ¼cktitelbild: Enantioselective Electrophilic Aromatic Nitration: A Chiral Auxiliary Approach (Angew. Chem. 4/2019). Angewandte Chemie, 2019, 131, 1231-1231.	2.0	0
54	Carbonyl-to-Alkyne Electron Donation Effects in up to 10-nm-Long, Unimolecular Oligo(p-phenylene) Tj ETQq0 0 0 rgBT /Overlock 10 Tf	2.0	0

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55	Nuclear Magnetic Resonance-Based Quality Assessment of Vermont-Grown Saffron (Crocus sativus) Tj ETQq1 1 0.784314 rgBT /Overlock	2.7	0
56	Concerted Rolling and Penetration of Peptides during Membrane Binding. Journal of Chemical Theory and Computation, 2022, 18, 3921-3929.	5.3	0