Guo-Hui Li

List of Publications by Year
in descending order

91 papers	2,528 citations	236925 25 h-index	254184 43 g-index
94 all docs	94 docs citations	94 times ranked	3971 citing authors

#	Article	IF	Citations
1	Multiscale simulations of large complexes in conjunction with cryo-EM analysis. Current Opinion in Structural Biology, 2022, 72, 27-32.	5.7	3
2	Stiffening Effect of Ceramide on Lipid Membranes Provides Non-Sacrificial Protection against Potent Chemical Damage. Langmuir, 2022, 38, 3522-3529.	3.5	1
3	ZDHHC18 negatively regulates cGASâ€mediated innate immunity through palmitoylation. EMBO Journal, 2022, 41, e109272.	7.8	26
4	A Rationally Designed Building Block of the Putative Magnetoreceptor MagR. Bioelectromagnetics, 2022, 43, 317-326.	1.6	5
5	Quality of force fields and sampling methods in simulating pepX peptides: a case study for intrinsically disordered proteins. Physical Chemistry Chemical Physics, 2021, 23, 2430-2437.	2.8	8
6	A double bilayer to study the nonequilibrium environmental response of GIRK2 in complex states. Physical Chemistry Chemical Physics, 2021, 23, 15784-15795.	2.8	1
7	A novel partially open state of SHP2 points to a â€œmultiple gearâ€•regulation mechanism. Journal of Biological Chemistry, 2021, 296, 100538.	3.4	18
8	The structural basis of function and regulation of neuronal cotransporters NKCC1 and KCC2. Communications Biology, 2021, 4, 226.	4.4	48
9	Phosphorylation of SNX27 by MAPK11/14 links cellular stressâ€“signaling pathways with endocytic recycling. Journal of Cell Biology, 2021, 220, .	5.2	30
10	Interaction energy prediction of organic molecules using deep tensor neural network. Chinese Journal of Chemical Physics, 2021, 34, 112-124.	1.3	1
11	Impact of Î”E_{ST} on Delayed Fluorescence Rate, Lifetime, and Intensity Ratio of Tetrahedral Cu(I) Complexes: Theoretical Simulation in Solution and Solid Phases. Journal of Physical Chemistry Letters, 2021, 12, 2232-2244.	4.6	6
12	Adaptively Iterative Multiscale Switching Simulation Strategy and Applications to Protein Folding and Structure Prediction. Journal of Physical Chemistry Letters, 2021, 12, 3151-3162.	4.6	5
13	Ceftazidime is a potential drug to inhibit SARS-CoV-2 infection in vitro by blocking spike proteinâ€“ACE2 interaction. Signal Transduction and Targeted Therapy, 2021, 6, 198.	17.1	31
14	Discovery of a cooperative mode of inhibiting RIPK1 kinase. Cell Discovery, 2021, 7, 41.	6.7	14
15	Induction and Monitoring of DNA Phase Separation in Living Cells by a Light-Switching Ruthenium Complex. Journal of the American Chemical Society, 2021, 143, 11370-11381.	13.7	19
16	Distinct chemokines selectively induce HIV-1 gp120-integrin Î±4Î²7 binding via triggering conformer-specific activation of Î±4Î²7. Signal Transduction and Targeted Therapy, 2021, 6, 265.	17.1	1
17	Effect of protein dimerization on ion conductivity of gramicidin a channel studied using polarizable force field. Chinese Journal of Chemical Physics, 2021, 34, 471-479.	1.3	0
18	Allosteric inhibition of SARS-CoV-2 3CL protease by colloidal bismuth subcitrate. Chemical Science, 2021, 12, 14098-14102.	7.4	19

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19	Zipper head mechanism of telomere synthesis by human telomerase. Cell Research, 2021, 31, 1275-1290.	12.0	19
20	Mechanisms of distinctive mismatch tolerance between Rad51 and Dmc1 in homologous recombination. Nucleic Acids Research, 2021, 49, 13135-13149.	14.5	17
21	Large-Scale Biomolecular Conformational Transitions Explored by a Combined Elastic Network Model and Enhanced Sampling Molecular Dynamics. Journal of Physical Chemistry Letters, 2020, 11, 325-332.	4.6	11
22	Probing cell membrane damage using a molecular rotor probe with membrane-to-nucleus translocation. Materials Horizons, 2020, 7, 3226-3233.	12.2	34
23	Structural insights into telomere protection and homeostasis regulation by yeast CST complex. Nature Structural and Molecular Biology, 2020, 27, 752-762.	8.2	23
24	Molecular Dynamics Simulation-assisted Ionic Liquid Screening for Deep Coverage Proteome Analysis. Molecular and Cellular Proteomics, 2020, 19, 1724-1737.	3.8	24
25	Distinct Interaction of Lytic Polysaccharide Monooxygenase with Cellulose Revealed by Computational and Biochemical Studies. Journal of Physical Chemistry Letters, 2020, 11, 3987-3992.	4.6	21
26	Higher Accuracy Achieved for Proteinâ€“Ligand Binding Pose Prediction by Elastic Network Model-Based Ensemble Docking. Journal of Chemical Information and Modeling, 2020, 60, 2939-2950.	5.4	13
27	Sur-X, a novel peptide, kills colorectal cancer cells by targeting survivin-XIAP complex. Journal of Experimental and Clinical Cancer Research, 2020, 39, 82.	8.6	9
28	Coevolution of Eukaryote-like Vps4 and ESCRT-III Subunits in the Asgard Archaea. MBio, 2020, 11, .	4.1	23
29	Mechanism of ligand activation of a eukaryotic cyclic nucleotideâ˜gated channel. Nature Structural and Molecular Biology, 2020, 27, 625-634.	8.2	40
30	Different regions of synaptic vesicle membrane regulate VAMP2 conformation for the SNARE assembly. Nature Communications, 2020, 11, 1531.	12.8	30
31	Small-Molecule Antagonist Targeting Exportin-1 via Rational Structure-Based Discovery. Journal of Medicinal Chemistry, 2020, 63, 3881-3895.	6.4	17
32	Molecular chirality mediated amyloid formation on phospholipid surfaces. Chemical Science, 2020, 11, 7369-7378.	7.4	16
33	NLRP6 self-assembles into a linear molecular platform following LPS binding and ATP stimulation. Scientific Reports, 2020, 10, 198.	3.3	23
34	Arbitrary Resolution with Two Bead Types Coarse-Grained Strategy and Applications to Protein Recognition. Journal of Physical Chemistry Letters, 2020, 11, 3263-3270.	4.6	3
35	Structural and functional insights into the tetrameric photosystem I from heterocyst-forming cyanobacteria. Nature Plants, 2019, 5, 1087-1097.	9.3	57
36	Î±-Ketoglutarate-Activated NF-ÎºB Signaling Promotes Compensatory Glucose Uptake and Brain Tumor Development. Molecular Cell, 2019, 76, 148-162.e7.	9.7	94

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37	Interwoven Molecular Chains Obtained by Ionic Self-Assembly of Two Iron(III) Porphyrins with Opposite and Mismatched Charges. ACS Applied Materials & Interfaces, 2019, 11, 34203-34211.	8.0	11
38	Advances in enhanced sampling molecular dynamics simulations for biomolecules. Chinese Journal of Chemical Physics, 2019, 32, 277-286.	1.3	28
39	Quantitative Lysine Reactivity Profiling Reveals Conformational Inhibition Dynamics and Potency of Aurora A Kinase Inhibitors. Analytical Chemistry, 2019, 91, 13222-13229.	6.5	13
40	UDP-glucose accelerates SNAI1 mRNA decay and impairs lung cancer metastasis. Nature, 2019, 571, 127-131.	27.8	140
41	NRDE2 negatively regulates exosome functions by inhibiting MTR4 recruitment and exosome interaction. Genes and Development, 2019, 33, 536-549.	5.9	34
42	<scp>ALYREF</scp> links 3â€²â€end processing to nuclear export of nonâ€polyadenylated <scp>mRNA</scp> s. EMBO Journal, 2019, 38, .	7.8	30
43	Chinese Spring Festival Editorial. Journal of Physical Chemistry Letters, 2019, 10, 701-701.	4.6	3
44	Stereoselective catalysis controlled by a native leucine or variant isoleucine wingâ€gatekeeper in 2â€haloacid dehalogenase. FEBS Letters, 2019, 593, 308-318.	2.8	1
45	Polarizable atomic multipole-based force field for DOPC and POPE membrane lipids. Molecular Physics, 2018, 116, 1037-1050.	1.7	9
46	Benzoxazinone-containing 3,5-dimethylisoxazole derivatives as BET bromodomain inhibitors for treatment of castration-resistant prostate cancer. European Journal of Medicinal Chemistry, 2018, 152, 542-559.	5.5	21
47	Integrating Multiple Accelerated Molecular Dynamics To Improve Accuracy of Free Energy Calculations. Journal of Chemical Theory and Computation, 2018, 14, 1216-1227.	5.3	28
48	Y08060: A Selective BET Inhibitor for Treatment of Prostate Cancer. ACS Medicinal Chemistry Letters, 2018, 9, 262-267.	2.8	14
49	Cholesterol modulating the orientation of His17 in hepatitis C virus p7 (5a) viroporin â€“ A molecular dynamic simulation study. Chinese Chemical Letters, 2018, 29, 719-723.	9.0	4
50	Intramembrane ionic proteinâ€“lipid interaction regulates integrin structure and function. PLoS Biology, 2018, 16, e2006525.	5.6	11
51	Higher Accuracy Achieved in the Simulations of Protein Structure Refinement, Protein Folding, and Intrinsically Disordered Proteins Using Polarizable Force Fields. Journal of Physical Chemistry Letters, 2018, 9, 7110-7116.	4.6	24
52	Structural insight into precursor tRNA processing by yeast ribonuclease P. Science, 2018, 362, .	12.6	59
53	Saikosaponin D from Radix Bupleuri suppresses triple-negative breast cancer cell growth by targeting Î²-catenin signaling. Biomedicine and Pharmacotherapy, 2018, 108, 724-733.	5.6	46
54	A Polarizable Atomic Multipole-Based Force Field for Molecular Dynamics Simulations of Anionic Lipids. Molecules, 2018, 23, 77.	3.8	8

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55	Integrin Î±4Î²7 switches its ligand specificity via distinct conformer-specific activation. Journal of Cell Biology, 2018, 217, 2799-2812.	5.2	29
56	mRNAs are sorted for export or degradation before passing through nuclear speckles. Nucleic Acids Research, 2018, 46, 8404-8416.	14.5	22
57	Macrophage-Associated PGK1 Phosphorylation Promotes Aerobic Glycolysis and Tumorigenesis. Molecular Cell, 2018, 71, 201-215.e7.	9.7	211
58	Prediction of molecular energy using deep tensor neural networks. Communications in Information and Systems, 2018, 18, 229-250.	0.5	2
59	Polarizable force field development for lipids and their efficient applications in membrane proteins. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2017, 7, e1312.	14.6	11
60	Inert Gas Deactivates Protein Activity by Aggregation. Scientific Reports, 2017, 7, 10176.	3.3	25
61	A salt-bridge switch in the molecular recognition between RS receptor and RGD ligand from the ABEEM ÏƒÎ€ molecular dynamics simulations. Molecular Simulation, 2017, 43, 1045-1055.	2.0	1
62	ALYREF mainly binds to the 5â€² and the 3â€² regions of the mRNA in vivo. Nucleic Acids Research, 2017, 45, 9640-9653.	14.5	87
63	Exosome cofactor <scp>hMTR</scp>4 competes with export adaptor <scp>ALYREF</scp> to ensure balanced nuclear <scp>RNA</scp> pools for degradation and export. EMBO Journal, 2017, 36, 2870-2886.	7.8	82
64	Stereoselective Stabilization of Polymeric Vitamin E Conjugate Micelles. Biomacromolecules, 2017, 18, 4349-4356.	5.4	37
65	Recent Developments in Using Molecular Dynamics Simulation Techniques to Study Biomolecules. Wuli Huaxue Xuebao/ Acta Physico - Chimica Sinica, 2017, 33, 1354-1365.	4.9	14
66	Prevalent Accumulation of Non-Optimal Codons through Somatic Mutations in Human Cancers. PLoS ONE, 2016, 11, e0160463.	2.5	7
67	The Effect of Codon Mismatch on the Protein Translation System. PLoS ONE, 2016, 11, e0148302.	2.5	5
68	Free energy simulations with the AMOEBA polarizable force field and metadynamics on GPU platform. Journal of Computational Chemistry, 2016, 37, 614-622.	3.3	12
69	Validation of polarizable force field parameters for nucleic acids by inter-molecular interactions. Frontiers of Chemical Science and Engineering, 2016, 10, 203-212.	4.4	5
70	Some polarisable force fields for molecular dynamics simulations of lipids, and bilayers. Molecular Simulation, 2016, 42, 820-826.	2.0	2
71	Understanding enzyme reactions using enhanced sampling techniques. Molecular Simulation, 2016, 42, 846-854.	2.0	0
72	Multiscale Simulations on Spectral Tuning and the Photoisomerization Mechanism in Fluorescent RNA Spinach. Journal of Chemical Theory and Computation, 2016, 12, 5453-5464.	5.3	11

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73	Mediation mechanism of tyrosine 185 on the retinal isomerization equilibrium and the proton release channel in the seven-transmembrane receptor bacteriorhodopsin. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1786-1795.	1.0	6
74	Wedelolactone enhances osteoblastogenesis by regulating Wnt/Î²-catenin signaling pathway but suppresses osteoclastogenesis by NF-Î¹B/c-fos/NFATc1 pathway. Scientific Reports, 2016, 6, 32260.	3.3	36
75	Accurate Evaluation of Ion Conductivity of the Gramicidin A Channel Using a Polarizable Force Field without Any Corrections. Journal of Chemical Theory and Computation, 2016, 12, 2973-2982.	5.3	41
76	Nuclear AURKA acquires kinase-independent transactivating function to enhance breast cancer stem cell phenotype. Nature Communications, 2016, 7, 10180.	12.8	142
77	Structural basis for activity regulation of MLL family methyltransferases. Nature, 2016, 530, 447-452.	27.8	189
78	Coarse-Grained Modeling of Nucleic Acids Using Anisotropic Gayâ€“Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2016, 12, 676-693.	5.3	47
79	Hypotaurine evokes a malignant phenotype in glioma through aberrant hypoxic signaling. Oncotarget, 2016, 7, 15200-15214.	1.8	30
80	Computational discovery and experimental verification of tyrosine kinase inhibitor pazopanib for the reversal of memory and cognitive deficits in rat model neurodegeneration. Chemical Science, 2015, 6, 2812-2821.	7.4	27
81	Mechanistic insight into the functional transition of the enzyme guanylate kinase induced by a single mutation. Scientific Reports, 2015, 5, 8405.	3.3	4
82	Ultrafast Tracking of a Single Live Virion During the Invagination of a Cell Membrane. Small, 2015, 11, 2782-2788.	10.0	27
83	An anisotropic coarseâ€grained model based on <scp>G</scp>ayâ€“<scp>B</scp>erne and electric multipole potentials and its application to simulate a DMPC bilayer in an implicit solvent model. Journal of Computational Chemistry, 2015, 36, 1103-1113.	3.3	16
84	Insights into the molecular recognition of the granuphilin C2A domain with PI(4,5)P2. Chemistry and Physics of Lipids, 2015, 186, 61-67.	3.2	24
85	Bridging the Missing Link between Structure and Fidelity of the RNA-Dependent RNA Polymerase from Poliovirus through Free Energy Simulations. Journal of Chemical Theory and Computation, 2014, 10, 5195-5205.	5.3	5
86	Anisotropic Coarse-Grained Model for Proteins Based On Gayâ€“Berne and Electric Multipole Potentials. Journal of Chemical Theory and Computation, 2014, 10, 731-750.	5.3	44
87	Theoretical Study on the UVR8 Photoreceptor: Sensing Ultraviolet-B by Tryptophan and Dissociation of Homodimer. Journal of Chemical Theory and Computation, 2014, 10, 3319-3330.	5.3	17
88	A Sub-Element in PRE enhances nuclear export of intronless mRNAs by recruiting the TREX complex via ZC3H18. Nucleic Acids Research, 2014, 42, 7305-7318.	14.5	49
89	UNDERSTANDING THE MOLECULAR MECHANISM OF BINDING MODES OF AURORA A INHIBITORS BY LONG TIME SCALE GPU DYNAMICS. Journal of Theoretical and Computational Chemistry, 2013, 12, 1341003.	1.8	11
90	Photoelectron spectroscopy of ammonia via a fast predissociative state. Faraday Discussions, 2000, 115, 127-136.	3.2	9

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91	Moderate and strong static magnetic fields directly affect EGFR kinase domain orientation to inhibit cancer cell proliferation. Oncotarget, 0, 7, 41527-41539.	1.8	45