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	Macrophage-Associated PGK1 Phosphorylation Promotes Aerobic Glycolysis and Tumorigenesis. Molecular Cell, 2018, 71, 201-215.e7.	9.7	211
2	Structural basis for activity regulation of MLL family methyltransferases. Nature, 2016, 530, 447-452.	27.8	189
3	Nuclear AURKA acquires kinase-independent transactivating function to enhance breast cancer stem cell phenotype. Nature Communications, 2016, 7, 10180.	12.8	142
4	UDP-glucose accelerates SNAI1 mRNA decay and impairs lung cancer metastasis. Nature, 2019, 571, 127-131.	27.8	140
5	Î±-Ketoglutarate-Activated NF-Î²B Signaling Promotes Compensatory Glucose Uptake and Brain Tumor Development. Molecular Cell, 2019, 76, 148-162.e7.	9.7	94
6	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
7	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
8	Structural insight into precursor tRNA processing by yeast ribonuclease P. Science, 2018, 362, .	12.6	59
9	Structural and functional insights into the tetrameric photosystem I from heterocyst-forming cyanobacteria. Nature Plants, 2019, 5, 1087-1097.	9.3	57
10	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
11	The structural basis of function and regulation of neuronal cotransporters NKCC1 and KCC2. Communications Biology, 2021, 4, 226.	4.4	48
12	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
13	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
14	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
15	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
16	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
17	Mechanism of ligand activation of a eukaryotic cyclic nucleotideâ^'gated channel. Nature Structural and Molecular Biology, 2020, 27, 625-634.	8.2	40
18	Stereoselective Stabilization of Polymeric Vitamin E Conjugate Micelles. Biomacromolecules, 2017, 18, 4349-4356.	5.4	37

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19	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
20	NRDE2 negatively regulates exosome functions by inhibiting MTR4 recruitment and exosome interaction. Genes and Development, 2019, 33, 536-549.	5.9	34
21	Probing cell membrane damage using a molecular rotor probe with membrane-to-nucleus translocation. Materials Horizons, 2020, 7, 3226-3233.	12.2	34
22	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
23	<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
24	Different regions of synaptic vesicle membrane regulate VAMP2 conformation for the SNARE assembly. Nature Communications, 2020, 11, 1531.	12.8	30
25	Phosphorylation of SNX27 by MAPK11/14 links cellular stressâ€“signaling pathways with endocytic recycling. Journal of Cell Biology, 2021, 220, .	5.2	30
26	Hypotaurine evokes a malignant phenotype in glioma through aberrant hypoxic signaling. Oncotarget, 2016, 7, 15200-15214.	1.8	30
27	Integrin Î±4Î²7 switches its ligand specificity via distinct conformer-specific activation. Journal of Cell Biology, 2018, 217, 2799-2812.	5.2	29
28	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
29	Advances in enhanced sampling molecular dynamics simulations for biomolecules. Chinese Journal of Chemical Physics, 2019, 32, 277-286.	1.3	28
30	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
31	Ultrafast Tracking of a Single Live Virion During the Invagination of a Cell Membrane. Small, 2015, 11, 2782-2788.	10.0	27
32	ZDHHC18 negatively regulates cGASâ€mediated innate immunity through palmitoylation. EMBO Journal, 2022, 41, e109272.	7.8	26
33	Inert Gas Deactivates Protein Activity by Aggregation. Scientific Reports, 2017, 7, 10176.	3.3	25
34	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
35	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
36	Molecular Dynamics Simulation-assisted Ionic Liquid Screening for Deep Coverage Proteome Analysis. Molecular and Cellular Proteomics, 2020, 19, 1724-1737.	3.8	24

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37	Structural insights into telomere protection and homeostasis regulation by yeast CST complex. Nature Structural and Molecular Biology, 2020, 27, 752-762.	8.2	23
38	Coevolution of Eukaryote-like Vps4 and ESCRT-III Subunits in the Asgard Archaea. MBio, 2020, 11, .	4.1	23
39	NLRP6 self-assembles into a linear molecular platform following LPS binding and ATP stimulation. Scientific Reports, 2020, 10, 198.	3.3	23
40	mRNAs are sorted for export or degradation before passing through nuclear speckles. Nucleic Acids Research, 2018, 46, 8404-8416.	14.5	22
41	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
42	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
43	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
44	Allosteric inhibition of SARS-CoV-2 3CL protease by colloidal bismuth subcitrate. Chemical Science, 2021, 12, 14098-14102.	7.4	19
45	Zipper head mechanism of telomere synthesis by human telomerase. Cell Research, 2021, 31, 1275-1290.	12.0	19
46	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
47	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
48	Small-Molecule Antagonist Targeting Exportin-1 via Rational Structure-Based Discovery. Journal of Medicinal Chemistry, 2020, 63, 3881-3895.	6.4	17
49	Mechanisms of distinctive mismatch tolerance between Rad51 and Dmc1 in homologous recombination. Nucleic Acids Research, 2021, 49, 13135-13149.	14.5	17
50	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
51	Molecular chirality mediated amyloid formation on phospholipid surfaces. Chemical Science, 2020, 11, 7369-7378.	7.4	16
52	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
53	Y08060: A Selective BET Inhibitor for Treatment of Prostate Cancer. ACS Medicinal Chemistry Letters, 2018, 9, 262-267.	2.8	14
54	Discovery of a cooperative mode of inhibiting RIPK1 kinase. Cell Discovery, 2021, 7, 41.	6.7	14

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55	Quantitative Lysine Reactivity Profiling Reveals Conformational Inhibition Dynamics and Potency of Aurora A Kinase Inhibitors. Analytical Chemistry, 2019, 91, 13222-13229.	6.5	13
56	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
57	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
58	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
59	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
60	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
61	Intramembrane ionic proteinâ€“lipid interaction regulates integrin structure and function. PLoS Biology, 2018, 16, e2006525.	5.6	11
62	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
63	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
64	Photoelectron spectroscopy of ammonia via a fast predissociative state. Faraday Discussions, 2000, 115, 127-136.	3.2	9
65	Polarizable atomic multipole-based force field for DOPC and POPE membrane lipids. Molecular Physics, 2018, 116, 1037-1050.	1.7	9
66	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
67	A Polarizable Atomic Multipole-Based Force Field for Molecular Dynamics Simulations of Anionic Lipids. Molecules, 2018, 23, 77.	3.8	8
68	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
69	Prevalent Accumulation of Non-Optimal Codons through Somatic Mutations in Human Cancers. PLoS ONE, 2016, 11, e0160463.	2.5	7
70	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
71	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
72	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

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73	The Effect of Codon Mismatch on the Protein Translation System. PLoS ONE, 2016, 11, e0148302.	2.5	5
74	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
75	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
76	A Rationally Designed Building Block of the Putative Magnetoreceptor MagR. Bioelectromagnetics, 2022, 43, 317-326.	1.6	5
77	Mechanistic insight into the functional transition of the enzyme guanylate kinase induced by a single mutation. Scientific Reports, 2015, 5, 8405.	3.3	4
78	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
79	Chinese Spring Festival Editorial. Journal of Physical Chemistry Letters, 2019, 10, 701-701.	4.6	3
80	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
81	Multiscale simulations of large complexes in conjunction with cryo-EM analysis. Current Opinion in Structural Biology, 2022, 72, 27-32.	5.7	3
82	Some polarisable force fields for molecular dynamics simulations of lipids, and bilayers. Molecular Simulation, 2016, 42, 820-826.	2.0	2
83	Prediction of molecular energy using deep tensor neural networks. Communications in Information and Systems, 2018, 18, 229-250.	0.5	2
84	A salt-bridge switch in the molecular recognition between RS receptor and RGD ligand from the ABEEM ÏƒÏ€ molecular dynamics simulations. Molecular Simulation, 2017, 43, 1045-1055.	2.0	1
85	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
86	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
87	Interaction energy prediction of organic molecules using deep tensor neural network. Chinese Journal of Chemical Physics, 2021, 34, 112-124.	1.3	1
88	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
89	Stiffening Effect of Ceramide on Lipid Membranes Provides Non-Sacrificial Protection against Potent Chemical Damage. Langmuir, 2022, 38, 3522-3529.	3.5	1
90	Understanding enzyme reactions using enhanced sampling techniques. Molecular Simulation, 2016, 42, 846-854.	2.0	0

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91	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