Xiaolin Cheng

List of Publications by Year
in descending order

109	3,320	147801 31	182427 51
papers	citations	h-index	g-index

112	112	112	4573
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Computational and Experimental Approaches to Investigate Lipid Nanoparticles as Drug and Gene Delivery Systems. Current Topics in Medicinal Chemistry, 2021, 21, 92-114.	2.1	16
2	Facilitative lysosomal transport of bile acids alleviates ER stress in mouse hematopoietic precursors. Nature Communications, 2021, 12, 1248.	12.8	11
3	Structural Insights into gp16 ATPase in the Bacteriophage Ï•29 DNA Packaging Motor. Biochemistry, 2021, 60, 886-897.	2.5	7
4	Activated nanoscale actin-binding domain motion in the cateninâ€“cadherin complex revealed by neutron spin echo spectroscopy. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	8
5	Reply to: Insufficient evidence for ageing in protein dynamics. Nature Physics, 2021, 17, 775-776.	16.7	3
6	Mechanistic Insights into the Allosteric Inhibition of Androgen Receptors by Binding Function 3 Antagonists from an Integrated Molecular Modeling Study. Journal of Chemical Information and Modeling, 2021, 61, 3477-3494.	5.4	4
7	Structural Insights into the Interactions of Digoxin and Na+/K+-ATPase and Other Targets for the Inhibition of Cancer Cell Proliferation. Molecules, 2021, 26, 3672.	3.8	9
8	Interaction of (+)-Strebloside and Its Derivatives with Na+/K+-ATPase and Other Targets. Molecules, 2021, 26, 5675.	3.8	6
9	Development of Murine Leukemia Virus Integrase-Derived Peptides That Bind Brd4 Extra-Terminal Domain as Candidates for Suppression of Acute Myeloid Leukemia. ACS Pharmacology and Translational Science, 2021, 4, 1628-1638.	4.9	9
10	Covalent inhibition of hAChE by organophosphates causes homodimer dissociation through long-range allosteric effects. Journal of Biological Chemistry, 2021, 297, 101007.	3.4	8
11	Computational investigation of the binding of a designed peptide to Î» light chain amyloid fibril. Physical Chemistry Chemical Physics, 2021, 23, 20634-20644.	2.8	2
12	Listeria monocytogenes upregulates mitochondrial calcium signalling to inhibit LC3-associated phagocytosis as a survival strategy. Nature Microbiology, 2021, 6, 366-379.	13.3	33
13	In Vitro and In Vivo Inhibition of MATE1 by Tyrosine Kinase Inhibitors. Pharmaceutics, 2021, 13, 2004.	4.5	9
14	Cytotoxic and non-cytotoxic cardiac glycosides isolated from the combined flowers, leaves, and twigs of Streblus asper. Bioorganic and Medicinal Chemistry, 2020, 28, 115301.	3.0	14
15	Direct structural evidence supporting a revolving mechanism in DNA packaging motors. Biophysics Reports, 2020, 6, 155-158.	0.8	1
16	Carotenoids promote lateral packing and condensation of lipid membranes. Physical Chemistry Chemical Physics, 2020, 22, 12281-12293.	2.8	24
17	Semi-synthetic cinnamodial analogues: Structural insights into the insecticidal and antifeedant activities of drimane sesquiterpenes against the mosquito Aedes aegypti. PLoS Neglected Tropical Diseases, 2020, 14, e0008073.	3.0	6
18	The structures of polyunsaturated lipid bilayers by joint refinement of neutron and X-ray scattering data. Chemistry and Physics of Lipids, 2020, 229, 104892.	3.2	21

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19	A computational study of effects on membrane recruitment of the polar linkers in Vitamin E derivatives. Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129655.	2.4	1
20	Rational design, synthesis, and evaluation of uncharged, â€œsmartâ€•bis-oxime antidotes of organophosphate-inhibited human acetylcholinesterase. Journal of Biological Chemistry, 2020, 295, 4079-4092.	3.4	24
21	Na⁺/K⁺-ATPase-Targeted Cytotoxicity of (+)-Digoxin and Several Semisynthetic Derivatives. Journal of Natural Products, 2020, 83, 638-648.	3.0	23
22	Rational Design of Small Molecules to Enhance Genome Editing Efficiency by Selectively Targeting Distinct Functional States of CRISPR-Cas12a. Bioconjugate Chemistry, 2020, 31, 542-546.	3.6	9
23	SCNrank: spectral clustering for network-based ranking to reveal potential drug targets and its application in pancreatic ductal adenocarcinoma. BMC Medical Genomics, 2020, 13, 50.	1.5	11
24	A Multifunctional Cosolvent Pair Reveals Molecular Principles of Biomass Deconstruction. Journal of the American Chemical Society, 2019, 141, 12545-12557.	13.7	73
25	Structurally Modified Cyclopenta[b]benzofuran Analogues Isolated from Aglaia perviridis. Journal of Natural Products, 2019, 82, 2870-2877.	3.0	11
26	STarFish: A Stacked Ensemble Target Fishing Approach and its Application to Natural Products. Journal of Chemical Information and Modeling, 2019, 59, 4906-4920.	5.4	27
27	Computationally Guided Discovery and Experimental Validation of Indole-3-acetic Acid Synthesis Pathways. ACS Chemical Biology, 2019, 14, 2867-2875.	3.4	8
28	Insecticidal and Antifeedant Activities of Malagasy Medicinal Plant (Cinnamosma sp.) Extracts and Drimane-Type Sesquiterpenes against Aedes aegypti Mosquitoes. Insects, 2019, 10, 373.	2.2	17
29	Generation of the configurational ensemble of an intrinsically disordered protein from unbiased molecular dynamics simulation. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 20446-20452.	7.1	88
30	Branched-Chain Fatty Acid Content Modulates Structure, Fluidity, and Phase in Model Microbial Cell Membranes. Journal of Physical Chemistry B, 2019, 123, 5814-5821.	2.6	27
31	A new crystal form of human acetylcholinesterase for exploratory room-temperature crystallography studies. Chemico-Biological Interactions, 2019, 309, 108698.	4.0	82
32	Productive reorientation of a bound oxime reactivator revealed in room temperature X-ray structures of native and VX-inhibited human acetylcholinesterase. Journal of Biological Chemistry, 2019, 294, 10607-10618.	3.4	13
33	Controlling the Revolving and Rotating Motion Direction of Asymmetric Hexameric Nanomotor by Arginine Finger and Channel Chirality. ACS Nano, 2019, 13, 6207-6223.	14.6	17
34	Biological Membrane Organization and Cellular Signaling. Chemical Reviews, 2019, 119, 5849-5880.	47.7	112
35	21. Molecular dynamics simulation studies of small molecules interacting with cell membranes. , 2019, , 603-630.		1
36	Lipid Rafts: Buffers of Cell Membrane Physical Properties. Journal of Physical Chemistry B, 2019, 123, 2050-2056.	2.6	40

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37	Heterohexamers Formed by CcmK3 and CcmK4 Increase the Complexity of Beta Carboxysome Shells. Plant Physiology, 2019, 179, 156-167.	4.8	61
38	Abstract 4257: Integrated network analysis reveals potentially novel molecular pathways mechanism and therapeutic targets of pancreatic ductal adenocarcinoma. , 2019, , .		0
39	Temperature-dependent phase behaviour of tetrahydrofuranâ€“water alters solubilization of xylan to improve co-production of furfurals from lignocellulosic biomass. Green Chemistry, 2018, 20, 1612-1620.	9.0	39
40	Temperature-Dependent Lipid Extraction from Membranes by Boron Nitride Nanosheets. ACS Nano, 2018, 12, 2764-2772.	14.6	44
41	Synthesis and biological evaluation of aminothiazoles against Histoplasma capsulatum and Cryptococcus neoformans. Bioorganic and Medicinal Chemistry, 2018, 26, 2251-2261.	3.0	6
42	Effects of carotenoids on lipid bilayers. Physical Chemistry Chemical Physics, 2018, 20, 3795-3804.	2.8	19
43	Ordering of lipid membranes altered by boron nitride nanosheets. Physical Chemistry Chemical Physics, 2018, 20, 3903-3910.	2.8	22
44	Neutron scattering in the biological sciences: progress and prospects. Acta Crystallographica Section D: Structural Biology, 2018, 74, 1129-1168.	2.3	47
45	Structural investigation of the enantioselectivity and thermostability mechanisms of esterase RhEst1. Journal of Molecular Graphics and Modelling, 2018, 85, 182-189.	2.4	6
46	Lipid extraction by boron nitride nanosheets from liquid-ordered and liquid-disordered nanodomains. Nanoscale, 2018, 10, 14073-14081.	5.6	6
47	The Effect of Organophosphate (OP)â€Induced Structural Changes in Acetylcholinesterase on Kinetics of OP Inhibition and Oxime Reactivation. FASEB Journal, 2018, 32, 526.40.	0.5	0
48	Dynamics of Organophosphateâ€Induced Structural Changes in Acetylcholinesterase Revealed by Timeâ€Resolved Smallâ€Angle Xâ€Ray Scattering and Inelastic Neutron Scattering. FASEB Journal, 2018, 32, 527.7.	0.5	0
49	Crystallographic studies of human acetylcholinesterase inhibition by organophosphates and reactivation by oximes. FASEB Journal, 2018, 32, 527.10.	0.5	0
50	Quasielastic neutron scattering in biology: Theory and applications. Biochimica Et Biophysica Acta - General Subjects, 2017, 1861, 3638-3650.	2.4	15
51	The tilt-dependent potential of mean force of a pair of DNA oligomers from all-atom molecular dynamics simulations. Journal of Physics Condensed Matter, 2017, 29, 084002.	1.8	8
52	Description of Hydration Water in Protein (GFP) Solution. Biophysical Journal, 2017, 112, 201a.	0.5	1
53	Probing the structural requirements of polybasic peptides for effective and specific amyloid reactivity. Amyloid: the International Journal of Experimental and Clinical Investigation: the Official Journal of the International Society of Amyloidosis, 2017, 24, 30-31.	3.0	22
54	Bacillus subtilis Lipid Extract, A Branched-Chain Fatty Acid Model Membrane. Journal of Physical Chemistry Letters, 2017, 8, 4214-4217.	4.6	42

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55	Structural relaxation, viscosity, and network connectivity in a hydrogen bonding liquid. Physical Chemistry Chemical Physics, 2017, 19, 25859-25869.	2.8	22
56	Modeling of the Passive Permeation of Mercury and Methylmercury Complexes Through a Bacterial Cytoplasmic Membrane. Environmental Science & Technology, 2017, 51, 10595-10604.	10.0	15
57	Organosolv-Water Cosolvent Phase Separation on Cellulose and its Influence on the Physical Deconstruction of Cellulose: A Molecular Dynamics Analysis. Scientific Reports, 2017, 7, 14494.	3.3	29
58	Serendipitous inhibition of AÎ² and rVÎ»6Wil amyloid fibril growth by bi-functional peptides. Amyloid: the International Journal of Experimental and Clinical Investigation: the Official Journal of the International Society of Amyloidosis, 2017, 24, 32-33.	3.0	0
59	Description of Hydration Water in Protein (Green Fluorescent Protein) Solution. Journal of the American Chemical Society, 2017, 139, 1098-1105.	13.7	68
60	The in vivo structure of biological membranes and evidence for lipid domains. PLoS Biology, 2017, 15, e2002214.	5.6	123
61	Structure and Function of Photosystem Iâ€“[FeFe] Hydrogenase Protein Fusions: An All-Atom Molecular Dynamics Study. Journal of Physical Chemistry B, 2016, 120, 599-609.	2.6	10
62	Behavior of Bilayer Leaflets in Asymmetric Model Membranes: Atomistic Simulation Studies. Journal of Physical Chemistry B, 2016, 120, 8438-8448.	2.6	19
63	Morphology-Induced Defects Enhance Lipid Transfer Rates. Langmuir, 2016, 32, 9757-9764.	3.5	11
64	Generalized Ensemble Sampling of Enzyme Reaction Free Energy Pathways. Methods in Enzymology, 2016, 577, 57-74.	1.0	3
65	Secondary structure propensity and chirality of the amyloidophilic peptide p5 and its analogues impacts ligand binding - In vitro characterization. Biochemistry and Biophysics Reports, 2016, 8, 89-99.	1.3	9
66	Local Phase Separation of Co-solvents Enhances Pretreatment of Biomass for Bioenergy Applications. Journal of the American Chemical Society, 2016, 138, 10869-10878.	13.7	89
67	Limitations in current acetylcholinesterase structureâ€“based design of oxime antidotes for organophosphate poisoning. Annals of the New York Academy of Sciences, 2016, 1378, 41-49.	3.8	17
68	Relative Binding Affinities of Monolignols to Horseradish Peroxidase. Journal of Physical Chemistry B, 2016, 120, 7635-7640.	2.6	6
69	Determination of functional collective motions in a protein at atomic resolution using coherent neutron scattering. Science Advances, 2016, 2, e1600886.	10.3	30
70	Comparative exploration of hydrogen sulfide and water transmembrane free energy surfaces via orthogonal space tempering free energy sampling. Journal of Computational Chemistry, 2016, 37, 567-574.	3.3	11
71	Theoretical Study of the Initial Stages of Self-Assembly of a Carboxysomeâ€™s Facet. ACS Nano, 2016, 10, 5751-5758.	14.6	19
72	Enhanced sampling simulation analysis of the structure of lignin in the THFâ€“water miscibility gap. Physical Chemistry Chemical Physics, 2016, 18, 6394-6398.	2.8	24

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73	Molecular Driving Forces behind the Tetrahydrofuranâ€“Water Miscibility Gap. Journal of Physical Chemistry B, 2016, 120, 740-747.	2.6	30
74	The dynamics of single protein molecules is non-equilibrium and self-similar over thirteen decades in time. Nature Physics, 2016, 12, 171-174.	16.7	140
75	Cosolvent pretreatment in cellulosic biofuel production: effect of tetrahydrofuran-water on lignin structure and dynamics. Green Chemistry, 2016, 18, 1268-1277.	9.0	122
76	Preclinical Validation of the Heparin-Reactive Peptide p5+14 as a Molecular Imaging Agent for Visceral Amyloidosis. Molecules, 2015, 20, 7657-7682.	3.8	30
77	Molecular dynamics simulation studies of the wild type and E92Q/N155H mutant of Elvitegravir-resistance HIV-1 integrase. Interdisciplinary Sciences, Computational Life Sciences, 2015, 7, 36-42.	3.6	9
78	Molecular Dynamics Investigation of the Substrate Binding Mechanism in Carboxylesterase. Biochemistry, 2015, 54, 1841-1848.	2.5	25
79	Lateral organization, bilayer asymmetry, and inter-leaflet coupling of biological membranes. Chemistry and Physics of Lipids, 2015, 192, 87-99.	3.2	104
80	Interactions of the Anticancer Drug Tamoxifen with Lipid Membranes. Biophysical Journal, 2015, 108, 2492-2501.	0.5	55
81	Mechanical Properties of Nanoscopic Lipid Domains. Journal of the American Chemical Society, 2015, 137, 15772-15780.	13.7	108
82	Rational design of a carboxylic esterase RhEst1 based on computational analysis of substrate binding. Journal of Molecular Graphics and Modelling, 2015, 62, 319-324.	2.4	8
83	Structural and mechanical properties of cardiolipin lipid bilayers determined using neutron spin echo, small angle neutron and X-ray scattering, and molecular dynamics simulations. Soft Matter, 2015, 11, 130-138.	2.7	65
84	The Role of Histone Tails in the Nucleosome: A Computational Study. Biophysical Journal, 2014, 107, 2911-2922.	0.5	70
85	Simulation of a cellulose fiber in ionic liquid suggests a synergistic approach to dissolution. Cellulose, 2014, 21, 983-997.	4.9	58
86	The molecular structure of a phosphatidylserine bilayer determined by scattering and molecular dynamics simulations. Soft Matter, 2014, 10, 3716.	2.7	84
87	Coarse-Grain Model for Natural Cellulose Fibrils in Explicit Water. Journal of Physical Chemistry B, 2014, 118, 3026-3034.	2.6	22
88	Structure and Dynamics of a Compact State of a Multidomain Protein, the Mercuric Ion Reductase. Biophysical Journal, 2014, 107, 393-400.	0.5	19
89	Replica-Exchange Molecular Dynamics Simulations of Cellulose Solvated in Water and in the Ionic Liquid 1-Butyl-3-Methylimidazolium Chloride. Journal of Physical Chemistry B, 2014, 118, 11037-11049.	2.6	29
90	Simulation analysis of the cellulase Cel7A carbohydrate binding module on the surface of the cellulose Iβ. Cellulose, 2014, 21, 951-971.	4.9	19

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91	All-Atom Molecular Dynamics Simulation of a Photosystem I/Detergent Complex. Journal of Physical Chemistry B, 2014, 118, 11633-11645.	2.6	13
92	Analysis of the solution structure of Thermosynechococcus elongatus photosystem I in n-dodecyl-Î²-d-maltoside using small-angle neutron scattering and molecular dynamics simulation. Archives of Biochemistry and Biophysics, 2014, 550-551, 50-57.	3.0	23
93	Enantioselective Electrophilic Trifluoromethylthiolation of Î²â€Ketoesters: A Case of Reactivity and Selectivity Bias for Organocatalysis. Angewandte Chemie - International Edition, 2013, 52, 12860-12864.	13.8	203
94	AFMPB: An adaptive fast multipole Poissonâ€“Boltzmann solver for calculating electrostatics in biomolecular systems. Computer Physics Communications, 2013, 184, 2618-2619.	7.5	5
95	Ab Initio Study of Molecular Interactions in Cellulose Iβ. Journal of Physical Chemistry B, 2013, 117, 10430-10443.	2.6	22
96	Synthesis, docking, and biological studies of phenanthrene Î²-diketo acids as novel HIV-1 integrase inhibitors. Bioorganic and Medicinal Chemistry Letters, 2013, 23, 6146-6151.	2.2	35
97	Impact of Resistance Mutations on Inhibitor Binding to HIV-1 Integrase. Journal of Chemical Information and Modeling, 2013, 53, 3297-3307.	5.4	14
98	Mathematical and Numerical Aspects of the Adaptive Fast Multipole Poisson-Boltzmann Solver. Communications in Computational Physics, 2013, 13, 107-128.	1.7	12
99	Surface Hydration Amplifies Single-Well Protein Atom Diffusion Propagating into the Macromolecular Core. Physical Review Letters, 2012, 108, 238102.	7.8	45
100	Interactions between Ether Phospholipids and Cholesterol As Determined by Scattering and Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2012, 116, 14829-14838.	2.6	36
101	Molecular Dynamics. Methods in Molecular Biology, 2012, 929, 243-285.	0.9	36
102	A Solvent-Free Coarse Grain Model for Crystalline and Amorphous Cellulose Fibrils. Journal of Chemical Theory and Computation, 2011, 7, 2539-2548.	5.3	52
103	AFMPB: An adaptive fast multipole Poissonâ€“Boltzmann solver for calculating electrostatics in biomolecular systems. Computer Physics Communications, 2010, 181, 1150-1160.	7.5	42
104	Atomistic Simulation of Lignocellulosic Biomass and Associated Cellulosomal Protein Complexes. ACS Symposium Series, 2010, , 55-73.	0.5	4
105	Molecular-Dynamics Simulations of ELICâ€”a Prokaryotic Homologue of the Nicotinic Acetylcholine Receptor. Biophysical Journal, 2009, 96, 4502-4513.	0.5	36
106	An Explicit, Multi-Factor Credit Default Swap Pricing Model with Correlated Factors. Journal of Financial and Quantitative Analysis, 2008, 43, 123-160.	3.5	53
107	Improved Conformational Sampling through an Efficient Combination of Mean-Field Simulation Approaches. Journal of Physical Chemistry B, 2004, 108, 426-437.	2.6	20
108	Lines of communication within and between catalytic subunits of human acetylcholinesterase revealed by cryo- and room-temperature X-ray crystallography and by Small Angle X-ray Scattering (SAXS). , 0, , .		0

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109	Accelerating structure-based design of rapid uncharged reactivators of organophosphate-inhibited human acetylcholinesterase by joint X-ray/neutron mechanistic studies. , 0, , .		0