Ray Luo

List of Publications by Year
in descending order

131 papers	17,605 citations	61984 43 h-index	13771 129 g-index
135 all docs	135 docs citations	135 times ranked	18330 citing authors

#	Article	IF	Citations
1	The Hippo pathway kinases LATS1 and LATS2 attenuate cellular responses to heavy metals through phosphorylating MTF1. Nature Cell Biology, 2022, 24, 74-87.	10.3	22
2	Motif-dependent immune co-receptor interactome profiling by photoaffinity chemical proteomics. Cell Chemical Biology, 2022, 29, 1024-1036.e5.	5.2	8
3	Stress tensor and constant pressure simulation for polarizable Gaussian multipole model. Journal of Chemical Physics, 2022, 156, 114114.	3.0	10
4	Heparin-Assisted Amyloidogenesis Uncovered through Molecular Dynamics Simulations. ACS Omega, 2022, 7, 15132-15144.	3.5	7
5	PyRESP: A Program for Electrostatic Parameterizations of Additive and Induced Dipole Polarizable Force Fields. Journal of Chemical Theory and Computation, 2022, 18, 3654-3670.	5.3	12
6	Engineering Embdenâ€“Meyerhofâ€“Parnas Glycolysis to Generate Noncanonical Reducing Power. ACS Catalysis, 2022, 12, 8582-8592.	11.2	5
7	Development of a Pantetheine Force Field Library for Molecular Modeling. Journal of Chemical Information and Modeling, 2021, 61, 856-868.	5.4	11
8	Recent Force Field Strategies for Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2021, 61, 1037-1047.	5.4	67
9	Estimating the Roles of Protonation and Electronic Polarization in Absolute Binding Affinity Simulations. Journal of Chemical Theory and Computation, 2021, 17, 2541-2555.	5.3	11
10	Recent Developments in Free Energy Calculations for Drug Discovery. Frontiers in Molecular Biosciences, 2021, 8, 712085.	3.5	56
11	Machine-Learned Molecular Surface and Its Application to Implicit Solvent Simulations. Journal of Chemical Theory and Computation, 2021, 17, 6214-6224.	5.3	4
12	Growth-Based, High-Throughput Selection for NADH Preference in an Oxygen-Dependent Biocatalyst. ACS Synthetic Biology, 2021, 10, 2359-2370.	3.8	10
13	A 2,3-dialkoxynaphthalene-based naphthocage. Chemical Communications, 2020, 56, 888-891.	4.1	11
14	Elucidation of <scp>WW</scp> domain ligand binding specificities in the Hippo pathway reveals <scp>STXBP</scp> 4 as <scp>YAP</scp> inhibitor. EMBO Journal, 2020, 39, e102406.	7.8	23
15	In Vivo, High-Throughput Selection of Thermostable Cyclohexanone Monooxygenase (CHMO). Catalysts, 2020, 10, 935.	3.5	2
16	Efficient formulation of polarizable Gaussian multipole electrostatics for biomolecular simulations. Journal of Chemical Physics, 2020, 153, 114116.	3.0	19
17	Molecular Basis for Polyketide Ketoreductaseâ€“Substrate Interactions. International Journal of Molecular Sciences, 2020, 21, 7562.	4.1	12
18	Leveraging Oxidative Stress to Regulate Redox Balance-Based, In Vivo Growth Selections for Oxygenase Engineering. ACS Synthetic Biology, 2020, 9, 3124-3133.	3.8	10

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19	Environment-Specific Force Field for Intrinsically Disordered and Ordered Proteins. Journal of Chemical Information and Modeling, 2020, 60, 2257-2267.	5.4	55
20	Well-Balanced Force Field ff03CMAP for Folded and Disordered Proteins. Journal of Chemical Theory and Computation, 2019, 15, 6769-6780.	5.3	43
21	Extensive tests and evaluation of the CHARMM36IDPSFF force field for intrinsically disordered proteins and folded proteins. Physical Chemistry Chemical Physics, 2019, 21, 21918-21931.	2.8	37
22	Improved Poissonâ€“Boltzmann Methods for High-Performance Computing. Journal of Chemical Theory and Computation, 2019, 15, 6190-6202.	5.3	10
23	Molecular basis for interactions between an acyl carrier protein and a ketosynthase. Nature Chemical Biology, 2019, 15, 669-671.	8.0	41
24	Heterogeneous Dielectric Implicit Membrane Model for the Calculation of MMPBSA Binding Free Energies. Journal of Chemical Information and Modeling, 2019, 59, 3041-3056.	5.4	27
25	Computational structural enzymology methodologies for the study and engineering of fatty acid synthases, polyketide synthases and nonribosomal peptide synthetases. Methods in Enzymology, 2019, 622, 375-409.	1.0	11
26	Dynamical important residue network (DIRN): network inference via conformational change. Bioinformatics, 2019, 35, 4664-4670.	4.1	12
27	An efficient secondâ€order poissonâ€“boltzmann method. Journal of Computational Chemistry, 2019, 40, 1257-1269.	3.3	7
28	Development of Polarizable Gaussian Model for Molecular Mechanical Calculations I: Atomic Polarizability Parameterization To Reproduce ab Initio Anisotropy. Journal of Chemical Theory and Computation, 2019, 15, 1146-1158.	5.3	26
29	Robustness and Efficiency of Poissonâ€“Boltzmann Modeling on Graphics Processing Units. Journal of Chemical Information and Modeling, 2019, 59, 409-420.	5.4	9
30	Computational Analysis for the Rational Design of Anti-Amyloid Beta (AÎ²) Antibodies. Journal of Physical Chemistry B, 2018, 122, 4521-4536.	2.6	8
31	An Oxetane-Based Polyketide Surrogate To Probe Substrate Binding in a Polyketide Synthase. Journal of the American Chemical Society, 2018, 140, 4961-4964.	13.7	21
32	Engineering a Coenzyme A Detour To Expand the Product Scope and Enhance the Selectivity of the Ehrlich Pathway. ACS Synthetic Biology, 2018, 7, 2758-2764.	3.8	1
33	Regulation of the Hippo Pathway by Phosphatidic Acid-Mediated Lipid-Protein Interaction. Molecular Cell, 2018, 72, 328-340.e8.	9.7	74
34	Computational Studies of Intrinsically Disordered Proteins. Journal of Physical Chemistry B, 2018, 122, 10455-10469.	2.6	24
35	Improved Accuracy and Convergence of Intrinsically Disordered Protein Molecular Dynamics Simulations Using the ff14IDPSFF Force Field. Biophysical Journal, 2018, 114, 432a.	0.5	1
36	Intrinsically disordered proteinâ€specific force field <scp>CHARMM</scp>36<scp>IDPSFF</scp>. Chemical Biology and Drug Design, 2018, 92, 1722-1735.	3.2	62

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37	Development of a High-Throughput, In Vivo Selection Platform for NADPH-Dependent Reactions Based on Redox Balance Principles. ACS Synthetic Biology, 2018, 7, 1715-1721.	3.8	33
38	Order-disorder transition of intrinsically disordered kinase inducible transactivation domain of CREB. Journal of Chemical Physics, 2018, 148, 225101.	3.0	5
39	Crystal Structure of StnA for the Biosynthesis of Antitumor Drug Streptonigrin Reveals a Unique Substrate Binding Mode. Scientific Reports, 2017, 7, 40254.	3.3	5
40	The IDP-Specific Force Field ff14IDPSFF Improves the Conformer Sampling of Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2017, 57, 1166-1178.	5.4	157
41	Allosteric Autoinhibition Pathway in Transcription Factor ERG: Dynamics Network and Mutant Experimental Evaluations. Journal of Chemical Information and Modeling, 2017, 57, 1153-1165.	5.4	12
42	A Continuum Poissonâ€“Boltzmann Model for Membrane Channel Proteins. Journal of Chemical Theory and Computation, 2017, 13, 3398-3412.	5.3	19
43	Conformation dynamics of the intrinsically disordered protein c-Myb with the ff99IDPs force field. RSC Advances, 2017, 7, 29713-29721.	3.6	17
44	Numerical interpretation of molecular surface field in dielectric modeling of solvation. Journal of Computational Chemistry, 2017, 38, 1057-1070.	3.3	10
45	Ionic Solution: What Goes Right and Wrong with Continuum Solvation Modeling. Journal of Physical Chemistry B, 2017, 121, 11169-11179.	2.6	9
46	Acceleration of Linear Finite-Difference Poissonâ€“Boltzmann Methods on Graphics Processing Units. Journal of Chemical Theory and Computation, 2017, 13, 3378-3387.	5.3	13
47	Allosteric pathways in tetrahydrofolate sensing riboswitch with dynamics correlation network. Molecular BioSystems, 2017, 13, 156-164.	2.9	6
48	ff14IDPs force field improving the conformation sampling of intrinsically disordered proteins. Chemical Biology and Drug Design, 2017, 89, 5-15.	3.2	67
49	Exploring a multi-scale method for molecular simulation in continuum solvent model: Explicit simulation of continuum solvent as an incompressible fluid. Journal of Chemical Physics, 2017, 147, 214112.	3.0	3
50	Recent Developments and Applications of the MMPBSA Method. Frontiers in Molecular Biosciences, 2017, 4, 87.	3.5	374
51	Dynamics Correlation Network for Allosteric Switching of PreQ1 Riboswitch. Scientific Reports, 2016, 6, 31005.	3.3	24
52	Synergistic Allosteric Mechanism of Fructose-1,6-bisphosphate and Serine for Pyruvate Kinase M2 via Dynamics Fluctuation Network Analysis. Journal of Chemical Information and Modeling, 2016, 56, 1184-1192.	5.4	33
53	Calculating proteinâ€“ligand binding affinities with MMPBSA: Method and error analysis. Journal of Computational Chemistry, 2016, 37, 2436-2446.	3.3	169
54	Modeling Membrane Proteinâ€“Ligand Binding Interactions: The Human Purinergic Platelet Receptor. Journal of Physical Chemistry B, 2016, 120, 12293-12304.	2.6	24

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55	Synergistic Modification Induced Specific Recognition between Histone and TRIM24 via Fluctuation Correlation Network Analysis. Scientific Reports, 2016, 6, 24587.	3.3	15
56	Charge Central Interpretation of the Full Nonlinear PB Equation: Implications for Accurate and Scalable Modeling of Solvation Interactions. Journal of Physical Chemistry B, 2016, 120, 8707-8721.	2.6	8
57	Structural Insights into Anthranilate Priming during Type II Polyketide Biosynthesis. ACS Chemical Biology, 2016, 11, 95-103.	3.4	25
58	Recognition Mechanism between Lac Repressor and DNA with Correlation Network Analysis. Journal of Physical Chemistry B, 2015, 119, 2844-2856.	2.6	12
59	Comprehensive Structural and Biochemical Analysis of the Terminal Myxalamid Reductase Domain for the Engineered Production of Primary Alcohols. Chemistry and Biology, 2015, 22, 1018-1029.	6.0	56
60	A semi-implicit augmented IIM for Navierâ€“Stokes equations with open, traction, or free boundary conditions. Journal of Computational Physics, 2015, 297, 182-193.	3.8	10
61	Test and Evaluation of ff99IDPs Force Field for Intrinsically Disordered Proteins. Journal of Chemical Information and Modeling, 2015, 55, 1021-1029.	5.4	68
62	Applications of MMPBSA to Membrane Proteins I: Efficient Numerical Solutions of Periodic Poissonâ€“Boltzmann Equation. Journal of Chemical Information and Modeling, 2015, 55, 2187-2199.	5.4	27
63	Biological applications of classical electrostatics methods. Journal of Theoretical and Computational Chemistry, 2014, 13, 1440008.	1.8	16
64	Recent progress in adapting Poissonâ€“Boltzmann methods to molecular simulations. Journal of Theoretical and Computational Chemistry, 2014, 13, 1430001.	1.8	25
65	New Force Field on Modeling Intrinsically Disordered Proteins. Chemical Biology and Drug Design, 2014, 84, 253-269.	3.2	110
66	Specific Recognition Mechanism between RNA and the KH3 Domain of Nova-2 Protein. Journal of Physical Chemistry B, 2014, 118, 12426-12434.	2.6	7
67	A multi-scale method for dynamics simulation in continuum solvent models. I: Finite-difference algorithm for Navierâ€“Stokes equation. Chemical Physics Letters, 2014, 616-617, 67-74.	2.6	11
68	Numerical Poissonâ€“Boltzmann model for continuum membrane systems. Chemical Physics Letters, 2013, 555, 274-281.	2.6	26
69	Electrostatic forces in the Poisson-Boltzmann systems. Journal of Chemical Physics, 2013, 139, 094106.	3.0	27
70	Exploring a charge-central strategy in the solution of Poisson's equation for biomolecular applications. Physical Chemistry Chemical Physics, 2013, 15, 129-141.	2.8	17
71	Kink turn sRNA folding upon L7Ae binding using molecular dynamics simulations. Physical Chemistry Chemical Physics, 2013, 15, 18510.	2.8	13
72	Exploring accurate Poissonâ€“Boltzmann methods for biomolecular simulations. Computational and Theoretical Chemistry, 2013, 1024, 34-44.	2.5	35

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73	Conformational Selection and Induced Fit in Specific Antibody and Antigen Recognition: SPE7 as a Case Study. Journal of Physical Chemistry B, 2013, 117, 4912-4923.	2.6	36
74	Poissonâ€“Boltzmann Implicit Solvation Models. Annual Reports in Computational Chemistry, 2012, , 149-162.	1.7	12
75	Dielectric pressure in continuum electrostatic solvation of biomolecules. Physical Chemistry Chemical Physics, 2012, 14, 15917.	2.8	26
76	Reducing Grid Dependence in Finite-Difference Poissonâ€“Boltzmann Calculations. Journal of Chemical Theory and Computation, 2012, 8, 2741-2751.	5.3	58
77	Development of Polarizable Models for Molecular Mechanical Calculations. 3. Polarizable Water Models Conforming to Thole Polarization Screening Schemes. Journal of Physical Chemistry B, 2012, 116, 7999-8008.	2.6	49
78	Development of Polarizable Models for Molecular Mechanical Calculations. 4. van der Waals Parametrization. Journal of Physical Chemistry B, 2012, 116, 7088-7101.	2.6	60
79	Atomistic Mechanism of MicroRNA Translation Upregulation via Molecular Dynamics Simulations. PLoS ONE, 2012, 7, e43788.	2.5	13
80	Development of Polarizable Models for Molecular Mechanical Calculations II: Induced Dipole Models Significantly Improve Accuracy of Intermolecular Interaction Energies. Journal of Physical Chemistry B, 2011, 115, 3100-3111.	2.6	116
81	On-the-Fly Numerical Surface Integration for Finite-Difference Poissonâ€“Boltzmann Methods. Journal of Chemical Theory and Computation, 2011, 7, 3608-3619.	5.3	24
82	Development of Polarizable Models for Molecular Mechanical Calculations I: Parameterization of Atomic Polarizability. Journal of Physical Chemistry B, 2011, 115, 3091-3099.	2.6	137
83	Dielectric boundary force in numerical Poissonâ€“Boltzmann methods: Theory and numerical strategies. Chemical Physics Letters, 2011, 514, 368-373.	2.6	30
84	Exploring a coarse-grained distributive strategy for finite-difference Poissonâ€“Boltzmann calculations. Journal of Molecular Modeling, 2011, 17, 1985-1996.	1.8	13
85	Virtual screening using molecular simulations. Proteins: Structure, Function and Bioinformatics, 2011, 79, 1940-1951.	2.6	171
86	Assessment of linear finiteâ€difference Poissonâ€“Boltzmann solvers. Journal of Computational Chemistry, 2010, 31, 1689-1698.	3.3	73
87	A Revised Density Function for Molecular Surface Calculation in Continuum Solvent Models. Journal of Chemical Theory and Computation, 2010, 6, 1157-1169.	5.3	28
88	Performance of Nonlinear Finite-Difference Poissonâ^'Boltzmann Solvers. Journal of Chemical Theory and Computation, 2010, 6, 203-211.	5.3	89
89	Balancing Simulation Accuracy and Efficiency with the Amber United Atom Force Field. Journal of Physical Chemistry B, 2010, 114, 2886-2893.	2.6	8
90	Widespread but Small-Scale Changes in the Structural and Dynamic Properties of Vaccinia Virus Poly(A) Polymerase upon Association with Its Processivity Factor in Solution. Biochemistry, 2010, 49, 6247-6262.	2.5	4

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91	Quantitative analysis of Poissonâ€“Boltzmann implicit solvent in molecular dynamics. Physical Chemistry Chemical Physics, 2010, 12, 1194-1202.	2.8	43
92	On removal of charge singularity in Poissonâ€“Boltzmann equation. Journal of Chemical Physics, 2009, 130, 145101.	3.0	47
93	Structural and functional implications of p53 missense cancer mutations. PMC Biophysics, 2009, 2, 5.	2.3	17
94	Achieving energy conservation in Poissonâ€“Boltzmann molecular dynamics: Accuracy and precision with finite-difference algorithms. Chemical Physics Letters, 2009, 468, 112-118.	2.6	50
95	Molecular mechanisms of functional rescue mediated by P53 tumor suppressor mutations. Biophysical Chemistry, 2009, 145, 37-44.	2.8	10
96	Roles of Boundary Conditions in DNA Simulations: Analysis of Ion Distributions with the Finite-Difference Poisson-Boltzmann Method. Biophysical Journal, 2009, 97, 554-562.	0.5	26
97	Impact of low-frequency hotspot mutation R282Q on the structure of p53 DNA-binding domain as revealed by crystallography at 1.54â€…Ã… resolution. Acta Crystallographica Section D: Biological Crystallography, 2008, 64, 471-477.	2.5	8
98	All-Atom Computer Simulations of Amyloid Fibrils Disaggregation. Biophysical Journal, 2008, 95, 5037-5047.	0.5	29
99	Protein Stability Prediction:â€‰ A Poissonâ^'Boltzmann Approach. Journal of Physical Chemistry B, 2008, 112, 1875-1883.	2.6	20
100	Continuum Polarizable Force Field within the Poissonâ^'Boltzmann Framework. Journal of Physical Chemistry B, 2008, 112, 7675-7688.	2.6	26
101	Inhibition Kinetics and Emodin Cocrystal Structure of a Type II Polyketide Ketoreductase[,]. Biochemistry, 2008, 47, 1837-1847.	2.5	57
102	Continuum treatment of electronic polarization effect. Journal of Chemical Physics, 2007, 126, 094103.	3.0	20
103	Implicit Nonpolar Solvent Models. Journal of Physical Chemistry B, 2007, 111, 12263-12274.	2.6	206
104	Binding Induced Folding in p53â^'MDM2 Complex. Journal of the American Chemical Society, 2007, 129, 2930-2937.	13.7	107
105	Molecular Dynamics Simulations of p53 DNA-Binding Domain. Journal of Physical Chemistry B, 2007, 111, 11538-11545.	2.6	60
106	New-Generation Amber United-Atom Force Field. Journal of Physical Chemistry B, 2006, 110, 13166-13176.	2.6	176
107	How Well Does Poissonâ^'Boltzmann Implicit Solvent Agree with Explicit Solvent? A Quantitative Analysis. Journal of Physical Chemistry B, 2006, 110, 18680-18687.	2.6	153
108	Force field influences in Î²-hairpin folding simulations. Protein Science, 2006, 15, 2642-2655.	7.6	63

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109	Is Poisson-Boltzmann theory insufficient for protein folding simulations?. Journal of Chemical Physics, 2006, 124, 034902.	3.0	44
110	Functional Census of Mutation Sequence Spaces: The Example of p53 Cancer Rescue Mutants. IEEE/ACM Transactions on Computational Biology and Bioinformatics, 2006, 3, 114-125.	3.0	28
111	The Amber biomolecular simulation programs. Journal of Computational Chemistry, 2005, 26, 1668-1688.	3.3	7,742
112	Overcoming entropic barrier with coupled sampling at dual resolutions. Journal of Chemical Physics, 2005, 123, 194904.	3.0	49
113	Enhanced ab initio protein folding simulations in Poissonâ€“Boltzmann molecular dynamics with self-guiding forces. Journal of Molecular Graphics and Modelling, 2004, 22, 415-424.	2.4	46
114	Physical scoring function based on AMBER force field and Poisson-Boltzmann implicit solvent for protein structure prediction. Proteins: Structure, Function and Bioinformatics, 2004, 56, 475-486.	2.6	46
115	Interplay of secondary structures and side-chain contacts in the denatured state of BBA1. Journal of Chemical Physics, 2004, 121, 2412-2421.	3.0	20
116	A point-charge force field for molecular mechanics simulations of proteins based on condensed-phase quantum mechanical calculations. Journal of Computational Chemistry, 2003, 24, 1999-2012.	3.3	4,028
117	A Poissonâ€“Boltzmann dynamics method with nonperiodic boundary condition. Journal of Chemical Physics, 2003, 119, 11035-11047.	3.0	155
118	Accelerated Poisson-Boltzmann calculations for static and dynamic systems. Journal of Computational Chemistry, 2002, 23, 1244-1253.	3.3	421
119	Interpreting trends in the binding of cyclic ureas to HIV-1 protease. Journal of Molecular Biology, 2001, 309, 507-517.	4.2	39
120	The Physical Basis of Nucleic Acid Base Stacking in Water. Biophysical Journal, 2001, 80, 140-148.	0.5	87
121	An Analysis of the Interactions between the Semâ”5 SH3 Domain and Its Ligands Using Molecular Dynamics, Free Energy Calculations, and Sequence Analysis. Journal of the American Chemical Society, 2001, 123, 3986-3994.	13.7	130
122	Ligand-receptor docking with the Mining Minima optimizer. Journal of Computer-Aided Molecular Design, 2001, 15, 157-171.	2.9	51
123	Comparison of generalized born and poisson models: Energetics and dynamics of HIV protease. Journal of Computational Chemistry, 2000, 21, 295-309.	3.3	98
124	Modeling Molecular Recognition: Theory and Application. Journal of Biomolecular Structure and Dynamics, 2000, 17, 89-94.	3.5	5
125	Synthetic Adenine Receptors:Â Direct Calculation of Binding Affinity and Entropy. Journal of the American Chemical Society, 2000, 122, 2934-2937.	13.7	49
126	Nucleic acid base-pairing and N-methylacetamide self-association in chloroform: affinity and conformation. Biophysical Chemistry, 1999, 78, 183-193.	2.8	36

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127	Strength of Solvent-Exposed Salt-Bridges. Journal of Physical Chemistry B, 1999, 103, 727-736.	2.6	71
128	Computational Study of KNI-272, a Potent Inhibitor of HIV-1 Protease: On the Mechanism of Preorganization. Journal of Physical Chemistry B, 1999, 103, 1031-1044.	2.6	19
129	pKaShifts in Small Molecules and HIV Protease:Â Electrostatics and Conformation. Journal of the American Chemical Society, 1998, 120, 6138-6146.	13.7	55
130	Dielectric Screening Treatment of Electrostatic Solvation. Journal of Physical Chemistry B, 1997, 101, 11226-11236.	2.6	37
131	Confronting the problem of interconnected structural changes in the comparative modeling of proteins. Proteins: Structure, Function and Bioinformatics, 1995, 23, 327-336.	2.6	25