## Yun Luo

## List of Publications by Year in descending order

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58 papers	1,248 citations	567281 15 h-index	395702 33 g-index
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74 all docs	74 docs citations	74 times ranked	2237 citing authors

#	Article	IF	CITATIONS
1	Simulations of Anionic Lipid Membranes: Development of Interaction-Specific Ion Parameters and Validation Using NMR Data. Journal of Physical Chemistry B, 2013, 117, 10183-10192.	2.6	181
2	A mechanism for the activation of the mechanosensitive Piezo1 channel by the small molecule Yoda1. Nature Communications, 2019, 10, 4503.	12.8	136
3	Generalized scalable multiple copy algorithms for molecular dynamics simulations in NAMD. Computer Physics Communications, 2014, 185, 908-916.	7.5	115
4	Probing the gating mechanism of the mechanosensitive channel Piezo1 with the small molecule Yoda1. Nature Communications, 2018, 9, 2029.	12.8	104
5	UBE3A Regulates Synaptic Plasticity and Learning and Memory by Controlling SK2 Channel Endocytosis. Cell Reports, 2015, 12, 449-461.	6.4	101
6	Calculation of Free Energy Landscape in Multi-Dimensions with Hamiltonian-Exchange Umbrella Sampling on Petascale Supercomputer. Journal of Chemical Theory and Computation, 2012, 8, 4672-4680.	5.3	89
7	Mechanism of gating by calcium in connexin hemichannels. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E7986-E7995.	7.1	75
8	PRMT1-mediated FLT3 arginine methylation promotes maintenance of FLT3-ITD+ acute myeloid leukemia. Blood, 2019, 134, 548-560.	1.4	58
9	Can Relative Binding Free Energy Predict Selectivity of Reversible Covalent Inhibitors?. Journal of the American Chemical Society, 2017, 139, 17945-17952.	13.7	44
10	Molecular Mechanism of Resveratrol's Lipid Membrane Protection. Scientific Reports, 2018, 8, 1587.	3.3	37
11	Ranking Reversible Covalent Drugs: From Free Energy Perturbation to Fragment Docking. Journal of Chemical Information and Modeling, 2019, 59, 2093-2102.	5.4	35
12	Crowding-induced opening of the mechanosensitive Piezo1 channel in silico. Communications Biology, 2021, 4, 84.	4.4	35
13	Robust Determination of Protein Allosteric Signaling Pathways. Journal of Chemical Theory and Computation, 2019, 15, 2116-2126.	5.3	33
14	Targeting PRMT1-mediated FLT3 methylation disrupts maintenance of MLL-rearranged acute lymphoblastic leukemia. Blood, 2019, 134, 1257-1268.	1.4	30
15	Computational Studies of Molecular Permeation through Connexin26 Channels. Biophysical Journal, 2016, 110, 584-599.	0.5	17
16	Effects of bioactive constituents in the Traditional Chinese Medicinal formula Si–Wu–Tang on Nrf2 signaling and neoplastic cellular transformation. Phytomedicine, 2018, 40, 1-9.	5.3	17
17	Ginsenoside Rg1 prevents early diabetic retinopathy via reducing retinal ganglion cell layer and inner nuclear layer cell apoptosis in db/db mice. Annals of Translational Medicine, 2020, 8, 232-232.	1.7	17
18	Polymodal allosteric regulation of Type 1 Serine/Threonine Kinase Receptors via a conserved electrostatic lock. PLoS Computational Biology, 2017, 13, e1005711.	3.2	16

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19	The connexin26 human mutation N14K disrupts cytosolic intersubunit interactions and promotes channel opening. Journal of General Physiology, 2019, 151, 328-341.	1.9	16
20	Mechanism-Based and Computational-Driven Covalent Drug Design. Journal of Chemical Information and Modeling, 2021, 61, 5307-5311.	5.4	12
21	Uncovering Molecular Bases Underlying Bone Morphogenetic Protein Receptor Inhibitor Selectivity. PLoS ONE, 2015, 10, e0132221.	2.5	11
22	Ion Pairing and Dielectric Decrement in Glycosaminoglycan Brushes. Journal of Physical Chemistry B, 2021, 125, 2771-2780.	2.6	8
23	A novel voltage-clamp/dye uptake assay reveals saturable transport of molecules through CALHM1 and connexin channels. Journal of General Physiology, 2020, 152, .	1.9	8
24	PKA and Ube3a regulate SK2 channel trafficking to promote synaptic plasticity in hippocampus: Implications for Angelman Syndrome. Scientific Reports, 2020, 10, 9824.	3.3	7
25	Mechanical properties of anionic asymmetric bilayers from atomistic simulations. Journal of Chemical Physics, 2021, 154, 224701.	3.0	7
26	Insight into Molecular Mechanism for Activin A-Induced Bone Morphogenetic Protein Signaling. International Journal of Molecular Sciences, 2020, 21, 6498.	4.1	6
27	Alterations at Arg <sup>76</sup> of human connexin 46, a residue associated with cataract formation, cause loss of gap junction formation but preserve hemichannel function. American Journal of Physiology - Cell Physiology, 2018, 315, C623-C635.	4.6	5
28	Free energy and kinetics of cAMP permeation through connexin26 via applied voltage and milestoning. Biophysical Journal, 2021, 120, 2969-2983.	0.5	5
29	In silico prediction of ARB resistance: A first step in creating personalized ARB therapy. PLoS Computational Biology, 2020, 16, e1007719.	3.2	5
30	Investigating Protein–Protein Allosteric Network using Currentâ€Flow Scheme. Journal of Computational Chemistry, 2020, 41, 552-560.	3.3	3
31	Concepts, Practices, and Interactive Tutorial for Allosteric Network Analysis of Molecular Dynamics Simulations. Methods in Molecular Biology, 2021, 2302, 311-334.	0.9	2
32	Cancer Cell Metabolism Featuring Nrf2. Current Drug Discovery Technologies, 2020, 17, 263-271.	1.2	2
33	Ado-Trastuzumab Emtansine. AAPS Advances in the Pharmaceutical Sciences Series, 2015, , 203-223.	0.6	1
34	Resveratrol Protects Membranes from PLA1 and PLA2 Hydrolytic Attack. Biophysical Journal, 2018, 114, 259a.	0.5	1
35	Insights on Gating Functions of Cytosolic Domains of Connexin26 Hemichannels Revealed by a Human Pathogenic Mutation (N14K). Biophysical Journal, 2018, 114, 379a.	0.5	1
36	Targeting PRMT9 Suppresses Acute Myeloid Leukemia Maintenance. Blood, 2021, 138, 358-358.	1.4	1

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37	Computational Studies of Molecular Permeation through Connexin26 Channels. Biophysical Journal, 2014, 106, 556a.	0.5	0
38	Modeling the Structural Differences between Wild-Type and Polymorphic G Protein-Coupled Receptor Kinase 4 Gamma. Biophysical Journal, 2016, 110, 589a-590a.	0.5	0
39	Revealing Activation Mechanism of Alk2 Kinase Mutations in Fibrodysplasia Ossificans Progressiva (FOP). Biophysical Journal, 2016, 110, 206a.	0.5	O
40	A Molecular Dynamics Study of Michaelis Complex for Designing Selective Transition State Analog Inhibitors for Cysteine Protease calpain-2. Biophysical Journal, 2016, 110, 545a.	0.5	0
41	Using Current-Flow Scheme to Capture the Protein-Protein Binding Allostericity. Biophysical Journal, 2018, 114, 420a.	0.5	0
42	Structural Bases for Chemical and Mechanical Gating in the Piezo1 Channel. Biophysical Journal, 2019, 116, 478a-479a.	0.5	0
43	Molecular Dynamics Simulation of pH-Mediated Conformational Change in Connexin Channels. Biophysical Journal, 2021, 120, 228a.	0.5	0
44	An Open State Was Induced by Mimicking Mechanosensitive Piezo1 Channel Clusters in Molecular Dynamic Simulations. Biophysical Journal, 2021, 120, 228a.	0.5	0
45	In Silico Transmission of Cyclic Amp through Connexin 26 via Milestoning and External Electric Field Molecular Dynamics Simulations. Biophysical Journal, 2021, 120, 178a.	0.5	O
46	Elucidation of the structural determinants of ARB binding to the human AT1R (1173.4). FASEB Journal, 2014, 28, 1173.4.	0.5	0
47	Comparative structural biology of human and opossum AT 1 Rs reveals different ARB binding sites. FASEB Journal, 2015, 29, 971.1.	0.5	0
48	G proteinâ€coupled receptor kinase 4 gammaâ€mediated activation of NFâ€PB. FASEB Journal, 2015, 29, 934.2.	0.5	0
49	Abstract 5252: Skin cancer prevention by traditional Chinese medicinal formula Si-Wu-Tang and its constituents. , 2016, , .		0
50	Modeling Angiotensin IIâ€mediated activation of the Angiotensin II Type 1 Receptor. FASEB Journal, 2018, 32, 555.16.	0.5	0
51	A142V GRK4γ increased RHâ€kinase domain separation is dependent on interaction with the plasma membrane. FASEB Journal, 2018, 32, 687.4.	0.5	O
52	Structural determination of the mechanism of domain separation of Gâ€proteinâ€coupled receptor kinase 4g. FASEB Journal, 2019, 33, 668.7.	0.5	0
53	Ion Channels in Biophysics and Physiology: Methods & December 2021, 1349, 33-49. Channels. Advances in Experimental Medicine and Biology, 2021, 1349, 33-49.	1.6	O
54	Unifying Single-Channel Permeability From Rare-Event Sampling and Steady-State Flux. Frontiers in Molecular Biosciences, 2022, 9, 860933.	3.5	0

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55	In silico prediction of ARB resistance: A first step in creating personalized ARB therapy., 2020, 16, e1007719.		O
56	In silico prediction of ARB resistance: A first step in creating personalized ARB therapy. , 2020, $16$ , e $1007719$ .		0
57	In silico prediction of ARB resistance: A first step in creating personalized ARB therapy., 2020, 16, e1007719.		O
58	In silico prediction of ARB resistance: A first step in creating personalized ARB therapy. , 2020, 16, e1007719.		0