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List of Publications by Year
in descending order

65 papers	3,720 citations	147801 31 h-index	138484 58 g-index
78 all docs	78 docs citations	78 times ranked	4338 citing authors

#	Article	IF	Citations
1	Interpreting hydrogen-deuterium exchange experiments with molecular simulations: Tutorials and applications of the HDXer ensemble reweighting software [Article v1.0]. Living Journal of Computational Molecular Science, 2022, 3, .	6.4	3
2	Bivalent recognition of fatty acyl-CoA by a human integral membrane palmitoyltransferase. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, .	7.1	15
3	Asymmetric drug binding in an ATP-loaded inward-facing state of an ABC transporter. Nature Chemical Biology, 2022, 18, 226-235.	8.0	15
4	Structure of the Shaker Kv channel and mechanism of slow C-type inactivation. Science Advances, 2022, 8, eabm7814.	10.3	49
5	Conserved binding site in the N-lobe of prokaryotic MATE transporters suggests a role for Na+ in ion-coupled drug efflux. Journal of Biological Chemistry, 2021, 296, 100262.	3.4	8
6	On the Role of a Conserved Methionine in the Na+-Coupling Mechanism of a Neurotransmitter Transporter Homolog. Neurochemical Research, 2021, , 1.	3.3	4
7	Membrane transporter dimerization driven by differential lipid solvation energetics of dissociated and associated states. ELife, 2021, 10, .	6.0	39
8	Corrections in the CHARMM36 Parametrization of Chloride Interactions with Proteins, Lipids, and Alkali Cations, and Extension to Other Halide Anions. Journal of Chemical Theory and Computation, 2021, 17, 6240-6261.	5.3	7
9	Conserved binding site in the N-lobe of prokaryotic MATE transporters suggests a role for Na in ion-coupled drug efflux. Journal of Biological Chemistry, 2021, , .	3.4	2
10	Force-Correction Analysis Method for Derivation of Multidimensional Free-Energy Landscapes from Adaptively Biased Replica Simulations. Journal of Chemical Theory and Computation, 2021, 17, 6775-6788.	5.3	7
11	Direct Derivation of Free Energies of Membrane Deformation and Other Solvent Density Variations From Enhanced Sampling Molecular Dynamics. Journal of Computational Chemistry, 2020, 41, 449-459.	3.3	26
12	DHHC20 Palmitoyl-Transferase Reshapes the Membrane to Foster Catalysis. Biophysical Journal, 2020, 118, 980-988.	0.5	10
13	The structure of human ATG9A and its interplay with the lipid bilayer. Autophagy, 2020, 16, 2292-2293.	9.1	6
14	An embedded lipid in the multidrug transporter LmrP suggests a mechanism for polyspecificity. Nature Structural and Molecular Biology, 2020, 27, 829-835.	8.2	57
15	Bedaquiline inhibits the yeast and human mitochondrial ATP synthases. Communications Biology, 2020, 3, 452.	4.4	32
16	Structure and Mechanism of DHHC Protein Acyltransferases. Journal of Molecular Biology, 2020, 432, 4983-4998.	4.2	36
17	Structure of Human ATG9A, the Only Transmembrane Protein of the Core Autophagy Machinery. Cell Reports, 2020, 31, 107837.	6.4	108
18	New Molecular-Mechanics Model for Simulations of Hydrogen Fluoride in Chemistry and Biology. Journal of Chemical Theory and Computation, 2020, 16, 5105-5126.	5.3	15

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19	Interpretation of HDX Data by Maximum-Entropy Reweighting of Simulated Structural Ensembles. Biophysical Journal, 2020, 118, 1649-1664.	0.5	28
20	Membrane physiologists of all kinds meet at Woods Hole. Journal of General Physiology, 2019, 151, 273-273.	1.9	0
21	Molecular mechanisms of human P2X3 receptor channel activation and modulation by divalent cation bound ATP. ELife, 2019, 8, .	6.0	30
22	Large-scale state-dependent membrane remodeling by a transporter protein. ELife, 2019, 8, .	6.0	42
23	ÂÂMitochondrial ATP synthase dimers spontaneously associate due to a long-range membrane-induced forceÂ. Journal of General Physiology, 2018, 150, 763-770.	1.9	56
24	Membrane plasticity facilitates recognition of the inhibitor oligomycin by the mitochondrial ATP synthase rotor. Biochimica Et Biophysica Acta - Bioenergetics, 2018, 1859, 789-796.	1.0	6
25	High-resolution cryo-EM analysis of the yeast ATP synthase in a lipid membrane. Science, 2018, 360, .	12.6	163
26	The prokaryotic Na+/Ca2+ exchanger NCX_Mj transports Na+ and Ca2+ in a 3:1 stoichiometry. Journal of General Physiology, 2018, 150, 51-65.	1.9	27
27	TRPV1 pore turret dictates distinct DkTx and capsaicin gating. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E11837-E11846.	7.1	45
28	Confidence Analysis of DEER Data and Its Structural Interpretation with Ensemble-Biased Metadynamics. Biophysical Journal, 2018, 115, 1200-1216.	0.5	38
29	Broadly conserved Na ⁺ -binding site in the N-lobe of prokaryotic multidrug MATE transporters. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E6172-E6181.	7.1	25
30	Predicted Structures of the Proton-Bound Membrane-Embedded Rotor Rings of the Saccharomyces cerevisiae and Escherichia coli ATP Synthases. Journal of Physical Chemistry B, 2017, 121, 3297-3307.	2.6	6
31	Asymmetry of inverted-topology repeats in the AE1 anion exchanger suggests an elevator-like mechanism. Journal of General Physiology, 2017, 149, 1149-1164.	1.9	32
32	Atomistic simulations indicate the c-subunit ring of the F1Fo ATP synthase is not the mitochondrial permeability transition pore. ELife, 2017, 6, .	6.0	71
33	Atomicâ€resolution dissection of the energetics and mechanism of isomerization of hydrated <scp>ATP</scp>â€<scp>M</scp>g²⁺ through the <scp>SOMA</scp> string method. Journal of Computational Chemistry, 2016, 37, 575-586.	3.3	8
34	Mechanism of extracellular ion exchange and binding-site occlusion in a sodium/calcium exchanger. Nature Structural and Molecular Biology, 2016, 23, 590-599.	8.2	75
35	Structure and mechanism of the ATP synthase membrane motor inferred from quantitative integrative modeling. Journal of General Physiology, 2016, 148, 441-457.	1.9	17
36	Structural insights into the mechanism of activation of the TRPV1 channel by a membrane-bound tarantula toxin. ELife, 2016, 5, .	6.0	71

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37	Ensemble-Biased Metadynamics: A Molecular Simulation Method to Sample Experimental Distributions. Biophysical Journal, 2015, 108, 2779-2782.	0.5	71
38	On the principle of ion selectivity in Na ⁺ /H ⁺ -coupled membrane proteins: Experimental and theoretical studies of an ATP synthase rotor. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, E1057-66.	7.1	41
39	Coupling of remote alternating-access transport mechanisms for protons and substrates in the multidrug efflux pump AcrB. ELife, 2014, 3, .	6.0	137
40	Channeling your inner energy. Nature Structural and Molecular Biology, 2014, 21, 575-577.	8.2	1
41	Sodium recognition by the Na ⁺ /Ca ²⁺ exchanger in the outward-facing conformation. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, E5354-62.	7.1	59
42	High-resolution structure and mechanism of an F/V-hybrid rotor ring in a Na+-coupled ATP synthase. Nature Communications, 2014, 5, 5286.	12.8	68
43	Ceramideâ€“lipid interactions studied by MD simulations and solid-state NMR. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2511-2519.	2.6	16
44	String Method for Calculation of Minimum Free-Energy Paths in Cartesian Space in Freely Tumbling Systems. Journal of Chemical Theory and Computation, 2013, 9, 4140-4154.	5.3	26
45	A New Type of Na+-Driven ATP Synthase Membrane Rotor with a Two-Carboxylate Ion-Coupling Motif. PLoS Biology, 2013, 11, e1001596.	5.6	61
46	Two-state dynamics of the SH3â€“SH2 tandem of Abl kinase and the allosteric role of the N-cap. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, E3372-80.	7.1	33
47	Structure of the c10 ring of the yeast mitochondrial ATP synthase in the open conformation. Nature Structural and Molecular Biology, 2012, 19, 485-491.	8.2	116
48	Structure of the yeast F ₁ F _o -ATP synthase dimer and its role in shaping the mitochondrial cristae. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 13602-13607.	7.1	413
49	Engineering rotor ring stoichiometries in the ATP synthase. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, E1599-608.	7.1	89
50	Promiscuous archaeal ATP synthase concurrently coupled to Na ⁺ and H ⁺ translocation. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 947-952.	7.1	113
51	GRIFFIN: A Versatile Methodology for Optimization of Proteinâ^'Lipid Interfaces for Membrane Protein Simulations. Journal of Chemical Theory and Computation, 2011, 7, 1167-1176.	5.3	60
52	ATP Synthase â€“ A Paradigmatic Molecular Machine. , 2011, , 208-238.		20
53	Modeling and simulation of ion-coupled and ATP-driven membrane proteins. Current Opinion in Structural Biology, 2011, 21, 173-179.	5.7	19
54	Evidence for an allosteric mechanism of substrate release from membrane-transporter accessory binding proteins. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, E1285-92.	7.1	34

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55	Structural and energetic basis for H+ versus Na+ binding selectivity in ATP synthase Fo rotors. Biochimica Et Biophysica Acta - Bioenergetics, 2010, 1797, 763-772.	1.0	58
56	Microscopic rotary mechanism of ion translocation in the Fo complex of ATP synthases. Nature Chemical Biology, 2010, 6, 891-899.	8.0	142
57	On the Question of Hydronium Binding to ATP-Synthase Membrane Rotors. Biophysical Journal, 2010, 99, L53-L55.	0.5	19
58	On the Structure of the Proton-Binding Site in the Fo Rotor of Chloroplast ATP Synthases. Journal of Molecular Biology, 2010, 395, 20-27.	4.2	43
59	High-resolution structure of the rotor ring of a proton-dependent ATP synthase. Nature Structural and Molecular Biology, 2009, 16, 1068-1073.	8.2	194
60	Complete Ion-Coordination Structure in the Rotor Ring of Na+-Dependent F-ATP Synthases. Journal of Molecular Biology, 2009, 391, 498-507.	4.2	98
61	Characterization of conformational equilibria through Hamiltonian and temperature replica-exchange simulations: Assessing entropic and environmental effects. Journal of Computational Chemistry, 2007, 28, 1634-1647.	3.3	44
62	Conformational sampling and dynamics of membrane proteins from 10-nanosecond computer simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 783-791.	2.6	92
63	Electrostatics of Ion Stabilization in a ClC Chloride Channel Homologue from Escherichia coli. Journal of Molecular Biology, 2004, 339, 981-1000.	4.2	111
64	Acquisition of siderophores in Gram-negative bacteria. Nature Reviews Molecular Cell Biology, 2003, 4, 105-116.	37.0	349
65	Differential ion dehydration energetics explains selectivity in the non-canonical lysosomal K+ channel TMEM175. ELife, 0, 11, .	6.0	9