Toby W Allen

List of Publications by Year
in descending order

72 papers	5,326 citations	94433 37 h-index	95266 68 g-index
74 all docs	74 docs citations	74 times ranked	4758 citing authors

#	Article	IF	Citations
1	Energetics of ion conduction through the gramicidin channel. Proceedings of the National Academy of Sciences of the United States of America, 2004, 101, 117-122.	7.1	371
2	Theoretical and computational models of biological ion channels. Quarterly Reviews of Biophysics, 2004, 37, 15-103.	5.7	362
3	On the thermodynamic stability of a charged arginine side chain in a transmembrane helix. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 4943-4948.	7.1	254
4	The Different Interactions of Lysine and Arginine Side Chains with Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 11906-11920.	2.6	245
5	Permeation of Ions Across the Potassium Channel: Brownian Dynamics Studies. Biophysical Journal, 1999, 77, 2517-2533.	0.5	190
6	The role of tryptophan side chains in membrane protein anchoring and hydrophobic mismatch. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 864-876.	2.6	182
7	Molecular dynamics â€" potential of mean force calculations as a tool for understanding ion permeation and selectivity in narrow channels. Biophysical Chemistry, 2006, 124, 251-267.	2.8	181
8	Mechanisms of Permeation and Selectivity in Calcium Channels. Biophysical Journal, 2001, 80, 195-214.	0.5	171
9	Mechanism of potassium-channel selectivity revealed by Na+ and Li+ binding sites within the KcsA pore. Nature Structural and Molecular Biology, 2009, 16, 1317-1324.	8.2	158
10	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. Journal of Membrane Biology, 2015, 248, 611-640.	2.1	157
11	Molecular Dynamics Study of the KcsA Potassium Channel. Biophysical Journal, 1999, 77, 2502-2516.	0.5	152
12	On the Importance of Atomic Fluctuations, Protein Flexibility, and Solvent in Ion Permeation. Journal of General Physiology, 2004, 124, 679-690.	1.9	141
13	The potassium channel: Structure, selectivity and diffusion. Journal of Chemical Physics, 2000, 112, 8191-8204.	3.0	134
14	Conducting-State Properties of the KcsA Potassium Channel from Molecular and Brownian Dynamics Simulations. Biophysical Journal, 2002, 82, 628-645.	0.5	134
15	Ion Permeation through a Narrow Channel: Using Gramicidin to Ascertain All-Atom Molecular Dynamics Potential of Mean Force Methodology and Biomolecular Force Fields. Biophysical Journal, 2006, 90, 3447-3468.	0.5	133
16	Structure of Gramicidin A in a Lipid Bilayer Environment Determined Using Molecular Dynamics Simulations and Solid-State NMR Data. Journal of the American Chemical Society, 2003, 125, 9868-9877.	13.7	123
17	Study of Ionic Currents across a Model Membrane Channel Using Brownian Dynamics. Biophysical Journal, 1998, 75, 793-809.	0.5	113
18	Potential of Mean Force and pK_a Profile Calculation for a Lipid Membrane-Exposed Arginine Side Chain. Journal of Physical Chemistry B, 2008, 112, 9574-9587.	2.6	107

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19	Gramicidin A Channel as a Test Ground for Molecular Dynamics Force Fields. Biophysical Journal, 2003, 84, 2159-2168.	0.5	105
20	Assessing Atomistic and Coarse-Grained Force Fields for Proteinâ˜'Lipid Interactions: the Formidable Challenge of an Ionizable Side Chain in a Membrane. Journal of Physical Chemistry B, 2008, 112, 9588-9602.	2.6	103
21	Ion conduction and conformational flexibility of a bacterial voltage-gated sodium channel. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 3454-3459.	7.1	95
22	Ion-Induced Defect Permeation of Lipid Membranes. Biophysical Journal, 2014, 106, 586-597.	0.5	93
23	Modeling Diverse Range of Potassium Channels with Brownian Dynamics. Biophysical Journal, 2002, 83, 263-277.	0.5	89
24	The effect of hydrophobic and hydrophilic channel walls on the structure and diffusion of water and ions. Journal of Chemical Physics, 1999, 111, 7985-7999.	3.0	88
25	Local anesthetic and antiepileptic drug access and binding to a bacterial voltage-gated sodium channel. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 13057-13062.	7.1	87
26	Atomistic Simulations of Membrane Ion Channel Conduction, Gating, and Modulation. Chemical Reviews, 2019, 119, 7737-7832.	47.7	87
27	Is Arginine Charged in a Membrane?. Biophysical Journal, 2008, 94, L11-L13.	0.5	81
28	On the selective ion binding hypothesis for potassium channels. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 17963-17968.	7.1	80
29	Origins of ion selectivity in potassium channels from the perspective of channel block. Journal of General Physiology, 2011, 137, 405-413.	1.9	66
30	The role of membrane thickness in charged proteinâ€“lipid interactions. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 135-145.	2.6	66
31	Molecular dynamics estimates of ion diffusion in model hydrophobic and KcsA potassium channels. Biophysical Chemistry, 2000, 86, 1-14.	2.8	62
32	Reservoir Boundaries in Brownian Dynamics Simulations of Ion Channels. Biophysical Journal, 2002, 82, 1975-1984.	0.5	60
33	String method solution of the gating pathways for a pentameric ligand-gated ion channel. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E4158-E4167.	7.1	60
34	Towards a Structural View of Drug Binding to hERG K + Channels. Trends in Pharmacological Sciences, 2017, 38, 899-907.	8.7	56
35	Electrostatics of Deformable Lipid Membranes. Biophysical Journal, 2010, 98, 2904-2913.	0.5	49
36	A selectivity filter at the intracellular end of the acid-sensing ion channel pore. ELife, 2017, 6, .	6.0	48

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37	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. Journal of Chemical Theory and Computation, 2012, 8, 618-628.	5.3	47
38	Ball-and-chain inactivation in a calcium-gated potassium channel. Nature, 2020, 580, 288-293.	27.8	45
39	On the role of anionic lipids in charged protein interactions with membranes. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1673-1683.	2.6	44
40	The determinants of hydrophobic mismatch response for transmembrane helices. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 851-863.	2.6	40
41	The electrostatics of solvent and membrane interfaces and the role of electronic polarizability. Journal of Chemical Physics, 2010, 132, 185101.	3.0	38
42	Evidence for Leaflet-Dependent Redistribution of Charged Molecules in Fluid Supported Phospholipid Bilayers. Langmuir, 2008, 24, 13250-13253.	3.5	35
43	A model of calcium channels. Biochimica Et Biophysica Acta - Biomembranes, 2000, 1509, 1-6.	2.6	33
44	Modeling Charged Protein Side Chains in Lipid Membranes. Journal of General Physiology, 2007, 130, 237-240.	1.9	32
45	Molecular and Brownian dynamics study of ion selectivity and conductivity in the potassium channel. Chemical Physics Letters, 1999, 313, 358-365.	2.6	31
46	Selectivity filter ion binding affinity determines inactivation in a potassium channel. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 29968-29978.	7.1	29
47	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. Journal of Chemical Theory and Computation, 2021, 17, 1726-1741.	5.3	26
48	The Potassium Ion Channel:Â Comparison of Linear Scaling Semiempirical and Molecular Mechanics Representations of the Electrostatic Potential. Journal of Physical Chemistry B, 2001, 105, 12674-12679.	2.6	25
49	Bennett's acceptance ratio and histogram analysis methods enhanced by umbrella sampling along a reaction coordinate in configurational space. Journal of Chemical Physics, 2012, 136, 164103.	3.0	25
50	Cholesterol depletion inhibits Na+,K+-ATPase activity in a near-native membrane environment. Journal of Biological Chemistry, 2019, 294, 5956-5969.	3.4	25
51	Comment on â€œFree energy simulations of single and double ion occupancy in gramicidin Aâ€•[J. Chem. Phys. 126, 105103 (2007)]. Journal of Chemical Physics, 2008, 128, 227101.	3.0	21
52	Selective ion permeation involves complexation with carboxylates and lysine in a model human sodium channel. PLoS Computational Biology, 2018, 14, e1006398.	3.2	21
53	Estimation of Potentials of Mean Force from Nonequilibrium Pulling Simulations Using Both Minh-Adib Estimator and Weighted Histogram Analysis Method. Journal of Chemical Theory and Computation, 2016, 12, 1000-1010.	5.3	20
54	Identification of Electric-Field-Dependent Steps in the Na+,K+-Pump Cycle. Biophysical Journal, 2014, 107, 1352-1363.	0.5	18

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55	The voltage-sensitive dye RH421 detects a Na+,K+-ATPase conformational change at the membrane surface. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 813-823.	2.6	13
56	Computational models for predictive cardiac ion channel pharmacology. Drug Discovery Today: Disease Models, 2014, 14, 3-10.	1.2	12
57	Molecular Dynamics Simulations Based on Polarizable Models Show that Ion Permeation Interconverts between Different Mechanisms as a Function of Membrane Thickness. Journal of Physical Chemistry B, 2021, 125, 1020-1035.	2.6	12
58	Determinants of ion selectivity in ASIC1a- and ASIC2a-containing acid-sensing ion channels. Journal of General Physiology, 2020, 152, .	1.9	11
59	Understanding Sodium Channel Function and Modulation Using Atomistic Simulations of Bacterial Channel Structures. Current Topics in Membranes, 2016, 78, 145-182.	0.9	9
60	Positronium states in three-dimensional QED. Physical Review D, 1996, 53, 5842-5855.	4.7	8
61	Comparison of permeation mechanisms in sodium-selective ion channels. Neuroscience Letters, 2019, 700, 3-8.	2.1	6
62	Simulating ion channel activation mechanisms using swarms of trajectories. Journal of Computational Chemistry, 2020, 41, 387-401.	3.3	5
63	Conformational Dynamics in a Nicotinic Receptor Homologue Probed by Simulations. Biophysical Journal, 2011, 100, 272a.	0.5	3
64	Vector positronium states in three-dimensional QED. Physical Review D, 1997, 55, 4954-4966.	4.7	2
65	Chapter 15 Charged Protein Side Chain Movement in Lipid Bilayers Explored with Free Energy Simulation. Current Topics in Membranes, 2008, , 405-459.	0.9	2
66	Multi-Ion Mechanism of Potassium Channel Rejection of Na and Li Ions. Biophysical Journal, 2010, 98, 331a.	0.5	1
67	Long Molecular Dynamics Simulations of the Voltage-Gated Sodium Channel, NavAb. Biophysical Journal, 2013, 104, 137a.	0.5	1
68	In Honour of Professor Cristobal dos Remedios on behalf of the MAWA Trust. Biophysical Reviews, 2020, 12, 765-766.	3.2	1
69	Membrane protein structure and function. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 125.	2.6	0
70	Uncovering the Links Between Conformational Flexibility and Function for a Bacterial Voltage-Gated Sodium Channel. Biophysical Journal, 2014, 106, 130a.	0.5	0
71	Structure and Dynamics of the Mthk K+ Channel Selectivity Filter duringÂGating. Biophysical Journal, 2015, 108, 119a.	0.5	0
72	A Selectivity Filter at the Lower End of ASIC1a. Biophysical Journal, 2017, 112, 476a-477a.	0.5	0