Toby W Allen

List of Publications by Year in Descending Order

67 papers	4,483 citations	37 h-index	66 g-index
74 ext. papers	4,962 ext. citations	5.6 avg, IF	5.68 L-index

#	Paper	IF	Citations
67	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	3.4	3
66	Polarization Effects in Water-Mediated Selective Cation Transport across a Narrow Transmembrane Channel. *Journal of Chemical Theory and Computation*, **2021**, 17, 1726-1741	6.4	7
65	Ball-and-chain inactivation in a calcium-gated potassium channel. *Nature*, **2020**, 580, 288-293	50.4	20
64	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	11.5	11
63	Simulating ion channel activation mechanisms using swarms of trajectories. *Journal of Computational Chemistry*, **2020**, 41, 387-401	3.5	4
62	Determinants of ion selectivity in ASIC1a- and ASIC2a-containing acid-sensing ion channels. *Journal of General Physiology*, **2020**, 152,	3.4	5
61	In Honour of Professor Cristobal dos Remedios on behalf of the MAWA Trust. *Biophysical Reviews*, **2020**, 12, 765-766	3.7	0
60	Atomistic Simulations of Membrane Ion Channel Conduction, Gating, and Modulation. *Chemical Reviews*, **2019**, 119, 7737-7832	68.1	46
59	Cholesterol depletion inhibits Na,K-ATPase activity in a near-native membrane environment. *Journal of Biological Chemistry*, **2019**, 294, 5956-5969	5.4	17
58	Comparison of permeation mechanisms in sodium-selective ion channels. *Neuroscience Letters*, **2019**, 700, 3-8	3.3	3
57	Selective ion permeation involves complexation with carboxylates and lysine in a model human sodium channel. *PLoS Computational Biology*, **2018**, 14, e1006398	5	10
56	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	3.8	10
55	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	11.5	37
54	Towards a Structural View of Drug Binding to hERG K Channels. *Trends in Pharmacological Sciences*, **2017**, 38, 899-907	13.2	37
53	A selectivity filter at the intracellular end of the acid-sensing ion channel pore. *ELife*, **2017**, 6,	8.9	27
52	Understanding Sodium Channel Function and Modulation Using Atomistic Simulations of Bacterial Channel Structures. *Current Topics in Membranes*, **2016**, 78, 145-82	2.2	5
51	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, 1000-10	6.4	19

50	Membrane Protein Structure, Function, and Dynamics: a Perspective from Experiments and Theory. *Journal of Membrane Biology*, **2015**, 248, 611-40	2.3	101
49	Ion-induced defect permeation of lipid membranes. *Biophysical Journal*, **2014**, 106, 586-97	2.9	77
48	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, 13057-62	11.5	67
47	Computational Models for Predictive Cardiac Ion Channel Pharmacology. *Drug Discovery Today: Disease Models*, **2014**, 14, 3-10	1.3	11
46	Identification of electric-field-dependent steps in the Na(+),K(+)-pump cycle. *Biophysical Journal*, **2014**, 107, 1352-63	2.9	15
45	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, 3454-9	11.5	77
44	The different interactions of lysine and arginine side chains with lipid membranes. *Journal of Physical Chemistry B*, **2013**, 117, 11906-20	3.4	176
43	The role of tryptophan side chains in membrane protein anchoring and hydrophobic mismatch. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 864-76	3.8	130
42	The determinants of hydrophobic mismatch response for transmembrane helices. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 851-63	3.8	35
41	The role of membrane thickness in charged protein-lipid interactions. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 135-45	3.8	55
40	Membrane protein structure and function. *Biochimica Et Biophysica Acta - Biomembranes*, **2012**, 1818, 125	3.8	
39	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. *Journal of Chemical Theory and Computation*, **2012**, 8, 618-28	6.4	42
38	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	3.9	21
37	Conformational Dynamics in a Nicotinic Receptor Homologue Probed by Simulations. *Biophysical Journal*, **2011**, 100, 272a	2.9	3
36	On the role of anionic lipids in charged protein interactions with membranes. *Biochimica Et Biophysica Acta - Biomembranes*, **2011**, 1808, 1673-83	3.8	34
35	Origins of ion selectivity in potassium channels from the perspective of channel block. *Journal of General Physiology*, **2011**, 137, 405-13	3.4	60
34	On the selective ion binding hypothesis for potassium channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2011**, 108, 17963-8	11.5	72
33	The electrostatics of solvent and membrane interfaces and the role of electronic polarizability. *Journal of Chemical Physics*, **2010**, 132, 185101	3.9	37

32	Electrostatics of deformable lipid membranes. *Biophysical Journal*, **2010**, 98, 2904-13	2.9	42
31	Mechanism of potassium-channel selectivity revealed by Na(+) and Li(+) binding sites within the KcsA pore. *Nature Structural and Molecular Biology*, **2009**, 16, 1317-24	17.6	131
30	Assessing atomistic and coarse-grained force fields for protein-lipid interactions: the formidable challenge of an ionizable side chain in a membrane. *Journal of Physical Chemistry B*, **2008**, 112, 9588-602	3.4	99
29	Potential of mean force and pKa profile calculation for a lipid membrane-exposed arginine side chain. *Journal of Physical Chemistry B*, **2008**, 112, 9574-87	3.4	102
28	Is arginine charged in a membrane?. *Biophysical Journal*, **2008**, 94, L11-3	2.9	74
27	Evidence for leaflet-dependent redistribution of charged molecules in fluid supported phospholipid bilayers. *Langmuir*, **2008**, 24, 13250-3	4	34
26	Comment on "Free energy simulations of single and double ion occupancy in gramicidin A" [J. Chem. Phys. 126, 105103 (2007)]. *Journal of Chemical Physics*, **2008**, 128, 227101; author reply 227102	3.9	19
25	Chapter 15 Charged Protein Side Chain Movement in Lipid Bilayers Explored with Free Energy Simulation. *Current Topics in Membranes*, **2008**, 405-459	2.2	2
24	Modeling charged protein side chains in lipid membranes. *Journal of General Physiology*, **2007**, 130, 237-40	3.4	31
23	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, 4943-8	11.5	221
22	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, 3447-68	2.9	123
21	Molecular dynamics - potential of mean force calculations as a tool for understanding ion permeation and selectivity in narrow channels. *Biophysical Chemistry*, **2006**, 124, 251-67	3.5	155
20	Energetics of ion conduction through the gramicidin channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2004**, 101, 117-22	11.5	335
19	Theoretical and computational models of biological ion channels. *Quarterly Reviews of Biophysics*, **2004**, 37, 15-103	7	321
18	On the importance of atomic fluctuations, protein flexibility, and solvent in ion permeation. *Journal of General Physiology*, **2004**, 124, 679-90	3.4	127
17	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, 9868-77	16.4	115
16	Gramicidin A channel as a test ground for molecular dynamics force fields. *Biophysical Journal*, **2003** , 84, 2159-68	2.9	102
15	Modeling diverse range of potassium channels with Brownian dynamics. *Biophysical Journal*, **2002**, 83, 263-77	2.9	83

14	Conducting-state properties of the KcsA potassium channel from molecular and Brownian dynamics simulations. *Biophysical Journal*, **2002**, 82, 628-45	2.9	120
13	Reservoir boundaries in Brownian dynamics simulations of ion channels. *Biophysical Journal*, **2002**, 82, 1975-84	2.9	53
12	Mechanisms of permeation and selectivity in calcium channels. *Biophysical Journal*, **2001**, 80, 195-214	2.9	151
11	The Potassium Ion Channel: Comparison of Linear Scaling Semiempirical and Molecular Mechanics Representations of the Electrostatic Potential. *Journal of Physical Chemistry B*, **2001**, 105, 12674-12679	3.4	24
10	Molecular dynamics estimates of ion diffusion in model hydrophobic and KcsA potassium channels. *Biophysical Chemistry*, **2000**, 86, 1-14	3.5	57
9	A model of calcium channels. *Biochimica Et Biophysica Acta - Biomembranes*, **2000**, 1509, 1-6	3.8	29
8	The potassium channel: Structure, selectivity and diffusion. *Journal of Chemical Physics*, **2000**, 112, 8191-8204	3.9	122
7	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	3.9	79
6	Molecular and Brownian dynamics study of ion selectivity and conductivity in the potassium channel. *Chemical Physics Letters*, **1999**, 313, 358-365	2.5	31
5	Molecular dynamics study of the KcsA potassium channel. *Biophysical Journal*, **1999**, 77, 2502-16	2.9	138
4	Permeation of ions across the potassium channel: Brownian dynamics studies. *Biophysical Journal*, **1999**, 77, 2517-33	2.9	176
3	Study of ionic currents across a model membrane channel using Brownian dynamics. *Biophysical Journal*, **1998**, 75, 793-809	2.9	101
2	Vector positronium states in three-dimensional QED. *Physical Review D*, **1997**, 55, 4954-4966	4.9	2
1	Positronium states in three-dimensional QED. *Physical Review D*, **1996**, 53, 5842-5855	4.9	8