Phillip James Stansfeld

List of Publications by Year
in descending order

142	6,751	61977	76898
papers	citations	43 h-index	74 g-index

165	165	165	7966
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The role of interfacial lipids in stabilizing membrane protein oligomers. Nature, 2017, 541, 421-424.	27.8	344
2	MemProtMD: Automated Insertion of Membrane Protein Structures into Explicit Lipid Membranes. Structure, 2015, 23, 1350-1361.	3.3	257
3	From Coarse Grained to Atomistic: A Serial Multiscale Approach to Membrane Protein Simulations. Journal of Chemical Theory and Computation, 2011, 7, 1157-1166.	5.3	240
4	Structural basis for outer membrane lipopolysaccharide insertion. Nature, 2014, 511, 52-56.	27.8	239
5	Structural basis of outer membrane protein insertion by the BAM complex. Nature, 2016, 531, 64-69.	27.8	234
6	The SARS-COV-2 Spike Protein Binds Sialic Acids and Enables Rapid Detection in a Lateral Flow Point of Care Diagnostic Device. ACS Central Science, 2020, 6, 2046-2052.	11.3	222
7	Structures of ABCB10, a human ATP-binding cassette transporter in apo- and nucleotide-bound states. Proceedings of the National Academy of Sciences of the United States of America, 2013, 110, 9710-9715.	7.1	219
8	Structure of the TatC core of the twin-arginine protein transport system. Nature, 2012, 492, 210-214.	27.8	164
9	The pore structure and gating mechanism of K2P channels. EMBO Journal, 2011, 30, 3607-3619.	7.8	162
10	Molecular Simulation Approaches to Membrane Proteins. Structure, 2011, 19, 1562-1572.	3.3	152
11	Lipidbook: A Public Repository for Force-Field Parameters Used in Membrane Simulations. Journal of Membrane Biology, 2010, 236, 255-258.	2.1	145
12	The MemProtMD database: a resource for membrane-embedded protein structures and their lipid interactions. Nucleic Acids Research, 2019, 47, D390-D397.	14.5	143
13	Structural Features of the Glutamate Binding Site in Recombinant NR1/NR2A N-Methyl-d-aspartate Receptors Determined by Site-Directed Mutagenesis and Molecular Modeling. Molecular Pharmacology, 2005, 67, 1470-1484.	2.3	138
14	Structures of the stator complex that drives rotation of the bacterial flagellum. Nature Microbiology, 2020, 5, 1553-1564.	13.3	131
15	PIP₂-Binding Site in Kir Channels: Definition by Multiscale Biomolecular Simulations. Biochemistry, 2009, 48, 10926-10933.	2.5	127
16	Structural basis of lipoprotein signal peptidase II action and inhibition by the antibiotic globomycin. Science, 2016, 351, 876-880.	12.6	111
17	The structural basis of lipid scrambling and inactivation in the endoplasmic reticulum scramblase TMEM16K. Nature Communications, 2019, 10, 3956.	12.8	101
18	Drug block of the hERG potassium channel: Insight from modeling. Proteins: Structure, Function and Bioinformatics, 2007, 68, 568-580.	2.6	100

#	Article	IF	Citations
19	Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association. Journal of Physical Chemistry B, 2017, 121, 3364-3375.	2.6	93
20	The Structural Basis of ZMPSTE24-Dependent Laminopathies. Science, 2013, 339, 1604-1607.	12.6	89
21	Mechanistic Insight into Human ether-Ã-go-go-related Gene (hERG) K+ Channel Deactivation Gating from the Solution Structure of the EAG Domain. Journal of Biological Chemistry, 2011, 286, 6184-6191.	3.4	87
22	New insights into KATP channel gene mutations and neonatal diabetes mellitus. Nature Reviews Endocrinology, 2020, 16, 378-393.	9.6	87
23	Drug Binding Interactions in the Inner Cavity of hERG Channels: Molecular Insights from Structure-Activity Relationships of Clofilium and Ibutilide Analogs. Molecular Pharmacology, 2006, 69, 509-519.	2.3	84
24	Functional analysis of missense variants in the TRESK (KCNK18) K+ channel. Scientific Reports, 2012, 2, 237.	3.3	82
25	In Situ Structure of an Intact Lipopolysaccharide-Bound Bacterial Surface Layer. Cell, 2020, 180, 348-358.e15.	28.9	79
26	Multiscale Simulations Reveal Conserved Patterns of Lipid Interactions with Aquaporins. Structure, 2013, 21, 810-819.	3.3	74
27	Lipopolysaccharide is Inserted into the Outer Membrane through An Intramembrane Hole, AÂLumen Gate, and the Lateral Opening of LptD. Structure, 2015, 23, 496-504.	3.3	71
28	Insights into Membrane Proteinâ€“Lipid Interactions from Free Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5727-5736.	5.3	70
29	A Specific Two-pore Domain Potassium Channel Blocker Defines the Structure of the TASK-1 Open Pore. Journal of Biological Chemistry, 2011, 286, 13977-13984.	3.4	69
30	PyLipID: A Python Package for Analysis of Proteinâ€“Lipid Interactions from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 1188-1201.	5.3	69
31	Structural Analysis of the G-Box Domain of the Microcephaly Protein CPAP Suggests a Role in Centriole Architecture. Structure, 2013, 21, 2069-2077.	3.3	66
32	Structure and mechanism of bactericidal mammalian perforin-2, an ancient agent of innate immunity. Science Advances, 2020, 6, eaax8286.	10.3	66
33	The pore structure and gating mechanism of K2P channels. EMBO Journal, 2011, 30, 4515-4515.	7.8	65
34	CG2AT2: an Enhanced Fragment-Based Approach for Serial Multi-scale Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 6472-6482.	5.3	64
35	Simulation-Based Prediction of Phosphatidylinositol 4,5-Bisphosphate Binding to an Ion Channel. Biochemistry, 2013, 52, 279-281.	2.5	63
36	Assembling the Tat protein translocase. ELife, 2016, 5, .	6.0	62

#	Article	IF	Citations
37	Structural basis of proton-coupled potassium transport in the KUP family. Nature Communications, 2020, 11, 626.	12.8	60
38	Biophysical and Computational Studies of Membrane Penetration by the GRP1 Pleckstrin Homology Domain. Structure, 2011, 19, 1338-1346.	3.3	56
39	Structure, substrate recognition and initiation of hyaluronan synthase. Nature, 2022, 604, 195-201.	27.8	53
40	Structural insights into the mechanism of the membrane integral N-acyltransferase step in bacterial lipoprotein synthesis. Nature Communications, 2017, 8, 15952.	12.8	52
41	A heuristic derived from analysis of the ion channel structural proteome permits the rapid identification of hydrophobic gates. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 13989-13995.	7.1	52
42	Insight into the Mechanism of Inactivation and pH Sensitivity in Potassium Channels from Molecular Dynamics Simulations. Biochemistry, 2008, 47, 7414-7422.	2.5	50
43	Side pockets provide the basis for a new mechanism of Kv channelâ€“specific inhibition. Nature Chemical Biology, 2013, 9, 507-513.	8.0	50
44	A bipartite structural organization defines the SERINC family of HIV-1 restriction factors. Nature Structural and Molecular Biology, 2020, 27, 78-83.	8.2	50
45	Identification and assessment of cardiolipin interactions with E. coli inner membrane proteins. Science Advances, 2021, 7, .	10.3	49
46	Water and hydrophobic gates in ion channels and nanopores. Faraday Discussions, 2018, 209, 231-247.	3.2	48
47	The energetics of proteinâ€“lipid interactions as viewed by molecular simulations. Biochemical Society Transactions, 2020, 48, 25-37.	3.4	48
48	Crystal structure of undecaprenyl-pyrophosphate phosphatase and its role in peptidoglycan biosynthesis. Nature Communications, 2018, 9, 1078.	12.8	47
49	Complete structure of the chemosensory array core signalling unit in an E. coli minicell strain. Nature Communications, 2020, 11, 743.	12.8	47
50	Targeting of proteins to the twinâ€arginine translocation pathway. Molecular Microbiology, 2020, 113, 861-871.	2.5	47
51	A lipid gating mechanism for the channel-forming O antigen ABC transporter. Nature Communications, 2019, 10, 824.	12.8	44
52	Multiple lipid binding sites determine the affinity of PH domains for phosphoinositide-containing membranes. Science Advances, 2020, 6, eaay5736.	10.3	44
53	Dimerization of the EphA1 Receptor Tyrosine Kinase Transmembrane Domain: Insights into the Mechanism of Receptor Activation. Biochemistry, 2014, 53, 6641-6652.	2.5	43
54	A Coarse Grained Model for a Lipid Membrane with Physiological Composition and Leaflet Asymmetry. PLoS ONE, 2015, 10, e0144814.	2.5	43

#	Article	IF	Citations
55	Molecular mechanisms for drug interactions with hERG that cause long QT syndrome. Expert Opinion on Drug Metabolism and Toxicology, 2006, 2, 81-94.	3.3	41
56	Dynamics of an LPS translocon induced by substrate and an antimicrobial peptide. Nature Chemical Biology, 2021, 17, 187-195.	8.0	41
57	Activation Gating of hERG Potassium Channels. Journal of Biological Chemistry, 2007, 282, 31972-31981.	3.4	40
58	Balancing Force Field Proteinâ€“Lipid Interactions To Capture Transmembrane Helixâ€“Helix Association. Journal of Chemical Theory and Computation, 2018, 14, 1706-1715.	5.3	40
59	Mechanism of lipid droplet formation by the yeast Sei1/Ldb16 Seipin complex. Nature Communications, 2021, 12, 5892.	12.8	40
60	Lipid binding attenuates channel closure of the outer membrane protein OmpF. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 6691-6696.	7.1	39
61	State-independent intracellular access of quaternary ammonium blockers to the pore of TREK-1. Channels, 2012, 6, 473-478.	2.8	37
62	Structure and Function of the Escherichia coli Tol-Pal Stator Protein TolR. Journal of Biological Chemistry, 2015, 290, 26675-26687.	3.4	35
63	Structure and dynamics of the E. coli chemotaxis core signaling complex by cryo-electron tomography and molecular simulations. Communications Biology, 2020, 3, 24.	4.4	35
64	Structural Determinants for High-Affinity Block of hERG Potassium Channels. Novartis Foundation Symposium, 2008, , 136-154.	1.1	34
65	Interactions of the EphA2 Kinase Domain with PIPs in Membranes: Implications for Receptor Function. Structure, 2018, 26, 1025-1034.e2.	3.3	33
66	A Massâ€Spectrometryâ€Based Approach to Distinguish Annular and Specific Lipid Binding to Membrane Proteins. Angewandte Chemie - International Edition, 2020, 59, 3523-3528.	13.8	33
67	Structures of monomeric and oligomeric forms of the Toxoplasma gondii perforin-like protein 1. Science Advances, 2018, 4, eaaq0762.	10.3	32
68	Insights into bacterial cell division from a structure of EnvC bound to the FtsX periplasmic domain. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 28355-28365.	7.1	32
69	Ternary structure reveals mechanism of a membrane diacylglycerol kinase. Nature Communications, 2015, 6, 10140.	12.8	30
70	The selectivity, voltage-dependence and acid sensitivity of the tandem pore potassium channel TASK-1: contributions of the pore domains. Pflugers Archiv European Journal of Physiology, 2007, 455, 333-348.	2.8	27
71	The TatC component of the twinâ€arginine protein translocase functions as an obligate oligomer. Molecular Microbiology, 2015, 98, 111-129.	2.5	27
72	A BEST example of channel structure annotation by molecular simulation. Channels, 2017, 11, 347-353.	2.8	26

#	Article	IF	Citations
73	Sharing Data from Molecular Simulations. Journal of Chemical Information and Modeling, 2019, 59, 4093-4099.	5.4	26
74	Structural analysis of P. falciparum KAHRP and PfEMP1 complexes with host erythrocyte spectrin suggests a model for cytoadherent knob protrusions. PLoS Pathogens, 2017, 13, e1006552.	4.7	26
75	The response of the tandem pore potassium channel TASKâ€3 (K_{2P}9.1) to voltage: gating at the cytoplasmic mouth. Journal of Physiology, 2009, 587, 4769-4783.	2.9	25
76	Structural basis of lipopolysaccharide maturation by the O-antigen ligase. Nature, 2022, 604, 371-376.	27.8	25
77	Chapter 12 Molecular Modeling and Simulation Studies of Ion Channel Structures, Dynamics and Mechanisms. Methods in Cell Biology, 2008, 90, 233-265.	1.1	24
78	Substrate-triggered position switching of TatA and TatB during Tat transport in Escherichia coli. Open Biology, 2017, 7, 170091.	3.6	24
79	Conformational dynamics of a G proteinâ€“coupled receptor helix 8 in lipid membranes. Science Advances, 2020, 6, eaav8207.	10.3	24
80	Structural basis for substrate specificity and regulation of nucleotide sugar transporters in the lipid bilayer. Nature Communications, 2019, 10, 4657.	12.8	23
81	Evaluating inositol phospholipid interactions with inward rectifier potassium channels and characterising their role in disease. Communications Chemistry, 2020, 3, .	4.5	23
82	Structural biology of Tat protein transport. Current Opinion in Structural Biology, 2014, 27, 32-37.	5.7	22
83	Relative Affinities of Proteinâ€“Cholesterol Interactions from Equilibrium Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2021, 17, 6548-6558.	5.3	21
84	The Unconventional Cytoplasmic Sensing Mechanism for Ethanol Chemotaxis in Bacillus subtilis. MBio, 2020, 11, .	4.1	20
85	The molecular basis for an allosteric inhibition of K+-flux gating in K2P channels. ELife, 2019, 8, .	6.0	20
86	Peptidoglycan biosynthesis is driven by lipid transfer along enzyme-substrate affinity gradients. Nature Communications, 2022, 13, 2278.	12.8	20
87	A conserved tryptophan at the membraneâ€“water interface acts as a gatekeeper for Kir6.2/SUR1 channels and causes neonatal diabetes when mutated. Journal of Physiology, 2011, 589, 3071-3083.	2.9	19
88	Switching Cytolytic Nanopores into Antimicrobial Fractal Ruptures by a Single Side Chain Mutation. ACS Nano, 2021, 15, 9679-9689.	14.6	17
89	Computational studies of membrane proteins: from sequence to structure to simulation. Current Opinion in Structural Biology, 2017, 45, 133-141.	5.7	16
90	Atomistic mechanism of transmembrane helix association. PLoS Computational Biology, 2020, 16, e1007919.	3.2	16

#	Article	IF	Citations
91	Ion-Blocking Sites of the Kir2.1 Channel Revealed by Multiscale Modeling. Biochemistry, 2009, 48, 8758-8763.	2.5	15
92	Direct Gating of ATP-activated Ion Channels (P2X2 Receptors) by Lipophilic Attachment at the Outer End of the Second Transmembrane Domain. Journal of Biological Chemistry, 2014, 289, 618-626.	3.4	15
93	Interaction of lipids with the neurotensin receptor 1. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1278-1287.	2.6	15
94	Characterizing Membrane Association and Periplasmic Transfer of Bacterial Lipoproteins through Molecular Dynamics Simulations. Structure, 2020, 28, 475-487.e3.	3.3	15
95	Cryo-EM Structures of CusA Reveal a Mechanism of Metal-Ion Export. MBio, 2021, 12, .	4.1	15
96	An outer-pore gate modulates the pharmacology of the TMEM16A channel. Proceedings of the National Academy of Sciences of the United States of America, 2021, 118, .	7.1	15
97	Calmodulin Regulates Human Ether Ã Go-Go 1 (hEAG1) Potassium Channels through Interactions of the Eag Domain with the Cyclic Nucleotide Binding Homology Domain. Journal of Biological Chemistry, 2016, 291, 17907-17918.	3.4	14
98	Simulations of the BM2 Proton Channel Transmembrane Domain from Influenza Virus B. Biochemistry, 2009, 48, 9949-9951.	2.5	13
99	Structural basis of trehalose recognition by the mycobacterial LpqY-SugABC transporter. Journal of Biological Chemistry, 2021, 296, 100307.	3.4	13
100	High-resolution mapping of metal ions reveals principles of surface layer assembly in Caulobacter crescentus cells. Structure, 2022, 30, 215-228.e5.	3.3	12
101	Membrane Binding of Antimicrobial Peptides Is Modulated by Lipid Charge Modification. Journal of Chemical Theory and Computation, 2021, 17, 1218-1228.	5.3	10
102	Deciphering ion transport and ATPase coupling in the intersubunit tunnel of KdpFABC. Nature Communications, 2021, 12, 5098.	12.8	10
103	NaViA: a program for the visual analysis of complex mass spectra. Bioinformatics, 2021, 37, 4876-4878.	4.1	9
104	A Bacterial Inflammation Sensor Regulates c-di-GMP Signaling, Adhesion, and Biofilm Formation. MBio, 2021, 12, e0017321.	4.1	9
105	A Leucine Zipper Motif Essential for Gating of Hyperpolarization-activated Channels. Journal of Biological Chemistry, 2012, 287, 40150-40160.	3.4	8
106	The centriolar protein CPAP G-box: an amyloid fibril in a single domain. Biochemical Society Transactions, 2015, 43, 838-843.	3.4	7
107	Interactions of a Bacterial Cu(I)-ATPase with a Complex Lipid Environment. Biochemistry, 2018, 57, 4063-4073.	2.5	6
108	Alternative Architecture of the E. coli Chemosensory Array. Biomolecules, 2021, 11, 495.	4.0	6

#	Article	IF	Citations
109	From Bench to Biomolecular Simulation: Phospholipid Modulation of Potassium Channels. Journal of Molecular Biology, 2021, 433, 167105.	4.2	4
110	Conformational dynamics of the membrane enzyme LspA upon antibiotic and substrate binding. Biophysical Journal, 2022, 121, 2078-2083.	0.5	4
111	MemProtMD: Membrane Protein Structures and Simulations. Biophysical Journal, 2014, 106, 634a.	0.5	2
112	A Massâ€Spectrometryâ€Based Approach to Distinguish Annular and Specific Lipid Binding to Membrane Proteins. Angewandte Chemie, 2020, 132, 3551-3556.	2.0	2
113	Identification and Characterization of Specific Proteinâ€“Lipid Interactions Using Molecular Simulation. Methods in Molecular Biology, 2021, 2315, 121-139.	0.9	2
114	Mechanistic Insight into hERG Channel Deactivation Gating from the Solution Structure of the eag Domain. Biophysical Journal, 2011, 100, 425a.	0.5	1
115	Towards Dynamic Pharmacophore Models by Coarse Grained Molecular Dynamics. Biophysical Journal, 2018, 114, 558a.	0.5	1
116	A Newly Available Tool for Functional Annotation of Ion Channel Structures Based on Molecular Dynamics Simulations. Biophysical Journal, 2018, 114, 134a.	0.5	1
117	Homology Models Applied to Toxicology. , 0, , 433-468.		0
118	Investigating the PIP2 Binding Site in Kir Channels Via Multi-Scale Biomolecular Simulations. Biophysical Journal, 2010, 98, 698a.	0.5	0
119	Multiscale Simulations of Lipid Interactions with Integral Membrane Proteins: Aquaporins. Biophysical Journal, 2011, 100, 204a.	0.5	0
120	PIP2-Binding to an Open State Model of Kir1.1 Probed by Multiscale Biomolecular Simulations. Biophysical Journal, 2011, 100, 431a.	0.5	0
121	Biomolecular Simulations of Kir Channel Gating and Membrane Phospholipid Interactions. Biophysical Journal, 2011, 100, 431a.	0.5	0
122	Functional Analysis of Mutations in the TRESK K2P Potassium Channel Associated with â€˜migraine with Auraâ€™. Biophysical Journal, 2011, 100, 279a.	0.5	0
123	Multiscale Simulations of Signalling at Membranes. Biophysical Journal, 2012, 102, 7a.	0.5	0
124	A Coarse Grain Model for a Lipid Membrane with Physiological Composition and Leaflet Asymmetry. Biophysical Journal, 2012, 102, 172a.	0.5	0
125	Memprotmd: Adding the Grease to Membrane Protein Structures. Biophysical Journal, 2012, 102, 469a.	0.5	0
126	Memprotmd: Restoring Membrane Protein Structures to their Bilayer Environments. Biophysical Journal, 2013, 104, 384a.	0.5	0

#	Article	IF	Citations
127	Deciphering Metastable EphA1 Transmembrane Helices Association using PMF Calculations and Multiscale Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 117a.	0.5	0
128	Dynamics of Transition Metal Transporting P-Type ATPases in Native Membranes. Biophysical Journal, 2014, 106, 100a.	0.5	0
129	Memprotmd: Protein-Lipid Interactions of Phospholipid Biosynthetic Enzymes and Development of the Web Database. Biophysical Journal, 2016, 110, 572a.	0.5	0
130	Towards Dynamic Pharmacophore Models by Coarse Grain Molecular Dynamics. Biophysical Journal, 2017, 112, 448a.	0.5	0
131	Molecular Simulations of Bacterial Lipoprotein Biogenesis. Biophysical Journal, 2017, 112, 65a.	0.5	0
132	Coupling Form and Function: How the Oligomerisation Symmetry of the SAS-6 Protein Contributes to the Architecture of Centriole Organelles. Symmetry, 2017, 9, 74.	2.2	0
133	Mechanism of Assembly of a Transmembrane Helix Dimer from All-Atom Simulation. Biophysical Journal, 2018, 114, 244a-245a.	0.5	0
134	Functional Annotation of Ion Channel Structures: Predicting Pore Solvation States Based on Local Radius and Hydrophobicity. Biophysical Journal, 2019, 116, 241a.	0.5	0
135	Investigating Protein-Lipid Interactions of MthK and Native Bacterial Membrane Lipids. Biophysical Journal, 2020, 118, 554a.	0.5	0
136	Molecular Mechanism of Modulation of the TMEM16A Channel by Anthracene-9-Carboxylic Acid: Implications for Channel Gating. Biophysical Journal, 2020, 118, 325a.	0.5	0
137	Greasing the Gears of Mechanosensitive Piezo Channels with Phosphoinositides and Cholesterol. Biophysical Journal, 2020, 119, 1467-1469.	0.5	0
138	Cationic Antimicrobial Peptides have Reduced Binding to MprF-Modified Membranes. Biophysical Journal, 2020, 118, 237a.	0.5	0
139	Conformational Dynamics of the Membrane Enzyme LspA using EPR and MD. Biophysical Journal, 2020, 118, 178a.	0.5	0
140	Investigating the Conformational Dynamics of the Outer Membrane LPS Translocon LptDE. Biophysical Journal, 2020, 118, 26a.	0.5	0
141	Structural Understanding of Ion Channels in Atomic Detail. RSC Drug Discovery Series, 2014, , 56-82.	0.3	0
142	Structural, Functional and Computational Studies of Membrane Recognition by Plasmodium Perforin-Like Proteins 1 and 2. Journal of Molecular Biology, 2022, 434, 167642.	4.2	0