# Phillip James Stansfeld

## List of Publications by Citations



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|---|---|---|---|
| 125 papers | 4,560 citations | 37 h-index | 64 g-index |
| 165 ext. papers | 5,798 ext. citations | 9 avg, IF | 5.88 L-index |

| # | Paper | IF | Citations |
|---|---|---|---|
| 125 | The role of interfacial lipids in stabilizing membrane protein oligomers. *Nature*, **2017**, 541, 421-424 | 50.4 | 238 |
| 124 | MemProtMD: Automated Insertion of Membrane Protein Structures into Explicit Lipid Membranes. *Structure*, **2015**, 23, 1350-61 | 5.2 | 204 |
| 123 | From Coarse Grained to Atomistic: A Serial Multiscale Approach to Membrane Protein Simulations. *Journal of Chemical Theory and Computation*, **2011**, 7, 1157-66 | 6.4 | 200 |
| 122 | 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, 9710-5 | 11.5 | 193 |
| 121 | Structural basis of outer membrane protein insertion by the BAM complex. *Nature*, **2016**, 531, 64-9 | 50.4 | 182 |
| 120 | Structural basis for outer membrane lipopolysaccharide insertion. *Nature*, **2014**, 511, 52-6 | 50.4 | 181 |
| 119 | Molecular simulation approaches to membrane proteins. *Structure*, **2011**, 19, 1562-72 | 5.2 | 136 |
| 118 | Lipidbook: a public repository for force-field parameters used in membrane simulations. *Journal of Membrane Biology*, **2010**, 236, 255-8 | 2.3 | 131 |
| 117 | The pore structure and gating mechanism of K2P channels. *EMBO Journal*, **2011**, 30, 3607-19 | 13 | 129 |
| 116 | Structure of the TatC core of the twin-arginine protein transport system. *Nature*, **2012**, 492, 210-4 | 50.4 | 126 |
| 115 | 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, 1470-84 | 4.3 | 124 |
| 114 | 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 | 16.8 | 116 |
| 113 | PIP(2)-binding site in Kir channels: definition by multiscale biomolecular simulations. *Biochemistry*, **2009**, 48, 10926-33 | 3.2 | 108 |
| 112 | Drug block of the hERG potassium channel: insight from modeling. *Proteins: Structure, Function and Bioinformatics*, **2007**, 68, 568-80 | 4.2 | 87 |
| 111 | Mechanistic insight into human ether-□go-go-related gene (hERG) K+ channel deactivation gating from the solution structure of the EAG domain. *Journal of Biological Chemistry*, **2011**, 286, 6184-91 | 5.4 | 78 |
| 110 | Structural basis of lipoprotein signal peptidase II action and inhibition by the antibiotic globomycin. *Science*, **2016**, 351, 876-80 | 33.3 | 77 |
| 109 | The structural basis of ZMPSTE24-dependent laminopathies. *Science*, **2013**, 339, 1604-7 | 33.3 | 75 |

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|---|---|---|---|
| 108 | 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, 509-19 | 4.2 | 72 |
| 107 | Functional analysis of missense variants in the TRESK (KCNK18) K channel. *Scientific Reports*, **2012**, 2, 237 | 4.9 | 70 |
| 106 | The MemProtMD database: a resource for membrane-embedded protein structures and their lipid interactions. *Nucleic Acids Research*, **2019**, 47, D390-D397 | 20.1 | 70 |
| 105 | Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association. *Journal of Physical Chemistry B*, **2017**, 121, 3364-3375 | 3.4 | 69 |
| 104 | Multiscale simulations reveal conserved patterns of lipid interactions with aquaporins. *Structure*, **2013**, 21, 810-9 | 5.2 | 64 |
| 103 | A specific two-pore domain potassium channel blocker defines the structure of the TASK-1 open pore. *Journal of Biological Chemistry*, **2011**, 286, 13977-84 | 5.4 | 62 |
| 102 | Structures of the stator complex that drives rotation of the bacterial flagellum. *Nature Microbiology* , **2020**, 5, 1553-1564 | 26.6 | 61 |
| 101 | Structural analysis of the G-box domain of the microcephaly protein CPAP suggests a role in centriole architecture. *Structure*, **2013**, 21, 2069-77 | 5.2 | 59 |
| 100 | The structural basis of lipid scrambling and inactivation in the endoplasmic reticulum scramblase TMEM16K. *Nature Communications*, **2019**, 10, 3956 | 17.4 | 55 |
| 99 | Simulation-based prediction of phosphatidylinositol 4,5-bisphosphate binding to an ion channel. *Biochemistry*, **2013**, 52, 279-81 | 3.2 | 54 |
| 98 | Lipopolysaccharide is inserted into the outer membrane through an intramembrane hole, a lumen gate, and the lateral opening of LptD. *Structure*, **2015**, 23, 496-504 | 5.2 | 53 |
| 97 | Biophysical and computational studies of membrane penetration by the GRP1 pleckstrin homology domain. *Structure*, **2011**, 19, 1338-46 | 5.2 | 50 |
| 96 | Insight into the mechanism of inactivation and pH sensitivity in potassium channels from molecular dynamics simulations. *Biochemistry*, **2008**, 47, 7414-22 | 3.2 | 46 |
| 95 | Side pockets provide the basis for a new mechanism of Kv channel-specific inhibition. *Nature Chemical Biology*, **2013**, 9, 507-13 | 11.7 | 43 |
| 94 | New insights into K channel gene mutations and neonatal diabetes mellitus. *Nature Reviews Endocrinology*, **2020**, 16, 378-393 | 15.2 | 41 |
| 93 | Structural insights into the mechanism of the membrane integral N-acyltransferase step in bacterial lipoprotein synthesis. *Nature Communications*, **2017**, 8, 15952 | 17.4 | 40 |
| 92 | Assembling the Tat protein translocase. *ELife*, **2016**, 5, | 8.9 | 39 |
| 91 | A Coarse Grained Model for a Lipid Membrane with Physiological Composition and Leaflet Asymmetry. *PLoS ONE*, **2015**, 10, e0144814 | 3.7 | 38 |

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|---|---|---|---|
| 90 | Molecular mechanisms for drug interactions with hERG that cause long QT syndrome. *Expert Opinion on Drug Metabolism and Toxicology*, **2006**, 2, 81-94 | 5.5 | 38 |
| 89 | In Situ Structure of an Intact Lipopolysaccharide-Bound Bacterial Surface Layer. *Cell*, **2020**, 180, 348-358.e15 | 36.2 | 37 |
| 88 | Structural basis of proton-coupled potassium transport in the KUP family. *Nature Communications*, **2020**, 11, 626 | 17.4 | 35 |
| 87 | State-independent intracellular access of quaternary ammonium blockers to the pore of TREK-1. *Channels*, **2012**, 6, 473-8 | 3 | 34 |
| 86 | Activation gating of hERG potassium channels: S6 glycines are not required as gating hinges. *Journal of Biological Chemistry*, **2007**, 282, 31972-81 | 5.4 | 34 |
| 85 | A bipartite structural organization defines the SERINC family of HIV-1 restriction factors. *Nature Structural and Molecular Biology*, **2020**, 27, 78-83 | 17.6 | 34 |
| 84 | A lipid gating mechanism for the channel-forming O antigen ABC transporter. *Nature Communications*, **2019**, 10, 824 | 17.4 | 34 |
| 83 | Insights into Membrane Protein-Lipid Interactions from Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2019**, 15, 5727-5736 | 6.4 | 33 |
| 82 | Structure and mechanism of bactericidal mammalian perforin-2, an ancient agent of innate immunity. *Science Advances*, **2020**, 6, eaax8286 | 14.3 | 32 |
| 81 | Dimerization of the EphA1 receptor tyrosine kinase transmembrane domain: Insights into the mechanism of receptor activation. *Biochemistry*, **2014**, 53, 6641-52 | 3.2 | 32 |
| 80 | Crystal structure of undecaprenyl-pyrophosphate phosphatase and its role in peptidoglycan biosynthesis. *Nature Communications*, **2018**, 9, 1078 | 17.4 | 31 |
| 79 | Water and hydrophobic gates in ion channels and nanopores. *Faraday Discussions*, **2018**, 209, 231-247 | 3.6 | 28 |
| 78 | Ternary structure reveals mechanism of a membrane diacylglycerol kinase. *Nature Communications*, **2015**, 6, 10140 | 17.4 | 27 |
| 77 | 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, 333-48 | 4.6 | 25 |
| 76 | Balancing Force Field Protein-Lipid Interactions To Capture Transmembrane Helix-Helix Association. *Journal of Chemical Theory and Computation*, **2018**, 14, 1706-1715 | 6.4 | 24 |
| 75 | Structural Determinants for High-Affinity Block of hERG Potassium Channels. *Novartis Foundation Symposium*, **2008**, 136-154 | | 24 |
| 74 | 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 | 11.5 | 23 |
| 73 | Targeting of proteins to the twin-arginine translocation pathway. *Molecular Microbiology*, **2020**, 113, 861-871 | 4.1 | 22 |

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|---|---|---|---|
| 72 | The response of the tandem pore potassium channel TASK-3 (K(2P)9.1) to voltage: gating at the cytoplasmic mouth. *Journal of Physiology*, **2009**, 587, 4769-83 | 3.9 | 22 |
| 71 | Molecular modeling and simulation studies of ion channel structures, dynamics and mechanisms. *Methods in Cell Biology*, **2008**, 90, 233-65 | 1.8 | 22 |
| 70 | The energetics of protein-lipid interactions as viewed by molecular simulations. *Biochemical Society Transactions*, **2020**, 48, 25-37 | 5.1 | 22 |
| 69 | 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 | 11.5 | 21 |
| 68 | Structures of monomeric and oligomeric forms of the perforin-like protein 1. *Science Advances*, **2018**, 4, eaaq0762 | 14.3 | 20 |
| 67 | Interactions of the EphA2 Kinase Domain with PIPs in Membranes: Implications for Receptor Function. *Structure*, **2018**, 26, 1025-1034.e2 | 5.2 | 20 |
| 66 | The TatC component of the twin-arginine protein translocase functions as an obligate oligomer. *Molecular Microbiology*, **2015**, 98, 111-29 | 4.1 | 20 |
| 65 | A BEST example of channel structure annotation by molecular simulation. *Channels*, **2017**, 11, 347-353 | 3 | 19 |
| 64 | Complete structure of the chemosensory array core signalling unit in an E. coli minicell strain. *Nature Communications*, **2020**, 11, 743 | 17.4 | 19 |
| 63 | Structural biology of Tat protein transport. *Current Opinion in Structural Biology*, **2014**, 27, 32-7 | 8.1 | 19 |
| 62 | 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 | 7.6 | 18 |
| 61 | A Mass-Spectrometry-Based Approach to Distinguish Annular and Specific Lipid Binding to Membrane Proteins. *Angewandte Chemie - International Edition*, **2020**, 59, 3523-3528 | 16.4 | 18 |
| 60 | Dynamics of an LPS translocon induced by substrate and an antimicrobial peptide. *Nature Chemical Biology*, **2021**, 17, 187-195 | 11.7 | 18 |
| 59 | Multiple lipid binding sites determine the affinity of PH domains for phosphoinositide-containing membranes. *Science Advances*, **2020**, 6, eaay5736 | 14.3 | 17 |
| 58 | Substrate-triggered position switching of TatA and TatB during Tat transport in. *Open Biology*, **2017**, 7, | 7 | 16 |
| 57 | Structure and function of the Escherichia coli Tol-Pal stator protein TolR. *Journal of Biological Chemistry*, **2015**, 290, 26675-87 | 5.4 | 16 |
| 56 | The molecular basis for an allosteric inhibition of K-flux gating in K channels. *ELife*, **2019**, 8, | 8.9 | 16 |
| 55 | Structure and dynamics of the E. coli chemotaxis core signaling complex by cryo-electron tomography and molecular simulations. *Communications Biology*, **2020**, 3, 24 | 6.7 | 16 |

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| 54 | Computational studies of membrane proteins: from sequence to structure to simulation. *Current Opinion in Structural Biology*, **2017**, 45, 133-141 | 8.1 | 15 |
| 53 | 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, 618-26 | 5.4 | 14 |
| 52 | Ion-blocking sites of the Kir2.1 channel revealed by multiscale modeling. *Biochemistry*, **2009**, 48, 8758-63 | 3.2 | 14 |
| 51 | CG2AT2: an Enhanced Fragment-Based Approach for Serial Multi-scale Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6472-6482 | 6.4 | 14 |
| 50 | A conserved tryptophan at the membrane-water interface acts as a gatekeeper for Kir6.2/SUR1 channels and causes neonatal diabetes when mutated. *Journal of Physiology*, **2011**, 589, 3071-83 | 3.9 | 13 |
| 49 | Interaction of lipids with the neurotensin receptor 1. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1278-87 | 3.8 | 12 |
| 48 | Simulations of the BM2 proton channel transmembrane domain from influenza virus B. *Biochemistry*, **2009**, 48, 9949-51 | 3.2 | 12 |
| 47 | Sharing Data from Molecular Simulations. *Journal of Chemical Information and Modeling*, **2019**, 59, 4093-4099 | 4.3 | 11 |
| 46 | Characterizing Membrane Association and Periplasmic Transfer of Bacterial Lipoproteins through Molecular Dynamics Simulations. *Structure*, **2020**, 28, 475-487.e3 | 5.2 | 11 |
| 45 | Calmodulin Regulates Human Ether □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, 17907-18 | 5.4 | 11 |
| 44 | Structural basis for substrate specificity and regulation of nucleotide sugar transporters in the lipid bilayer. *Nature Communications*, **2019**, 10, 4657 | 17.4 | 10 |
| 43 | PyLipID: A Python Package for Analysis of Protein-Lipid Interactions from Molecular Dynamics Simulations.. *Journal of Chemical Theory and Computation*, **2022**, | 6.4 | 10 |
| 42 | The Unconventional Cytoplasmic Sensing Mechanism for Ethanol Chemotaxis in Bacillus subtilis. *MBio*, **2020**, 11, | 7.8 | 10 |
| 41 | Conformational dynamics of a G protein-coupled receptor helix 8 in lipid membranes. *Science Advances*, **2020**, 6, eaav8207 | 14.3 | 10 |
| 40 | 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 | 11.5 | 9 |
| 39 | The structural basis of lipid scrambling and inactivation in the endoplasmic reticulum scramblase TMEM16K | | 9 |
| 38 | Switching Cytolytic Nanopores into Antimicrobial Fractal Ruptures by a Single Side Chain Mutation. *ACS Nano*, **2021**, 15, 9679-9689 | 16.7 | 9 |
| 37 | Evaluating inositol phospholipid interactions with inward rectifier potassium channels and characterising their role in disease. *Communications Chemistry*, **2020**, 3, | 6.3 | 8 |

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| 36 | Identification and assessment of cardiolipin interactions with inner membrane proteins. *Science Advances*, **2021**, 7, | 14.3 | 7 |
| 35 | The centriolar protein CPAP G-box: an amyloid fibril in a single domain. *Biochemical Society Transactions*, **2015**, 43, 838-43 | 5.1 | 6 |
| 34 | A leucine zipper motif essential for gating of hyperpolarization-activated channels. *Journal of Biological Chemistry*, **2012**, 287, 40150-60 | 5.4 | 6 |
| 33 | Mechanism of lipid droplet formation by the yeast Sei1/Ldb16 Seipin complex. *Nature Communications*, **2021**, 12, 5892 | 17.4 | 5 |
| 32 | 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, | 11.5 | 5 |
| 31 | Structure, substrate recognition and initiation of hyaluronan synthase.. *Nature*, **2022**, | 50.4 | 5 |
| 30 | Atomistic mechanism of transmembrane helix association. *PLoS Computational Biology*, **2020**, 16, e1007519 | 3 | 4 |
| 29 | Structures of the stator complex that drives rotation of the bacterial flagellum | | 4 |
| 28 | CG2AT2: An Enhanced Fragment-based approach for Serial Multi-scale Molecular Dynamics simulations | | 4 |
| 27 | Cryo-EM Structures of CusA Reveal a Mechanism of Metal-Ion Export. *MBio*, **2021**, 12, | 7.8 | 4 |
| 26 | Interactions of a Bacterial Cu(I)-ATPase with a Complex Lipid Environment. *Biochemistry*, **2018**, 57, 4063-4073 | 3.2 | 3 |
| 25 | Substrate-triggered position-switching of TatA and TatB is an essential step in the Escherichia coli Tat protein export pathway | | 3 |
| 24 | Identification and assessment of cardiolipin interactions with E. coli inner membrane proteins | | 3 |
| 23 | NaViA: A Program for the Visual Analysis of Complex Mass Spectra. *Bioinformatics*, **2021**, | 7.2 | 3 |
| 22 | PyLipID: A Python package for analysis of protein-lipid interactions from MD simulations | | 3 |
| 21 | Relative Affinities of Protein-Cholesterol Interactions from Equilibrium Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6548-6558 | 6.4 | 3 |
| 20 | Structural basis of trehalose recognition by the mycobacterial LpqY-SugABC transporter. *Journal of Biological Chemistry*, **2021**, 296, 100307 | 5.4 | 3 |
| 19 | The pore structure and gating mechanism of K2P channels. *EMBO Journal*, **2011**, 30, 4515-4515 | 13 | 2 |

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|---|---|---|---|
| 18 | High-resolution mapping of metal ions reveals principles of surface layer assembly in Caulobacter crescentus cells. *Structure*, **2021**, | 5.2 | 2 |
| 17 | Alternative Architecture of the Chemosensory Array. *Biomolecules*, **2021**, 11, | 5.9 | 2 |
| 16 | Membrane Binding of Antimicrobial Peptides Is Modulated by Lipid Charge Modification. *Journal of Chemical Theory and Computation*, **2021**, 17, 1218-1228 | 6.4 | 2 |
| 15 | Deciphering ion transport and ATPase coupling in the intersubunit tunnel of KdpFABC. *Nature Communications*, **2021**, 12, 5098 | 17.4 | 2 |
| 14 | Identification and Characterization of Specific Protein-Lipid Interactions Using Molecular Simulation. *Methods in Molecular Biology*, **2021**, 2315, 121-139 | 1.4 | 2 |
| 13 | A Heuristic Derived from Analysis of the Ion Channel Structural Proteome Permits the Rapid Identification of Hydrophobic Gates | | 1 |
| 12 | Evaluating Inositol phospholipid interactions with Inward Rectifier Potassium Channels and characterising their role in Disease | | 1 |
| 11 | Insights into Membrane Protein-Lipid Interactions from Free Energy Calculations | | 1 |
| 10 | A Mass-Spectrometry-Based Approach to Distinguish Annular and Specific Lipid Binding to Membrane Proteins. *Angewandte Chemie*, **2020**, 132, 3551-3556 | 3.6 | 1 |
| 9 | The dynamic interplay of PIP2 and ATP in the regulation of the KATP channel | | 1 |
| 8 | A Bacterial Inflammation Sensor Regulates c-di-GMP Signaling, Adhesion, and Biofilm Formation. *MBio*, **2021**, 12, e0017321 | 7.8 | 1 |
| 7 | From Bench to Biomolecular Simulation: Phospholipid Modulation of Potassium Channels. *Journal of Molecular Biology*, **2021**, 433, 167105 | 6.5 | 1 |
| 6 | Peptidoglycan biosynthesis is driven by lipid transfer along enzyme-substrate affinity gradients.. *Nature Communications*, **2022**, 13, 2278 | 17.4 | 1 |
| 5 | Coupling Form and Function: How the Oligomerisation Symmetry of the SAS-6 Protein Contributes to the Architecture of Centriole Organelles. *Symmetry*, **2017**, 9, 74 | 2.7 | |
| 4 | Memprotmd: Adding the Grease to Membrane Protein Structures. *Biophysical Journal*, **2012**, 102, 469a | 2.9 | |
| 3 | Homology Models Applied to Toxicology433-468 | | |
| 2 | Greasing the Gears of Mechanosensitive Piezo Channels with Phosphoinositides and Cholesterol. *Biophysical Journal*, **2020**, 119, 1467-1469 | 2.9 | |
| 1 | Structural, Functional and Computational Studies of Membrane Recognition by Plasmodium Perforin-Like Proteins 1 and 2. *Journal of Molecular Biology*, **2022**, 434, 167642 | 6.5 | |