Mark S P Sansom

List of Publications by Year in Descending Order

530 papers	25,998 citations	83 h-index	129 g-index
572 ext. papers	29,054 ext. citations	6.5 avg, IF	7.41 L-index

#	Paper	IF	Citations
530	Structural insights into the Venus flytrap mechanosensitive ion channel Flycatcher1.. *Nature Communications*, **2022**, 13, 850	16.9	0
529	PyLipID: A Python Package for Analysis of Protein-Lipid Interactions from Molecular Dynamics Simulations.. *Journal of Chemical Theory and Computation*, **2022**,	6.2	2
528	Molecular Simulations of Hydrophobic Gating of Pentameric Ligand Gated Ion Channels: Insights into Water and Ions. *Journal of Physical Chemistry B*, **2021**, 125, 981-994	3.3	4
527	Membrane Binding of Antimicrobial Peptides Is Modulated by Lipid Charge Modification. *Journal of Chemical Theory and Computation*, **2021**, 17, 1218-1228	6.2	2
526	Binding of Ca-independent C2 domains to lipid membranes: A multi-scale molecular dynamics study. *Structure*, **2021**, 29, 1200-1213.e2	5	1
525	Modulation of adenosine A2a receptor oligomerization by receptor activation and PIP interactions. *Structure*, **2021**, 29, 1312-1325.e3	5	1
524	Identification and assessment of cardiolipin interactions with inner membrane proteins. *Science Advances*, **2021**, 7,	13.9	5
523	Membrane-binding mechanism of the EEA1 FYVE domain revealed by multi-scale molecular dynamics simulations. *PLoS Computational Biology*, **2021**, 17, e1008807	4.8	1
522	Influence of water models on water movement through AQP1. *Journal of Chemical Physics*, **2021**, 155, 154502	3.8	1
521	Effect of Water Models on Transmembrane Self-Assembled Cyclic Peptide Nanotubes. *ACS Nano*, **2021**, 15, 7053-7064	16.4	2
520	Membrane Interactions of □Synuclein Revealed by Multiscale Molecular Dynamics Simulations, Markov State Models, and NMR. *Journal of Physical Chemistry B*, **2021**, 125, 2929-2941	3.3	0
519	Switching Cytolytic Nanopores into Antimicrobial Fractal Ruptures by a Single Side Chain Mutation. *ACS Nano*, **2021**, 15, 9679-9689	16.4	6
518	Structure, mechanism, and inhibition of Hedgehog acyltransferase. *Molecular Cell*, **2021**,	17	1
517	Relative Affinities of Protein-Cholesterol Interactions from Equilibrium Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2021**, 17, 6548-6558	6.2	2
516	Identification and Characterization of Specific Protein-Lipid Interactions Using Molecular Simulation. *Methods in Molecular Biology*, **2021**, 2315, 121-139	1.4	1
515	Lipid Interactions of a Ciliary Membrane TRP Channel: Simulation and Structural Studies of Polycystin-2. *Structure*, **2020**, 28, 169-184.e5	5	18
514	Lipid-Dependent Regulation of Ion Channels and G Protein-Coupled Receptors: Insights from Structures and Simulations. *Annual Review of Pharmacology and Toxicology*, **2020**, 60, 31-50	17.4	53

513	Electric Field Induced Wetting of a Hydrophobic Gate in a Model Nanopore Based on the 5-HT Receptor Channel. *ACS Nano*, **2020**, 14, 10480-10491	16.4	7
512	Mechanisms of activation and desensitization of full-length glycine receptor in lipid nanodiscs. *Nature Communications*, **2020**, 11, 3752	16.9	25
511	Water in Nanopores and Biological Channels: A Molecular Simulation Perspective. *Chemical Reviews* , **2020**, 120, 10298-10335	66.4	40
510	Coarse-Grained Simulations Suggest the Epsin N-Terminal Homology Domain Can Sense Membrane Curvature without Its Terminal Amphipathic Helix. *ACS Nano*, **2020**,	16.4	3
509	The MscS-like channel YnaI has a gating mechanism based on flexible pore helices. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 28754-28762	11.1	15
508	The Glycosphingolipid GM3 Modulates Conformational Dynamics of the Glucagon Receptor. *Biophysical Journal*, **2020**, 119, 300-313	0.5	8
507	Atomistic mechanism of transmembrane helix association. *PLoS Computational Biology*, **2020**, 16, e1007918	4.8	3
506	Multiple lipid binding sites determine the affinity of PH domains for phosphoinositide-containing membranes. *Science Advances*, **2020**, 6, eaay5736	13.9	14
505	Induced Polarization in Molecular Dynamics Simulations of the 5-HT Receptor Channel. *Journal of the American Chemical Society*, **2020**, 142, 9415-9427	16	14
504	Defining how multiple lipid species interact with inward rectifier potassium (Kir2) channels. *Proceedings of the National Academy of Sciences of the United States of America*, **2020**, 117, 7803-7813	11.1	37
503	The energetics of protein-lipid interactions as viewed by molecular simulations. *Biochemical Society Transactions*, **2020**, 48, 25-37	5	20
502	Local frustration determines loop opening during the catalytic cycle of an oxidoreductase. *ELife*, **2020**, 9,	8.6	4
501	Insights into Membrane Protein-Lipid Interactions from Free Energy Calculations. *Journal of Chemical Theory and Computation*, **2019**, 15, 5727-5736	6.2	31
500	The morphogen Sonic hedgehog inhibits its receptor Patched by a pincer grasp mechanism. *Nature Chemical Biology*, **2019**, 15, 975-982	11.3	32
499	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	11.1	21
498	CHAP: A Versatile Tool for the Structural and Functional Annotation of Ion Channel Pores. *Journal of Molecular Biology*, **2019**, 431, 3353-3365	6.3	44
497	Structures of the otopetrin proton channels Otop1 and Otop3. *Nature Structural and Molecular Biology*, **2019**, 26, 518-525	17.2	24
496	Lipid Bilayer Composition Influences the Activity of the Antimicrobial Peptide Dermcidin Channel. *Biophysical Journal*, **2019**, 116, 1658-1666	0.5	11

495	Computational Virology: Molecular Simulations of Virus Dynamics and Interactions. *Advances in Experimental Medicine and Biology*, **2019**, 1215, 201-233	3.4	6
494	Membrane Recognition and Binding by the Phosphatidylinositol Phosphate Kinase PIP5K1A: A Multiscale Simulation Study. *Structure*, **2019**, 27, 1336-1346.e2	5	7
493	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. *Wiley Interdisciplinary Reviews: Computational Molecular Science*, **2019**, 9, e1393	7.6	65
492	A lipid gating mechanism for the channel-forming O antigen ABC transporter. *Nature Communications*, **2019**, 10, 824	16.9	34
491	Structure and Dynamics of Cinnamycin-Lipid Complexes: Mechanisms of Selectivity for Phosphatidylethanolamine Lipids. *ACS Omega*, **2019**, 4, 18889-18899	3.8	5
490	More Favorable Palmitic Acid Over Palmitoleic Acid Modification of Wnt3 Ensures Its Localization and Activity in Plasma Membrane Domains. *Frontiers in Cell and Developmental Biology*, **2019**, 7, 281	5.4	6
489	State-dependent Lipid Interactions with the A2a Receptor Revealed by MD Simulations Using In Vivo-Mimetic Membranes. *Structure*, **2019**, 27, 392-403.e3	5	40
488	The MemProtMD database: a resource for membrane-embedded protein structures and their lipid interactions. *Nucleic Acids Research*, **2019**, 47, D390-D397	19.4	70
487	Cholesterol Interaction Sites on the Transmembrane Domain of the Hedgehog Signal Transducer and Class F G Protein-Coupled Receptor Smoothened. *Structure*, **2019**, 27, 549-559.e2	5	44
486	Computational Modeling of Realistic Cell Membranes. *Chemical Reviews*, **2019**, 119, 6184-6226	66.4	244
485	A Newly Available Tool for Functional Annotation of Ion Channel Structures Based on Molecular Dynamics Simulations. *Biophysical Journal*, **2018**, 114, 134a	0.5	1
484	Water and hydrophobic gates in ion channels and nanopores. *Faraday Discussions*, **2018**, 209, 231-247	3.4	29
483	Balancing Force Field Protein-Lipid Interactions To Capture Transmembrane Helix-Helix Association. *Journal of Chemical Theory and Computation*, **2018**, 14, 1706-1715	6.2	22
482	Modes of Interaction of Pleckstrin Homology Domains with Membranes: Toward a Computational Biochemistry of Membrane Recognition. *Journal of Molecular Biology*, **2018**, 430, 372-388	6.3	25
481	Distinctive phosphoinositide- and Ca-binding properties of normal and cognitive performance-linked variant forms of KIBRA C2 domain. *Journal of Biological Chemistry*, **2018**, 293, 9335-9344	5	5
480	Electric-Field-Driven Translocation of ssDNA through Hydrophobic Nanopores. *ACS Nano*, **2018**, 12, 8208-8213	14.1	11
479	PtdIns(4,5)P stabilizes active states of GPCRs and enhances selectivity of G-protein coupling. *Nature*, **2018**, 559, 423-427	47.5	136
478	How nanoscale protein interactions determine the mesoscale dynamic organisation of bacterial outer membrane proteins. *Nature Communications*, **2018**, 9, 2846	16.9	31

477	Interactions of the EphA2 Kinase Domain with PIPs in Membranes: Implications for Receptor Function. *Structure*, **2018**, 26, 1025-1034.e2	5	20
476	Interactions of a Bacterial Cu(I)-ATPase with a Complex Lipid Environment. *Biochemistry*, **2018**, 57, 4063-4073	3.0	3
475	The effect of mutations in the lid region of Thermomyces lanuginosus lipase on interactions with triglyceride surfaces: A multi-scale simulation study. *Chemistry and Physics of Lipids*, **2018**, 211, 4-15	3.6	13
474	State Dependent Interactions of Lipids with GPCR Revealed by MD Simulations using In Vivo-Mimetic Membranes. *Biophysical Journal*, **2018**, 114, 274a	0.5	2
473	Cryo-EM reveals two distinct serotonin-bound conformations of full-length 5-HT receptor. *Nature*, **2018**, 563, 270-274	47.5	63
472	Analyzing protein topology based on Laguerre tessellation of a pore-traversing water network. *Scientific Reports*, **2018**, 8, 13540	4.7	4
471	The modelling and enhancement of water hydrodynamics: general discussion. *Faraday Discussions*, **2018**, 209, 273-285	3.4	1
470	Structure and function of natural proteins for water transport: general discussion. *Faraday Discussions*, **2018**, 209, 83-95	3.4	2
469	Biomimetic water channels: general discussion. *Faraday Discussions*, **2018**, 209, 205-229	3.4	7
468	Cryo-EM structure of the mechanically activated ion channel OSCA1.2. *ELife*, **2018**, 7,	8.6	61
467	Asymmetric mechanosensitivity in a eukaryotic ion channel. *Proceedings of the National Academy of Sciences of the United States of America*, **2017**, 114, E8343-E8351	11.1	34
466	Dynamic role of the tether helix in PIP-dependent gating of a G protein-gated potassium channel. *Journal of General Physiology*, **2017**, 149, 799-811	3.2	25
465	The effects of stretch activation on ionic selectivity of the TREK-2 K2P K channel. *Channels*, **2017**, 11, 482-486	2.8	4
464	Protein crowding and lipid complexity influence the nanoscale dynamic organization of ion channels in cell membranes. *Scientific Reports*, **2017**, 7, 16647	4.7	45
463	Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association. *Journal of Physical Chemistry B*, **2017**, 121, 3364-3375	3.3	68
462	The Integrin Receptor in Biologically Relevant Bilayers: Insights from Molecular Dynamics Simulations. *Journal of Membrane Biology*, **2017**, 250, 337-351	2.1	18
461	Effect of the Southeast Asian Ovalocytosis Deletion on the Conformational Dynamics of Signal-Anchor Transmembrane Segment 1 of Red Cell Anion Exchanger 1 (AE1, Band 3, or SLC4A1). *Biochemistry*, **2017**, 56, 712-722	3.1	5
460	Voltage Gating of a Biomimetic Nanopore: Electrowetting of a Hydrophobic Barrier. *ACS Nano*, **2017**, 11, 1840-1847	16.4	37

459	Dynamic interactions between a membrane binding protein and lipids induce fluctuating diffusivity. *Science Advances*, **2017**, 3, e1601871	13.9	39
458	Biomimetic Phospholipid Membrane Organization on Graphene and Graphene Oxide Surfaces: A Molecular Dynamics Simulation Study. *ACS Nano*, **2017**, 11, 1613-1625	16.4	53
457	Bilayer-Mediated Structural Transitions Control Mechanosensitivity of the TREK-2 K2P Channel. *Structure*, **2017**, 25, 708-718.e2	5	43
456	Stability and dynamics of membrane-spanning DNA nanopores. *Nature Communications*, **2017**, 8, 14784	16.9	33
455	A BEST example of channel structure annotation by molecular simulation. *Channels*, **2017**, 11, 347-353	2.8	18
454	Interfacial activation of M37 lipase: A multi-scale simulation study. *Biochimica Et Biophysica Acta - Biomembranes*, **2017**, 1859, 340-349	3.6	13
453	Structure and lipid-binding properties of the kindlin-3 pleckstrin homology domain. *Biochemical Journal*, **2017**, 474, 539-556	3.7	28
452	Functional Annotation of Ion Channel Structures by Molecular Simulation. *Structure*, **2016**, 24, 2207-2216	5	41
451	Conformational Changes in the Epidermal Growth Factor Receptor: Role of the Transmembrane Domain Investigated by Coarse-Grained MetaDynamics Free Energy Calculations. *Journal of the American Chemical Society*, **2016**, 138, 10611-22	16	64
450	Structural basis of Smoothened regulation by its extracellular domains. *Nature*, **2016**, 535, 517-522	47.5	229
449	Lipid-Loving ANTs: Molecular Simulations of Cardiolipin Interactions and the Organization of the Adenine Nucleotide Translocase in Model Mitochondrial Membranes. *Biochemistry*, **2016**, 55, 6238-6249	3.1	52
448	Molecular dynamics simulations of membrane proteins and their interactions: from nanoscale to mesoscale. *Current Opinion in Structural Biology*, **2016**, 40, 8-16	7.9	83
447	Association of Peripheral Membrane Proteins with Membranes: Free Energy of Binding of GRP1 PH Domain with Phosphatidylinositol Phosphate-Containing Model Bilayers. *Journal of Physical Chemistry Letters*, **2016**, 7, 1219-24	6.3	32
446	Computational virology: From the inside out. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1610-8	3.6	37
445	Why do the outer membrane proteins OmpF from E. coli and OprP from P. aeruginosa prefer trimers? Simulation studies. *Journal of Molecular Graphics and Modelling*, **2016**, 65, 1-7	2.8	9
444	The Role of the Membrane in the Structure and Biophysical Robustness of the Dengue Virion Envelope. *Structure*, **2016**, 24, 375-82	5	62
443	Structures of the EphA2 Receptor at the Membrane: Role of Lipid Interactions. *Structure*, **2016**, 24, 337-47	5	26
442	Lipid Bilayer Membrane Perturbation by Embedded Nanopores: A Simulation Study. *ACS Nano*, **2016**, 10, 3693-701	16.4	31

441	Lipid interaction sites on channels, transporters and receptors: Recent insights from molecular dynamics simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 2390-2400	3.6	110
440	Molecular simulations of glycolipids: Towards mammalian cell membrane models. *Biochimie*, **2016**, 120, 105-9	4.4	20
439	Multiscale Simulations Suggest a Mechanism for the Association of the Dok7 PH Domain with PIP-Containing Membranes. *PLoS Computational Biology*, **2016**, 12, e1005028	4.8	18
438	On the interpretation of reflectivity data from lipid bilayers in terms of molecular-dynamics models. *Acta Crystallographica Section D: Structural Biology*, **2016**, 72, 1227-1240	5.3	8
437	Super-complexes of adhesion GPCRs and neural guidance receptors. *Nature Communications*, **2016**, 7, 11184	16.9	49
436	Accurate Prediction of Ligand Affinities for a Proton-Dependent Oligopeptide Transporter. *Cell Chemical Biology*, **2016**, 23, 299-309	7.9	26
435	Band 3, the human red cell chloride/bicarbonate anion exchanger (AE1, SLC4A1), in a structural context. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1507-32	3.6	97
434	Free Energy Landscape of Lipid Interactions with Regulatory Binding Sites on the Transmembrane Domain of the EGF Receptor. *Journal of Physical Chemistry B*, **2016**, 120, 8154-63	3.3	43
433	Interactions of Pleckstrin Homology Domains with Membranes: Adding Back the Bilayer via High-Throughput Molecular Dynamics. *Structure*, **2016**, 24, 1421-1431	5	48
432	Membrane Compartmentalization Reducing the Mobility of Lipids and Proteins within a Model Plasma Membrane. *Journal of Physical Chemistry B*, **2016**, 120, 8873-81	3.3	22
431	Membrane stiffness is modified by integral membrane proteins. *Soft Matter*, **2016**, 12, 7792-7803	3.5	50
430	Roles of Interleaflet Coupling and Hydrophobic Mismatch in Lipid Membrane Phase-Separation Kinetics. *Journal of the American Chemical Society*, **2016**, 138, 11633-42	16	36
429	Proton currents constrain structural models of voltage sensor activation. *ELife*, **2016**, 5,	8.6	20
428	Anomalous Dynamics of a Lipid Recognition Protein on a Membrane Surface. *Scientific Reports*, **2015**, 5, 18245	4.7	34
427	Nothing to sneeze at: a dynamic and integrative computational model of an influenza A virion. *Structure*, **2015**, 23, 584-597	5	67
426	Molecular dynamics simulations of the bacterial UraA H+-uracil symporter in lipid bilayers reveal a closed state and a selective interaction with cardiolipin. *PLoS Computational Biology*, **2015**, 11, e1004123	4.8	29
425	Modeling Suggests TRPC3 Hydrogen Bonding and Not Phosphorylation Contributes to the Ataxia Phenotype of the Moonwalker Mouse. *Biochemistry*, **2015**, 54, 4033-41	3.1	7
424	The juxtamembrane regions of human receptor tyrosine kinases exhibit conserved interaction sites with anionic lipids. *Scientific Reports*, **2015**, 5, 9198	4.7	68

423	MemProtMD: Automated Insertion of Membrane Protein Structures into Explicit Lipid Membranes. *Structure*, **2015**, 23, 1350-61	5	204
422	Alchembed: A Computational Method for Incorporating Multiple Proteins into Complex Lipid Geometries. *Journal of Chemical Theory and Computation*, **2015**, 11, 2743-2754	6.2	37
421	Capsaicin interaction with TRPV1 channels in a lipid bilayer: molecular dynamics simulation. *Biophysical Journal*, **2015**, 108, 1425-1434	0.5	63
420	K2P channel gating mechanisms revealed by structures of TREK-2 and a complex with Prozac. *Science*, **2015**, 347, 1256-9	32.2	193
419	Molecular simulation studies of hydrophobic gating in nanopores and ion channels. *Biochemical Society Transactions*, **2015**, 43, 146-50	5	21
418	Organization and Dynamics of Receptor Proteins in a Plasma Membrane. *Journal of the American Chemical Society*, **2015**, 137, 14694-704	16	78
417	Gating-like Motions and Wall Porosity in a DNA Nanopore Scaffold Revealed by Molecular Simulations. *ACS Nano*, **2015**, 9, 11209-17	16.4	37
416	Interactions of the EGFR juxtamembrane domain with PIP2-containing lipid bilayers: Insights from multiscale molecular dynamics simulations. *Biochimica Et Biophysica Acta - General Subjects*, **2015**, 1850, 1017-1025	3.9	47
415	Hydrophobic gating in ion channels. *Journal of Molecular Biology*, **2015**, 427, 121-30	6.3	171
414	Interactions of lipids and detergents with a viral ion channel protein: molecular dynamics simulation studies. *Journal of Physical Chemistry B*, **2015**, 119, 764-72	3.3	18
413	A Coarse Grained Model for a Lipid Membrane with Physiological Composition and Leaflet Asymmetry. *PLoS ONE*, **2015**, 10, e0144814	3.6	37
412	Epock: rapid analysis of protein pocket dynamics. *Bioinformatics*, **2015**, 31, 1478-80	6.8	52
411	Supramolecular assemblies underpin turnover of outer membrane proteins in bacteria. *Nature*, **2015**, 523, 333-6	47.5	118
410	The role of lipids in mechanosensation. *Nature Structural and Molecular Biology*, **2015**, 22, 991-8	17.2	109
409	Crystal Structures of the Extracellular Domain from PepT1 and PepT2 Provide Novel Insights into Mammalian Peptide Transport. *Structure*, **2015**, 23, 1889-1899	5	30
408	Ternary structure reveals mechanism of a membrane diacylglycerol kinase. *Nature Communications*, **2015**, 6, 10140	16.9	27
407	Influence of lipids on the hydrophobic barrier within the pore of the TWIK-1 K2P channel. *Channels*, **2015**, 9, 44-9	2.8	15
406	Crystal structure of the sodium-proton antiporter NhaA dimer and new mechanistic insights. *Journal of General Physiology*, **2014**, 144, 529-44	3.2	58

405	Lipid clustering correlates with membrane curvature as revealed by molecular simulations of complex lipid bilayers. *PLoS Computational Biology*, **2014**, 10, e1003911	4.8	158
404	The free energy landscape of dimerization of a membrane protein, NanC. *PLoS Computational Biology*, **2014**, 10, e1003417	4.8	22
403	A multiscale approach to modelling drug metabolism by membrane-bound cytochrome P450 enzymes. *PLoS Computational Biology*, **2014**, 10, e1003714	4.8	36
402	NRas slows the rate at which a model lipid bilayer phase separates. *Faraday Discussions*, **2014**, 169, 209-23	3.4	16
401	Insights into the structural nature of the transition state in the Kir channel gating pathway. *Channels*, **2014**, 8, 551-5	2.8	1
400	A conformational landscape for alginate secretion across the outer membrane of Pseudomonas aeruginosa. *Acta Crystallographica Section D: Biological Crystallography*, **2014**, 70, 2054-68		36
399	The role of 2-methyl-2, 4-pentanediol in sodium dodecyl sulfate micelle dissociation unveiled by dynamic light scattering and molecular dynamics simulations. *Colloids and Surfaces B: Biointerfaces*, **2014**, 114, 357-62	5.8	6
398	Flexible gates generate occluded intermediates in the transport cycle of LacY. *Journal of Molecular Biology*, **2014**, 426, 735-51	6.3	49
397	Primary and secondary dimer interfaces of the fibroblast growth factor receptor 3 transmembrane domain: characterization via multiscale molecular dynamics simulations. *Biochemistry*, **2014**, 53, 323-32	3.1	20
396	Designing a hydrophobic barrier within biomimetic nanopores. *ACS Nano*, **2014**, 8, 11268-79	16.4	25
395	Interactions of peripheral proteins with model membranes as viewed by molecular dynamics simulations. *Biochemical Society Transactions*, **2014**, 42, 1418-24	5	29
394	Methodologies for the analysis of instantaneous lipid diffusion in MD simulations of large membrane systems. *Faraday Discussions*, **2014**, 169, 455-75	3.4	26
393	Sidekick for Membrane Simulations: Automated Ensemble Molecular Dynamics Simulations of Transmembrane Helices. *Journal of Chemical Theory and Computation*, **2014**, 10, 2165-75	6.2	22
392	State-dependent network connectivity determines gating in a K+ channel. *Structure*, **2014**, 22, 1037-46	5	7
391	Interactions of phosphatase and tensin homologue (PTEN) proteins with phosphatidylinositol phosphates: insights from molecular dynamics simulations of PTEN and voltage sensitive phosphatase. *Biochemistry*, **2014**, 53, 1724-32	3.1	33
390	Dimerization of the EphA1 receptor tyrosine kinase transmembrane domain: Insights into the mechanism of receptor activation. *Biochemistry*, **2014**, 53, 6641-52	3.1	32
389	Iain Campbell – a personal recollection. *Structure*, **2014**, 22, 507-8	5	0
388	Molecular mechanism of ligand recognition by membrane transport protein, Mhp1. *EMBO Journal*, **2014**, 33, 1831-44	12.6	44

387	A hydrophobic barrier deep within the inner pore of the TWIK-1 K2P potassium channel. *Nature Communications*, **2014**, 5, 4377	16.9	82
386	Control of KirBac3.1 potassium channel gating at the interface between cytoplasmic domains. *Journal of Biological Chemistry*, **2014**, 289, 143-51	5	16
385	Interactions of the auxilin-1 PTEN-like domain with model membranes result in nanoclustering of phosphatidyl inositol phosphates. *Biophysical Journal*, **2013**, 105, 137-45	0.5	22
384	Energetics of Multi-Ion Conduction Pathways in Potassium Ion Channels. *Journal of Chemical Theory and Computation*, **2013**, 9, 5176-5189	6.2	32
383	The pore of voltage-gated potassium ion channels is strained when closed. *Nature Communications*, **2013**, 4, 1872	16.9	44
382	Detailed Examination of a Single Conduction Event in a Potassium Channel. *Journal of Physical Chemistry Letters*, **2013**, 4, 3104-3109	6.3	6
381	The structural basis of ZMPSTE24-dependent laminopathies. *Science*, **2013**, 339, 1604-7	32.2	74
380	Simulation-based prediction of phosphatidylinositol 4,5-bisphosphate binding to an ion channel. *Biochemistry*, **2013**, 52, 279-81	3.1	54
379	Dodecyl maltoside protects membrane proteins in vacuo. *Biophysical Journal*, **2013**, 105, 648-56	0.5	19
378	Defining the membrane-associated state of the PTEN tumor suppressor protein. *Biophysical Journal* , **2013**, 104, 613-21	0.5	34
377	Multiscale simulations reveal conserved patterns of lipid interactions with aquaporins. *Structure*, **2013**, 21, 810-9	5	64
376	Membrane perturbation by carbon nanotube insertion: pathways to internalization. *Small*, **2013**, 9, 3639-468	11.8	59
375	Side pockets provide the basis for a new mechanism of Kv channel-specific inhibition. *Nature Chemical Biology*, **2013**, 9, 507-13	11.3	44
374	Stability and membrane interactions of an autotransport protein: MD simulations of the Hia translocator domain in a complex membrane environment. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 715-23	3.6	23
373	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	11.1	191
372	Reduced lateral mobility of lipids and proteins in crowded membranes. *PLoS Computational Biology*, **2013**, 9, e1003033	4.8	119
371	Formation of raft-like assemblies within clusters of influenza hemagglutinin observed by MD simulations. *PLoS Computational Biology*, **2013**, 9, e1003034	4.8	41
370	Conformational changes in talin on binding to anionic phospholipid membranes facilitate signaling by integrin transmembrane helices. *PLoS Computational Biology*, **2013**, 9, e1003316	4.8	23

369	Structural model for the protein-translocating element of the twin-arginine transport system. *Proceedings of the National Academy of Sciences of the United States of America*, **2013**, 110, E1092-101	11.1	71
368	Diffusion, Aggregation and Penetration: Modelling the Complex Cell Envelope of E.coli. *IFMBE Proceedings*, **2013**, 376-379	0.2	
367	Tetrameric structure of SUR2B revealed by electron microscopy of oriented single particles. *FEBS Journal*, **2013**, 280, 1051-63	5.4	8
366	Characterization and optimization of a novel protein refolding methodology. *MATEC Web of Conferences*, **2013**, 3, 01004	0.3	
365	Local Lipid Reorganization by a Transmembrane Protein Domain. *Journal of Physical Chemistry Letters*, **2012**, 3, 3498-502	6.3	28
364	Multiscale simulations of the antimicrobial peptide maculatin 1.1: water permeation through disordered aggregates. *Journal of Physical Chemistry B*, **2012**, 116, 8485-93	3.3	27
363	Biomimetic design of a brush-like nanopore: simulation studies. *Journal of Physical Chemistry B*, **2012**, 116, 462-8	3.3	18
362	Designing biomimetic pores based on carbon nanotubes. *Proceedings of the National Academy of Sciences of the United States of America*, **2012**, 109, 6939-44	11.1	66
361	Bendix: intuitive helix geometry analysis and abstraction. *Bioinformatics*, **2012**, 28, 2193-4	6.8	86
360	Finding a needle in a haystack: the role of electrostatics in target lipid recognition by PH domains. *PLoS Computational Biology*, **2012**, 8, e1002617	4.8	32
359	Mechanism of bacterial signal transduction revealed by molecular dynamics of Tsr dimers and trimers of dimers in lipid vesicles. *PLoS Computational Biology*, **2012**, 8, e1002685	4.8	33
358	Locating a plausible binding site for an open-channel blocker, GlyH-101, in the pore of the cystic fibrosis transmembrane conductance regulator. *Molecular Pharmacology*, **2012**, 82, 1042-55	4.1	35
357	State-independent intracellular access of quaternary ammonium blockers to the pore of TREK-1. *Channels*, **2012**, 6, 473-8	2.8	34
356	Louise Johnson (1940-2012). *Nature*, **2012**, 490, 488	47.5	
355	A novel congenital myasthenic syndrome due to decreased acetylcholine receptor ion-channel conductance. *Brain*, **2012**, 135, 1070-80	10.9	16
354	A universally conserved residue in the SUR1 subunit of the KATP channel is essential for translating nucleotide binding at SUR1 into channel opening. *Journal of Physiology*, **2012**, 590, 5025-36	3.8	10
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