Mark S P Sansom

List of Publications by Year
in descending order

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524 papers	32,160 citations	3762 89 h-index	9942 141 g-index
572 all docs	572 docs citations	572 times ranked	21911 citing authors

#	Article	IF	Citations
1	HOLE: A program for the analysis of the pore dimensions of ion channel structural models. Journal of Molecular Graphics, 1996, 14, 354-360.	1.1	1,425
2	Computational Modeling of Realistic Cell Membranes. Chemical Reviews, 2019, 119, 6184-6226.	49.9	502
3	Liquid-vapor oscillations of water in hydrophobic nanopores. Proceedings of the National Academy of Sciences of the United States of America, 2003, 100, 7063-7068.	7.6	415
4	Acquisition of siderophores in Gram-negative bacteria. Nature Reviews Molecular Cell Biology, 2003, 4, 105-116.	37.5	349
5	Proline-induced Distortions of Transmembrane Helices. Journal of Molecular Biology, 2002, 323, 951-960.	4.1	345
6	Amino acid distributions in integral membrane protein structures. Biochimica Et Biophysica Acta - Biomembranes, 2001, 1512, 1-14.	2.7	332
7	Insertion and Assembly of Membrane Proteins via Simulation. Journal of the American Chemical Society, 2006, 128, 2697-2704.	14.4	314
8	Coarse-grained molecular dynamics simulations of membrane proteins and peptides. Journal of Structural Biology, 2007, 157, 593-605.	2.9	303
9	Structural basis of Smoothened regulation by its extracellular domains. Nature, 2016, 535, 517-522.	36.5	300
10	Membrane proteins: molecular dynamics simulations. Current Opinion in Structural Biology, 2008, 18, 425-431.	5.9	297
11	Hinges, swivels and switches: the role of prolines in signalling via transmembrane Î±-helices. Trends in Pharmacological Sciences, 2000, 21, 445-451.	7.0	293
12	A Hydrophobic Gating Mechanism for Nanopores. Journal of Physical Chemistry B, 2001, 105, 12902-12905.	2.7	290
13	Molecular Basis of Alternating Access Membrane Transport by the Sodium-Hydantoin Transporter Mhp1. Science, 2010, 328, 470-473.	12.9	283
14	Crystal structure of a prokaryotic homologue of the mammalian oligopeptide-proton symporters, PepT1 and PepT2. EMBO Journal, 2011, 30, 417-426.	7.7	269
15	Structure and Orientation of the Mammalian Antibacterial Peptide Cecropin P1 within Phospholipid Membranes. Journal of Molecular Biology, 1996, 258, 860-870.	4.1	262
16	Simulations of Ion Permeation Through a Potassium Channel: Molecular Dynamics of KcsA in a Phospholipid Bilayer. Biophysical Journal, 2000, 78, 557-570.	0.5	261
17	MemProtMD: Automated Insertion of Membrane Protein Structures into Explicit Lipid Membranes. Structure, 2015, 23, 1350-1361.	3.4	257
18	Hydrophobic Gating in Ion Channels. Journal of Molecular Biology, 2015, 427, 121-130.	4.1	254

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19	From Coarse Grained to Atomistic: A Serial Multiscale Approach to Membrane Protein Simulations. Journal of Chemical Theory and Computation, 2011, 7, 1157-1166.	5.5	240
20	PtdIns(4,5)P2 stabilizes active states of GPCRs and enhances selectivity of G-protein coupling. Nature, 2018, 559, 423-427.	36.5	236
21	The influence of geometry, surface character, and flexibility on the permeation of ions and water through biological pores. Physical Biology, 2004, 1, 42-52.	1.8	227
22	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.	7.6	219
23	Alamethicin Helices in a Bilayer and in Solution: Molecular Dynamics Simulations. Biophysical Journal, 1999, 76, 40-49.	0.5	201
24	Coarse-Grained MD Simulations of Membrane Protein-Bilayer Self-Assembly. Structure, 2008, 16, 621-630.	3.4	199
25	Lipid Clustering Correlates with Membrane Curvature as Revealed by Molecular Simulations of Complex Lipid Bilayers. PLoS Computational Biology, 2014, 10, e1003911.	3.2	189
26	Simulation approaches to ion channel structureâ€“function relationships. Quarterly Reviews of Biophysics, 2001, 34, 473-561.	5.5	186
27	Not Ions Alone:Â Barriers to Ion Permeation in Nanopores and Channels. Journal of the American Chemical Society, 2004, 126, 14694-14695.	14.4	181
28	Functional analysis of a structural model of the ATP-binding site of the KATP channel Kir6.2 subunit. EMBO Journal, 2005, 24, 229-239.	7.7	177
29	A hydrophobic gate in an ion channel: the closed state of the nicotinic acetylcholine receptor. Physical Biology, 2006, 3, 147-159.	1.8	177
30	Multiscale methods for macromolecular simulations. Current Opinion in Structural Biology, 2008, 18, 630-640.	5.9	175
31	Properties of integral membrane protein structures: Derivation of an implicit membrane potential. Proteins: Structure, Function and Bioinformatics, 2005, 59, 252-265.	3.1	174
32	Membrane simulations: bigger and better?. Current Opinion in Structural Biology, 2000, 10, 174-181.	5.9	173
33	An Alamethicin Channel in a Lipid Bilayer: Molecular Dynamics Simulations. Biophysical Journal, 1999, 76, 1757-1769.	0.5	172
34	Supramolecular assemblies underpin turnover of outer membrane proteins in bacteria. Nature, 2015, 523, 333-336.	36.5	170
35	Lipid Properties and the Orientation of Aromatic Residues in OmpF, Influenza M2, and Alamethicin Systems:â€‰ Molecular Dynamics Simulations. Biochemistry, 1998, 37, 17554-17561.	2.6	166
36	Structure of the TatC core of the twin-arginine protein transport system. Nature, 2012, 492, 210-214.	36.5	164

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37	The pore structure and gating mechanism of K2P channels. EMBO Journal, 2011, 30, 3607-3619.	7.7	162
38	The structure and organization within the membrane of the helices composing the pore-forming domain of Bacillus thuringiensis Â-endotoxin are consistent with an "umbrella-like" structure of the pore. Proceedings of the National Academy of Sciences of the United States of America, 1998, 95, 12289-12294.	7.6	161
39	Outer membrane protein G: Engineering a quiet pore for biosensing. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 6272-6277.	7.6	160
40	An aqueous H+ permeation pathway in the voltage-gated proton channel Hv1. Nature Structural and Molecular Biology, 2010, 17, 869-875.	8.2	160
41	The role of lipids in mechanosensation. Nature Structural and Molecular Biology, 2015, 22, 991-998.	8.2	160
42	Setting up and optimization of membrane protein simulations. European Biophysics Journal, 2002, 31, 217-227.	2.3	157
43	3-D structural and functional characterization of the purified KATPchannel complex Kir6.2-SUR1. EMBO Journal, 2005, 24, 4166-4175.	7.7	156
44	Band 3, the human red cell chloride/bicarbonate anion exchanger (AE1, SLC4A1), in a structural context. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1507-1532.	2.7	154
45	Molecular Simulation Approaches to Membrane Proteins. Structure, 2011, 19, 1562-1572.	3.4	152
46	Water at the nanoscale. Nature, 2001, 414, 157-159.	36.5	150
47	The Influenza A Virus M2 Channel: A Molecular Modeling and Simulation Study. Virology, 1997, 233, 163-173.	2.4	146
48	Lipidbook: A Public Repository for Force-Field Parameters Used in Membrane Simulations. Journal of Membrane Biology, 2010, 236, 255-258.	2.3	145
49	Reduced Lateral Mobility of Lipids and Proteins in Crowded Membranes. PLoS Computational Biology, 2013, 9, e1003033.	3.2	145
50	Lipid interaction sites on channels, transporters and receptors: Recent insights from molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2390-2400.	2.7	143
51	The MemProtMD database: a resource for membrane-embedded protein structures and their lipid interactions. Nucleic Acids Research, 2019, 47, D390-D397.	14.5	143
52	Blocking of Carbon Nanotube Based Nanoinjectors by Lipids: A Simulation Study. Nano Letters, 2008, 8, 2751-2756.	9.4	139
53	Proline-induced hinges in transmembrane helices: Possible roles in ion channel gating. Proteins: Structure, Function and Bioinformatics, 2001, 44, 63-72.	3.1	138
54	K+ versus Na+ Ions in a K Channel Selectivity Filter: A Simulation Study. Biophysical Journal, 2002, 83, 633-645.	0.5	137

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55	Structure and Dynamics of the Membrane-Bound Cytochrome P450 2C9. PLoS Computational Biology, 2011, 7, e1002152.	3.2	134
56	Potassium channels: structures, models, simulations. Biochimica Et Biophysica Acta - Biomembranes, 2002, 1565, 294-307.	2.7	132
57	Molecular dynamics simulations of membrane proteins and their interactions: from nanoscale to mesoscale. Current Opinion in Structural Biology, 2016, 40, 8-16.	5.9	131
58	Membrane Protein Dynamics versus Environment: Simulations of OmpA in a Micelle and in a Bilayer. Journal of Molecular Biology, 2003, 329, 1035-1053.	4.1	130
59	Homology Modeling and Molecular Dynamics Simulation Studies of an Inward Rectifier Potassium Channel. Biophysical Journal, 2000, 78, 2929-2942.	0.5	127
60	PIP₂-Binding Site in Kir Channels: Definition by Multiscale Biomolecular Simulations. Biochemistry, 2009, 48, 10926-10933.	2.6	127
61	Analysis and Evaluation of Channel Models: Simulations of Alamethicin. Biophysical Journal, 2002, 83, 2393-2407.	0.5	123
62	Carbon Nanotube/Detergent Interactions via Coarse-Grained Molecular Dynamics. Nano Letters, 2007, 7, 1923-1928.	9.4	121
63	Water in Nanopores and Biological Channels: A Molecular Simulation Perspective. Chemical Reviews, 2020, 120, 10298-10335.	49.9	121
64	Exploring the Electronic and Mechanical Properties of Protein Using Conducting Atomic Force Microscopy. Journal of the American Chemical Society, 2004, 126, 5601-5609.	14.4	120
65	Viral ion channels: structure and function. Biochimica Et Biophysica Acta - Biomembranes, 2002, 1561, 27-45.	2.7	119
66	Ion channel gating: insights via molecular simulations. FEBS Letters, 2003, 555, 85-90.	2.8	119
67	Simulation studies of the interaction of antimicrobial peptides and lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 1999, 1462, 185-200.	2.7	118
68	Cryo-EM structure of the mechanically activated ion channel OSCA1.2. ELife, 2018, 7, .	6.0	118
69	Transmembrane helix prediction: a comparative evaluation and analysis. Protein Engineering, Design and Selection, 2005, 18, 295-308.	2.2	117
70	Coarse-grained simulation: a high-throughput computational approach to membrane proteins. Biochemical Society Transactions, 2008, 36, 27-32.	3.5	117
71	Lipid-Dependent Regulation of Ion Channels and G Proteinâ€“Coupled Receptors: Insights from Structures and Simulations. Annual Review of Pharmacology and Toxicology, 2020, 60, 31-50.	9.8	117
72	Aggregation of Model Membrane Proteins, Modulated by Hydrophobic Mismatch, Membrane Curvature, and Protein Class. Biophysical Journal, 2011, 101, 691-699.	0.5	115

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73	Bendix: intuitive helix geometry analysis and abstraction. Bioinformatics, 2012, 28, 2193-2194.	4.2	115
74	An atomic detail model for the human ATP binding cassette transporter Pâ€glycoprotein derived from disulphide crossâ€linking and homology modeling. FASEB Journal, 2003, 17, 2287-2289.	0.5	112
75	Biomolecular simulations: From dynamics and mechanisms to computational assays of biological activity. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2019, 9, e1393.	15.8	110
76	Ion-channel gating mechanisms: model identification and parameter estimation from single channel recordings. Proceedings of the Royal Society of London Series B, Containing Papers of A Biological Character, 1989, 236, 385-416.	1.7	108
77	Potassium Channel, Ions, and Water: Simulation Studies Based on the High Resolution X-Ray Structure of KcsA. Biophysical Journal, 2003, 85, 2787-2800.	0.5	107
78	A hydrophobic barrier deep within the inner pore of the TWIK-1 K2P potassium channel. Nature Communications, 2014, 5, 4377.	13.2	107
79	Interactions of Î±-helices with lipid bilayers: a review of simulation studies. Biophysical Chemistry, 1999, 76, 161-183.	2.9	105
80	Lipid-Protein Interactions of Integral Membrane Proteins: A Comparative Simulation Study. Biophysical Journal, 2004, 87, 3737-3749.	0.5	104
81	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, 10611-10622.	14.4	103
82	Properties of ion channels formed by Staphylococcus aureus Î´-toxin. Biochimica Et Biophysica Acta - Biomembranes, 1988, 942, 280-294.	2.7	101
83	Bilayer deformation by the Kv channel voltage sensor domain revealed by self-assembly simulations. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 2631-2636.	7.6	100
84	Carbon nanotube self-assembly with lipids and detergent: a molecular dynamics study. Nanotechnology, 2009, 20, 045101.	2.7	100
85	A gating mutation at the internal mouth of the Kir6.2 pore is associated with DEND syndrome. EMBO Reports, 2005, 6, 470-475.	4.5	99
86	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.	7.6	99
87	Exploring Models of the Influenza A M2 Channel: MD Simulations in a Phospholipid Bilayer. Biophysical Journal, 2000, 78, 55-69.	0.5	98
88	Cryo-EM reveals two distinct serotonin-bound conformations of full-length 5-HT3A receptor. Nature, 2018, 563, 270-274.	36.5	98
89	CHAP: A Versatile Tool for the Structural and Functional Annotation of Ion Channel Pores. Journal of Molecular Biology, 2019, 431, 3353-3365.	4.1	97
90	How Does a Voltage Sensor Interact with a Lipid Bilayer? Simulations of a Potassium Channel Domain. Structure, 2007, 15, 235-244.	3.4	96

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91	Convergence and Sampling in Determining Free Energy Landscapes for Membrane Protein Association. Journal of Physical Chemistry B, 2017, 121, 3364-3375.	2.7	93
92	OmpA: A Pore or Not a Pore? Simulation and Modeling Studies. Biophysical Journal, 2002, 83, 763-775.	0.5	92
93	Molecular Dynamics Simulations of the Bacterial Outer Membrane Protein FhuA: A Comparative Study of the Ferrichrome-Free and Bound States. Biophysical Journal, 2003, 85, 1406-1420.	0.5	92
94	Conformational sampling and dynamics of membrane proteins from 10-nanosecond computer simulations. Proteins: Structure, Function and Bioinformatics, 2004, 57, 783-791.	3.1	92
95	Structure of a KirBac potassium channel with an open bundle crossing indicates a mechanism of channel gating. Nature Structural and Molecular Biology, 2012, 19, 158-163.	8.2	92
96	Organization and Dynamics of Receptor Proteins in a Plasma Membrane. Journal of the American Chemical Society, 2015, 137, 14694-14704.	14.4	91
97	Nothing to Sneeze At: A Dynamic and Integrative Computational Model of an Influenza A Virion. Structure, 2015, 23, 584-597.	3.4	90
98	Membrane stiffness is modified by integral membrane proteins. Soft Matter, 2016, 12, 7792-7803.	2.8	90
99	The juxtamembrane regions of human receptor tyrosine kinases exhibit conserved interaction sites with anionic lipids. Scientific Reports, 2015, 5, 9198.	3.4	89
100	Ion channels formed by HIV-1 Vpu: a modelling and simulation study. FEBS Letters, 1997, 405, 299-304.	2.8	88
101	Molecular dynamics studies of AChBP with nicotine and carbamylcholine: the role of water in the binding pocket. Protein Engineering, Design and Selection, 2007, 20, 353-359.	2.2	88
102	Molecular Dynamics Simulations of the Ligand-Binding Domain of the Ionotropic Glutamate Receptor GluR2. Biophysical Journal, 2002, 82, 676-683.	0.5	87
103	Coarse-Grained Molecular Dynamics Simulations of the Energetics of Helix Insertion into a Lipid Bilayer. Biochemistry, 2008, 47, 11321-11331.	2.6	87
104	MD Simulations of Spontaneous Membrane Protein/Detergent Micelle Formation. Journal of the American Chemical Society, 2004, 126, 15948-15949.	14.4	85
105	Engineering Stabilized Ion Channels:Â Covalent Dimers of Alamethicinâ€. Biochemistry, 1996, 35, 6225-6232.	2.6	84
106	Simulations of ion channels â€“ watching ions and water move. Trends in Biochemical Sciences, 2000, 25, 368-374.	6.2	84
107	Super-complexes of adhesion GPCRs and neural guidance receptors. Nature Communications, 2016, 7, 11184.	13.2	84
108	Influenza virus M2 protein: a molecular modelling study of the ion channel. Protein Engineering, Design and Selection, 1993, 6, 65-74.	2.2	83

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109	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.	7.6	83
110	Helixâ^'Helix Interactions in Membrane Proteins: Coarse-Grained Simulations of Glycophorin A Helix Dimerization. Biochemistry, 2008, 47, 10503-10512.	2.6	82
111	Molecular Dynamics Simulations of the Dimerization of Transmembrane Î±-Helices. Accounts of Chemical Research, 2010, 43, 388-396.	16.1	82
112	Functional analysis of missense variants in the TRESK (KCNK18) K+ channel. Scientific Reports, 2012, 2, 237.	3.4	82
113	Epock: rapid analysis of protein pocket dynamics. Bioinformatics, 2015, 31, 1478-1480.	4.2	81
114	The Role of the Membrane in the Structure and Biophysical Robustness of the Dengue Virion Envelope. Structure, 2016, 24, 375-382.	3.4	81
115	State-dependent Lipid Interactions with the A2a Receptor Revealed by MD Simulations Using InÂVivo-Mimetic Membranes. Structure, 2019, 27, 392-403.e3.	3.4	80
116	Potassium and sodium ions in a potassium channel studied by molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2001, 1510, 1-9.	2.7	79
117	Crystal structure of the sodiumâ€“proton antiporter NhaA dimer and new mechanistic insights. Journal of General Physiology, 2014, 144, 529-544.	1.9	79
118	Molecular mechanism of ligand recognition by membrane transport protein, Mhp1. EMBO Journal, 2014, 33, 1831-1844.	7.7	79
119	Changes in Transmembrane Helix Alignment by Arginine Residues Revealed by Solid-State NMR Experiments and Coarse-Grained MD Simulations. Journal of the American Chemical Society, 2010, 132, 5803-5811.	14.4	78
120	Designing biomimetic pores based on carbon nanotubes. Proceedings of the National Academy of Sciences of the United States of America, 2012, 109, 6939-6944.	7.6	78
121	Anionic Phospholipid Interactions with the Potassium Channel KcsA: Simulation Studies. Biophysical Journal, 2006, 90, 822-830.	0.5	77
122	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.	3.4	77
123	Electrostatics and the Ion Selectivity of Ligand-Gated Channels. Biophysical Journal, 1998, 75, 1211-1222.	0.5	76
124	The interaction of C₆₀and its derivatives with a lipid bilayer via molecular dynamics simulations. Nanotechnology, 2009, 20, 115102.	2.7	76
125	Identification of the PIP2-binding site on Kir6.2 by molecular modelling and functional analysis. EMBO Journal, 2007, 26, 3749-3759.	7.7	75
126	Surface Binding of Alamethicin Stabilizes its Helical Structure: Molecular Dynamics Simulations. Biophysical Journal, 1999, 76, 3186-3191.	0.5	74

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127	Identification of residues contributing to the ATP binding site of Kir6.2. EMBO Journal, 2003, 22, 2903-2912.	7.7	74
128	Potassium channel regulation. EMBO Reports, 2003, 4, 1038-1042.	4.5	74
129	A Generalized Born Implicit-Membrane Representation Compared to Experimental Insertion Free Energies. Biophysical Journal, 2007, 92, 2338-2349.	0.5	74
130	Multiscale Simulations Reveal Conserved Patterns of Lipid Interactions with Aquaporins. Structure, 2013, 21, 810-819.	3.4	74
131	Capsaicin Interaction with TRPV1 Channels in a Lipid Bilayer: Molecular Dynamics Simulation. Biophysical Journal, 2015, 108, 1425-1434.	0.5	74
132	Mechanisms of activation and desensitization of full-length glycine receptor in lipid nanodiscs. Nature Communications, 2020, 11, 3752.	13.2	74
133	Structure and Dynamics of K Channel Pore-Lining Helices: A Comparative Simulation Study. Biophysical Journal, 2000, 78, 79-92.	0.5	72
134	Side-Chain Ionization States in a Potassium Channel. Biophysical Journal, 2001, 80, 1210-1219.	0.5	71
135	Conformational Change in an MFS Protein: MD Simulations of LacY. Structure, 2007, 15, 873-884.	3.4	70
136	Flexible Gates Generate Occluded Intermediates in the Transport Cycle of LacY. Journal of Molecular Biology, 2014, 426, 735-751.	4.1	70
137	Insights into Membrane Proteinâ€“Lipid Interactions from Free Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5727-5736.	5.5	70
138	Self-Assembly of a Simple Membrane Protein: Coarse-Grained Molecular Dynamics Simulations of the Influenza M2 Channel. Biophysical Journal, 2008, 95, 3790-3801.	0.5	69
139	Kv Channel Gating Requires a Compatible S4-S5 Linker and Bottom Part of S6, Constrained by Non-interacting Residues. Journal of General Physiology, 2008, 132, 667-680.	1.9	69
140	Cystic Fibrosis Transmembrane Conductance Regulator: Using Differential Reactivity toward Channel-Permeant and Channel-Impermeant Thiol-Reactive Probes To Test a Molecular Model for the Pore. Biochemistry, 2009, 48, 10078-10088.	2.6	69
141	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.	3.5	69
142	Functional Annotation of Ion Channel Structures by Molecular Simulation. Structure, 2016, 24, 2207-2216.	3.4	69
143	PyLipID: A Python Package for Analysis of Proteinâ€“Lipid Interactions from Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2022, 18, 1188-1201.	5.5	69
144	Conformational dynamics of helix S6 from Shaker potassium channel: Simulation studies. Biopolymers, 2002, 64, 303-313.	2.2	68

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145	Coarse-Grained Simulations of the Membrane-Active Antimicrobial Peptide Maculatin 1.1. Biophysical Journal, 2008, 95, 3802-3815.	0.5	68
146	Interactions of Pleckstrin Homology Domains with Membranes: Adding Back the Bilayer via High-Throughput Molecular Dynamics. Structure, 2016, 24, 1421-1431.	3.4	68
147	Protein crowding and lipid complexity influence the nanoscale dynamic organization of ion channels in cell membranes. Scientific Reports, 2017, 7, 16647.	3.4	68
148	Asymmetric Switching in a Homodimeric ABC Transporter: A Simulation Study. PLoS Computational Biology, 2010, 6, e1000762.	3.2	67
149	Interdomain dynamics and ligand binding: molecular dynamics simulations of glutamine binding protein. FEBS Letters, 2003, 550, 168-174.	2.8	66
150	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.	2.5	66
151	Biomimetic Phospholipid Membrane Organization on Graphene and Graphene Oxide Surfaces: A Molecular Dynamics Simulation Study. ACS Nano, 2017, 11, 1613-1625.	15.1	66
152	Secondary structure in oligomers of carbohydrate amino acids. Chemical Communications, 1998, , 2041-2042.	4.2	65
153	Flexibility in a Drug Transport Accessory Protein: Molecular Dynamics Simulations of MexA. Biophysical Journal, 2006, 91, 558-564.	0.5	65
154	Transmembrane Helixâ˜Helix Interactions:â€‰ Comparative Simulations of the Glycophorin A Dimer. Biochemistry, 2006, 45, 14298-14310.	2.6	65
155	The pore structure and gating mechanism of K2P channels. EMBO Journal, 2011, 30, 4515-4515.	7.7	65
156	Proline residues in transmembrane helices of channel and transport proteins: a molecular modelling study. Protein Engineering, Design and Selection, 1992, 5, 53-60.	2.2	64
157	DNA and lipid bilayers: self-assembly and insertion. Journal of the Royal Society Interface, 2008, 5, 241-250.	3.5	64
158	Membrane Perturbation by Carbon Nanotube Insertion: Pathways to Internalization. Small, 2013, 9, 3639-3646.	11.1	64
159	Bilayer-Mediated Structural Transitions Control Mechanosensitivity of the TREK-2 K2P Channel. Structure, 2017, 25, 708-718.e2.	3.4	64
160	Defining the Transmembrane Helix of M2 Protein from Influenza A by Molecular Dynamics Simulations in a Lipid Bilayer. Biophysical Journal, 1999, 76, 1886-1896.	0.5	63
161	H Bonding at the Helix-Bundle Crossing Controls Gating in Kir Potassium Channels. Neuron, 2007, 55, 602-614.	8.2	63
162	The Selectivity of K+ Ion Channels: Testing the Hypotheses. Biophysical Journal, 2008, 95, 5062-5072.	0.5	63

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163	Simulation-Based Prediction of Phosphatidylinositol 4,5-Bisphosphate Binding to an Ion Channel. Biochemistry, 2013, 52, 279-281.	2.6	63
164	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.	2.6	63
165	The properties of ion channels formed by zervamicins. European Biophysics Journal, 1992, 21, 117-28.	2.3	62
166	Multiscale simulations suggest a mechanism for integrin inside-out activation. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 11890-11895.	7.6	62
167	The simulation approach to bacterial outer membrane proteins (Review). Molecular Membrane Biology, 2004, 21, 151-161.	1.9	61
168	Focus on Kir6.2: a key component of the ATP-sensitive potassium channel. Journal of Molecular and Cellular Cardiology, 2005, 38, 927-936.	1.8	61
169	Simulations of anion transport through OprP reveal the molecular basis for high affinity and selectivity for phosphate. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 21614-21618.	7.6	61
170	Stability and dynamics of membrane-spanning DNA nanopores. Nature Communications, 2017, 8, 14784.	13.2	61
171	The Flexing/Twirling Helix:Â Exploring the Flexibility about Molecular Hinges Formed by Proline and Glycine Motifs in Transmembrane Helices. Journal of Physical Chemistry B, 2003, 107, 627-636.	2.7	60
172	Filter Flexibility in a Mammalian K Channel: Models and Simulations of Kir6.2 Mutants. Biophysical Journal, 2003, 84, 2345-2356.	0.5	60
173	Filter Flexibility and Distortion in a Bacterial Inward Rectifier K+ Channel: Simulation Studies of KirBac1.1. Biophysical Journal, 2004, 87, 256-267.	0.5	60
174	Cysteine-scanning Mutagenesis and Disulfide Mapping Studies of the Conserved Domain of the Twin-arginine Translocase TatB Component. Journal of Biological Chemistry, 2006, 281, 34072-34085.	3.5	60
175	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, 8154-8163.	2.7	60
176	Dynamics and Function in a Bacterial ABC Transporter:Â Simulation Studies of the BtuCDF System and Its Componentsâ€. Biochemistry, 2007, 46, 2767-2778.	2.6	59
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