D Peter Tieleman

List of Publications by Year
in descending order

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306	31,919	5558 82	4750 169
papers	citations	h-index	g-index

325	325	325	19979
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	The MARTINI Force Field:â€‰ Coarse Grained Model for Biomolecular Simulations. Journal of Physical Chemistry B, 2007, 111, 7812-7824.	1.2	4,650
2	The MARTINI Coarse-Grained Force Field: Extension to Proteins. Journal of Chemical Theory and Computation, 2008, 4, 819-834.	2.3	2,178
3	Improved Parameters for the Martini Coarse-Grained Protein Force Field. Journal of Chemical Theory and Computation, 2013, 9, 687-697.	2.3	1,181
4	Perspective on the Martini model. Chemical Society Reviews, 2013, 42, 6801.	18.7	1,008
5	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2144-2155.	2.3	847
6	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	6.6	734
7	A computer perspective of membranes: molecular dynamics studies of lipid bilayer systems. BBA - Biomembranes, 1997, 1331, 235-270.	7.9	695
8	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. Journal of Chemical Theory and Computation, 2014, 10, 676-690.	2.3	566
9	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
10	Effect of Lipid Peroxidation on the Properties of Lipid Bilayers: A Molecular Dynamics Study. Biophysical Journal, 2007, 93, 4225-4236.	0.2	502
11	Computational Modeling of Realistic Cell Membranes. Chemical Reviews, 2019, 119, 6184-6226.	23.0	502
12	Distribution of Amino Acids in a Lipid Bilayer from Computer Simulations. Biophysical Journal, 2008, 94, 3393-3404.	0.2	486
13	Molecular dynamics simulations of a fully hydrated dipalmitoylphosphatidylcholine bilayer with different macroscopic boundary conditions and parameters. Journal of Chemical Physics, 1996, 105, 4871-4880.	1.2	467
14	Computer simulation study of fullerene translocation through lipid membranes. Nature Nanotechnology, 2008, 3, 363-368.	15.6	459
15	Setting up and running molecular dynamics simulations of membrane proteins. Methods, 2007, 41, 475-488.	1.9	428
16	Simulation of Pore Formation in Lipid Bilayers by Mechanical Stress and Electric Fields. Journal of the American Chemical Society, 2003, 125, 6382-6383.	6.6	417
17	Lipids on the move: Simulations of membrane pores, domains, stalks and curves. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 149-168.	1.4	400
18	The molecular basis of electroporation. , 2004, 5, 10.		355

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19	A Molecular Dynamics Study of the Pores Formed by Escherichia coli OmpF Porin in a Fully Hydrated Palmitoyloleoylphosphatidylcholine Bilayer. Biophysical Journal, 1998, 74, 2786-2801.	0.2	346
20	Methodological Issues in Lipid Bilayer Simulations. Journal of Physical Chemistry B, 2003, 107, 9424-9433.	1.2	337
21	Emerging Diversity in Lipidâ€“Protein Interactions. Chemical Reviews, 2019, 119, 5775-5848.	23.0	299
22	Lipidâ€“Protein Interactions Are Unique Fingerprints for Membrane Proteins. ACS Central Science, 2018, 4, 709-717.	5.3	274
23	Molecular Dynamics Simulations of Dodecylphosphocholine Micelles at Three Different Aggregate Sizes:Â Micellar Structure and Chain Relaxation. Journal of Physical Chemistry B, 2000, 104, 6380-6388.	1.2	273
24	Molecular Dynamics Simulation of the Kinetics of Spontaneous Micelle Formation. Journal of Physical Chemistry B, 2000, 104, 12165-12173.	1.2	269
25	Molecular View of Cholesterol Flip-Flop and Chemical Potential in Different Membrane Environments. Journal of the American Chemical Society, 2009, 131, 12714-12720.	6.6	256
26	The molecular mechanism of lipid monolayer collapse. Proceedings of the National Academy of Sciences of the United States of America, 2008, 105, 10803-10808.	3.3	245
27	Partitioning of Amino Acid Side Chains into Lipid Bilayers: Results from Computer Simulations and Comparison to Experiment. Journal of General Physiology, 2007, 129, 371-377.	0.9	244
28	Martini Coarse-Grained Force Field: Extension to DNA. Journal of Chemical Theory and Computation, 2015, 11, 3932-3945.	2.3	239
29	Lipid Nanoparticles Containing siRNA Synthesized by Microfluidic Mixing Exhibit an Electron-Dense Nanostructured Core. Journal of Physical Chemistry C, 2012, 116, 18440-18450.	1.5	232
30	Computer simulations of membrane proteins. Biochimica Et Biophysica Acta - Biomembranes, 2004, 1666, 158-189.	1.4	217
31	An Electrostatic/Hydrogen Bond Switch as the Basis for the Specific Interaction of Phosphatidic Acid with Proteins. Journal of Biological Chemistry, 2007, 282, 11356-11364.	1.6	214
32	Lipids Out of Equilibrium:Â Energetics of Desorption and Pore Mediated Flip-Flop. Journal of the American Chemical Society, 2006, 128, 12462-12467.	6.6	202
33	Alamethicin Helices in a Bilayer and in Solution: Molecular Dynamics Simulations. Biophysical Journal, 1999, 76, 40-49.	0.2	201
34	Adhesion Forces of Lipids in a Phospholipid Membrane Studied by Molecular Dynamics Simulations. Biophysical Journal, 1998, 74, 931-943.	0.2	199
35	Simulation approaches to ion channel structureâ€“function relationships. Quarterly Reviews of Biophysics, 2001, 34, 473-561.	2.4	186
36	A consistent potential energy parameter set for lipids: dipalmitoylphosphatidylcholine as a benchmark of the GROMOS96 45A3 force field. European Biophysics Journal, 2003, 32, 67-77.	1.2	181

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37	Statistical Convergence of Equilibrium Properties in Simulations of Molecular Solutes Embedded in Lipid Bilayers. Journal of Chemical Theory and Computation, 2011, 7, 4175-4188.	2.3	175
38	Molecular Dynamics Simulation of a Palmitoyl-Oleoyl Phosphatidylserine Bilayer with Na+ Counterions and NaCl. Biophysical Journal, 2004, 86, 1601-1609.	0.2	173
39	An Alamethicin Channel in a Lipid Bilayer: Molecular Dynamics Simulations. Biophysical Journal, 1999, 76, 1757-1769.	0.2	172
40	The ryanodine receptor store-sensing gate controls Ca2+ waves and Ca2+-triggered arrhythmias. Nature Medicine, 2014, 20, 184-192.	15.2	172
41	Structural and functional diversity calls for a new classification of ABC transporters. FEBS Letters, 2020, 594, 3767-3775.	1.3	169
42	Lipid Properties and the Orientation of Aromatic Residues in OmpF, Influenza M2, and Alamethicin Systems:â€‰ Molecular Dynamics Simulations. Biochemistry, 1998, 37, 17554-17561.	1.2	166
43	Atomistic Simulations of Pore Formation and Closure in Lipid Bilayers. Biophysical Journal, 2014, 106, 210-219.	0.2	166
44	Pressureâ˜Area Isotherm of a Lipid Monolayer from Molecular Dynamics Simulations. Langmuir, 2007, 23, 12617-12623.	1.6	161
45	Thermodynamic Analysis of the Effect of Cholesterol on Dipalmitoylphosphatidylcholine Lipid Membranes. Journal of the American Chemical Society, 2009, 131, 1972-1978.	6.6	157
46	Computer simulations of lipid membrane domains. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 1765-1776.	1.4	157
47	The mechanism of ABC transporters: general lessons from structural and functional studies of an antigenic peptide transporter. FASEB Journal, 2009, 23, 1287-1302.	0.2	155
48	Conical Lipids in Flat Bilayers Induce Packing Defects Similar to that Induced by Positive Curvature. Biophysical Journal, 2013, 104, 585-593.	0.2	149
49	Membrane protein simulations with a united-atom lipid and all-atom protein model: lipidâ€“protein interactions, side chain transfer free energies and model proteins. Journal of Physics Condensed Matter, 2006, 18, S1221-S1234.	0.7	148
50	Computational and experimental approaches for investigating nanoparticle-based drug delivery systems. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1688-1709.	1.4	142
51	ATP-binding cassette transporters in Escherichia coli. Biochimica Et Biophysica Acta - Biomembranes, 2008, 1778, 1757-1771.	1.4	139
52	Proline-induced hinges in transmembrane helices: Possible roles in ion channel gating. Proteins: Structure, Function and Bioinformatics, 2001, 44, 63-72.	1.5	138
53	K+ versus Na+ Ions in a K Channel Selectivity Filter: A Simulation Study. Biophysical Journal, 2002, 83, 633-645.	0.2	137
54	Nanopore Formation and Phosphatidylserine Externalization in a Phospholipid Bilayer at High Transmembrane Potential. Journal of the American Chemical Society, 2006, 128, 6288-6289.	6.6	137

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55	Computer Simulation of the Distribution of Hexane in a Lipid Bilayer:Â Spatially Resolved Free Energy, Entropy, and Enthalpy Profiles. Journal of the American Chemical Society, 2006, 128, 125-130.	6.6	135
56	Nanopore-facilitated, voltage-driven phosphatidylserine translocation in lipid bilayersâ€"in cells andin silico. Physical Biology, 2006, 3, 233-247.	0.8	135
57	Analysis and Evaluation of Channel Models: Simulations of Alamethicin. Biophysical Journal, 2002, 83, 2393-2407.	0.2	123
58	Molecular Dynamics Simulation of a Polyunsaturated Lipid Bilayer Susceptible to Lipid Peroxidation. Journal of Physical Chemistry B, 2004, 108, 7170-7179.	1.2	123
59	Self-association of Transmembrane Î±-Helices in Model Membranes. Journal of Biological Chemistry, 2005, 280, 39324-39331.	1.6	123
60	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	13.5	122
61	Water Defect and Pore Formation in Atomistic and Coarse-Grained Lipid Membranes: Pushing the Limits of Coarse Graining. Journal of Chemical Theory and Computation, 2011, 7, 2981-2988.	2.3	121
62	Simulation studies of the interaction of antimicrobial peptides and lipid bilayers. Biochimica Et Biophysica Acta - Biomembranes, 1999, 1462, 185-200.	1.4	118
63	2H-NMR Study and Molecular Dynamics Simulation of the Location, Alignment, and Mobility of Pyrene in POPC Bilayers. Biophysical Journal, 2005, 88, 1818-1827.	0.2	117
64	Voltage-Dependent Insertion of Alamethicin at Phospholipid/Water and Octane/Water Interfaces. Biophysical Journal, 2001, 80, 331-346.	0.2	116
65	Electroporating Fields Target Oxidatively Damaged Areas in the Cell Membrane. PLoS ONE, 2009, 4, e7966.	1.1	116
66	Structures of Neat and Hydrated 1-Octanol from Computer Simulations. Journal of the American Chemical Society, 2002, 124, 15085-15093.	6.6	113
67	Molecular Dynamics Simulations of Pentapeptides at Interfaces:Â Salt Bridge and Cationâ^'Ï€ Interactionsâ€. Biochemistry, 2003, 42, 8976-8987.	1.2	112
68	Free energy of WALP23 dimer association in DMPC, DPPC, and DOPC bilayers. Chemistry and Physics of Lipids, 2013, 169, 95-105.	1.5	111
69	Thermodynamics of flip-flop and desorption for a systematic series of phosphatidylcholine lipids. Soft Matter, 2009, 5, 3295.	1.2	108
70	Molecular View of Phase Coexistence in Lipid Monolayers. Journal of the American Chemical Society, 2012, 134, 17543-17553.	6.6	102
71	Calculation of the water-cyclohexane transfer free energies of neutral amino acid side-chain analogs using the OPLS all-atom force field. Journal of Computational Chemistry, 2003, 24, 1930-1935.	1.5	101
72	Force Fields for Classical Molecular Dynamics. Methods in Molecular Biology, 2013, 924, 197-213.	0.4	101

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73	Microsecond Molecular Dynamics Simulations of Lipid Mixing. Langmuir, 2014, 30, 11993-12001.	1.6	101
74	Alamethicin in lipid bilayers: Combined use of X-ray scattering and MD simulations. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 1387-1397.	1.4	99
75	Exploring Models of the Influenza A M2 Channel: MD Simulations in a Phospholipid Bilayer. Biophysical Journal, 2000, 78, 55-69.	0.2	98
76	The Molecular Mechanism of Monolayer-Bilayer Transformations of Lung Surfactant from Molecular Dynamics Simulations. Biophysical Journal, 2007, 93, 3775-3782.	0.2	97
77	Computer Simulation of Antimicrobial Peptides. Current Medicinal Chemistry, 2007, 14, 2789-2798.	1.2	94
78	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. Journal of Chemical Theory and Computation, 2015, 11, 2278-2291.	2.3	94
79	Molecular simulation of rapid translocation of cholesterol, diacylglycerol, and ceramide in model raft and nonraft membranes. Journal of Lipid Research, 2012, 53, 421-429.	2.0	91
80	Water Permeation through Gramicidin A: Desformylation and the Double Helix: A Molecular Dynamics Study. Biophysical Journal, 2002, 82, 2934-2942.	0.2	89
81	Interactions of the designed antimicrobial peptide MB21 and truncated dermaseptin S3 with lipid bilayers: molecular-dynamics simulations. Biochemical Journal, 2003, 370, 233-243.	1.7	89
82	Structural arrangement of the transmission interface in the antigen ABC transport complex TAP. Proceedings of the National Academy of Sciences of the United States of America, 2009, 106, 5551-5556.	3.3	86
83	Transfer of Arginine into Lipid Bilayers Is Nonadditive. Biophysical Journal, 2011, 101, 110-117.	0.2	86
84	Molecular dynamics simulations of peptides from BPTI: A closer look at amideâ€"aromatic interactions. Journal of Biomolecular NMR, 1996, 8, 229-238.	1.6	84
85	The molecular structure of a phosphatidylserine bilayer determined by scattering and molecular dynamics simulations. Soft Matter, 2014, 10, 3716.	1.2	84
86	Conformational Transitions Induced by the Binding of MgATP to the Vitamin B12 ATP-binding Cassette (ABC) Transporter BtuCD. Journal of Biological Chemistry, 2004, 279, 45013-45019.	1.6	82
87	Hydrophobicity scales: a thermodynamic looking glass into lipidâ€"protein interactions. Trends in Biochemical Sciences, 2011, 36, 653-662.	3.7	81
88	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3262-3275.	1.2	81
89	Pâ€glycoprotein models of the apo and ATPâ€bound states based on homology with Sav1866 and MalK. FEBS Letters, 2007, 581, 4217-4222.	1.3	80
90	Hydrophobic association of Â-helices, steric dewetting, and enthalpic barriers to protein folding. Proceedings of the National Academy of Sciences of the United States of America, 2007, 104, 6206-6210.	3.3	78

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91	Antimicrobial Peptide Simulations and the Influence of Force Field on the Free Energy for Pore Formation in Lipid Bilayers. Journal of Chemical Theory and Computation, 2016, 12, 4524-4533.	2.3	78
92	The Importance of Membrane Defectsâ€"Lessons from Simulations. Accounts of Chemical Research, 2014, 47, 2244-2251.	7.6	77
93	Molecular Dynamics Simulation of Spontaneous Membrane Fusion during a Cubic-Hexagonal Phase Transition. Biophysical Journal, 2002, 83, 2386-2392.	0.2	76
94	Combination of the CHARMM27 force field with unitedâ€atom lipid force fields. Journal of Computational Chemistry, 2011, 32, 1400-1410.	1.5	75
95	Surface Binding of Alamethicin Stabilizes its Helical Structure: Molecular Dynamics Simulations. Biophysical Journal, 1999, 76, 3186-3191.	0.2	74
96	Direct Simulation of Protein-Mediated Vesicle Fusion: Lung Surfactant Protein B. Biophysical Journal, 2010, 99, 2134-2142.	0.2	71
97	Improving Internal Peptide Dynamics in the Coarse-Grained MARTINI Model: Toward Large-Scale Simulations of Amyloid- and Elastin-like Peptides. Journal of Chemical Theory and Computation, 2012, 8, 1774-1785.	2.3	69
98	Computer simulations of the phase separation in model membranes. Faraday Discussions, 2013, 161, 63-75.	1.6	69
99	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 3282-3292.	2.3	67
100	Comment on â€œOn using a too large integration time step in molecular dynamics simulations of coarse-grained molecular modelsâ€• by M. Winger, D. Trzesniak, R. Baron and W. F. van Gunsteren, Phys. Chem. Chem. Phys., 2009, 11, 1934. Physical Chemistry Chemical Physics, 2010, 12, 2254.	1.3	66
101	Interaction of Pristine and Functionalized Carbon Nanotubes with Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 12113-12123.	1.2	66
102	A Salt-Bridge Motif Involved in Ligand Binding and Large-Scale Domain Motions of the Maltose-Binding Protein. Biophysical Journal, 2005, 89, 3362-3371.	0.2	65
103	Structural basis for antibacterial peptide selfâ€immunity by the bacterial ABC transporter McjD. EMBO Journal, 2017, 36, 3062-3079.	3.5	64
104	Defining the Transmembrane Helix of M2 Protein from Influenza A by Molecular Dynamics Simulations in a Lipid Bilayer. Biophysical Journal, 1999, 76, 1886-1896.	0.2	63
105	Membranes and water: an interesting relationship. Faraday Discussions, 1996, 103, 191.	1.6	62
106	Cholesterol Flip-Flop in Heterogeneous Membranes. Journal of Chemical Theory and Computation, 2019, 15, 2064-2070.	2.3	62
107	Molecular Structure of Membrane Tethers. Biophysical Journal, 2012, 102, 1866-1871.	0.2	61
108	Lipid-Protein Interactions Are a Unique Property and Defining Feature of G Protein-Coupled Receptors. Biophysical Journal, 2020, 118, 1887-1900.	0.2	61

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109	Constant pH simulations with the coarse-grained MARTINI model â€" Application to oleic acid aggregates. Canadian Journal of Chemistry, 2013, 91, 839-846.	0.6	59
110	Opening and Closing Motions in the Periplasmic Vitamin B12Binding Protein BtuFâ€. Biochemistry, 2006, 45, 13284-13292.	1.2	58
111	Two decades of Martini: Better beads, broader scope. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	6.2	58
112	Phase Separation in Atomistic Simulations of Model Membranes. Journal of the American Chemical Society, 2020, 142, 2844-2856.	6.6	57
113	Oleic Acid Phase Behavior from Molecular Dynamics Simulations. Langmuir, 2014, 30, 10661-10667.	1.6	56
114	Distribution of Pentachlorophenol in Phospholipid Bilayers: A Molecular Dynamics Study. Biophysical Journal, 2004, 86, 337-345.	0.2	55
115	Molecular Dynamics Simulation of a Lipid Diamond Cubic Phase. Journal of the American Chemical Society, 2001, 123, 12383-12391.	6.6	54
116	Lung Surfactant Protein SP-B Promotes Formation of Bilayer Reservoirs from Monolayer and Lipid Transfer between the Interface and Subphase. Biophysical Journal, 2011, 100, 1678-1687.	0.2	54
117	Curvatureâ€Induced Sorting of Lipids in Plasma Membrane Tethers. Advanced Theory and Simulations, 2018, 1, 1800034.	1.3	54
118	Structure and dynamics of the pore-lining helix of the nicotinic receptor: MD simulations in water, lipid bilayers, and transbilayer bundles. , 2000, 39, 47-55.		53
119	Orientation and interactions of dipolar molecules during transport through OmpF porin. FEBS Letters, 2002, 528, 53-57.	1.3	53
120	The Dynamics of the MgATP-driven Closure of MalK, the Energy-transducing Subunit of the Maltose ABC Transporter. Journal of Biological Chemistry, 2006, 281, 28397-28407.	1.6	53
121	Simulation of the Coupling between Nucleotide Binding and Transmembrane Domains in the ATP Binding Cassette Transporter BtuCD. Biophysical Journal, 2007, 92, 2727-2734.	0.2	53
122	Lateral pressure profiles in lipid monolayers. Faraday Discussions, 2010, 144, 393-409.	1.6	51
123	Computer simulation of the KvAP voltage-gated potassium channel: steered molecular dynamics of the voltage sensor. FEBS Letters, 2004, 564, 325-332.	1.3	49
124	Docking of Î¼-Conotoxin GIIIA in the Sodium Channel Outer Vestibule. Channels, 2007, 1, 344-352.	1.5	49
125	Interactions of Key Charged Residues Contributing to Selective Block of Neuronal Sodium Channels by Î¼-Conotoxin KIIIA. Molecular Pharmacology, 2011, 80, 573-584.	1.0	49
126	Molecular simulation of multistate peptide dynamics: A comparison between microsecond timescale sampling and multiple shorter trajectories. Journal of Computational Chemistry, 2008, 29, 1740-1752.	1.5	48

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127	Molecular Dynamics Simulations of the Apo-, Holo-, and Acyl-forms of Escherichia coli Acyl Carrier Protein. Journal of Biological Chemistry, 2008, 283, 33620-33629.	1.6	48
128	Using the Wimleyâ€“White Hydrophobicity Scale as a Direct Quantitative Test of Force Fields: The MARTINI Coarse-Grained Model. Journal of Chemical Theory and Computation, 2011, 7, 2316-2324.	2.3	47
129	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. Journal of Chemical Theory and Computation, 2012, 8, 618-628.	2.3	47
130	Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). Journal of Biological Chemistry, 2015, 290, 22891-22906.	1.6	47
131	Molecular basis of voltage gating of OmpF porin. Biochemistry and Cell Biology, 2002, 80, 517-523.	0.9	46
132	Modifying the OPLS-AA force field to improve hydration free energies for several amino acid side chains using new atomic charges and an off-plane charge model for aromatic residues. Journal of Computational Chemistry, 2007, 28, 689-697.	1.5	46
133	Modulating interactions between ligand-coated nanoparticles and phase-separated lipid bilayers by varying the ligand density and the surface charge. Nanoscale, 2018, 10, 2481-2491.	2.8	46
134	Ionizable amino lipid interactions with POPC: implications for lipid nanoparticle function. Nanoscale, 2019, 11, 14141-14146.	2.8	46
135	COMPUTER SIMULATIONS OF TRANSPORT THROUGH MEMBRANES: PASSIVE DIFFUSION, PORES, CHANNELS AND TRANSPORTERS. Clinical and Experimental Pharmacology and Physiology, 2006, 33, 893-903.	0.9	45
136	Computer simulations of lung surfactant. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2431-2440.	1.4	45
137	Activation of the bacterial thermosensor DesK involves a serine zipper dimerization motif that is modulated by bilayer thickness. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 6353-6358.	3.3	44
138	Phospholipid Chain Interactions with Cholesterol Drive Domain Formation in Lipid Membranes. Biophysical Journal, 2018, 114, 2595-2605.	0.2	44
139	Interpretation of 2H-NMR Experiments on the Orientation of the Transmembrane Helix WALP23 by Computer Simulations. Biophysical Journal, 2010, 99, 1455-1464.	0.2	43
140	The Heterodimeric ABC Transporter EfrCD Mediates Multidrug Efflux in Enterococcus faecalis. Antimicrobial Agents and Chemotherapy, 2016, 60, 5400-5411.	1.4	43
141	Composition Fluctuations in Lipid Bilayers. Biophysical Journal, 2017, 113, 2750-2761.	0.2	42
142	Pores Formed by the Nicotinic Receptor M2Î´ Peptide: A Molecular Dynamics Simulation Study. Biophysical Journal, 2003, 84, 14-27.	0.2	41
143	Residue G346 in Transmembrane Segment Six is Involved in Inter-Domain Communication in P-Glycoprotein. Biochemistry, 2007, 46, 9899-9910.	1.2	41
144	Molecular dynamics simulations of antimicrobial peptides: From membrane binding to trans-membrane channels. International Journal of Quantum Chemistry, 2001, 83, 166-179.	1.0	40

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145	Molecular dynamics study of the effect of cholesterol on the properties of lipid monolayers at low surface tensions. Physical Chemistry Chemical Physics, 2009, 11, 1916.	1.3	40
146	Molecular Dynamics Simulation of the Evolution of Hydrophobic Defects in One Monolayer of a Phosphatidylcholine Bilayer: Relevance for Membrane Fusion Mechanisms. Biophysical Journal, 2002, 83, 1501-1510.	0.2	39
147	Computer simulation of partitioning of ten pentapeptides Ace-WLXLL at the cyclohexane/water and phospholipid/water interfaces. , 2005, 6, 30.		39
148	Direct Simulation of Transmembrane Helix Association: Role of Asparagines. Biophysical Journal, 2004, 87, 1650-1656.	0.2	37
149	The TatA Subunit of Escherichia coli Twin-Arginine Translocase Has an N-in Topology. Biochemistry, 2007, 46, 7396-7404.	1.2	35
150	Structural Basis for Autoinhibition of CTP:Phosphocholine Cytidylyltransferase (CCT), the Regulatory Enzyme in Phosphatidylcholine Synthesis, by Its Membrane-binding Amphipathic Helix. Journal of Biological Chemistry, 2014, 289, 1742-1755.	1.6	35
151	Mechanism of Helix Nucleation and Propagation:Â Microscopic View from Microsecond Time Scale MD Simulations. Journal of Physical Chemistry B, 2005, 109, 20064-20067.	1.2	34
152	The Mechanism of Collapse of Heterogeneous Lipid Monolayers. Biophysical Journal, 2014, 107, 1136-1145.	0.2	34
153	Chapter 8 Interactions between Small Molecules and Lipid Bilayers. Current Topics in Membranes, 2008, , 227-256.	0.5	33
154	Molecular Simulations of Lipid Flip-Flop in the Presence of Model Transmembrane Helices. Biochemistry, 2010, 49, 7665-7673.	1.2	33
155	Molecular Models of Nanodiscs. Journal of Chemical Theory and Computation, 2015, 11, 4923-4932.	2.3	33
156	Structural and Functional Basis for Lipid Synergy on the Activity of the Antibacterial Peptide ABC Transporter McjD. Journal of Biological Chemistry, 2016, 291, 21656-21668.	1.6	33
157	Parameterization of Palmitoylated Cysteine, Farnesylated Cysteine, Geranylgeranylated Cysteine, and Myristoylated Glycine for the Martini Force Field. Journal of Physical Chemistry B, 2017, 121, 11132-11143.	1.2	33
158	Low-q Bicelles Are Mixed Micelles. Journal of Physical Chemistry Letters, 2018, 9, 4469-4473.	2.1	33
159	Conformational choreography of a molecular switch region in myelin basic proteinâ€"Molecular dynamics shows induced folding and secondary structure type conversion upon threonyl phosphorylation in both aqueous and membrane-associated environments. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 674-683.	1.4	31
160	Coarse-grained molecular dynamics simulations reveal lipid access pathways in P-glycoprotein. Journal of General Physiology, 2018, 150, 417-429.	0.9	31
161	Changes in the dynamics of the cardiac troponin C molecule explain the effects of Ca2+-sensitizing mutations. Journal of Biological Chemistry, 2017, 292, 11915-11926.	1.6	30
162	Holoâ€BtuF stabilizes the open conformation of the vitamin B12 ABC transporter BtuCD. Proteins: Structure, Function and Bioinformatics, 2010, 78, 738-753.	1.5	28

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163	Alamethicin channels in a membrane: molecular dynamics simulations. Faraday Discussions, 1999, 111, 209-223.	1.6	27
164	Transmembrane Helix 12 Modulates Progression of the ATP Catalytic Cycle in ABCB1. Biochemistry, 2009, 48, 6249-6258.	1.2	27
165	The Human Transporter Associated with Antigen Processing. Journal of Biological Chemistry, 2012, 287, 28099-28111.	1.6	26
166	Structure of Transmembrane Helix 8 and Possible Membrane Defects in CFTR. Biophysical Journal, 2018, 114, 1751-1754.	0.2	26
167	Molecular dynamics simulations of bovine lactoferricin: turning a helix into a sheet. BioMetals, 2004, 17, 217-223.	1.8	25
168	Disrupting a key hydrophobic pair in the oligomerization interface of the actinoporins impairs their poreâ€forming activity. Protein Science, 2017, 26, 550-565.	3.1	25
169	The ugly, bad, and good stories of large-scale biomolecular simulations. Current Opinion in Structural Biology, 2022, 73, 102338.	2.6	25
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