D Peter Tieleman

List of Publications by Year
in descending order

306 papers	31,919 citations	5574 82 h-index	4774 169 g-index
325 all docs	325 docs citations	325 times ranked	19979 citing authors

#	Article	IF	Citations
1	Two decades of Martini: Better beads, broader scope. Wiley Interdisciplinary Reviews: Computational Molecular Science, 2023, 13, .	14.6	58
2	Effects of Lid Domain Structural Changes on the Interactions between Peripheral Myelin Protein 2 and a Lipid Bilayer. Journal of Physical Chemistry Letters, 2022, 13, 991-996.	4.6	1
3	Can two wrongs make a right? F508del-CFTR ion channel rescue by second-site mutations in its transmembrane domains. Journal of Biological Chemistry, 2022, 298, 101615.	3.4	4
4	A molecular switch controls the impact of cholesterol on a Kir channel. Proceedings of the National Academy of Sciences of the United States of America, 2022, 119, e2109431119.	7.1	9
5	The ugly, bad, and good stories of large-scale biomolecular simulations. Current Opinion in Structural Biology, 2022, 73, 102338.	5.7	25
6	Supramolecular Organization of SARS-CoV and SARS-CoV-2 Virions Revealed by Coarse-Grained Models of Intact Virus Envelopes. Journal of Chemical Information and Modeling, 2022, 62, 176-186.	5.4	25
7	Effects of cholesterol and PIP2 on interactions between glycophorin A and Band 3 in lipid bilayers. Biophysical Journal, 2022, 121, 2069-2077.	0.5	1
8	Curvature-based sorting of eight lipid types in asymmetric buckled plasma membrane models. Biophysical Journal, 2022, 121, 2060-2068.	0.5	8
9	Computational Insights into the Role of Cholesterol in Inverted Hexagonal Phase Stabilization and Endosomal Drug Release. Langmuir, 2022, 38, 7462-7471.	3.5	11
10	Lipid distributions and transleaflet cholesterol migration near heterogeneous surfaces in asymmetric bilayers. Faraday Discussions, 2021, 232, 103-113.	3.2	2
11	Refinement of a cryo-EM structure of hERG: Bridging structure and function. Biophysical Journal, 2021, 120, 738-748.	0.5	5
12	Lipid regulation of hERG1 channel function. Nature Communications, 2021, 12, 1409.	12.8	9
13	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	19.0	557
14	Identification of PUFA interaction sites on the cardiac potassium channel KCNQ1. Journal of General Physiology, 2021, 153, .	1.9	22
15	ProLint: a web-based framework for the automated data analysis and visualization of lipidâ€“protein interactions. Nucleic Acids Research, 2021, 49, W544-W550.	14.5	23
16	Mutagenic Analysis of the Putative ABCC6 Substrate-Binding Cavity Using a New Homology Model. International Journal of Molecular Sciences, 2021, 22, 6910.	4.1	8
17	Modulation of Phospholipid Bilayer Properties by Simvastatin. Journal of Physical Chemistry B, 2021, 125, 8406-8418.	2.6	5
18	Insights into lipid-protein interactions from computer simulations. Biophysical Reviews, 2021, 13, 1019-1027.	3.2	13

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19	Evaluation of all-atom force fields in viral capsid simulations and properties. RSC Advances, 2021, 12, 216-220.	3.6	0
20	Structural and functional diversity calls for a new classification of ABC transporters. FEBS Letters, 2020, 594, 3767-3775.	2.8	169
21	Computer simulations of a heterogeneous membrane with enhanced sampling techniques. Journal of Chemical Physics, 2020, 153, 144110.	3.0	10
22	Location of the Hydrophobic Surfactant Proteins, SP-B and SP-C, in Fluid-Phase Bilayers. Journal of Physical Chemistry B, 2020, 124, 6763-6774.	2.6	11
23	Atomistic Simulations on Interactions between Amphiphilic Janus Nanoparticles and Lipid Bilayers: Effects of Lipid Ordering and Leaflet Asymmetry. Journal of Physical Chemistry B, 2020, 124, 4466-4475.	2.6	12
24	Lipid-Protein Interactions Are a Unique Property and Defining Feature of G Protein-Coupled Receptors. Biophysical Journal, 2020, 118, 1887-1900.	0.5	61
25	Phase Separation in Atomistic Simulations of Model Membranes. Journal of the American Chemical Society, 2020, 142, 2844-2856.	13.7	57
26	Interactions between Band 3 Anion Exchanger and Lipid Nanodomains in Ternary Lipid Bilayers: Atomistic Simulations. Journal of Physical Chemistry B, 2020, 124, 3054-3064.	2.6	9
27	Structural Properties of Inverted Hexagonal Phase: A Hybrid Computational and Experimental Approach. Langmuir, 2020, 36, 6668-6680.	3.5	9
28	Ionizable amino lipid interactions with POPC: implications for lipid nanoparticle function. Nanoscale, 2019, 11, 14141-14146.	5.6	46
29	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. Cell, 2019, 179, 1098-1111.e23.	28.9	122
30	Molecular Ordering in Lipid Monolayers: An Atomistic Simulation. Langmuir, 2019, 35, 13782-13790.	3.5	3
31	Membrane Remodeling by the Lytic Fragment ofÂSticholysinII: Implications for the Toroidal PoreÂModel. Biophysical Journal, 2019, 117, 1563-1576.	0.5	12
32	The Fluidity of Phosphocholine and Maltoside Micelles and the Effect of CHAPS. Biophysical Journal, 2019, 116, 1682-1691.	0.5	1
33	In vitro analyses of suspected arrhythmogenic thin filament variants as a cause of sudden cardiac death in infants. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 6969-6974.	7.1	16
34	NMRâ€“ and MD simulationâ€“based structural characterization of the membrane-associating FATC domain of ataxia telangiectasia mutated. Journal of Biological Chemistry, 2019, 294, 7098-7112.	3.4	7
35	Lipid Bilayer Structure Refinement with Saxs/Sans Based Restrained Ensemble Molecular Dynamics. Biophysical Journal, 2019, 116, 164a.	0.5	1
36	Emerging Diversity in Lipidâ€“Protein Interactions. Chemical Reviews, 2019, 119, 5775-5848.	47.7	299

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37	19. Simulations of biological membranes with the Martini model. , 2019, , 551-568.		0
38	Computational Modeling of Realistic Cell Membranes. Chemical Reviews, 2019, 119, 6184-6226.	47.7	502
39	Cholesterol Flip-Flop in Heterogeneous Membranes. Journal of Chemical Theory and Computation, 2019, 15, 2064-2070.	5.3	62
40	An auto-inhibitory helix in CTP:phosphocholine cytidylyltransferase hijacks the catalytic residue and constrains a pliable, domain-bridging helix pair. Journal of Biological Chemistry, 2018, 293, 7070-7084.	3.4	12
41	Coarse-grained molecular dynamics simulations reveal lipid access pathways in P-glycoprotein. Journal of General Physiology, 2018, 150, 417-429.	1.9	31
42	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.	5.6	46
43	Structure of Transmembrane Helix 8 and Possible Membrane Defects in CFTR. Biophysical Journal, 2018, 114, 1751-1754.	0.5	26
44	Effect of late endosomal DOBMP lipid and traditional model lipids of electrophysiology on the anthrax toxin channel activity. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2192-2203.	2.6	4
45	Regulation of Shigella Effector Kinase OspG through Modulation of Its Dynamic Properties. Journal of Molecular Biology, 2018, 430, 2096-2112.	4.2	8
46	Low-q Bicelles Are Mixed Micelles. Journal of Physical Chemistry Letters, 2018, 9, 4469-4473.	4.6	33
47	Cyclooxygenase 1 Lipid Interactions Revealed by All-Atom and Coarse-Grained Molecular Dynamics Simulations. Biophysical Journal, 2018, 114, 617a.	0.5	1
48	Phospholipid Chain Interactions with Cholesterol Drive Domain Formation in Lipid Membranes. Biophysical Journal, 2018, 114, 2595-2605.	0.5	44
49	Lipidâ€“Protein Interactions Are Unique Fingerprints for Membrane Proteins. ACS Central Science, 2018, 4, 709-717.	11.3	274
50	Curvatureâ€Induced Sorting of Lipids in Plasma Membrane Tethers. Advanced Theory and Simulations, 2018, 1, 1800034.	2.8	54
51	Molecular Dynamics Simulations. , 2018, , 1-7.		0
52	Dimerization, a Key Step for Pore Formation of Fragaceatoxin C, an Actinoporin from the Sea Anemone Actinia Fragacea. Biophysical Journal, 2017, 112, 524a-525a.	0.5	0
53	Lipid Mixing in Model Membranes. Biophysical Journal, 2017, 112, 82a-83a.	0.5	0
54	Molecular Views of a Eukaryotic Plasma Membrane Model. Biophysical Journal, 2017, 112, 138a.	0.5	0

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55	Disrupting a key hydrophobic pair in the oligomerization interface of the actinoporins impairs their poreâ€forming activity. Protein Science, 2017, 26, 550-565.	7.6	25
56	Structural basis for antibacterial peptide selfâ€immunity by the bacterial ABC transporter McjD. EMBO Journal, 2017, 36, 3062-3079.	7.8	64
57	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.	3.4	30
58	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.	2.6	33
59	Antimicrobial Peptides in the Cross Hairs of Computer Simulations. Biophysical Journal, 2017, 113, 1-3.	0.5	19
60	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2017, 121, 3262-3275.	2.6	81
61	Conformational flexibility of PL12 family heparinases: structure and substrate specificity of heparinase III fromBacteroides thetaiotaomicron(BT4657). Glycobiology, 2017, 27, 176-187.	2.5	14
62	Composition Fluctuations in Lipid Bilayers. Biophysical Journal, 2017, 113, 2750-2761.	0.5	42
63	Characterization of Zebrafish Cardiac and Slow Skeletal Troponin C Paralogs by MD Simulation andÂITC. Biophysical Journal, 2016, 111, 38-49.	0.5	16
64	The Heterodimeric ABC Transporter EfrCD Mediates Multidrug Efflux in Enterococcus faecalis. Antimicrobial Agents and Chemotherapy, 2016, 60, 5400-5411.	3.2	43
65	Structure and Stability of Carbohydrateâ€“Lipid Interactions. Methylmannose Polysaccharideâ€“Fatty Acid Complexes. ChemBioChem, 2016, 17, 1571-1578.	2.6	5
66	Computer simulations of lung surfactant. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2431-2440.	2.6	45
67	Probing catalytic rate enhancement during intramembrane proteolysis. Biological Chemistry, 2016, 397, 907-919.	2.5	6
68	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.	3.4	33
69	Biophysical experiments and simulation in nanoparticle-based drug delivery systems. Journal of Drug Targeting, 2016, 24, 768-773.	4.4	8
70	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.	5.3	78
71	Role of Influenza M2 Protein Clustering on the Induced Curvature of Model Membranes. Biophysical Journal, 2016, 110, 322a.	0.5	0
72	Development of Lipid-Based Drug Delivery Systems for Gene Therapy: Physicochemical Characterization of Charged Lipid Interactions. Biophysical Journal, 2016, 110, 247a.	0.5	0

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73	Functional Divergence in Teleost Cardiac Troponin Paralogs Guides Variation in the Interaction of TnI Switch Region with TnC. Genome Biology and Evolution, 2016, 8, 994-1011.	2.5	13
74	Two-Dimensional Potentials of Mean Force of Nile Red in Intact and Damaged Model Bilayers. Application to Calculations of Fluorescence Spectra. Journal of Chemical Theory and Computation, 2016, 12, 364-371.	5.3	11
75	Computational and experimental approaches for investigating nanoparticle-based drug delivery systems. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1688-1709.	2.6	142
76	Membrane Curvature Induced via Influenza M2 Protein Clusters. Biophysical Journal, 2015, 108, 468a-469a.	0.5	0
77	Localization of Lipids to the Cavity and Transmembrane Domain of ATP-Binding Cassette Transporter ABCB10, as Revealed by Molecular Dynamics Simulations. Biophysical Journal, 2015, 108, 252a.	0.5	0
78	Computational Lipidomics and the Lipid Organization of Cell Envelopes. Biophysical Journal, 2015, 108, 342a.	0.5	0
79	Landscapes of Membrane Protein Interactions from High-Throughput MD Simulations using the Daft Approach. Biophysical Journal, 2015, 108, 526a.	0.5	0
80	Computational Studies of Nile Red in Lipid Bilayers. Biophysical Journal, 2015, 108, 467a.	0.5	0
81	Molecular Models of Nanodiscs for Studying Membrane Proteins. Biophysical Journal, 2015, 108, 467a.	0.5	0
82	Computer Simulations of Lipid Flip-Flop and Membrane Asymmetry. Biophysical Journal, 2015, 108, 1a.	0.5	0
83	Simulation Study of Composition Fluctuations in Lipid Bilayers. Biophysical Journal, 2015, 108, 411a.	0.5	0
84	Martini Coarse-Grained Force Field: Extension to DNA. Journal of Chemical Theory and Computation, 2015, 11, 3932-3945.	5.3	239
85	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. Journal of Chemical Theory and Computation, 2015, 11, 2144-2155.	5.3	847
86	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.	7.1	44
87	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. Journal of Chemical Theory and Computation, 2015, 11, 2278-2291.	5.3	94
88	Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). Journal of Biological Chemistry, 2015, 290, 22891-22906.	3.4	47
89	Molecular Models of Nanodiscs. Journal of Chemical Theory and Computation, 2015, 11, 4923-4932.	5.3	33
90	Conformational Changes of the Antibacterial Peptide ATP Binding Cassette Transporter McjD Revealed by Molecular Dynamics Simulations. Biochemistry, 2015, 54, 5989-5998.	2.5	21

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91	Computer Simulations of Phase Separation in Lipid Bilayers and Monolayers. Methods in Molecular Biology, 2015, 1232, 307-322.	0.9	10
92	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.	3.4	35
93	Development of Coarse-Grained Martini Model for Nucleic Acid Structures. Biophysical Journal, 2014, 106, 704a.	0.5	0
94	Going Backward: An Efficient Multiscale Approach using Reverse Transformation. Biophysical Journal, 2014, 106, 640a.	0.5	2
95	Optimizing Drug Release: Bilayer to Inverted Hexagonal Phase Transition of Cationic XTC2 and Anionic DSPS Lipid System is Influenced by pH, Temperature, and Salt Concentration. Biophysical Journal, 2014, 106, 700a.	0.5	0
96	The molecular structure of a phosphatidylserine bilayer determined by scattering and molecular dynamics simulations. Soft Matter, 2014, 10, 3716.	2.7	84
97	Investigating the Domains' Motions of an Asymmetric ABC Transporter. Biophysical Journal, 2014, 106, 790a.	0.5	0
98	The ryanodine receptor store-sensing gate controls Ca2+ waves and Ca2+-triggered arrhythmias. Nature Medicine, 2014, 20, 184-192.	30.7	172
99	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.	5.3	566
100	Density based visualization for molecular simulation. Faraday Discussions, 2014, 169, 225-243.	3.2	17
101	The Mechanism of Collapse of Heterogeneous Lipid Monolayers. Biophysical Journal, 2014, 107, 1136-1145.	0.5	34
102	Lipid Organization of the Plasma Membrane. Journal of the American Chemical Society, 2014, 136, 14554-14559.	13.7	734
103	Oleic Acid Phase Behavior from Molecular Dynamics Simulations. Langmuir, 2014, 30, 10661-10667.	3.5	56
104	The Importance of Membrane Defectsâ€"Lessons from Simulations. Accounts of Chemical Research, 2014, 47, 2244-2251.	15.6	77
105	Effect of confinement on DNA, solvent and counterion dynamics in a model biological nanopore. Nanoscale, 2014, 6, 9006-9016.	5.6	17
106	Microsecond Molecular Dynamics Simulations of Lipid Mixing. Langmuir, 2014, 30, 11993-12001.	3.5	101
107	Potential of Mean Force Calculations for Nile Red in Lipid Bilayers. Biophysical Journal, 2014, 106, 703a.	0.5	0
108	Coarse-Grained Modeling of DNA-Vesicle Systems with the Martini Force Field. Biophysical Journal, 2014, 106, 803a.	0.5	1

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109	Atomistic Simulations of Pore Formation and Closure in Lipid Bilayers. Biophysical Journal, 2014, 106, 210-219.	0.5	166
110	SIMtoEXP: Software for Comparing Simulations to Experimental Scattering Data. Biophysical Journal, 2014, 106, 384a.	0.5	2
111	Monolayer-Bilayer Transformations with Phase Coexistence. Biophysical Journal, 2014, 106, 709a.	0.5	0
112	Molecular Dynamics Studies on Structural Changes in NK-Lysin and Saposins A, C, and D. Biophysical Journal, 2014, 106, 51a.	0.5	1
113	Modelling of the Interaction between Cationic Lipid Dlin-Kc2-Dma (XTC2) and Anionic Lipid Distearoylphosphatidylserine (DSPS). Biophysical Journal, 2014, 106, 700a-701a.	0.5	0
114	Molecular Dynamics Study of Self-Assembled Lipid Nano-Particles for Drug Delivery. Biophysical Journal, 2014, 106, 616a.	0.5	0
115	Characterization of the Immersion Properties of the Peripheral Membrane Anchor of the FATC Domain of the Kinase â€œTarget of Rapamycinâ€•by NMR, Oriented CD Spectroscopy, and MD Simulations. Journal of Physical Chemistry B, 2014, 118, 4817-4831.	2.6	14
116	Role of M2 Influenza Protein on Viral Budding and Scission. Biophysical Journal, 2014, 106, 98a.	0.5	0
117	Perspective on the Martini model. Chemical Society Reviews, 2013, 42, 6801.	38.1	1,008
118	Simulation Studies on the Role of the M2 Protein in Viral Budding. Biophysical Journal, 2013, 104, 414a.	0.5	0
119	Molecular View of Phase Coexistence in Model Membranes. Biophysical Journal, 2013, 104, 590a.	0.5	0
120	Molecular Models of the Closed State of the Cystic Fibrosis Transmembrane Conductance Regulator (CFTR). Biophysical Journal, 2013, 104, 625a.	0.5	0
121	Temperature Controlled Helix-Helix Interactions in Desk Minimal Sensor. Biophysical Journal, 2013, 104, 409a.	0.5	0
122	Atomistic Simulations of Wimleyâ€“White Pentapeptides: Sampling of Structure and Dynamics in Solution. Journal of Chemical Theory and Computation, 2013, 9, 1657-1666.	5.3	8
123	Interaction of Pristine and Functionalized Carbon Nanotubes with Lipid Membranes. Journal of Physical Chemistry B, 2013, 117, 12113-12123.	2.6	66
124	Constant pH simulations with the coarse-grained MARTINI model â€” Application to oleic acid aggregates. Canadian Journal of Chemistry, 2013, 91, 839-846.	1.1	59
125	Computer simulations of the phase separation in model membranes. Faraday Discussions, 2013, 161, 63-75.	3.2	69
126	Improved Parameters for the Martini Coarse-Grained Protein Force Field. Journal of Chemical Theory and Computation, 2013, 9, 687-697.	5.3	1,181

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127	Simulations of Lipid Monolayers. Methods in Molecular Biology, 2013, 924, 431-444.	0.9	10
128	Ternary Lipid Domain Formation using Atomistic Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 591a.	0.5	0
129	Thermodynamics of Oleic Acid Aggregation from Coarse-Grained Molecular Dynamics Simulations. Biophysical Journal, 2013, 104, 169a-170a.	0.5	0
130	Effect of Lipid Bilayers on Prion Peptide Aggregation: Insights from Coarse-Grained Molecular Simulations. Biophysical Journal, 2013, 104, 395a.	0.5	0
131	Parameterization and Molecular Dynamics Simulations of Nile Red. Biophysical Journal, 2013, 104, 83a.	0.5	1
132	Fatty Acid Aggregates Simulated using Constant pH Molecular Dynamics with a Coarse-Grained Model. Biophysical Journal, 2013, 104, 169a.	0.5	1
133	Computer simulations of lipid membrane domains. Biochimica Et Biophysica Acta - Biomembranes, 2013, 1828, 1765-1776.	2.6	157
134	Conical Lipids in Flat Bilayers Induce Packing Defects Similar to that Induced by Positive Curvature. Biophysical Journal, 2013, 104, 585-593.	0.5	149
135	Free energy of WALP23 dimer association in DMPC, DPPC, and DOPC bilayers. Chemistry and Physics of Lipids, 2013, 169, 95-105.	3.2	111
136	Force Fields for Classical Molecular Dynamics. Methods in Molecular Biology, 2013, 924, 197-213.	0.9	101
137	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. Journal of Chemical Theory and Computation, 2013, 9, 3282-3292.	5.3	67
138	Molecular simulation of rapid translocation of cholesterol, diacylglycerol, and ceramide in model raft and nonraft membranes. Journal of Lipid Research, 2012, 53, 421-429.	4.2	91
139	The Human Transporter Associated with Antigen Processing. Journal of Biological Chemistry, 2012, 287, 28099-28111.	3.4	26
140	Challenges in analysing and visualizing large-scale molecular dynamics simulations: domain and defect formation in lung surfactant monolayers. Journal of Physics: Conference Series, 2012, 385, 012002.	0.4	4
141	Molecular Simulations Investigations of the Role of the M2 Influenza Protein in Viral Budding. Biophysical Journal, 2012, 102, 398a.	0.5	0
142	Lipid Nanoparticles Containing siRNA Synthesized by Microfluidic Mixing Exhibit an Electron-Dense Nanostructured Core. Journal of Physical Chemistry C, 2012, 116, 18440-18450.	3.1	232
143	Investigation of the Signal Sensing Mechanism by the Bacterial Thermosensor Desk using Molecular Dynamics Methods. Biophysical Journal, 2012, 102, 495a.	0.5	0
144	Deriving Transferable Parameters for the Coarse-Grained Martini Model: Application to Amyloid-Like and Elastin-Like Peptides. Biophysical Journal, 2012, 102, 732a.	0.5	0

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145	Simulating Pores in Saturated Phosphatidylcholine Lipid Bilayers. Biophysical Journal, 2012, 102, 289a.	0.5	0
146	Molecular View of Phase Coexistence in Lipid Monolayers. Journal of the American Chemical Society, 2012, 134, 17543-17553.	13.7	102
147	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. Journal of Chemical Theory and Computation, 2012, 8, 618-628.	5.3	47
148	Tailoring Î¼-Conotoxin-KIIIA to Selectively Inhibit NaV1.7. Biophysical Journal, 2012, 102, 325a.	0.5	0
149	The Transporter Associated with Antigen Processing: Molecular Models to Describe the Transport Cycle. Biophysical Journal, 2012, 102, 661a.	0.5	0
150	Sampling Issues in Atomistic Simulations of Peptides at Cyclohexane/Water and POPC/Water Interfaces. Biophysical Journal, 2012, 102, 492a.	0.5	0
151	Simulation Study of Domains in Lipid Monolayers. Biophysical Journal, 2012, 102, 240a-241a.	0.5	2
152	Computer Simulations of the Interactions Between Cationic and Anionic Lipids in Lipid Nano Particles for Drug Delivery. Biophysical Journal, 2012, 102, 396a.	0.5	0
153	Molecular Structure of Membrane Tethers. Biophysical Journal, 2012, 102, 1866-1871.	0.5	61
154	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.	5.3	69
155	ABC Transporters. , 2011, , 183-198.		1
156	Simulation Study on the Properties of Cationic Lipid Bilayers and Vesicles. Biophysical Journal, 2011, 100, 311a.	0.5	0
157	The Role of Domains and Proteins in the Function of Lung Surfactant. Biophysical Journal, 2011, 100, 640a.	0.5	0
158	Simulation Studies of Wimley-White Peptides. Biophysical Journal, 2011, 100, 149a.	0.5	0
159	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.	0.5	54
160	Transfer of Arginine into Lipid Bilayers Is Nonadditive. Biophysical Journal, 2011, 101, 110-117.	0.5	86
161	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.	5.3	47
162	The Human Transporter Associated with Antigen Processing (TAP): A Computational Study Focused on the Nucleotide Binding Domains. Biophysical Journal, 2011, 100, 205a.	0.5	0

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163	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.	2.6	31
164	Statistical Convergence of Equilibrium Properties in Simulations of Molecular Solutes Embedded in Lipid Bilayers. Journal of Chemical Theory and Computation, 2011, 7, 4175-4188.	5.3	175
165	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.	5.3	121
166	Hydrophobicity scales: a thermodynamic looking glass into lipidâ€"protein interactions. Trends in Biochemical Sciences, 2011, 36, 653-662.	7.5	81
167	Combination of the CHARMM27 force field with unitedâ€atom lipid force fields. Journal of Computational Chemistry, 2011, 32, 1400-1410.	3.3	75
168	Interactions of Key Charged Residues Contributing to Selective Block of Neuronal Sodium Channels by Î¼-Conotoxin KIIIA. Molecular Pharmacology, 2011, 80, 573-584.	2.3	49
169	Orientation of Î¼-Conotoxin PIIIA in a Sodium Channel Vestibule, Based on Voltage Dependence of Its Binding. Molecular Pharmacology, 2011, 80, 219-227.	2.3	23
170	Holoâ€BtuF stabilizes the open conformation of the vitamin B12 ABC transporter BtuCD. Proteins: Structure, Function and Bioinformatics, 2010, 78, 738-753.	2.6	28
171	Molecular Dynamics Simulations of Î²-Ketoacyl-, Î²-Hydroxyacyl-, andtrans-2-Enoyl-Acyl Carrier Proteins ofEscherichia coli. Biochemistry, 2010, 49, 2860-2868.	2.5	11
172	Molecular dynamics simulations reveal that AEDANS is an inert fluorescent probe for the study of membrane proteins. European Biophysics Journal, 2010, 39, 229-239.	2.2	5
173	Molecular Dynamics Simulations of Ceramide Flip-Flop and Desorption inÂLipid Rafts. Biophysical Journal, 2010, 98, 76a.	0.5	0
174	Simulation Studies on Interactions of Lung Surfactant Protein SP-B with Lipid Monolayers and Vesicles. Biophysical Journal, 2010, 98, 90a.	0.5	0
175	Interpretation of 2H-NMR Experiments on the Orientation of the Transmembrane Helix WALP23 by Computer Simulations. Biophysical Journal, 2010, 99, 1455-1464.	0.5	43
176	Direct Simulation of Protein-Mediated Vesicle Fusion: Lung Surfactant Protein B. Biophysical Journal, 2010, 99, 2134-2142.	0.5	71
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