D Peter Tieleman

List of Publications by Year in Descending Order

250 papers	25,231 citations	78 h-index	156 g-index
325 ext. papers	28,909 ext. citations	4.8 avg, IF	7.3 L-index

#	Paper	IF	Citations
250	Effects of Lid Domain Structural Changes on the Interactions between Peripheral Myelin Protein 2 and a Lipid Bilayer.. *Journal of Physical Chemistry Letters*, **2022**, 991-996	6.4	
249	Can two wrongs make a right? F508del-CFTR ion channel rescue by second-site mutations in its transmembrane domains.. *Journal of Biological Chemistry*, **2022**, 101615	5.4	0
248	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	11.5	3
247	The ugly, bad, and good stories of large-scale biomolecular simulations.. *Current Opinion in Structural Biology*, **2022**, 73, 102338	8.1	1
246	Insights into lipid-protein interactions from computer simulations.. *Biophysical Reviews*, **2021**, 13, 1019-1027	3.7	0
245	Evaluation of all-atom force fields in viral capsid simulations and properties.. *RSC Advances*, **2021**, 12, 216-220	3.7	
244	Lipid regulation of hERG1 channel function. *Nature Communications*, **2021**, 12, 1409	17.4	2
243	Martini 3: a general purpose force field for coarse-grained molecular dynamics. *Nature Methods*, **2021**, 18, 382-388	21.6	124
242	Identification of PUFA interaction sites on the cardiac potassium channel KCNQ1. *Journal of General Physiology*, **2021**, 153,	3.4	4
241	ProLint: a web-based framework for the automated data analysis and visualization of lipid-protein interactions. *Nucleic Acids Research*, **2021**, 49, W544-W550	20.1	8
240	Mutagenic Analysis of the Putative ABCC6 Substrate-Binding Cavity Using a New Homology Model. *International Journal of Molecular Sciences*, **2021**, 22,	6.3	3
239	Modulation of Phospholipid Bilayer Properties by Simvastatin. *Journal of Physical Chemistry B*, **2021** , 125, 8406-8418	3.4	1
238	Lipid distributions and transleaflet cholesterol migration near heterogeneous surfaces in asymmetric bilayers. *Faraday Discussions*, **2021**,	3.6	1
237	Refinement of a cryo-EM structure of hERG: Bridging structure and function. *Biophysical Journal*, **2021**, 120, 738-748	2.9	2
236	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*, **2021**,	6.1	3
235	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	3.4	5
234	Lipid-Protein Interactions Are a Unique Property and Defining Feature of G Protein-Coupled Receptors. *Biophysical Journal*, **2020**, 118, 1887-1900	2.9	27

233	Phase Separation in Atomistic Simulations of Model Membranes. *Journal of the American Chemical Society*, **2020**, 142, 2844-2856	16.4	28
232	Interactions between Band 3 Anion Exchanger and Lipid Nanodomains in Ternary Lipid Bilayers: Atomistic Simulations. *Journal of Physical Chemistry B*, **2020**, 124, 3054-3064	3.4	4
231	Structural Properties of Inverted Hexagonal Phase: A Hybrid Computational and Experimental Approach. *Langmuir*, **2020**, 36, 6668-6680	4	2
230	Structural and functional diversity calls for a new classification of ABC transporters. *FEBS Letters*, **2020**, 594, 3767-3775	3.8	66
229	Computer simulations of a heterogeneous membrane with enhanced sampling techniques. *Journal of Chemical Physics*, **2020**, 153, 144110	3.9	5
228	Location of the Hydrophobic Surfactant Proteins, SP-B and SP-C, in Fluid-Phase Bilayers. *Journal of Physical Chemistry B*, **2020**, 124, 6763-6774	3.4	7
227	Molecular Ordering in Lipid Monolayers: An Atomistic Simulation. *Langmuir*, **2019**, 35, 13782-13790	4	2
226	Membrane Remodeling by the Lytic Fragment of SticholysinII: Implications for the Toroidal Pore Model. *Biophysical Journal*, **2019**, 117, 1563-1576	2.9	8
225	The Fluidity of Phosphocholine and Maltoside Micelles and the Effect of CHAPS. *Biophysical Journal* , **2019**, 116, 1682-1691	2.9	
224	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	11.5	13
223	NMR- and MD simulation-based structural characterization of the membrane-associating FATC domain of ataxia telangiectasia mutated. *Journal of Biological Chemistry*, **2019**, 294, 7098-7112	5.4	3
222	Ionizable amino lipid interactions with POPC: implications for lipid nanoparticle function. *Nanoscale* , **2019**, 11, 14141-14146	7.7	23
221	Atoms to Phenotypes: Molecular Design Principles of Cellular Energy Metabolism. *Cell*, **2019**, 179, 1098-1111.e23	36.1	83
220	Emerging Diversity in Lipid-Protein Interactions. *Chemical Reviews*, **2019**, 119, 5775-5848	68.1	163
219	19. Simulations of biological membranes with the Martini model **2019**, 551-568		
218	Computational Modeling of Realistic Cell Membranes. *Chemical Reviews*, **2019**, 119, 6184-6226	68.1	265
217	Cholesterol Flip-Flop in Heterogeneous Membranes. *Journal of Chemical Theory and Computation*, **2019**, 15, 2064-2070	6.4	32
216	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	5.4	10

215	Coarse-grained molecular dynamics simulations reveal lipid access pathways in P-glycoprotein. *Journal of General Physiology*, **2018**, 150, 417-429	3.4	18
214	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	7.7	33
213	Structure of Transmembrane Helix 8 and Possible Membrane Defects in CFTR. *Biophysical Journal*, **2018**, 114, 1751-1754	2.9	15
212	Low- q Bicelles Are Mixed Micelles. *Journal of Physical Chemistry Letters*, **2018**, 9, 4469-4473	6.4	21
211	Phospholipid Chain Interactions with Cholesterol Drive Domain Formation in Lipid Membranes. *Biophysical Journal*, **2018**, 114, 2595-2605	2.9	33
210	Lipid-Protein Interactions Are Unique Fingerprints for Membrane Proteins. *ACS Central Science*, **2018**, 4, 709-717	16.8	139
209	Curvature-Induced Sorting of Lipids in Plasma Membrane Tethers. *Advanced Theory and Simulations*, **2018**, 1, 1800034	3.5	28
208	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	3.8	4
207	Regulation of Shigella Effector Kinase OspG through Modulation of Its Dynamic Properties. *Journal of Molecular Biology*, **2018**, 430, 2096-2112	6.5	5
206	Disrupting a key hydrophobic pair in the oligomerization interface of the actinoporins impairs their pore-forming activity. *Protein Science*, **2017**, 26, 550-565	6.3	21
205	Structural basis for antibacterial peptide self-immunity by the bacterial ABC transporter McjD. *EMBO Journal*, **2017**, 36, 3062-3079	13	41
204	Changes in the dynamics of the cardiac troponin C molecule explain the effects of Ca-sensitizing mutations. *Journal of Biological Chemistry*, **2017**, 292, 11915-11926	5.4	15
203	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	3.4	13
202	Antimicrobial Peptides in the Cross Hairs of Computer Simulations. *Biophysical Journal*, **2017**, 113, 1-3	2.9	16
201	Ganglioside-Lipid and Ganglioside-Protein Interactions Revealed by Coarse-Grained and Atomistic Molecular Dynamics Simulations. *Journal of Physical Chemistry B*, **2017**, 121, 3262-3275	3.4	60
200	Conformational flexibility of PL12 family heparinases: structure and substrate specificity of heparinase III from Bacteroides thetaiotaomicron (BT4657). *Glycobiology*, **2017**, 27, 176-187	5.8	10
199	Composition Fluctuations in Lipid Bilayers. *Biophysical Journal*, **2017**, 113, 2750-2761	2.9	31
198	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	5.4	22

197	Biophysical experiments and simulation in nanoparticle-based drug delivery systems. *Journal of Drug Targeting*, **2016**, 24, 768-773	5.4	8
196	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, 4524-33	6.4	59
195	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	3.9	8
194	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, 364-71	6.4	9
193	Computational and experimental approaches for investigating nanoparticle-based drug delivery systems. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1688-709	3.8	108
192	Characterization of Zebrafish Cardiac and Slow Skeletal Troponin C Paralogs by MD Simulation and ITC. *Biophysical Journal*, **2016**, 111, 38-49	2.9	10
191	The Heterodimeric ABC Transporter EfrCD Mediates Multidrug Efflux in Enterococcus faecalis. *Antimicrobial Agents and Chemotherapy*, **2016**, 60, 5400-11	5.9	33
190	Structure and Stability of Carbohydrate-Lipid Interactions. Methylmannose Polysaccharide-Fatty Acid Complexes. *ChemBioChem*, **2016**, 17, 1571-8	3.8	1
189	Computer simulations of lung surfactant. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 2431-2440	3.8	35
188	Probing catalytic rate enhancement during intramembrane proteolysis. *Biological Chemistry*, **2016**, 397, 907-19	4.5	4
187	Martini Coarse-Grained Force Field: Extension to DNA. *Journal of Chemical Theory and Computation*, **2015**, 11, 3932-45	6.4	156
186	Computational Lipidomics with insane: A Versatile Tool for Generating Custom Membranes for Molecular Simulations. *Journal of Chemical Theory and Computation*, **2015**, 11, 2144-55	6.4	504
185	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, 6353-8	11.5	37
184	High-Throughput Simulations of Dimer and Trimer Assembly of Membrane Proteins. The DAFT Approach. *Journal of Chemical Theory and Computation*, **2015**, 11, 2278-91	6.4	73
183	Cystic Fibrosis Transmembrane Conductance Regulator (CFTR): CLOSED AND OPEN STATE CHANNEL MODELS. *Journal of Biological Chemistry*, **2015**, 290, 22891-906	5.4	40
182	Molecular models of nanodiscs. *Journal of Chemical Theory and Computation*, **2015**, 11, 4923-32	6.4	24
181	Conformational Changes of the Antibacterial Peptide ATP Binding Cassette Transporter McjD Revealed by Molecular Dynamics Simulations. *Biochemistry*, **2015**, 54, 5989-98	3.2	17
180	Computer simulations of phase separation in lipid bilayers and monolayers. *Methods in Molecular Biology*, **2015**, 1232, 307-22	1.4	9

179	The molecular structure of a phosphatidylserine bilayer determined by scattering and molecular dynamics simulations. *Soft Matter*, **2014**, 10, 3716-25	3.6	64
178	The ryanodine receptor store-sensing gate controls Ca2+ waves and Ca2+-triggered arrhythmias. *Nature Medicine*, **2014**, 20, 184-92	50.5	135
177	Going Backward: A Flexible Geometric Approach to Reverse Transformation from Coarse Grained to Atomistic Models. *Journal of Chemical Theory and Computation*, **2014**, 10, 676-90	6.4	378
176	Density based visualization for molecular simulation. *Faraday Discussions*, **2014**, 169, 225-43	3.6	12
175	The mechanism of collapse of heterogeneous lipid monolayers. *Biophysical Journal*, **2014**, 107, 1136-1145	2.9	27
174	Lipid organization of the plasma membrane. *Journal of the American Chemical Society*, **2014**, 136, 14554-9	26.4	519
173	Oleic acid phase behavior from molecular dynamics simulations. *Langmuir*, **2014**, 30, 10661-7	4	46
172	The importance of membrane defects-lessons from simulations. *Accounts of Chemical Research*, **2014**, 47, 2244-51	24.3	59
171	Effect of confinement on DNA, solvent and counterion dynamics in a model biological nanopore. *Nanoscale*, **2014**, 6, 9006-16	7.7	17
170	Microsecond molecular dynamics simulations of lipid mixing. *Langmuir*, **2014**, 30, 11993-2001	4	79
169	Atomistic simulations of pore formation and closure in lipid bilayers. *Biophysical Journal*, **2014**, 106, 210-9	2.9	129
168	SIMtoEXP: Software for Comparing Simulations to Experimental Scattering Data. *Biophysical Journal*, **2014**, 106, 384a	2.9	2
167	Characterization of the immersion properties of the peripheral membrane anchor of the FATC domain of the kinase "target of rapamycin" by NMR, oriented CD spectroscopy, and MD simulations. *Journal of Physical Chemistry B*, **2014**, 118, 4817-31	3.4	12
166	Protein Lipid Interactions from a Molecular Dynamics Simulation Point of View **2014**, 267-282		1
165	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, 1742-55	5.4	31
164	Going Backward: An Efficient Multiscale Approach using Reverse Transformation. *Biophysical Journal*, **2014**, 106, 640a	2.9	2
163	Perspective on the Martini model. *Chemical Society Reviews*, **2013**, 42, 6801-22	58.5	805
162	Atomistic Simulations of Wimley-White Pentapeptides: Sampling of Structure and Dynamics in Solution. *Journal of Chemical Theory and Computation*, **2013**, 9, 1657-66	6.4	8

161	Interaction of pristine and functionalized carbon nanotubes with lipid membranes. *Journal of Physical Chemistry B*, **2013**, 117, 12113-23	3.4	51
160	Constant pH simulations with the coarse-grained MARTINI model Application to oleic acid aggregates. *Canadian Journal of Chemistry*, **2013**, 91, 839-846	0.9	44
159	Computer simulations of the phase separation in model membranes. *Faraday Discussions*, **2013**, 161, 63-75; discussion 113-50	3.6	56
158	Improved Parameters for the Martini Coarse-Grained Protein Force Field. *Journal of Chemical Theory and Computation*, **2013**, 9, 687-97	6.4	782
157	Simulations of lipid monolayers. *Methods in Molecular Biology*, **2013**, 924, 431-44	1.4	9
156	Computer simulations of lipid membrane domains. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 1765-76	3.8	133
155	Conical lipids in flat bilayers induce packing defects similar to that induced by positive curvature. *Biophysical Journal*, **2013**, 104, 585-93	2.9	112
154	Free energy of WALP23 dimer association in DMPC, DPPC, and DOPC bilayers. *Chemistry and Physics of Lipids*, **2013**, 169, 95-105	3.7	92
153	Force fields for classical molecular dynamics. *Methods in Molecular Biology*, **2013**, 924, 197-213	1.4	69
152	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 3282-92	6.4	45
151	Lipid Nanoparticles Containing siRNA Synthesized by Microfluidic Mixing Exhibit an Electron-Dense Nanostructured Core. *Journal of Physical Chemistry C*, **2012**, 116, 18440-18450	3.8	151
150	Molecular view of phase coexistence in lipid monolayers. *Journal of the American Chemical Society*, **2012**, 134, 17543-53	16.4	83
149	The Role of Atomic Polarization in the Thermodynamics of Chloroform Partitioning to Lipid Bilayers. *Journal of Chemical Theory and Computation*, **2012**, 8, 618-28	6.4	42
148	Simulation Study of Domains in Lipid Monolayers. *Biophysical Journal*, **2012**, 102, 240a-241a	2.9	2
147	Molecular structure of membrane tethers. *Biophysical Journal*, **2012**, 102, 1866-71	2.9	54
146	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	6.4	63
145	Molecular simulation of rapid translocation of cholesterol, diacylglycerol, and ceramide in model raft and nonraft membranes. *Journal of Lipid Research*, **2012**, 53, 421-429	6.3	70
144	The human transporter associated with antigen processing: molecular models to describe peptide binding competent states. *Journal of Biological Chemistry*, **2012**, 287, 28099-111	5.4	22

143	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	0.3	2
142	Lung surfactant protein SP-B promotes formation of bilayer reservoirs from monolayer and lipid transfer between the interface and subphase. *Biophysical Journal*, **2011**, 100, 1678-87	2.9	49
141	Transfer of arginine into lipid bilayers is nonadditive. *Biophysical Journal*, **2011**, 101, 110-7	2.9	82
140	Using the Wimley-White Hydrophobicity Scale as a Direct Quantitative Test of Force Fields: The MARTINI Coarse-Grained Model. *Journal of Chemical Theory and Computation*, **2011**, 7, 2316-24	6.4	38
139	Conformational choreography of a molecular switch region in myelin basic protein--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, 674-83	3.8	28
138	Statistical Convergence of Equilibrium Properties in Simulations of Molecular Solutes Embedded in Lipid Bilayers. *Journal of Chemical Theory and Computation*, **2011**, 7, 4175-88	6.4	162
137	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, 2981-8	6.4	101
136	Hydrophobicity scales: a thermodynamic looking glass into lipid-protein interactions. *Trends in Biochemical Sciences*, **2011**, 36, 653-62	10.3	74
135	Combination of the CHARMM27 force field with united-atom lipid force fields. *Journal of Computational Chemistry*, **2011**, 32, 1400-10	3.5	57
134	ABC Transporters **2011**, 183-198		1
133	Interactions of key charged residues contributing to selective block of neuronal sodium channels by μ-conotoxin KIIIA. *Molecular Pharmacology*, **2011**, 80, 573-84	4.3	39
132	Orientation of μ-conotoxin PIIIA in a sodium channel vestibule, based on voltage dependence of its binding. *Molecular Pharmacology*, **2011**, 80, 219-27	4.3	22
131	Interpretation of 2H-NMR experiments on the orientation of the transmembrane helix WALP23 by computer simulations. *Biophysical Journal*, **2010**, 99, 1455-64	2.9	41
130	Direct simulation of protein-mediated vesicle fusion: lung surfactant protein B. *Biophysical Journal*, **2010**, 99, 2134-42	2.9	64
129	Molecular simulations of lipid flip-flop in the presence of model transmembrane helices. *Biochemistry*, **2010**, 49, 7665-73	3.2	31
128	Lateral pressure profiles in lipid monolayers. *Faraday Discussions*, **2010**, 144, 393-409; discussion 445-81	3.6	46
127	Comment on "On using a too large integration time step in molecular dynamics simulations of coarse-grained molecular models" 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, 2254-6; author reply 2257-8	3.6	60
126	Holo-BtuF stabilizes the open conformation of the vitamin B12 ABC transporter BtuCD. *Proteins: Structure, Function and Bioinformatics*, **2010**, 78, 738-53	4.2	24

125	Molecular dynamics simulations of beta-ketoacyl-, beta-hydroxyacyl-, and trans-2-enoyl-acyl carrier proteins of Escherichia coli. *Biochemistry*, **2010**, 49, 2860-8	3.2	10
124	Molecular dynamics simulations reveal that AEDANS is an inert fluorescent probe for the study of membrane proteins. *European Biophysics Journal*, **2010**, 39, 229-39	1.9	4
123	Electroporating fields target oxidatively damaged areas in the cell membrane. *PLoS ONE*, **2009**, 4, e7966	3.7	99
122	Molecular view of cholesterol flip-flop and chemical potential in different membrane environments. *Journal of the American Chemical Society*, **2009**, 131, 12714-20	16.4	222
121	Lipids on the move: simulations of membrane pores, domains, stalks and curves. *Biochimica Et Biophysica Acta - Biomembranes*, **2009**, 1788, 149-68	3.8	363
120	Alamethicin in lipid bilayers: combined use of X-ray scattering and MD simulations. *Biochimica Et Biophysica Acta - Biomembranes*, **2009**, 1788, 1387-97	3.8	85
119	Thermodynamics of flip-flop and desorption for a systematic series of phosphatidylcholine lipids. *Soft Matter*, **2009**, 5, 3295	3.6	97
118	Chapter 1 Free Energies of Lipid□lipid Interactions in Membranes. *Annual Reports in Computational Chemistry*, **2009**, 5, 3-21	1.8	1
117	Structure and Dynamics of Lipid Monolayers: Theory and Applications **2009**, 75-99		7
116	Transmembrane helix 12 modulates progression of the ATP catalytic cycle in ABCB1. *Biochemistry*, **2009**, 48, 6249-58	3.2	25
115	Thermodynamic analysis of the effect of cholesterol on dipalmitoylphosphatidylcholine lipid membranes. *Journal of the American Chemical Society*, **2009**, 131, 1972-8	16.4	133
114	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, 5551-6	11.5	78
113	The mechanism of ABC transporters: general lessons from structural and functional studies of an antigenic peptide transporter. *FASEB Journal*, **2009**, 23, 1287-302	0.9	135
112	Molecular dynamics study of the effect of cholesterol on the properties of lipid monolayers at low surface tensions. *Physical Chemistry Chemical Physics*, **2009**, 11, 1916-22	3.6	37
111	Computer simulation study of fullerene translocation through lipid membranes. *Nature Nanotechnology*, **2008**, 3, 363-8	28.7	411
110	Distribution of amino acids in a lipid bilayer from computer simulations. *Biophysical Journal*, **2008**, 94, 3393-404	2.9	434
109	Cytosolic region of TM6 in P-glycoprotein: topographical analysis and functional perturbation by site directed labeling. *Biochemistry*, **2008**, 47, 3615-24	3.2	17
108	Chapter 8 Interactions between Small Molecules and Lipid Bilayers. *Current Topics in Membranes*, **2008**, 227-256	2.2	29

107	The MARTINI Coarse-Grained Force Field: Extension to Proteins. *Journal of Chemical Theory and Computation*, **2008**, 4, 819-34	6.4	1717
106	ATP-binding cassette transporters in Escherichia coli. *Biochimica Et Biophysica Acta - Biomembranes*, **2008**, 1778, 1757-71	3.8	102
105	Structural proteomics of the cell envelope of Gram-negative bacteria. *Biochimica Et Biophysica Acta - Biomembranes*, **2008**, 1778, 1697	3.8	
104	Chapter 4 Molecular Dynamics Simulation of Lipid–Protein Interactions. *Current Topics in Membranes*, **2008**, 111-130	2.2	12
103	Water in Ion Channels and Pores—Simulation Studies. *Novartis Foundation Symposium*, **2008**, 66-83		8
102	The molecular mechanism of lipid monolayer collapse. *Proceedings of the National Academy of Sciences of the United States of America*, **2008**, 105, 10803-8	11.5	223
101	Molecular dynamics simulations of the Apo-, Holo-, and acyl-forms of Escherichia coli acyl carrier protein. *Journal of Biological Chemistry*, **2008**, 283, 33620-9	5.4	38
100	Structure and dynamics of the antifungal molecules Syringotoxin-B and Syringopeptin-25A from molecular dynamics simulation. *European Biophysics Journal*, **2008**, 37, 495-502	1.9	7
99	Molecular simulation of multistate peptide dynamics: a comparison between microsecond timescale sampling and multiple shorter trajectories. *Journal of Computational Chemistry*, **2008**, 29, 1740-52	3.5	47
98	Partitioning of amino acid side chains into lipid bilayers: results from computer simulations and comparison to experiment. *Journal of General Physiology*, **2007**, 129, 371-7	3.4	229
97	Simulation of the coupling between nucleotide binding and transmembrane domains in the ATP binding cassette transporter BtuCD. *Biophysical Journal*, **2007**, 92, 2727-34	2.9	48
96	Effect of lipid peroxidation on the properties of lipid bilayers: a molecular dynamics study. *Biophysical Journal*, **2007**, 93, 4225-36	2.9	407
95	The molecular mechanism of monolayer-bilayer transformations of lung surfactant from molecular dynamics simulations. *Biophysical Journal*, **2007**, 93, 3775-82	2.9	86
94	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, 689-97	3.5	42
93	Molecular dynamics simulations of biological membranes. *Chemistry and Physics of Lipids*, **2007**, 149, S4	3.7	
92	Residue G346 in transmembrane segment six is involved in inter-domain communication in P-glycoprotein. *Biochemistry*, **2007**, 46, 9899-910	3.2	37
91	The MARTINI force field: coarse grained model for biomolecular simulations. *Journal of Physical Chemistry B*, **2007**, 111, 7812-24	3.4	3596
90	Hydrophobic association of alpha-helices, steric dewetting, and enthalpic barriers to protein folding. *Proceedings of the National Academy of Sciences of the United States of America*, **2007**, 104, 6206-10	11.5	74

89	Computer simulation of antimicrobial peptides. *Current Medicinal Chemistry*, **2007**, 14, 2789-98	4.3	89
88	Docking of mu-conotoxin GIIIA in the sodium channel outer vestibule. *Channels*, **2007**, 1, 344-52	3	45
87	An electrostatic/hydrogen bond switch as the basis for the specific interaction of phosphatidic acid with proteins. *Journal of Biological Chemistry*, **2007**, 282, 11356-64	5.4	176
86	Setting up and running molecular dynamics simulations of membrane proteins. *Methods*, **2007**, 41, 475-88	4.6	364
85	Pressure-area isotherm of a lipid monolayer from molecular dynamics simulations. *Langmuir*, **2007**, 23, 12617-23	4	139
84	P-glycoprotein models of the apo and ATP-bound states based on homology with Sav1866 and MalK. *FEBS Letters*, **2007**, 581, 4217-22	3.8	77
83	The distribution and conformation of very long-chain plant wax components in a lipid bilayer. *Journal of Physical Chemistry B*, **2007**, 111, 8702-4	3.4	7
82	The TatA subunit of Escherichia coli twin-arginine translocase has an N-in topology. *Biochemistry*, **2007**, 46, 7396-404	3.2	34
81	Domain coupling in the ABC transporter system BtuCD/BtuF: molecular dynamics simulation, normal mode analysis and protein-protein docking **2007**,		1
80	Partitioning of Amino Acid Side Chains into Lipid Bilayers: Results from Computer Simulations and Comparison to Experiment. *Journal of Cell Biology*, **2007**, 177, i12-i12	7.3	1
79	Structural investigation of syringomycin-E using molecular dynamics simulation and NMR. *European Biophysics Journal*, **2006**, 35, 459-67	1.9	4
78	Nanopore-facilitated, voltage-driven phosphatidylserine translocation in lipid bilayers--in cells and in silico. *Physical Biology*, **2006**, 3, 233-47	3	119
77	The dynamics of the MgATP-driven closure of MalK, the energy-transducing subunit of the maltose ABC transporter. *Journal of Biological Chemistry*, **2006**, 281, 28397-407	5.4	53
76	Lipids out of equilibrium: energetics of desorption and pore mediated flip-flop. *Journal of the American Chemical Society*, **2006**, 128, 12462-7	16.4	187
75	Nanopore formation and phosphatidylserine externalization in a phospholipid bilayer at high transmembrane potential. *Journal of the American Chemical Society*, **2006**, 128, 6288-9	16.4	122
74	Computer simulation of the distribution of hexane in a lipid bilayer: spatially resolved free energy, entropy, and enthalpy profiles. *Journal of the American Chemical Society*, **2006**, 128, 125-30	16.4	121
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