D Peter Tieleman

List of Publications by Citations

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	The MARTINI force field: coarse grained model for biomolecular simulations. *Journal of Physical Chemistry B*, **2007**, 111, 7812-24	3.4	3596
249	The MARTINI Coarse-Grained Force Field: Extension to Proteins. *Journal of Chemical Theory and Computation*, **2008**, 4, 819-34	6.4	1717
248	Perspective on the Martini model. *Chemical Society Reviews*, **2013**, 42, 6801-22	58.5	805
247	Improved Parameters for the Martini Coarse-Grained Protein Force Field. *Journal of Chemical Theory and Computation*, **2013**, 9, 687-97	6.4	782
246	A computer perspective of membranes: molecular dynamics studies of lipid bilayer systems. *BBA - Biomembranes*, **1997**, 1331, 235-70		622
245	Lipid organization of the plasma membrane. *Journal of the American Chemical Society*, **2014**, 136, 14554-9	16.4	519
244	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
243	Molecular dynamics simulations of a fully hydrated dipalmitoylphosphatidylcholine bilayer with different macroscopic boundary conditions and parameters. *Journal of Chemical Physics*, **1996**, 105, 4871-4880	3.8	438
242	Distribution of amino acids in a lipid bilayer from computer simulations. *Biophysical Journal*, **2008**, 94, 3393-404	2.9	434
241	Computer simulation study of fullerene translocation through lipid membranes. *Nature Nanotechnology*, **2008**, 3, 363-8	28.7	411
240	Effect of lipid peroxidation on the properties of lipid bilayers: a molecular dynamics study. *Biophysical Journal*, **2007**, 93, 4225-36	2.9	407
239	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
238	Setting up and running molecular dynamics simulations of membrane proteins. *Methods*, **2007**, 41, 475-88	4.6	364
237	Lipids on the move: simulations of membrane pores, domains, stalks and curves. *Biochimica Et Biophysica Acta - Biomembranes*, **2009**, 1788, 149-68	3.8	363
236	Simulation of pore formation in lipid bilayers by mechanical stress and electric fields. *Journal of the American Chemical Society*, **2003**, 125, 6382-3	16.4	363
235	A molecular dynamics study of the pores formed by Escherichia coli OmpF porin in a fully hydrated palmitoyloleoylphosphatidylcholine bilayer. *Biophysical Journal*, **1998**, 74, 2786-801	2.9	318
234	Methodological Issues in Lipid Bilayer Simulations. *Journal of Physical Chemistry B*, **2003**, 107, 9424-9433	3.4	314

233	The molecular basis of electroporation. *BMC Biochemistry*, **2004**, 5, 10	4.8	309
232	Computational Modeling of Realistic Cell Membranes. *Chemical Reviews*, **2019**, 119, 6184-6226	68.1	265
231	Molecular Dynamics Simulations of Dodecylphosphocholine Micelles at Three Different Aggregate Sizes:Micellar Structure and Chain Relaxation. *Journal of Physical Chemistry B*, **2000**, 104, 6380-6388	3.4	250
230	Molecular Dynamics Simulation of the Kinetics of Spontaneous Micelle Formation. *Journal of Physical Chemistry B*, **2000**, 104, 12165-12173	3.4	248
229	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
228	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
227	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
226	Computer simulations of membrane proteins. *Biochimica Et Biophysica Acta - Biomembranes*, **2004**, 1666, 158-89	3.8	205
225	Alamethicin helices in a bilayer and in solution: molecular dynamics simulations. *Biophysical Journal*, **1999**, 76, 40-9	2.9	193
224	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
223	Adhesion forces of lipids in a phospholipid membrane studied by molecular dynamics simulations. *Biophysical Journal*, **1998**, 74, 931-43	2.9	181
222	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
221	Simulation approaches to ion channel structure-function relationships. *Quarterly Reviews of Biophysics*, **2001**, 34, 473-561	7	168
220	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	1.9	166
219	Emerging Diversity in Lipid-Protein Interactions. *Chemical Reviews*, **2019**, 119, 5775-5848	68.1	163
218	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
217	An alamethicin channel in a lipid bilayer: molecular dynamics simulations. *Biophysical Journal*, **1999**, 76, 1757-69	2.9	161
216	Molecular dynamics simulation of a palmitoyl-oleoyl phosphatidylserine bilayer with Na+ counterions and NaCl. *Biophysical Journal*, **2004**, 86, 1601-9	2.9	159

215	Martini Coarse-Grained Force Field: Extension to DNA. *Journal of Chemical Theory and Computation*, **2015**, 11, 3932-45	6.4	156
214	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
213	Lipid properties and the orientation of aromatic residues in OmpF, influenza M2, and alamethicin systems: molecular dynamics simulations. *Biochemistry*, **1998**, 37, 17554-61	3.2	151
212	Lipid-Protein Interactions Are Unique Fingerprints for Membrane Proteins. *ACS Central Science*, **2018**, 4, 709-717	16.8	139
211	Pressure-area isotherm of a lipid monolayer from molecular dynamics simulations. *Langmuir*, **2007**, 23, 12617-23	4	139
210	Membrane protein simulations with a united-atom lipid and all-atom protein model: lipid-protein interactions, side chain transfer free energies and model proteins. *Journal of Physics Condensed Matter*, **2006**, 18, S1221-34	1.8	138
209	The ryanodine receptor store-sensing gate controls Ca2+ waves and Ca2+-triggered arrhythmias. *Nature Medicine*, **2014**, 20, 184-92	50.5	135
208	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
207	Computer simulations of lipid membrane domains. *Biochimica Et Biophysica Acta - Biomembranes*, **2013**, 1828, 1765-76	3.8	133
206	Thermodynamic analysis of the effect of cholesterol on dipalmitoylphosphatidylcholine lipid membranes. *Journal of the American Chemical Society*, **2009**, 131, 1972-8	16.4	133
205	Atomistic simulations of pore formation and closure in lipid bilayers. *Biophysical Journal*, **2014**, 106, 210-9	2.9	129
204	Proline-induced hinges in transmembrane helices: possible roles in ion channel gating. *Proteins: Structure, Function and Bioinformatics*, **2001**, 44, 63-72	4.2	128
203	K(+) versus Na(+) ions in a K channel selectivity filter: a simulation study. *Biophysical Journal*, **2002**, 83, 633-45	2.9	124
202	Martini 3: a general purpose force field for coarse-grained molecular dynamics. *Nature Methods*, **2021**, 18, 382-388	21.6	124
201	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
200	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
199	Nanopore-facilitated, voltage-driven phosphatidylserine translocation in lipid bilayers--in cells and in silico. *Physical Biology*, **2006**, 3, 233-47	3	119
198	Analysis and evaluation of channel models: simulations of alamethicin. *Biophysical Journal*, **2002**, 83, 2393-407	2.9	117

197	Molecular Dynamics Simulation of a Polyunsaturated Lipid Bilayer Susceptible to Lipid Peroxidation. *Journal of Physical Chemistry B*, **2004**, 108, 7170-7179	3.4	116
196	Conical lipids in flat bilayers induce packing defects similar to that induced by positive curvature. *Biophysical Journal*, **2013**, 104, 585-93	2.9	112
195	Voltage-dependent insertion of alamethicin at phospholipid/water and octane/water interfaces. *Biophysical Journal*, **2001**, 80, 331-46	2.9	110
194	Computational and experimental approaches for investigating nanoparticle-based drug delivery systems. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1688-709	3.8	108
193	2H-NMR study and molecular dynamics simulation of the location, alignment, and mobility of pyrene in POPC bilayers. *Biophysical Journal*, **2005**, 88, 1818-27	2.9	108
192	Self-association of transmembrane alpha-helices in model membranes: importance of helix orientation and role of hydrophobic mismatch. *Journal of Biological Chemistry*, **2005**, 280, 39324-31	5.4	106
191	ATP-binding cassette transporters in Escherichia coli. *Biochimica Et Biophysica Acta - Biomembranes*, **2008**, 1778, 1757-71	3.8	102
190	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
189	Structures of neat and hydrated 1-octanol from computer simulations. *Journal of the American Chemical Society*, **2002**, 124, 15085-93	16.4	101
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185	Thermodynamics of flip-flop and desorption for a systematic series of phosphatidylcholine lipids. *Soft Matter*, **2009**, 5, 3295	3.6	97
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183	Exploring models of the influenza A M2 channel: MD simulations in a phospholipid bilayer. *Biophysical Journal*, **2000**, 78, 55-69	2.9	96
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180	The molecular mechanism of monolayer-bilayer transformations of lung surfactant from molecular dynamics simulations. *Biophysical Journal*, **2007**, 93, 3775-82	2.9	86

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176	Interactions of the designed antimicrobial peptide MB21 and truncated dermaseptin S3 with lipid bilayers: molecular-dynamics simulations. *Biochemical Journal*, **2003**, 370, 233-43	3.8	82
175	Water permeation through gramicidin A: desformylation and the double helix: a molecular dynamics study. *Biophysical Journal*, **2002**, 82, 2934-42	2.9	80
174	Microsecond molecular dynamics simulations of lipid mixing. *Langmuir*, **2014**, 30, 11993-2001	4	79
173	Molecular dynamics simulations of peptides from BPTI: a closer look at amide-aromatic interactions. *Journal of Biomolecular NMR*, **1996**, 8, 229-38	3	79
172	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
171	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
170	Conformational transitions induced by the binding of MgATP to the vitamin B12 ATP-binding cassette (ABC) transporter BtuCD. *Journal of Biological Chemistry*, **2004**, 279, 45013-9	5.4	76
169	Hydrophobicity scales: a thermodynamic looking glass into lipid-protein interactions. *Trends in Biochemical Sciences*, **2011**, 36, 653-62	10.3	74
168	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
167	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
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165	Surface binding of alamethicin stabilizes its helical structure: molecular dynamics simulations. *Biophysical Journal*, **1999**, 76, 3186-91	2.9	72
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163	Force fields for classical molecular dynamics. *Methods in Molecular Biology*, **2013**, 924, 197-213	1.4	69
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159	Direct simulation of protein-mediated vesicle fusion: lung surfactant protein B. *Biophysical Journal*, **2010**, 99, 2134-42	2.9	64
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157	A salt-bridge motif involved in ligand binding and large-scale domain motions of the maltose-binding protein. *Biophysical Journal*, **2005**, 89, 3362-71	2.9	61
156	Defining the transmembrane helix of M2 protein from influenza A by molecular dynamics simulations in a lipid bilayer. *Biophysical Journal*, **1999**, 76, 1886-96	2.9	61
155	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
154	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
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149	Opening and closing motions in the periplasmic vitamin B12 binding protein BtuF. *Biochemistry*, **2006**, 45, 13284-92	3.2	56
148	Membranes and water: an interesting relationship. *Faraday Discussions*, **1996**, 103, 191	3.6	55
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141	Orientation and interactions of dipolar molecules during transport through OmpF porin. *FEBS Letters*, **2002**, 528, 53-7	3.8	49
140	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
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137	Oleic acid phase behavior from molecular dynamics simulations. *Langmuir*, **2014**, 30, 10661-7	4	46
136	Lateral pressure profiles in lipid monolayers. *Faraday Discussions*, **2010**, 144, 393-409; discussion 445-81	3.6	46
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134	Improved Angle Potentials for Coarse-Grained Molecular Dynamics Simulations. *Journal of Chemical Theory and Computation*, **2013**, 9, 3282-92	6.4	45
133	Docking of mu-conotoxin GIIIA in the sodium channel outer vestibule. *Channels*, **2007**, 1, 344-52	3	45
132	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
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129	Structural basis for antibacterial peptide self-immunity by the bacterial ABC transporter McjD. *EMBO Journal*, **2017**, 36, 3062-3079	13	41
128	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
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124	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, 1501-10	2.9	39
123	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
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121	Pores formed by the nicotinic receptor m2delta Peptide: a molecular dynamics simulation study. *Biophysical Journal*, **2003**, 84, 14-27	2.9	38
120	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
119	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
118	Residue G346 in transmembrane segment six is involved in inter-domain communication in P-glycoprotein. *Biochemistry*, **2007**, 46, 9899-910	3.2	37
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114	Molecular dynamics simulations of antimicrobial peptides: From membrane binding to trans-membrane channels. *International Journal of Quantum Chemistry*, **2001**, 83, 166-179	2.1	36
113	Computer simulations of lung surfactant. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 2431-2440	3.6	35
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107	Cholesterol Flip-Flop in Heterogeneous Membranes. *Journal of Chemical Theory and Computation*, **2019**, 15, 2064-2070	6.4	32
106	Composition Fluctuations in Lipid Bilayers. *Biophysical Journal*, **2017**, 113, 2750-2761	2.9	31
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101	Curvature-Induced Sorting of Lipids in Plasma Membrane Tethers. *Advanced Theory and Simulations*, **2018**, 1, 1800034	3.5	28
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96	Molecular models of nanodiscs. *Journal of Chemical Theory and Computation*, **2015**, 11, 4923-32	6.4	24
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90	Orientation of ω-conotoxin PIIIA in a sodium channel vestibule, based on voltage dependence of its binding. *Molecular Pharmacology*, **2011**, 80, 219-27	4.3	22

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