List of Publications by Year in descending order

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216 papers	15,930 citations	10351 72 h-index	22102 113 g-index
228 all docs	228 docs citations	228 times ranked	15077 citing authors

#	Article	IF	Citations
1	Machine learning in the analysis of biomolecular simulations. Advances in Physics: X, 2022, 7, .	1.5	7
2	A cholesterol analog stabilizes the human Î² ₂ -adrenergic receptor nonlinearly with temperature. Science Signaling, 2022, 15, .	1.6	8
3	N-Glycosylation can selectively block or foster different receptorâ€“ligand binding modes. Scientific Reports, 2021, 11, 5239.	1.6	18
4	Martini 3: a general purpose force field for coarse-grained molecular dynamics. Nature Methods, 2021, 18, 382-388.	9.0	557
5	Seipin traps triacylglycerols to facilitate their nanoscale clustering in the endoplasmic reticulum membrane. PLoS Biology, 2021, 19, e3000998.	2.6	54
6	Complexity of seemingly simple lipid nanodiscs. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183420.	1.4	22
7	Cryo-EM structure of the complete and ligand-saturated insulin receptor ectodomain. Journal of Cell Biology, 2020, 219, .	2.3	84
8	Tail-Oxidized Cholesterol Enhances Membrane Permeability for Small Solutes. Langmuir, 2020, 36, 10438-10447.	1.6	24
9	Understanding the Functional Properties of Lipid Heterogeneity in Pulmonary Surfactant Monolayers at the Atomistic Level. Frontiers in Cell and Developmental Biology, 2020, 8, 581016.	1.8	18
10	Membrane-Dependent Binding and Entry Mechanism of Dopamine into Its Receptor. ACS Chemical Neuroscience, 2020, 11, 1914-1924.	1.7	21
11	Highâ€content imaging and structureâ€based predictions reveal functional differences between Niemannâ€Pick C1 variants. Traffic, 2020, 21, 386-397.	1.3	14
12	Pulmonary Surfactant Lipid Reorganization Induced by the Adsorption of the Oligomeric Surfactant Protein B Complex. Journal of Molecular Biology, 2020, 432, 3251-3268.	2.0	29
13	Crystalline Wax Esters Regulate the Evaporation Resistance of Tear Film Lipid Layers Associated with Dry Eye Syndrome. Journal of Physical Chemistry Letters, 2019, 10, 3893-3898.	2.1	17
14	An efficient auxin-inducible degron system with low basal degradation in human cells. Nature Methods, 2019, 16, 866-869.	9.0	117
15	The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers. Small, 2019, 15, e1805046.	5.2	35
16	Multiscale Simulations of Biological Membranes: The Challenge To Understand Biological Phenomena in a Living Substance. Chemical Reviews, 2019, 119, 5607-5774.	23.0	209
17	Understanding the Role of Lipids in Signaling Through Atomistic and Multiscale Simulations of Cell Membranes. Annual Review of Biophysics, 2019, 48, 421-439.	4.5	31
18	The Devil Is in the Details: What Do We Really Track in Single-Particle Tracking Experiments of Diffusion in Biological Membranes?. Journal of Physical Chemistry Letters, 2019, 10, 1005-1011.	2.1	13

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19	Bobbing of Oxysterols: Molecular Mechanism for Translocation of Tail-Oxidized Sterols through Biological Membranes. Journal of Physical Chemistry Letters, 2018, 9, 1118-1123.	2.1	24
20	Molecular mechanism for inhibition of twinfilin by phosphoinositides. Journal of Biological Chemistry, 2018, 293, 4818-4829.	1.6	15
21	How cardiolipin peroxidation alters the properties of the inner mitochondrial membrane?. Chemistry and Physics of Lipids, 2018, 214, 15-23.	1.5	35
22	Cholesterol Protects the Oxidized Lipid Bilayer from Water Injury: An All-Atom Molecular Dynamics Study. Journal of Membrane Biology, 2018, 251, 521-534.	1.0	12
23	Atomistic Model for Nearly Quantitative Simulations of Langmuir Monolayers. Langmuir, 2018, 34, 2565-2572.	1.6	53
24	Glucosylceramide modifies the LPS-induced inflammatory response in macrophages and the orientation of the LPS/TLR4 complex in silico. Scientific Reports, 2018, 8, 13600.	1.6	33
25	How to minimize dye-induced perturbations while studying biomembrane structure and dynamics: PEG linkers as a rational alternative. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 2436-2445.	1.4	31
26	Redox-coupled quinone dynamics in the respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E8413-E8420.	3.3	84
27	Negatively Charged Gangliosides Promote Membrane Association of Amphipathic Neurotransmitters. Neuroscience, 2018, 384, 214-223.	1.1	17
28	Quantitative Assessment of Methods Used To Obtain Rate Constants from Molecular Dynamics Simulationsâ€"Translocation of Cholesterol across Lipid Bilayers. Journal of Chemical Theory and Computation, 2018, 14, 3840-3848.	2.3	18
29	Long-chain GM1 gangliosides alter transmembrane domain registration through interdigitation. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 870-878.	1.4	20
30	Glycosylation and Lipids Working in Concert Direct CD2 Ectodomain Orientation and Presentation. Journal of Physical Chemistry Letters, 2017, 8, 1060-1066.	2.1	22
31	Effects of Membrane PEGylation on Entry and Location of Antifungal Drug Itraconazole and Their Pharmacological Implications. Molecular Pharmaceutics, 2017, 14, 1057-1070.	2.3	19
32	Calcium Assists Dopamine Release by Preventing Aggregation on the Inner Leaflet of Presynaptic Vesicles. ACS Chemical Neuroscience, 2017, 8, 1242-1250.	1.7	21
33	Calcium Directly Regulates Phosphatidylinositol 4,5-Bisphosphate Headgroup Conformation and Recognition. Journal of the American Chemical Society, 2017, 139, 4019-4024.	6.6	87
34	On Atomistic Models for Molecular Oxygen. Journal of Physical Chemistry B, 2017, 121, 518-528.	1.2	19
35	Mechanistic principles underlying regulation of the actin cytoskeleton by phosphoinositides. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E8977-E8986.	3.3	106
36	Diffusion of Integral Membrane Proteins in Protein-Rich Membranes. Journal of Physical Chemistry Letters, 2017, 8, 4308-4313.	2.1	65

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37	doGlycansâ€“Tools for Preparing Carbohydrate Structures for Atomistic Simulations of Glycoproteins, Glycolipids, and Carbohydrate Polymers for GROMACS. Journal of Chemical Information and Modeling, 2017, 57, 2401-2406.	2.5	71
38	Dynamics and energetics of the mammalian phosphatidylinositol transfer protein phospholipid exchange cycle. Journal of Biological Chemistry, 2017, 292, 14438-14455.	1.6	25
39	Nanoscale Membrane Domain Formation Driven by Cholesterol. Scientific Reports, 2017, 7, 1143.	1.6	83
40	The Integrin Receptor in Biologically Relevant Bilayers: Insights from Molecular Dynamics Simulations. Journal of Membrane Biology, 2017, 250, 337-351.	1.0	29
41	Phase Partitioning of GM1 and Its Bodipy-Labeled Analog Determine Their Different Binding to Cholera Toxin. Frontiers in Physiology, 2017, 8, 252.	1.3	34
42	Concerted regulation of npc2 binding to endosomal/lysosomal membranes by bis(monoacylglycero)phosphate and sphingomyelin. PLoS Computational Biology, 2017, 13, e1005831.	1.5	27
43	Excessive aggregation of membrane proteins in the Martini model. PLoS ONE, 2017, 12, e0187936.	1.1	147
44	The role of hydrophobic matching on transmembrane helix packing in cells. Cell Stress, 2017, 1, 90-106.	1.4	37
45	Selective effect of cell membrane on synaptic neurotransmission. Scientific Reports, 2016, 6, 19345.	1.6	48
46	Data including GROMACS input files for atomistic molecular dynamics simulations of mixed, asymmetric bilayers including molecular topologies, equilibrated structures, and force field for lipids compatible with OPLS-AA parameters. Data in Brief, 2016, 7, 1171-1174.	0.5	15
47	Atomistic determinants of co-enzyme Q reduction at the Qi-site of the cytochrome bc1 complex. Scientific Reports, 2016, 6, 33607.	1.6	23
48	Protein Crowding in Lipid Bilayers Gives Rise to Non-Gaussian Anomalous Lateral Diffusion of Phospholipids and Proteins. Physical Review X, 2016, 6, .	2.8	152
49	What Can We Learn about Cholesterolâ€™s Transmembrane Distribution Based on Cholesterol-Induced Changes in Membrane Dipole Potential?. Journal of Physical Chemistry Letters, 2016, 7, 4585-4590.	2.1	19
50	Lipid membranes: Theory and simulations bridged to experiments. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2251-2253.	1.4	12
51	Distribution and dynamics of quinones in the lipid bilayer mimicking the inner membrane of mitochondria. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2116-2122.	1.4	47
52	Interdigitation of long-chain sphingomyelin induces coupling of membrane leaflets in a cholesterol dependent manner. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 281-288.	1.4	76
53	Role of charged lipids in membrane structures â€” Insight given by simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2322-2333.	1.4	63
54	Cholesterol oxidation products and their biological importance. Chemistry and Physics of Lipids, 2016, 199, 144-160.	1.5	130

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55	Mechanism of allosteric regulation of Î²2-adrenergic receptor by cholesterol. ELife, 2016, 5, .	2.8	115
56	Building Synthetic Sterols Computationally â€“ Unlocking the Secrets of Evolution?. Frontiers in Bioengineering and Biotechnology, 2015, 3, 121.	2.0	5
57	PEGylated Liposomes as Carriers of Hydrophobic Porphyrins. Journal of Physical Chemistry B, 2015, 119, 6646-6657.	1.2	47
58	Cholesterol under oxidative stressâ€"How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols. Free Radical Biology and Medicine, 2015, 84, 30-41.	1.3	57
59	How Well Does BODIPY-Cholesteryl Ester Mimic Unlabeled Cholesteryl Esters in High Density Lipoprotein Particles?. Journal of Physical Chemistry B, 2015, 119, 15848-15856.	1.2	4
60	Proton-coupled electron transfer and the role of water molecules in proton pumping by cytochrome c oxidase. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 2040-2045.	3.3	59
61	Biogenesis of Nascent High Density Lipoprotein Particles. Structure, 2015, 23, 1153-1154.	1.6	3
62	How To Minimize Artifacts in Atomistic Simulations of Membrane Proteins, Whose Crystal Structure Is Heavily Engineered: Î²₂-Adrenergic Receptor in the Spotlight. Journal of Chemical Theory and Computation, 2015, 11, 3432-3445.	2.3	16
63	Oxidation of Cholesterol Does Not Alter Significantly Its Uptake into High-Density Lipoprotein Particles. Journal of Physical Chemistry B, 2015, 119, 4594-4600.	1.2	6
64	Role of subunit III and its lipids in the molecular mechanism of cytochrome c oxidase. Biochimica Et Biophysica Acta - Bioenergetics, 2015, 1847, 690-697.	0.5	24
65	Sec14-nodulin proteins and the patterning of phosphoinositide landmarks for developmental control of membrane morphogenesis. Molecular Biology of the Cell, 2015, 26, 1764-1781.	0.9	44
66	N -Glycosylation as determinant of epidermal growth factor receptor conformation in membranes. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 4334-4339.	3.3	135
67	PIP2 and Talin Join Forces to Activate Integrin. Journal of Physical Chemistry B, 2015, 119, 12381-12389.	1.2	27
68	Redox-induced activation of the proton pump in the respiratory complex I. Proceedings of the National Academy of Sciences of the United States of America, 2015, 112, 11571-11576.	3.3	122
69	How endoglucanase enzymes act on cellulose nanofibrils: role of amorphous regions revealed by atomistic simulations. Cellulose, 2015, 22, 2911-2925.	2.4	20
70	Experimental determination and computational interpretation of biophysical properties of lipid bilayers enriched by cholesteryl hemisuccinate. Biochimica Et Biophysica Acta - Biomembranes, 2015, 1848, 422-432.	1.4	45
71	Enzymatic Oxidation of Cholesterol: Properties and Functional Effects of Cholestenone in Cell Membranes. PLoS ONE, 2014, 9, e103743.	1.1	50
72	Co-Exposure with Fullerene May Strengthen Health Effects of Organic Industrial Chemicals. PLoS ONE, 2014, 9, e114490.	1.1	9

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73	How Anacetrapib Inhibits the Activity of the Cholesteryl Ester Transfer Protein? Perspective through Atomistic Simulations. PLoS Computational Biology, 2014, 10, e1003987.	1.5	17
74	The challenges of understanding glycolipid functions: An open outlook based on molecular simulations. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2014, 1841, 1130-1145.	1.2	35
75	Effect of PEGylation on Drug Entry into Lipid Bilayer. Journal of Physical Chemistry B, 2014, 118, 144-151.	1.2	26
76	How well does cholesteryl hemisuccinate mimic cholesterol in saturated phospholipid bilayers?. Journal of Molecular Modeling, 2014, 20, 2121.	0.8	44
77	How to link pyrene to its host lipid to minimize the extent of membrane perturbations and to optimize pyrene dimer formation. Chemistry and Physics of Lipids, 2014, 177, 19-25.	1.5	7
78	Cholesterol, sphingolipids, and glycolipids: What do we know about their role in raft-like membranes?. Chemistry and Physics of Lipids, 2014, 184, 82-104.	1.5	159
79	Cationic Au Nanoparticle Binding with Plasma Membrane-like Lipid Bilayers: Potential Mechanism for Spontaneous Permeation to Cells Revealed by Atomistic Simulations. Journal of Physical Chemistry C, 2014, 118, 11131-11141.	1.5	69
80	How To Tackle the Issues in Free Energy Simulations of Long Amphiphiles Interacting with Lipid Membranes: Convergence and Local Membrane Deformations. Journal of Physical Chemistry B, 2014, 118, 3572-3581.	1.2	61
81	Atomistic simulations of anionic Au144(SR)60 nanoparticles interacting with asymmetric model lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2852-2860.	1.4	46
82	Refined OPLS All-Atom Force Field for Saturated Phosphatidylcholine Bilayers at Full Hydration. Journal of Physical Chemistry B, 2014, 118, 4571-4581.	1.2	139
83	Can pyrene probes be used to measure lateral pressure profiles of lipid membranes? Perspective through atomistic simulations. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 1406-1411.	1.4	16
84	Modeling of Lipid Membranes and Lipoproteins. , 2014, , 299-318.		2
85	Parameterization of the prosthetic redox centers of the bacterial cytochrome bc 1 complex for atomistic molecular dynamics simulations. Theoretical Chemistry Accounts, 2013, 132, 1.	0.5	16
86	Key role of water in proton transfer at the Qo-site of the cytochrome bc1 complex predicted by atomistic molecular dynamics simulations. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 761-768.	0.5	39
87	Anomalous and normal diffusion of proteins and lipids in crowded lipid membranes. Faraday Discussions, 2013, 161, 397-417.	1.6	170
88	Atomistic simulations indicate cardiolipin to have an integral role in the structure of the cytochrome bc1 complex. Biochimica Et Biophysica Acta - Bioenergetics, 2013, 1827, 769-778.	0.5	54
89	Molecular lipidomics of exosomes released by PC-3 prostate cancer cells. Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids, 2013, 1831, 1302-1309.	1.2	546
90	Do Lipids Retard the Evaporation of the Tear Fluid?. , 2012, 53, 6442.		49

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91	Interfacial Tension and Surface Pressure of High Density Lipoprotein, LowÂDensity Lipoprotein, and Related Lipid Droplets. Biophysical Journal, 2012, 103, 1236-1244.	0.2	42
92	Mechanism for translocation of fluoroquinolones across lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2563-2571.	1.4	76
93	Role of Neutral Lipids in Tear Fluid Lipid Layer: Coarse-Grained Simulation Study. Langmuir, 2012, 28, 17092-17100.	1.6	27
94	The impact of lipid composition on the stability of the tear fluid lipid layer. Soft Matter, 2012, 8, 5826.	1.2	40
95	Interaction of Hematoporphyrin with Lipid Membranes. Journal of Physical Chemistry B, 2012, 116, 4889-4897.	1.2	36
96	Interaction of C70 fullerene with the Kv1.2 potassium channel. Physical Chemistry Chemical Physics, 2012, 14, 12526.	1.3	17
97	Strong preferences of dopamine and <scp>l</scp>â€dopa towards lipid head group: importance of lipid composition and implication for neurotransmitter metabolism. Journal of Neurochemistry, 2012, 122, 681-690.	2.1	51
98	Cationic Dimyristoylphosphatidylcholine and Dioleoyloxytrimethylammonium Propane Lipid Bilayers: Atomistic Insight for Structure and Dynamics. Journal of Physical Chemistry B, 2012, 116, 269-276.	1.2	25
99	Atomistic Simulations of Functional Au₁₄₄(SR)₆₀ Gold Nanoparticles in Aqueous Environment. Journal of Physical Chemistry C, 2012, 116, 9805-9815.	1.5	94
100	Revealing structural and dynamical properties of high density lipoproteins through molecular simulations. Soft Matter, 2012, 8, 1262-1267.	1.2	11
101	Lipid Exchange Mechanism of the Cholesteryl Ester Transfer Protein Clarified by Atomistic and Coarse-grained Simulations. PLoS Computational Biology, 2012, 8, e1002299.	1.5	49
102	Drug-Lipid Membrane Interaction Mechanisms Revealed Through Molecular Simulations. Current Physical Chemistry, 2012, 2, 379-400.	0.1	13
103	Effect of Galactosylceramide on the Dynamics of Cholesterol-Rich Lipid Membranes. Journal of Physical Chemistry B, 2011, 115, 14424-14434.	1.2	17
104	Properties of the Membrane Binding Component of Catechol-O-methyltransferase Revealed by Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 13541-13550.	1.2	15
105	Protein Shape Change Has a Major Effect on the Gating Energy of a Mechanosensitive Channel. Biophysical Journal, 2011, 100, 1651-1659.	0.2	48
106	Analysis of Twisting of Cellulose Nanofibrils in Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 3747-3755.	1.2	129
107	Low density lipoprotein: structure, dynamics, and interactions of apoB-100 with lipids. Soft Matter, 2011, 7, 8135.	1.2	47
108	A MARTINI Coarse-Grained Model of a Thermoset Polyester Coating. Macromolecules, 2011, 44, 6198-6208.	2.2	66

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109	N- and O-methylation of sphingomyelin markedly affects its membrane properties and interactions with cholesterol. Biochimica Et Biophysica Acta - Biomembranes, 2011, 1808, 1179-1186.	1.4	35
110	Lipid Simulations: A Perspective on Lipids in Action. Cold Spring Harbor Perspectives in Biology, 2011, 3, a004655-a004655.	2.3	35
111	Coarse-graining polymers with the MARTINI force-field: polystyrene as a benchmark case. Soft Matter, 2011, 7, 698-708.	1.2	216
112	Cholesterol modulates glycolipid conformation and receptor activity. Nature Chemical Biology, 2011, 7, 260-262.	3.9	194
113	Lessons from the biophysics of interfaces: Lung surfactant and tear fluid. Progress in Retinal and Eye Research, 2011, 30, 204-215.	7.3	46
114	Lateral sorting in model membranes by cholesterol-mediated hydrophobic matching. Proceedings of the National Academy of Sciences of the United States of America, 2011, 108, 16628-16633.	3.3	131
115	Association of Lipidome Remodeling in the Adipocyte Membrane with Acquired Obesity in Humans. PLoS Biology, 2011, 9, e1000623.	2.6	213
116	High Density Lipoprotein Structural Changes and Drug Response in Lipidomic Profiles following the Long-Term Fenofibrate Therapy in the FIELD Substudy. PLoS ONE, 2011, 6, e23589.	1.1	33
117	Defect-Mediated Trafficking across Cell Membranes: Insights from in Silico Modeling. Chemical Reviews, 2010, 110, 6077-6103.	23.0	171
118	Molecular Dynamics Simulations Reveal Fundamental Role of Water As Factor Determining Affinity of Binding of Î²-Blocker Nebivolol to Î²2-Adrenergic Receptor. Journal of Physical Chemistry B, 2010, 114, 8374-8386.	1.2	35
119	Role of Lipids in Spheroidal High Density Lipoproteins. PLoS Computational Biology, 2010, 6, e1000964.	1.5	81
120	Composition and lipid spatial distribution of HDL particles in subjects with low and high HDL-cholesterol. Journal of Lipid Research, 2010, 51, 2341-2351.	2.0	111
121	Free Volume Theory Applied to Lateral Diffusion in Langmuir Monolayers: Atomistic Simulations for a Protein-Free Model of Lung Surfactant. Langmuir, 2010, 26, 15436-15444.	1.6	42
122	Molecular Organization of the Tear Fluid Lipid Layer. Biophysical Journal, 2010, 99, 2559-2567.	0.2	67
123	Role of Glycolipids in Lipid Rafts: A View through Atomistic Molecular Dynamics Simulations with Galactosylceramide. Journal of Physical Chemistry B, 2010, 114, 7797-7807.	1.2	60
124	Effects of DPH on DPPCâ"Cholesterol Membranes with Varying Concentrations of Cholesterol: From Local Perturbations to Limitations in Fluorescence Anisotropy Experiments. Journal of Physical Chemistry B, 2010, 114, 2704-2711.	1.2	39
125	The hydrophobic effect and its role in cold denaturation. Cryobiology, 2010, 60, 91-99.	0.3	164
126	Reply to the comment by Graziano on â€œThe hydrophobic effect and its role in cold denaturationâ€• Cryobiology, 2010, 60, 356-357.	0.3	1

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127	Temperature-induced structural transition in-situ in porcine lens â€" Changes observed in void size distribution. Biochimica Et Biophysica Acta - Biomembranes, 2010, 1798, 958-965.	1.4	12
128	Membrane Proteins Diffuse as Dynamic Complexes with Lipids. Journal of the American Chemical Society, 2010, 132, 7574-7575.	6.6	157
129	Effect of Sphingomyelin Headgroup Size on Molecular Properties andÂInteractions with Cholesterol. Biophysical Journal, 2010, 99, 3300-3308.	0.2	75
130	Concerted diffusion of lipids in raft-like membranes. Faraday Discussions, 2010, 144, 411-430.	1.6	92
131	Cholesterol Induces Specific Spatial and Orientational Order in Cholesterol/Phospholipid Membranes. PLoS ONE, 2010, 5, e11162.	1.1	101
132	Calculation of the electrostatic potential of lipid bilayers from molecular dynamics simulations: Methodological issues. Journal of Chemical Physics, 2009, 130, 215107.	1.2	63
133	Desipramine induces disorder in cholesterol-rich membranes: implications for viral trafficking. Physical Biology, 2009, 6, 046004.	0.8	10
134	Conformational Changes and Slow Dynamics through Microsecond Polarized Atomistic Molecular Simulation of an Integral Kv1.2 Ion Channel. PLoS Computational Biology, 2009, 5, e1000289.	1.5	108
135	Systematic coarse graining from structure using internal states: Application to phospholipid/cholesterol bilayer. Journal of Chemical Physics, 2009, 131, 055101.	1.2	51
136	Effects of carbon nanoparticles on lipid membranes: a molecular simulation perspective. Soft Matter, 2009, 5, 4433.	1.2	116
137	Mitochondrial Membranes with Mono- and Divalent Salt: Changes Induced by Salt Ions on Structure and Dynamics. Journal of Physical Chemistry B, 2009, 113, 15513-15521.	1.2	41
138	Why is the sn-2 Chain of Monounsaturated Glycerophospholipids Usually Unsaturated whereas the sn-1 Chain Is Saturated? Studies of 1-Stearoyl-2-oleoyl-sn-glycero-3-phosphatidylcholine (SOPC) and 1-Oleoyl-2-stearoyl-sn-glycero-3-phosphatidylcholine (OSPC) Membranes with and without Cholesterol. Journal of Physical Chemistry B, 2009, 113, 8347-8356.	1.2	22
139	Probing Biomembranes with Positrons. Journal of Physical Chemistry B, 2009, 113, 1810-1812.	1.2	31
140	Ion Dynamics in Cationic Lipid Bilayer Systems in Saline Solutions. Journal of Physical Chemistry B, 2009, 113, 9226-9234.	1.2	38
141	Atom-scale molecular interactions in lipid raft mixtures. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 122-135.	1.4	74
142	Ordering effects of cholesterol and its analogues. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 97-121.	1.4	506
143	Ceramide-1-Phosphate, in Contrast to Ceramide, Is Not Segregated into Lateral Lipid Domains in Phosphatidylcholine Bilayers. Biophysical Journal, 2009, 96, 2216-2226.	0.2	21
144	Atomistic Simulations of Phosphatidylcholines and Cholesteryl Esters in High-Density Lipoprotein-Sized Lipid Droplet and Trilayer: Clues to Cholesteryl Ester Transport and Storage. Biophysical Journal, 2009, 96, 4099-4108.	0.2	33

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145	Intrinsic Potential of Cell Membranes: Opposite Effects of Lipid Transmembrane Asymmetry and Asymmetric Salt Ion Distribution. Journal of Physical Chemistry B, 2009, 113, 7194-7198.	1.2	23
146	Collective Dynamics in Lipid Membranes: From Pore Formation to Flip-Flops. , 2009, , 121-139.		3
147	Asymmetric nature of lateral pressure profiles in supported lipid membranes and its implications for membrane protein functions. Soft Matter, 2009, 5, 3258.	1.2	32
148	Multiscale modeling of emergent materials: biological and soft matter. Physical Chemistry Chemical Physics, 2009, 11, 1869.	1.3	243
149	3D Pressure Field in Lipid Membranes and Membrane-Protein Complexes. Physical Review Letters, 2009, 102, 078101.	2.9	180
150	Role of Cardiolipins in the Inner Mitochondrial Membrane: Insight Gained through Atom-Scale Simulations. Journal of Physical Chemistry B, 2009, 113, 3413-3422.	1.2	62
151	Visualization of Complex Processes in Lipid Systems Using Computer Simulations and Molecular Graphics. , 2009, 580, 317-338.		0
152	Realâ€Time Translocation of Fullerene Reveals Cell Contraction. Small, 2008, 4, 1986-1992.	5.2	43
153	BODIPYâ€Cholesterol: A New Tool to Visualize Sterol Trafficking in Living Cells and Organisms. Traffic, 2008, 9, 1839-1849.	1.3	221
154	Strain hardening, avalanches, and strain softening in dense cross-linked actin networks. Physical Review E, 2008, 77, 051913.	0.8	56
155	Complexes Comprised of Charged Dendrimers, Linear Polyelectrolytes, and Counterions: Insight through Coarse-Grained Molecular Dynamics Simulations. Macromolecules, 2008, 41, 4961-4968.	2.2	48
156	Structure of Spheroidal HDL Particles Revealed by Combined Atomistic and Coarse-Grained Simulations. Biophysical Journal, 2008, 94, 2306-2319.	0.2	80
157	Interplay of Unsaturated Phospholipids and Cholesterol in Membranes: Effect of the Double-Bond Position. Biophysical Journal, 2008, 95, 3295-3305.	0.2	132
158	Influence of Ethanol on Lipid Membranes:â€‰ From Lateral Pressure Profiles to Dynamics and Partitioning. Journal of Physical Chemistry B, 2008, 112, 4131-4139.	1.2	94
159	Lateral Diffusion in Lipid Membranes through Collective Flows. Journal of the American Chemical Society, 2008, 130, 44-45.	6.6	145
160	Microscopic Mechanism for Cold Denaturation. Physical Review Letters, 2008, 100, 118101.	2.9	114
161	Chapter 2 Electrostatics in Biomolecular Simulations: Where Are We Now and Where Are We Heading?. Current Topics in Membranes, 2008, 60, 49-89.	0.5	62
162	Role of phosphatidylglycerols in the stability of bacterial membranes. Biochimie, 2008, 90, 930-938.	1.3	106

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163	Membrane Potential and Electrostatics of Phospholipid Bilayers with Asymmetric Transmembrane Distribution of Anionic Lipids. Journal of Physical Chemistry B, 2008, 112, 4629-4634.	1.2	88
164	Modeling of the Triglyceride-Rich Core in Lipoprotein Particles. Journal of Physical Chemistry B, 2008, 112, 13772-13782.	1.2	50
165	Replacing the Cholesterol Hydroxyl Group with the Ketone Group Facilitates Sterol Flip-Flop and Promotes Membrane Fluidity. Journal of Physical Chemistry B, 2008, 112, 1946-1952.	1.2	74
166	Comparison of cholesterol and its direct precursors along the biosynthetic pathway: Effects of cholesterol, desmosterol and 7-dehydrocholesterol on saturated and unsaturated lipid bilayers. Journal of Chemical Physics, 2008, 129, 154508.	1.2	42
167	Significance of Cholesterol Methyl Groups. Journal of Physical Chemistry B, 2008, 112, 2922-2929.	1.2	54
168	Effect of NaCl and KCl on Phosphatidylcholine and Phosphatidylethanolamine Lipid Membranes:â€‰ Insight from Atomic-Scale Simulations for Understanding Salt-Induced Effects in the Plasma Membrane. Journal of Physical Chemistry B, 2008, 112, 1953-1962.	1.2	227
169	Influence ofcisdouble-bond parametrization on lipid membrane properties: How seemingly insignificant details in force-field change even qualitative trends. Journal of Chemical Physics, 2008, 129, 105103.	1.2	49
170	Systematic Approach to Coarse-Graining of Molecular Descriptions and Interactions with Applications to Lipid Membranes. , 2008, , 83-106.		1
171	Conformational analysis of lipid molecules by self-organizing maps. Journal of Chemical Physics, 2007, 126, 054707.	1.2	17
172	Coarse-grained model for phospholipid/cholesterol bilayer employing inverse Monte Carlo with thermodynamic constraints. Journal of Chemical Physics, 2007, 126, 075101.	1.2	63
173	Assessing the Nature of Lipid Raft Membranes. PLoS Computational Biology, 2007, 3, e34.	1.5	257
174	Reptational dynamics in dissipative particle dynamics simulations of polymer melts. Physical Review E, 2007, 75, 036713.	0.8	122
175	Role of sterol type on lateral pressure profiles of lipid membranes affecting membrane protein functionality: Comparison between cholesterol, desmosterol, 7-dehydrocholesterol and ketosterol. Journal of Structural Biology, 2007, 159, 311-323.	1.3	117
176	Polyunsaturation in Lipid Membranes:â€‰ Dynamic Properties and Lateral Pressure Profiles. Journal of Physical Chemistry B, 2007, 111, 3139-3150.	1.2	180
177	Effect of Double Bond Position on Lipid Bilayer Properties:â€‰ Insight through Atomistic Simulations. Journal of Physical Chemistry B, 2007, 111, 11162-11168.	1.2	65
178	Atomic-Scale Structure and Electrostatics of Anionic Palmitoyloleoylphosphatidylglycerol Lipid Bilayers with Na+ Counterions. Biophysical Journal, 2007, 92, 1114-1124.	0.2	178
179	Insight into the Putative Specific Interactions between Cholesterol, Sphingomyelin, and Palmitoyl-Oleoyl Phosphatidylcholine. Biophysical Journal, 2007, 92, 1125-1137.	0.2	122
180	Ion Leakage through Transient Water Pores in Protein-Free Lipid Membranes Driven by Transmembrane Ionic Charge Imbalance. Biophysical Journal, 2007, 92, 1878-1890.	0.2	108

#	Article	IF	Citations
181	What Happens if Cholesterol Is Made Smoother. Biophysical Journal, 2007, 92, 3346-3357.	0.2	99
182	Glycolipid Membranes through Atomistic Simulations:â€‰ Effect of Glucose and Galactose Head Groups on Lipid Bilayer Properties. Journal of Physical Chemistry B, 2007, 111, 10146-10154.	1.2	61
183	Free Pyrene Probes in Gel and Fluid Membranes:â€‰ Perspective through Atomistic Simulations. Journal of Physical Chemistry B, 2007, 111, 3640-3650.	1.2	54
184	Lipid Transmembrane Asymmetry and Intrinsic Membrane Potential:Â Two Sides of the Same Coin. Journal of the American Chemical Society, 2007, 129, 5358-5359.	6.6	83
185	Molecular Mechanism for Lipid Flip-Flops. Journal of Physical Chemistry B, 2007, 111, 13554-13559.	1.2	125
186	Long-range interactions and parallel scalability in molecular simulations. Computer Physics Communications, 2007, 176, 14-22.	3.0	39
187	Effect of replacement of cholesterol hydroxyl group by ketone group. Chemistry and Physics of Lipids, 2007, 149, S41-S42.	1.5	0
188	Under the Influence of Alcohol: The Effect of Ethanol and Methanol on Lipid Bilayers. Biophysical Journal, 2006, 90, 1121-1135.	0.2	321
189	Influence of Chain Length and Unsaturation on Sphingomyelin Bilayers. Biophysical Journal, 2006, 90, 851-863.	0.2	116
190	Atomistic Simulation Studies of Cholesteryl Oleates: Model for the Core of Lipoprotein Particles. Biophysical Journal, 2006, 90, 2247-2257.	0.2	23
191	Interaction of Fusidic Acid with Lipid Membranes: Implications to the Mechanism of Antibiotic Activity. Biophysical Journal, 2006, 91, 1787-1799.	0.2	23
192	Tilt:Â Major Factor in Sterols' Ordering Capability in Membranes. Journal of Physical Chemistry B, 2006, 110, 25562-25564.	1.2	118
193	Influence of Pyrene-Labeling on Fluid Lipid Membranes. Journal of Physical Chemistry B, 2006, 110, 15403-15410.	1.2	66
194	Significance of Sterol Structural Specificity. Journal of Biological Chemistry, 2006, 281, 348-355.	1.6	121
195	Molecular dynamics study of charged dendrimers in salt-free solution: Effect of counterions. Journal of Chemical Physics, 2006, 124, 094904.	1.2	73
196	Transient Ordered Domains in Single-Component Phospholipid Bilayers. Physical Review Letters, 2006, 97, 238102.	2.9	40
197	Structural effects of small molecules on phospholipid bilayers investigated by molecular simulations. Fluid Phase Equilibria, 2005, 228-229, 135-140.	1.4	20
198	Influence of DPH on the Structure and Dynamics of a DPPC Bilayer. Biophysical Journal, 2005, 88, 3398-3410.	0.2	110

#	Article	IF	Citations
199	Response to Comment by Almeida et al.: Free Area Theories for Lipid Bilayersâ€"Predictive or Not?. Biophysical Journal, 2005, 89, 745-752.	0.2	33
200	Effect of Monovalent Salt on Cationic Lipid Membranes As Revealed by Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2005, 109, 21126-21134.	1.2	67
201	Pore Formation Coupled to Ion Transport through Lipid Membranes as Induced by Transmembrane Ionic Charge Imbalance:â€‰ Atomistic Molecular Dynamics Study. Journal of the American Chemical Society, 2005, 127, 17570-17571.	6.6	190
202	Diffusion in Membranes. , 2005, , 471-509.		15
203	Exploring the effect of xenon on biomembranes. Cellular and Molecular Biology Letters, 2005, 10, 563-9.	2.7	21
204	Modeling glycolipids: take one. Cellular and Molecular Biology Letters, 2005, 10, 625-30.	2.7	13
205	Modeling Lipidâ€"Sterol Bilayers: Applications to Structural Evolution, Lateral Diffusion, and Rafts. Methods in Enzymology, 2004, 383, 198-229.	0.4	25
206	Structural effects of small molecules on phospholipid bilayers investigated by molecular simulations. Fluid Phase Equilibria, 2004, 225, 63-68.	1.4	39
207	Distribution, Orientation, and Dynamics of DPH Probes in DPPC Bilayer. Journal of Physical Chemistry B, 2004, 108, 13438-13448.	1.2	91
208	Coarse-grained model for phospholipid/cholesterol bilayer. Journal of Chemical Physics, 2004, 121, 9156-9165.	1.2	125
209	Impact of cholesterol on voids in phospholipid membranes. Journal of Chemical Physics, 2004, 121, 12676.	1.2	94
210	Lessons of Slicing Membranes: Interplay of Packing, Free Area, and Lateral Diffusion in Phospholipid/Cholesterol Bilayers. Biophysical Journal, 2004, 87, 1076-1091.	0.2	265
211	Lipid Bilayers Driven to a Wrong Lane in Molecular Dynamics Simulations by Subtle Changes in Long-Range Electrostatic Interactions. Journal of Physical Chemistry B, 2004, 108, 4485-4494.	1.2	196
212	Cationic DMPC/DMTAP Lipid Bilayers: Molecular Dynamics Study. Biophysical Journal, 2004, 86, 3461-3472.	0.2	156
213	Structure and Dynamics of Sphingomyelin Bilayer: Insight Gained through Systematic Comparison to Phosphatidylcholine. Biophysical Journal, 2004, 87, 2976-2989.	0.2	141
214	On Coarse-Graining by the Inverse Monte Carlo Method: Dissipative Particle Dynamics Simulations Made to a Precise Tool in Soft Matter Modeling. Soft Materials, 2002, 1, 121-137.	0.8	78
215	SoftSimu2002 - Novel Methods in Soft Matter Simulations. Applied Rheology, 2002, 12, 200-201.	3.5	0
216	Towards better integrators for dissipative particle dynamics simulations. Physical Review E, 2000, 62, R7611-R7614.	0.8	110