

Ilpo Tapio Vattulainen

List of Publications by Year in descending order

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Version: 2024-02-01

227
papers

15,755
citations

13332

70
h-index

26792

111
g-index

247
all docs

247
docs citations

247
times ranked

17229
citing authors

#	ARTICLE	IF	CITATIONS
1	Machine learning in the analysis of biomolecular simulations. <i>Advances in Physics: X</i> , 2022, 7, .	1.5	7
2	Dimerization of the pulmonary surfactant protein C in a membrane environment. <i>PLoS ONE</i> , 2022, 17, e0267155.	1.1	5
3	Maturation of the SARS-CoV-2 virus is regulated by dimerization of its main protease. <i>Computational and Structural Biotechnology Journal</i> , 2022, 20, 3336-3346.	1.9	5
4	A cholesterol analog stabilizes the human β_2 -adrenergic receptor nonlinearly with temperature. <i>Science Signaling</i> , 2022, 15, .	1.6	8
5	Antidepressant drugs act by directly binding to TRKB neurotrophin receptors. <i>Cell</i> , 2021, 184, 1299-1313.e19.	13.5	347
6	N-Glycosylation can selectively block or foster different receptor–ligand binding modes. <i>Scientific Reports</i> , 2021, 11, 5239.	1.6	18
7	Martini 3: a general purpose force field for coarse-grained molecular dynamics. <i>Nature Methods</i> , 2021, 18, 382-388.	9.0	557
8	Cholesterol–recognition motifs in the transmembrane domain of the tyrosine kinase receptor family: The case of TRKB. <i>European Journal of Neuroscience</i> , 2021, 53, 3311-3322.	1.2	15
9	Seipin traps triacylglycerols to facilitate their nanoscale clustering in the endoplasmic reticulum membrane. <i>PLoS Biology</i> , 2021, 19, e3000998.	2.6	54
10	SHANK3 conformation regulates direct actin binding and crosstalk with Rap1 signaling. <i>Current Biology</i> , 2021, 31, 4956-4970.e9.	1.8	14
11	The F1 loop of the talin head domain acts as a gatekeeper in integrin activation and clustering. <i>Journal of Cell Science</i> , 2020, 133, .	1.2	18
12	Complexity of seemingly simple lipid nanodiscs. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2020, 1862, 183420.	1.4	22
13	Cryo-EM structure of the complete and ligand-saturated insulin receptor ectodomain. <i>Journal of Cell Biology</i> , 2020, 219, .	2.3	84
14	Tail-Oxidized Cholesterol Enhances Membrane Permeability for Small Solutes. <i>Langmuir</i> , 2020, 36, 10438-10447.	1.6	24
15	Understanding the Functional Properties of Lipid Heterogeneity in Pulmonary Surfactant Monolayers at the Atomistic Level. <i>Frontiers in Cell and Developmental Biology</i> , 2020, 8, 581016.	1.8	18
16	Membrane-Dependent Binding and Entry Mechanism of Dopamine into Its Receptor. <i>ACS Chemical Neuroscience</i> , 2020, 11, 1914-1924.	1.7	21
17	High-content imaging and structure-based predictions reveal functional differences between Niemann–Pick C1 variants. <i>Traffic</i> , 2020, 21, 386-397.	1.3	14
18	The Na,K-ATPase acts upstream of phosphoinositide PI(4,5)P2 facilitating unconventional secretion of Fibroblast Growth Factor 2. <i>Communications Biology</i> , 2020, 3, 141.	2.0	21

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19	Pulmonary Surfactant Lipid Reorganization Induced by the Adsorption of the Oligomeric Surfactant Protein B Complex. <i>Journal of Molecular Biology</i> , 2020, 432, 3251-3268.	2.0	29
20	Cryo-EM, X-ray diffraction, and atomistic simulations reveal determinants for the formation of a supramolecular myelin-like proteolipid lattice. <i>Journal of Biological Chemistry</i> , 2020, 295, 8692-8705.	1.6	15
21	Mechanism of homodimeric cytokine receptor activation and dysregulation by oncogenic mutations. <i>Science</i> , 2020, 367, 643-652.	6.0	123
22	Crystalline Wax Esters Regulate the Evaporation Resistance of Tear Film Lipid Layers Associated with Dry Eye Syndrome. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 3893-3898.	2.1	17
23	An efficient auxin-inducible degron system with low basal degradation in human cells. <i>Nature Methods</i> , 2019, 16, 866-869.	9.0	117
24	Nanoparticle-Membrane Interactions: The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers (Small 23/2019). <i>Small</i> , 2019, 15, 1970124.	5.2	8
25	Reduced level of docosahexaenoic acid shifts GPCR neuroreceptors to less ordered membrane regions. <i>PLoS Computational Biology</i> , 2019, 15, e1007033.	1.5	25
26	The Role of Temperature and Lipid Charge on Intake/Uptake of Cationic Gold Nanoparticles into Lipid Bilayers. <i>Small</i> , 2019, 15, e1805046.	5.2	35
27	Multiscale Simulations of Biological Membranes: The Challenge To Understand Biological Phenomena in a Living Substance. <i>Chemical Reviews</i> , 2019, 119, 5607-5774.	23.0	209
28	Understanding the Role of Lipids in Signaling Through Atomistic and Multiscale Simulations of Cell Membranes. <i>Annual Review of Biophysics</i> , 2019, 48, 421-439.	4.5	31
29	The Devil Is in the Details: What Do We Really Track in Single-Particle Tracking Experiments of Diffusion in Biological Membranes?. <i>Journal of Physical Chemistry Letters</i> , 2019, 10, 1005-1011.	2.1	13
30	Mechanism of synergistic actin filament pointed end depolymerization by cyclase-associated protein and cofilin. <i>Nature Communications</i> , 2019, 10, 5320.	5.8	76
31	New Paradigms for the Mechanisms of Thrombopoietin Receptor Activation and Dysregulation By the JAK2V617F Mutation. <i>Blood</i> , 2019, 134, 2962-2962.	0.6	0
32	Bobbing of Oxysterols: Molecular Mechanism for Translocation of Tail-Oxidized Sterols through Biological Membranes. <i>Journal of Physical Chemistry Letters</i> , 2018, 9, 1118-1123.	2.1	24
33	Molecular mechanism for inhibition of twinfilin by phosphoinositides. <i>Journal of Biological Chemistry</i> , 2018, 293, 4818-4829.	1.6	15
34	How cardiolipin peroxidation alters the properties of the inner mitochondrial membrane?. <i>Chemistry and Physics of Lipids</i> , 2018, 214, 15-23.	1.5	35
35	Cholesterol Protects the Oxidized Lipid Bilayer from Water Injury: An All-Atom Molecular Dynamics Study. <i>Journal of Membrane Biology</i> , 2018, 251, 521-534.	1.0	12
36	Atomistic Model for Nearly Quantitative Simulations of Langmuir Monolayers. <i>Langmuir</i> , 2018, 34, 2565-2572.	1.6	53

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37	Assessment of mutation probabilities of KRAS G12 missense mutants and their long-timescale dynamics by atomistic molecular simulations and Markov state modeling. <i>PLoS Computational Biology</i> , 2018, 14, e1006458.	1.5	59
38	Glucosylceramide modifies the LPS-induced inflammatory response in macrophages and the orientation of the LPS/TLR4 complex in silico. <i>Scientific Reports</i> , 2018, 8, 13600.	1.6	33
39	Structural basis of actin monomer re-charging by cyclase-associated protein. <i>Nature Communications</i> , 2018, 9, 1892.	5.8	60
40	Structure and dynamics of a human myelin protein P2 portal region mutant indicate opening of the $\hat{\imath}^2$ barrel in fatty acid binding proteins. <i>BMC Structural Biology</i> , 2018, 18, 8.	2.3	19
41	How to minimize dye-induced perturbations while studying biomembrane structure and dynamics: PEG linkers as a rational alternative. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2018, 1860, 2436-2445.	1.4	31
42	A Ceramide-Regulated Element in the Late Endosomal Protein LAPT4B Controls Amino Acid Transporter Interaction. <i>ACS Central Science</i> , 2018, 4, 548-558.	5.3	29
43	Redox-coupled quinone dynamics in the respiratory complex I. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, E8413-E8420.	3.3	84
44	Negatively Charged Gangliosides Promote Membrane Association of Amphipathic Neurotransmitters. <i>Neuroscience</i> , 2018, 384, 214-223.	1.1	17
45	Quantitative Assessment of Methods Used To Obtain Rate Constants from Molecular Dynamics Simulations—Translocation of Cholesterol across Lipid Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 3840-3848.	2.3	18
46	Long-chain GM1 gangliosides alter transmembrane domain registration through interdigitation. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2017, 1859, 870-878.	1.4	20
47	Atomistic Molecular Dynamics Simulations of Mitochondrial DNA Polymerase $\hat{\imath}^3$: Novel Mechanisms of Function and Pathogenesis. <i>Biochemistry</i> , 2017, 56, 1227-1238.	1.2	3
48	Glycosylation and Lipids Working in Concert Direct CD2 Ectodomain Orientation and Presentation. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 1060-1066.	2.1	22
49	Effects of Membrane PEGylation on Entry and Location of Antifungal Drug Itraconazole and Their Pharmacological Implications. <i>Molecular Pharmaceutics</i> , 2017, 14, 1057-1070.	2.3	19
50	Calcium Assists Dopamine Release by Preventing Aggregation on the Inner Leaflet of Presynaptic Vesicles. <i>ACS Chemical Neuroscience</i> , 2017, 8, 1242-1250.	1.7	21
51	Calcium Directly Regulates Phosphatidylinositol 4,5-Bisphosphate Headgroup Conformation and Recognition. <i>Journal of the American Chemical Society</i> , 2017, 139, 4019-4024.	6.6	87
52	On Atomistic Models for Molecular Oxygen. <i>Journal of Physical Chemistry B</i> , 2017, 121, 518-528.	1.2	19
53	Mechanistic principles underlying regulation of the actin cytoskeleton by phosphoinositides. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E8977-E8986.	3.3	106
54	Diffusion of Integral Membrane Proteins in Protein-Rich Membranes. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4308-4313.	2.1	65

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55	<i>Glycans</i> Tools for Preparing Carbohydrate Structures for Atomistic Simulations of Glycoproteins, Glycolipids, and Carbohydrate Polymers for GROMACS. <i>Journal of Chemical Information and Modeling</i> , 2017, 57, 2401-2406.	2.5	71
56	Dynamics and energetics of the mammalian phosphatidylinositol transfer protein phospholipid exchange cycle. <i>Journal of Biological Chemistry</i> , 2017, 292, 14438-14455.	1.6	25
57	Nanoscale Membrane Domain Formation Driven by Cholesterol. <i>Scientific Reports</i> , 2017, 7, 1143.	1.6	83
58	Molecular mechanisms of Charcot-Marie-Tooth neuropathy linked to mutations in human myelin protein P2. <i>Scientific Reports</i> , 2017, 7, 6510.	1.6	33
59	The Integrin Receptor in Biologically Relevant Bilayers: Insights from Molecular Dynamics Simulations. <i>Journal of Membrane Biology</i> , 2017, 250, 337-351.	1.0	29
60	Phase Partitioning of GM1 and Its Bodipy-Labeled Analog Determine Their Different Binding to Cholera Toxin. <i>Frontiers in Physiology</i> , 2017, 8, 252.	1.3	34
61	Atomistic fingerprint of hyaluronan-CD44 binding. <i>PLoS Computational Biology</i> , 2017, 13, e1005663.	1.5	33
62	Concerted regulation of npc2 binding to endosomal/lysosomal membranes by bis(monoacylglycero)phosphate and sphingomyelin. <i>PLoS Computational Biology</i> , 2017, 13, e1005831.	1.5	27
63	Excessive aggregation of membrane proteins in the Martini model. <i>PLoS ONE</i> , 2017, 12, e0187936.	1.1	147
64	The role of hydrophobic matching on transmembrane helix packing in cells. <i>Cell Stress</i> , 2017, 1, 90-106.	1.4	37
65	Key steps in unconventional secretion of fibroblast growth factor 2 reconstituted with purified components. <i>ELife</i> , 2017, 6, .	2.8	63
66	Selective effect of cell membrane on synaptic neurotransmission. <i>Scientific Reports</i> , 2016, 6, 19345.	1.6	48
67	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. <i>Data in Brief</i> , 2016, 7, 1171-1174.	0.5	15
68	Atomistic determinants of co-enzyme Q reduction at the Qi-site of the cytochrome bc1 complex. <i>Scientific Reports</i> , 2016, 6, 33607.	1.6	23
69	Protein Crowding in Lipid Bilayers Gives Rise to Non-Gaussian Anomalous Lateral Diffusion of Phospholipids and Proteins. <i>Physical Review X</i> , 2016, 6, .	2.8	152
70	What Can We Learn about Cholesterol's Transmembrane Distribution Based on Cholesterol-Induced Changes in Membrane Dipole Potential?. <i>Journal of Physical Chemistry Letters</i> , 2016, 7, 4585-4590.	2.1	19
71	Lipid membranes: Theory and simulations bridged to experiments. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2251-2253.	1.4	12
72	Distribution and dynamics of quinones in the lipid bilayer mimicking the inner membrane of mitochondria. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2116-2122.	1.4	47

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73	Interdigitation of long-chain sphingomyelin induces coupling of membrane leaflets in a cholesterol dependent manner. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 281-288.	1.4	76
74	Role of charged lipids in membrane structures – Insight given by simulations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 2322-2333.	1.4	63
75	Cholesterol oxidation products and their biological importance. <i>Chemistry and Physics of Lipids</i> , 2016, 199, 144-160.	1.5	130
76	Mechanism of allosteric regulation of β_2 -adrenergic receptor by cholesterol. <i>ELife</i> , 2016, 5, .	2.8	115
77	Building Synthetic Sterols Computationally – “Unlocking the Secrets of Evolution?”. <i>Frontiers in Bioengineering and Biotechnology</i> , 2015, 3, 121.	2.0	5
78	Mutually Exclusive Roles of SHARPIN in Integrin Inactivation and NF- κ B Signaling. <i>PLoS ONE</i> , 2015, 10, e0143423.	1.1	24
79	PEGylated Liposomes as Carriers of Hydrophobic Porphyrins. <i>Journal of Physical Chemistry B</i> , 2015, 119, 6646-6657.	1.2	47
80	Cholesterol under oxidative stress – How lipid membranes sense oxidation as cholesterol is being replaced by oxysterols. <i>Free Radical Biology and Medicine</i> , 2015, 84, 30-41.	1.3	57
81	Apolipoprotein A-I mimetic peptide 4F blocks sphingomyelinase-induced LDL aggregation. <i>Journal of Lipid Research</i> , 2015, 56, 1206-1221.	2.0	20
82	How Well Does BODIPY-Cholesteryl Ester Mimic Unlabeled Cholesteryl Esters in High Density Lipoprotein Particles?. <i>Journal of Physical Chemistry B</i> , 2015, 119, 15848-15856.	1.2	4
83	Proton-coupled electron transfer and the role of water molecules in proton pumping by cytochrome <i>c</i> oxidase. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 2040-2045.	3.3	59
84	Biogenesis of Nascent High Density Lipoprotein Particles. <i>Structure</i> , 2015, 23, 1153-1154.	1.6	3
85	How To Minimize Artifacts in Atomistic Simulations of Membrane Proteins, Whose Crystal Structure Is Heavily Engineered: β_2 -Adrenergic Receptor in the Spotlight. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3432-3445.	2.3	16
86	Oxidation of Cholesterol Does Not Alter Significantly Its Uptake into High-Density Lipoprotein Particles. <i>Journal of Physical Chemistry B</i> , 2015, 119, 4594-4600.	1.2	6
87	Role of subunit III and its lipids in the molecular mechanism of cytochrome <i>c</i> oxidase. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2015, 1847, 690-697.	0.5	24
88	Sec14-nodulin proteins and the patterning of phosphoinositide landmarks for developmental control of membrane morphogenesis. <i>Molecular Biology of the Cell</i> , 2015, 26, 1764-1781.	0.9	44
89	<i>N</i> -Glycosylation as determinant of epidermal growth factor receptor conformation in membranes. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2015, 112, 4334-4339.	3.3	135
90	PIP2 and Talin Join Forces to Activate Integrin. <i>Journal of Physical Chemistry B</i> , 2015, 119, 12381-12389.	1.2	27

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91	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
92	How endoglucanase enzymes act on cellulose nanofibrils: role of amorphous regions revealed by atomistic simulations. Cellulose, 2015, 22, 2911-2925.	2.4	20
93	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
94	Dynamics of the Peripheral Membrane Protein P2 from Human Myelin Measured by Neutron Scattering—A Comparison between Wild-Type Protein and a Hinge Mutant. PLoS ONE, 2015, 10, e0128954.	1.1	17
95	Enzymatic Oxidation of Cholesterol: Properties and Functional Effects of Cholestenone in Cell Membranes. PLoS ONE, 2014, 9, e103743.	1.1	50
96	Co-Exposure with Fullerene May Strengthen Health Effects of Organic Industrial Chemicals. PLoS ONE, 2014, 9, e114490.	1.1	9
97	How Anacetrapib Inhibits the Activity of the Cholesteryl Ester Transfer Protein? Perspective through Atomistic Simulations. PLoS Computational Biology, 2014, 10, e1003987.	1.5	17
98	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
99	Effect of PEGylation on Drug Entry into Lipid Bilayer. Journal of Physical Chemistry B, 2014, 118, 144-151.	1.2	26
100	How well does cholesteryl hemisuccinate mimic cholesterol in saturated phospholipid bilayers?. Journal of Molecular Modeling, 2014, 20, 2121.	0.8	44
101	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
102	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
103	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
104	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
105	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
106	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
107	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
108	Modeling of Lipid Membranes and Lipoproteins. , 2014, , 299-318.		2

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109	Parameterization of the prosthetic redox centers of the bacterial cytochrome bc ₁ complex for atomistic molecular dynamics simulations. <i>Theoretical Chemistry Accounts</i> , 2013, 132, 1.	0.5	16
110	Key role of water in proton transfer at the Q _o -site of the cytochrome bc ₁ complex predicted by atomistic molecular dynamics simulations. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2013, 1827, 761-768.	0.5	39
111	Anomalous and normal diffusion of proteins and lipids in crowded lipid membranes. <i>Faraday Discussions</i> , 2013, 161, 397-417.	1.6	170
112	Atomistic simulations indicate cardiolipin to have an integral role in the structure of the cytochrome bc ₁ complex. <i>Biochimica Et Biophysica Acta - Bioenergetics</i> , 2013, 1827, 769-778.	0.5	54
113	Molecular lipidomics of exosomes released by PC-3 prostate cancer cells. <i>Biochimica Et Biophysica Acta - Molecular and Cell Biology of Lipids</i> , 2013, 1831, 1302-1309.	1.2	546
114	Do Lipids Retard the Evaporation of the Tear Fluid?. , 2012, 53, 6442.		49
115	Interfacial Tension and Surface Pressure of High Density Lipoprotein, Low Density Lipoprotein, and Related Lipid Droplets. <i>Biophysical Journal</i> , 2012, 103, 1236-1244.	0.2	42
116	Mechanism for translocation of fluoroquinolones across lipid membranes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2012, 1818, 2563-2571.	1.4	76
117	Role of Neutral Lipids in Tear Fluid Lipid Layer: Coarse-Grained Simulation Study. <i>Langmuir</i> , 2012, 28, 17092-17100.	1.6	27
118	The impact of lipid composition on the stability of the tear fluid lipid layer. <i>Soft Matter</i> , 2012, 8, 5826.	1.2	40
119	Interaction of Hematoporphyrin with Lipid Membranes. <i>Journal of Physical Chemistry B</i> , 2012, 116, 4889-4897.	1.2	36
120	Interaction of C70 fullerene with the Kv1.2 potassium channel. <i>Physical Chemistry Chemical Physics</i> , 2012, 14, 12526.	1.3	17
121	Strong preferences of dopamine and L-dopa towards lipid head group: importance of lipid composition and implication for neurotransmitter metabolism. <i>Journal of Neurochemistry</i> , 2012, 122, 681-690.	2.1	51
122	Cationic Dimyristoylphosphatidylcholine and Dioleoyloxytrimethylammonium Propane Lipid Bilayers: Atomistic Insight for Structure and Dynamics. <i>Journal of Physical Chemistry B</i> , 2012, 116, 269-276.	1.2	25
123	Atomistic Simulations of Functional Au ₁₄₄ (SR) ₆₀ Gold Nanoparticles in Aqueous Environment. <i>Journal of Physical Chemistry C</i> , 2012, 116, 9805-9815.	1.5	94
124	Mechanical properties of cellulose nanofibrils determined through atomistic molecular dynamics simulations. <i>Nordic Pulp and Paper Research Journal</i> , 2012, 27, 282-286.	0.3	27
125	Revealing structural and dynamical properties of high density lipoproteins through molecular simulations. <i>Soft Matter</i> , 2012, 8, 1262-1267.	1.2	11
126	Lipid Exchange Mechanism of the Cholesteryl Ester Transfer Protein Clarified by Atomistic and Coarse-grained Simulations. <i>PLoS Computational Biology</i> , 2012, 8, e1002299.	1.5	49

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127	Drug-Lipid Membrane Interaction Mechanisms Revealed Through Molecular Simulations. <i>Current Physical Chemistry</i> , 2012, 2, 379-400.	0.1	13
128	Effect of Galactosylceramide on the Dynamics of Cholesterol-Rich Lipid Membranes. <i>Journal of Physical Chemistry B</i> , 2011, 115, 14424-14434.	1.2	17
129	Properties of the Membrane Binding Component of Catechol- <i>O</i> -methyltransferase Revealed by Atomistic Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 13541-13550.	1.2	15
130	Protein Shape Change Has a Major Effect on the Gating Energy of a Mechanosensitive Channel. <i>Biophysical Journal</i> , 2011, 100, 1651-1659.	0.2	48
131	Analysis of Twisting of Cellulose Nanofibrils in Atomistic Molecular Dynamics Simulations. <i>Journal of Physical Chemistry B</i> , 2011, 115, 3747-3755.	1.2	129
132	Low density lipoprotein: structure, dynamics, and interactions of apoB-100 with lipids. <i>Soft Matter</i> , 2011, 7, 8135.	1.2	47
133	A MARTINI Coarse-Grained Model of a Thermoset Polyester Coating. <i>Macromolecules</i> , 2011, 44, 6198-6208.	2.2	66
134	N- and O-methylation of sphingomyelin markedly affects its membrane properties and interactions with cholesterol. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2011, 1808, 1179-1186.	1.4	35
135	Lipid Simulations: A Perspective on Lipids in Action. <i>Cold Spring Harbor Perspectives in Biology</i> , 2011, 3, a004655-a004655.	2.3	35
136	Coarse-graining polymers with the MARTINI force-field: polystyrene as a benchmark case. <i>Soft Matter</i> , 2011, 7, 698-708.	1.2	216
137	Cholesterol modulates glycolipid conformation and receptor activity. <i>Nature Chemical Biology</i> , 2011, 7, 260-262.	3.9	194
138	Lessons from the biophysics of interfaces: Lung surfactant and tear fluid. <i>Progress in Retinal and Eye Research</i> , 2011, 30, 204-215.	7.3	46
139	Lateral sorting in model membranes by cholesterol-mediated hydrophobic matching. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2011, 108, 16628-16633.	3.3	131
140	Association of Lipidome Remodeling in the Adipocyte Membrane with Acquired Obesity in Humans. <i>PLoS Biology</i> , 2011, 9, e1000623.	2.6	213
141	High Density Lipoprotein Structural Changes and Drug Response in Lipidomic Profiles following the Long-Term Fenofibrate Therapy in the FIELD Substudy. <i>PLoS ONE</i> , 2011, 6, e23589.	1.1	33
142	Defect-Mediated Trafficking across Cell Membranes: Insights from <i>in Silico</i> Modeling. <i>Chemical Reviews</i> , 2010, 110, 6077-6103.	23.0	171
143	Molecular Dynamics Simulations Reveal Fundamental Role of Water As Factor Determining Affinity of Binding of β -Blocker Nebivolol to β -Adrenergic Receptor. <i>Journal of Physical Chemistry B</i> , 2010, 114, 8374-8386.	1.2	35
144	Role of Lipids in Spheroidal High Density Lipoproteins. <i>PLoS Computational Biology</i> , 2010, 6, e1000964.	1.5	81

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145	Composition and lipid spatial distribution of HDL particles in subjects with low and high HDL-cholesterol. <i>Journal of Lipid Research</i> , 2010, 51, 2341-2351.	2.0	111
146	Free Volume Theory Applied to Lateral Diffusion in Langmuir Monolayers: Atomistic Simulations for a Protein-Free Model of Lung Surfactant. <i>Langmuir</i> , 2010, 26, 15436-15444.	1.6	42
147	Molecular Organization of the Tear Fluid Lipid Layer. <i>Biophysical Journal</i> , 2010, 99, 2559-2567.	0.2	67
148	Role of Glycolipids in Lipid Rafts: A View through Atomistic Molecular Dynamics Simulations with Galactosylceramide. <i>Journal of Physical Chemistry B</i> , 2010, 114, 7797-7807.	1.2	60
149	Effects of DPH on DPPC~Cholesterol Membranes with Varying Concentrations of Cholesterol: From Local Perturbations to Limitations in Fluorescence Anisotropy Experiments. <i>Journal of Physical Chemistry B</i> , 2010, 114, 2704-2711.	1.2	39
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