Tomasz Rog

List of Publications by Year in descending order

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166	10,162	28242	42364
papers	citations	55 h-index	92 g-index

172	172	172	11638
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	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
2	Ordering effects of cholesterol and its analogues. Biochimica Et Biophysica Acta - Biomembranes, 2009, 1788, 97-121.	1.4	506
3	Antidepressant drugs act by directly binding to TRKB neurotrophin receptors. Cell, 2021, 184, 1299-1313.e19.	13.5	347
4	Phosphatidylethanolamine-Phosphatidylglycerol Bilayer as a Model of the Inner Bacterial Membrane. Biophysical Journal, 2005, 88, 1091-1103.	0.2	278
5	Association of Lipidome Remodeling in the Adipocyte Membrane with Acquired Obesity in Humans. PLoS Biology, 2011, 9, e1000623.	2.6	213
6	Cholesterol Effects on the Phosphatidylcholine Bilayer Polar Region: A Molecular Simulation Study. Biophysical Journal, 2000, 78, 1376-1389.	0.2	212
7	Multiscale Simulations of Biological Membranes: The Challenge To Understand Biological Phenomena in a Living Substance. Chemical Reviews, 2019, 119, 5607-5774.	23.0	209
8	Cholesterol modulates glycolipid conformation and receptor activity. Nature Chemical Biology, 2011, 7, 260-262.	3.9	194
9	Atomic-Scale Structure and Electrostatics of Anionic Palmitoyloleoylphosphatidylglycerol Lipid Bilayers with Na+ Counterions. Biophysical Journal, 2007, 92, 1114-1124.	0.2	178
10	nMoldyn: A program package for a neutron scattering oriented analysis of molecular dynamics simulations. Journal of Computational Chemistry, 2003, 24, 657-667.	1.5	174
11	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
12	Cholesterol level affects surface charge of lipid membranes in saline solution. Scientific Reports, 2014, 4, 5005.	1.6	157
13	Effects of Phospholipid Unsaturation on the Membrane/Water Interface: A Molecular Simulation Study. Biophysical Journal, 2001, 81, 170-183.	0.2	150
14	Cholesterol Effects on the Phosphatidylcholine Bilayer Nonpolar Region: A Molecular Simulation Study. Biophysical Journal, 2001, 81, 2190-2202.	0.2	146
15	Lateral Diffusion in Lipid Membranes through Collective Flows. Journal of the American Chemical Society, 2008, 130, 44-45.	6.6	145
16	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
17	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
18	Interplay of Unsaturated Phospholipids and Cholesterol in Membranes: Effect of the Double-Bond Position. Biophysical Journal, 2008, 95, 3295-3305.	0.2	132

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19	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
20	Cholesterol oxidation products and their biological importance. Chemistry and Physics of Lipids, 2016, 199, 144-160.	1.5	130
21	Analysis of Twisting of Cellulose Nanofibrils in Atomistic Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 3747-3755.	1.2	129
22	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
23	Significance of Sterol Structural Specificity. Journal of Biological Chemistry, 2006, 281, 348-355.	1.6	121
24	Tilt:Â Major Factor in Sterols' Ordering Capability in Membranes. Journal of Physical Chemistry B, 2006, 110, 25562-25564.	1.2	118
25	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
26	Mechanism of allosteric regulation of Î²2-adrenergic receptor by cholesterol. ELife, 2016, 5, .	2.8	115
27	Toward Atomistic Resolution Structure of Phosphatidylcholine Headgroup and Glycerol Backbone at Different Ambient Conditions. Journal of Physical Chemistry B, 2015, 119, 15075-15088.	1.2	109
28	Role of phosphatidylglycerols in the stability of bacterial membranes. Biochimie, 2008, 90, 930-938.	1.3	106
29	Indocyanine Green-Loaded Liposomes for Light-Triggered Drug Release. Molecular Pharmaceutics, 2016, 13, 2095-2107.	2.3	102
30	Cholesterol Induces Specific Spatial and Orientational Order in Cholesterol/Phospholipid Membranes. PLoS ONE, 2010, 5, e11162.	1.1	101
31	What Happens if Cholesterol Is Made Smoother. Biophysical Journal, 2007, 92, 3346-3357.	0.2	99
32	Study of PEGylated Lipid Layers as a Model for PEGylated Liposome Surfaces: Molecular Dynamics Simulation and Langmuir Monolayer Studies. Langmuir, 2011, 27, 7788-7798.	1.6	95
33	Cholesterol-Sphingomyelin Interactions: A Molecular Dynamics Simulation Study. Biophysical Journal, 2006, 91, 3756-3767.	0.2	88
34	Calcium Directly Regulates Phosphatidylinositol 4,5-Bisphosphate Headgroup Conformation and Recognition. Journal of the American Chemical Society, 2017, 139, 4019-4024.	6.6	87
35	Dynamics of water at membrane surfaces: Effect of headgroup structure. Biointerphases, 2006, 1, 98-105.	0.6	82
36	Mechanism for translocation of fluoroquinolones across lipid membranes. Biochimica Et Biophysica Acta - Biomembranes, 2012, 1818, 2563-2571.	1.4	76

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37	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
38	Effect of Sphingomyelin Headgroup Size on Molecular Properties andÂInteractions with Cholesterol. Biophysical Journal, 2010, 99, 3300-3308.	0.2	75
39	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
40	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
41	The biophysical properties of ethanolamine plasmalogens revealed by atomistic molecular dynamics simulations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 97-103.	1.4	69
42	Cis and trans unsaturated phosphatidylcholine bilayers: A molecular dynamics simulation study. Chemistry and Physics of Lipids, 2016, 195, 12-20.	1.5	69
43	The dynamics of water at the phospholipid bilayer surface: a molecular dynamics simulation study. Chemical Physics Letters, 2002, 352, 323-327.	1.2	68
44	Syndecan-4 tunes cell mechanics by activating the kindlin-integrin-RhoA pathway. Nature Materials, 2020, 19, 669-678.	13.3	66
45	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
46	Topologies, structures and parameter files for lipid simulations in GROMACS with the OPLS-aa force field: DPPC, POPC, DOPC, PEPC, and cholesterol. Data in Brief, 2015, 5, 333-336.	0.5	65
47	Effects of Epicholesterol on the Phosphatidylcholine Bilayer: A Molecular Simulation Study. Biophysical Journal, 2003, 84, 1818-1826.	0.2	64
48	Molecular Dynamics Simulation of PEGylated Bilayer Interacting with Salt Ions: A Model of the Liposome Surface in the Bloodstream. Journal of Physical Chemistry B, 2012, 116, 4212-4219.	1.2	64
49	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
50	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
51	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
52	Cholesterol effects on the phospholipid condensation and packing in the bilayer: a molecular simulation study. FEBS Letters, 2001, 502, 68-71.	1.3	60
53	Effects of phospholipid unsaturation on the bilayer nonpolar region. Journal of Lipid Research, 2004, 45, 326-336.	2.0	60
54	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

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55	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
56	Effects of the Lipid Bilayer Phase State on the Water Membrane Interface. Journal of Physical Chemistry B, 2010, 114, 11784-11792.	1.2	58
57	Analysis of cause of failure of new targeting peptide in PEGylated liposome: Molecular modeling as rational design tool for nanomedicine. European Journal of Pharmaceutical Sciences, 2012, 46, 121-130.	1.9	58
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	A Perspective: Active Role of Lipids in Neurotransmitter Dynamics. Molecular Neurobiology, 2020, 57, 910-925.	1.9	56
60	Cholesterol effects on a mixed-chain phosphatidylcholine bilayer: a molecular dynamics simulation study. Biochimie, 2006, 88, 449-460.	1.3	54
61	Significance of Cholesterol Methyl Groups. Journal of Physical Chemistry B, 2008, 112, 2922-2929.	1.2	54
62	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
63	Mechanistic Understanding From Molecular Dynamics Simulation in Pharmaceutical Research 1: Drug Delivery. Frontiers in Molecular Biosciences, 2020, 7, 604770.	1.6	54
64	Non-polar interactions between cholesterol and phospholipids: a molecular dynamics simulation study. Biophysical Chemistry, 2004, 107, 151-164.	1.5	52
65	Water Isotope Effect on the Phosphatidylcholine Bilayer Properties: A Molecular Dynamics Simulation Study. Journal of Physical Chemistry B, 2009, 113, 2378-2387.	1.2	51
66	Study of Interaction Between PEG Carrier and Three Relevant Drug Molecules: Piroxicam, Paclitaxel, and Hematoporphyrin. Journal of Physical Chemistry B, 2012, 116, 7334-7341.	1.2	51
67	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
68	Enzymatic Oxidation of Cholesterol: Properties and Functional Effects of Cholestenone in Cell Membranes. PLoS ONE, 2014, 9, e103743.	1.1	50
69	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
70	Selective effect of cell membrane on synaptic neurotransmission. Scientific Reports, 2016, 6, 19345.	1.6	48
71	Molecular dynamics, crystallography and mutagenesis studies on the substrate gating mechanism of prolyl oligopeptidase. Biochimie, 2012, 94, 1398-1411.	1.3	47
72	PEGylated Liposomes as Carriers of Hydrophobic Porphyrins. Journal of Physical Chemistry B, 2015, 119, 6646-6657.	1.2	47

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73	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
74	Behavior of the DPH fluorescence probe in membranes perturbed by drugs. Chemistry and Physics of Lipids, 2019, 223, 104784.	1.5	47
75	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
76	How well does cholesteryl hemisuccinate mimic cholesterol in saturated phospholipid bilayers?. Journal of Molecular Modeling, 2014, 20, 2121.	0.8	44
77	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
78	The effect of light sensitizer localization on the stability of indocyanine green liposomes. Journal of Controlled Release, 2018, 284, 213-223.	4.8	43
79	Molecular dynamics simulation studies of lipid bilayer systems.. Acta Biochimica Polonica, 2000, 47, 601-611.	0.3	43
80	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
81	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
82	Transient Ordered Domains in Single-Component Phospholipid Bilayers. Physical Review Letters, 2006, 97, 238102.	2.9	40
83	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
84	Molecular Dynamics Simulations of the Bacterial ABC Transporter SAV1866 in the Closed Form. Journal of Physical Chemistry B, 2012, 116, 2934-2942.	1.2	38
85	Molecular dynamics simulations of charged and neutral lipid bilayers: treatment of electrostatic interactions.. Acta Biochimica Polonica, 2003, 50, 789-798.	0.3	37
86	Interaction of Hematoporphyrin with Lipid Membranes. Journal of Physical Chemistry B, 2012, 116, 4889-4897.	1.2	36
87	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
88	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
89	Lipid Simulations: A Perspective on Lipids in Action. Cold Spring Harbor Perspectives in Biology, 2011, 3, a004655-a004655.	2.3	35
90	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

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91	How cardiolipin peroxidation alters the properties of the inner mitochondrial membrane?. Chemistry and Physics of Lipids, 2018, 214, 15-23.	1.5	35
92	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
93	Tat(48-60) peptide amino acid sequence is not unique in its cell penetrating properties and cell-surface glycosaminoglycans inhibit its cellular uptake. Journal of Controlled Release, 2012, 158, 277-285.	4.8	33
94	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
95	Dehydroergosterol as an Analogue for Cholesterol: Why It Mimics Cholesterol So Wellâ€"or Does It?. Journal of Physical Chemistry B, 2014, 118, 7345-7357.	1.2	31
96	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
97	The Integrin Receptor in Biologically Relevant Bilayers: Insights from Molecular Dynamics Simulations. Journal of Membrane Biology, 2017, 250, 337-351.	1.0	29
98	Effects of a Carane Derivative Local Anesthetic on a Phospholipid Bilayer Studied by Molecular Dynamics Simulation. Biophysical Journal, 2003, 85, 1248-1258.	0.2	28
99	Use of Umbrella Sampling to Calculate the Entrance/Exit Pathway for Z-Pro-Prolinal Inhibitor in Prolyl Oligopeptidase. Journal of Chemical Theory and Computation, 2011, 7, 1583-1594.	2.3	28
100	Design of cholesterol arabinogalactan anchored liposomes for asialoglycoprotein receptor mediated targeting to hepatocellular carcinoma: In silic o modeling, in vitro and in vivo evaluation. International Journal of Pharmaceutics, 2016, 509, 149-158.	2.6	28
101	Mechanical properties of cellulose nanofibrils determined through atomistic molecular dynamics simulations. Nordic Pulp and Paper Research Journal, 2012, 27, 282-286.	0.3	27
102	PIP2 and Talin Join Forces to Activate Integrin. Journal of Physical Chemistry B, 2015, 119, 12381-12389.	1.2	27
103	Complex Behavior of Phosphatidylcholineâ€"Phosphatidic Acid Bilayers and Monolayers: Effect of Acyl Chain Unsaturation. Langmuir, 2019, 35, 5944-5956.	1.6	27
104	Effect of PEGylation on Drug Entry into Lipid Bilayer. Journal of Physical Chemistry B, 2014, 118, 144-151.	1.2	26
105	Molecular Dynamics Simulation of PEGylated Membranes with Cholesterol: Building Toward the DOXIL Formulation. Journal of Physical Chemistry C, 2014, 118, 15541-15549.	1.5	25
106	Dynamics and energetics of the mammalian phosphatidylinositol transfer protein phospholipid exchange cycle. Journal of Biological Chemistry, 2017, 292, 14438-14455.	1.6	25
107	Stearic Acid Spin Labels in Lipid Bilayers:â€‰ Insight through Atomistic Simulations. Journal of Physical Chemistry B, 2007, 111, 12447-12453.	1.2	24
108	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

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109	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
110	Tail-Oxidized Cholesterol Enhances Membrane Permeability for Small Solutes. Langmuir, 2020, 36, 10438-10447.	1.6	24
111	Influence of the disulfide bond configuration on the dynamics of the spin label attached to cytochrome c. Proteins: Structure, Function and Bioinformatics, 2006, 62, 1088-1100.	1.5	23
112	Atomistic determinants of co-enzyme Q reduction at the Qi-site of the cytochrome bc1 complex. Scientific Reports, 2016, 6, 33607.	1.6	23
113	Mechanistic Understanding from Molecular Dynamics in Pharmaceutical Research 2: Lipid Membrane in Drug Design. Pharmaceuticals, 2021, 14, 1062.	1.7	23
114	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
115	Glycosylation and Lipids Working in Concert Direct CD2 Ectodomain Orientation and Presentation. Journal of Physical Chemistry Letters, 2017, 8, 1060-1066.	2.1	22
116	Physiologically-relevant levels of sphingomyelin, but not GM1, induces a Î²-sheet-rich structure in the amyloid-Î²(1-42) monomer. Biochimica Et Biophysica Acta - Biomembranes, 2018, 1860, 1709-1720.	1.4	22
117	Complexity of seemingly simple lipid nanodiscs. Biochimica Et Biophysica Acta - Biomembranes, 2020, 1862, 183420.	1.4	22
118	Calcium Assists Dopamine Release by Preventing Aggregation on the Inner Leaflet of Presynaptic Vesicles. ACS Chemical Neuroscience, 2017, 8, 1242-1250.	1.7	21
119	Membrane-Dependent Binding and Entry Mechanism of Dopamine into Its Receptor. ACS Chemical Neuroscience, 2020, 11, 1914-1924.	1.7	21
120	Exploring the effect of xenon on biomembranes. Cellular and Molecular Biology Letters, 2005, 10, 563-9.	2.7	21
121	Effect of Phosphatidic Acid on Biomembrane: Experimental and Molecular Dynamics Simulations Study. Journal of Physical Chemistry B, 2015, 119, 10042-10051.	1.2	20
122	How endoglucanase enzymes act on cellulose nanofibrils: role of amorphous regions revealed by atomistic simulations. Cellulose, 2015, 22, 2911-2925.	2.4	20
123	Long-chain GM1 gangliosides alter transmembrane domain registration through interdigitation. Biochimica Et Biophysica Acta - Biomembranes, 2017, 1859, 870-878.	1.4	20
124	Membrane bound COMT isoform is an interfacial enzyme: general mechanism and new drug design paradigm. Chemical Communications, 2018, 54, 3440-3443.	2.2	20
125	Functionalized lipids and surfactants for specific applications. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2362-2379.	1.4	19
126	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

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127	Cholesteryl Hemisuccinate Is Not a Good Replacement for Cholesterol in Lipid Nanodiscs. Journal of Physical Chemistry B, 2019, 123, 9839-9845.	1.2	18
128	The F1 loop of the talin head domain acts as a gatekeeper in integrin activation and clustering. Journal of Cell Science, 2020, 133, .	1.2	18
129	Effect of Galactosylceramide on the Dynamics of Cholesterol-Rich Lipid Membranes. Journal of Physical Chemistry B, 2011, 115, 14424-14434.	1.2	17
130	How Anacetrapib Inhibits the Activity of the Cholesteryl Ester Transfer Protein? Perspective through Atomistic Simulations. PLoS Computational Biology, 2014, 10, e1003987.	1.5	17
131	Stearylated cycloarginine nanosystems for intracellular delivery â€“ simulations, formulation and proof of concept. RSC Advances, 2016, 6, 113538-113550.	1.7	17
132	A computational study suggests that replacing PEG with PMOZ may increase exposure of hydrophobic targeting moiety. European Journal of Pharmaceutical Sciences, 2017, 103, 128-135.	1.9	17
133	Negatively Charged Gangliosides Promote Membrane Association of Amphipathic Neurotransmitters. Neuroscience, 2018, 384, 214-223.	1.1	17
134	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
135	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
136	Effect of piroxicam on lipid membranes: Drug encapsulation and gastric toxicity aspects. European Journal of Pharmaceutical Sciences, 2017, 100, 116-125.	1.9	16
137	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
138	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
139	Identifying involvement of Lys251/Asp252 pair in electron transfer and associated proton transfer at the quinone reduction site of Rhodobacter capsulatus cytochrome bc1. Biochimica Et Biophysica Acta - Bioenergetics, 2016, 1857, 1661-1668.	0.5	15
140	Cholesterolâ€recognition motifs in the transmembrane domain of the tyrosine kinase receptor family: The case of TRKB. European Journal of Neuroscience, 2021, 53, 3311-3322.	1.2	15
141	Molecular Dynamics Simulation of Inverse-Phosphocholine Lipids. Journal of Physical Chemistry C, 2014, 118, 19444-19449.	1.5	14
142	Drug-Lipid Membrane Interaction Mechanisms Revealed Through Molecular Simulations. Current Physical Chemistry, 2012, 2, 379-400.	0.1	13
143	Molecular dynamics simulation studies of lipid bilayer systems. Acta Biochimica Polonica, 2000, 47, 601-11.	0.3	13
144	Modeling glycolipids: take one. Cellular and Molecular Biology Letters, 2005, 10, 625-30.	2.7	13

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145	Nonpolar interactions between transâ€membrane helical EGF peptide and phosphatidylcholines, sphingomyelins and cholesterol. Molecular dynamics simulation studies. Journal of Peptide Science, 2008, 14, 374-382.	0.8	12
146	Lipid membranes: Theory and simulations bridged to experiments. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2251-2253.	1.4	12
147	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
148	Cholesterol Reduces Partitioning of Antifungal Drug Itraconazole into Lipid Bilayers. Journal of Physical Chemistry B, 2020, 124, 2139-2148.	1.2	12
149	Molecular dynamics simulations of the enzyme Catechol-O-Methyltransferase: methodological issues. SAR and QSAR in Environmental Research, 2008, 19, 179-189.	1.0	11
150	Behavior of 2,6-Bis(decyloxy)naphthalene Inside Lipid Bilayer. Journal of Physical Chemistry B, 2010, 114, 15483-15494.	1.2	11
151	Molecular dynamics study of prolyl oligopeptidase with inhibitor in binding cavity. SAR and QSAR in Environmental Research, 2009, 20, 595-609.	1.0	10
152	Co-Exposure with Fullerene May Strengthen Health Effects of Organic Industrial Chemicals. PLoS ONE, 2014, 9, e114490.	1.1	9
153	Mechanistic Insight into How PEGylation Reduces the Efficacy of pH-Sensitive Liposomes from Molecular Dynamics Simulations. Molecular Pharmaceutics, 2021, 18, 2612-2621.	2.3	8
154	Conformations, orientations and time scales characterising dimyristoylphosphatidylcholine bilayer membrane. Molecular dynamics simulation studies.. Acta Biochimica Polonica, 1997, 44, 607-624.	0.3	8
155	Interactions of Magainin-2 Amide with Membrane Lipids. Lecture Notes in Computer Science, 2004, , 325-331.	1.0	7
156	Molecular Dynamics Simulations of Lipid Bilayers: Simple Recipe of How to Do It. Methods in Molecular Biology, 2013, 924, 407-429.	0.4	6
157	Rigorous Computational Study Reveals What Docking Overlooks: Double Trouble from Membrane Association in Protein Kinase C Modulators. Journal of Chemical Information and Modeling, 2020, 60, 5624-5633.	2.5	6
158	Cooperative Effects of an Antifungal Moiety and DMSO on Pore Formation over Lipid Membranes Revealed by Free Energy Calculations. Journal of Physical Chemistry B, 2020, 124, 8811-8821.	1.2	6
159	Examining the Effect of Charged Lipids on Mitochondrial Outer Membrane Dynamics Using Atomistic Simulations. Biomolecules, 2022, 12, 183.	1.8	6
160	Deuteration of Water Enables Selfâ€Organization of Phospholipidâ€Based Reverse Micelles. ChemPhysChem, 2010, 11, 590-598.	1.0	5
161	Building Synthetic Sterols Computationally â€“ Unlocking the Secrets of Evolution?. Frontiers in Bioengineering and Biotechnology, 2015, 3, 121.	2.0	5
162	Atomistic Molecular Dynamics Simulations of Mitochondrial DNA Polymerase Î³: Novel Mechanisms of Function and Pathogenesis. Biochemistry, 2017, 56, 1227-1238.	1.2	3

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163	Conformations, orientations and time scales characterising dimyristoylphosphatidylcholine bilayer membrane. Molecular dynamics simulation studies. Acta Biochimica Polonica, 1997, 44, 607-24.	0.3	3
164	Non-polar interactions between cholesterol and phospholipids: a molecular dynamics simulation study. Biophysical Chemistry, 2003, 107, 151-151.	1.5	1
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