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List of Publications by Year
in descending order

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206	25,721	22099	8370
papers	citations	59 h-index	147 g-index

226	226	226	19029
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Comparative Molecular Dynamics Simulation Studies of Realistic Eukaryotic, Prokaryotic, and Archaeal Membranes. Journal of Chemical Information and Modeling, 2022, 62, 1036-1051.	2.5	32
2	Structural basis of neuropeptide Y signaling through Y1 receptor. Nature Communications, 2022, 13, 853.	5.8	20
3	Foldable Detergents for Membrane Protein Study: Importance of Detergent Core Flexibility in Protein Stabilization. Chemistry - A European Journal, 2022, 28, .	1.7	13
4	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. Journal of Chemical Theory and Computation, 2022, 18, 479-493.	2.3	53
5	<scp>CHARMMâ€GUI</scp> Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. Journal of Computational Chemistry, 2022, 43, 359-375.	1.5	24
6	Molecular Condensate in a Membrane: A Tugging Game between Hydrophobicity and Polarity with Its Biological Significance. Langmuir, 2022, 38, 5955-5962.	1.6	1
7	Evolutionary balance between foldability and functionality of a glucose transporter. Nature Chemical Biology, 2022, 18, 713-723.	3.9	13
8	A systematic analysis of proteinâ€“carbohydrate interactions in the Protein Data Bank. Glycobiology, 2021, 31, 126-136.	1.3	13
9	Structure, Dynamics, and Interactions of GPI-Anchored Human Glypican-1 with Heparan Sulfates in a Membrane. Glycobiology, 2021, 31, 593-602.	1.3	6
10	Ligand-Binding-Site Refinement to Generate Reliable Holo Protein Structure Conformations from Apo Structures. Journal of Chemical Information and Modeling, 2021, 61, 535-546.	2.5	19
11	Influences of Vibrio cholerae Lipid A Types on LPS Bilayer Properties. Journal of Physical Chemistry B, 2021, 125, 2105-2112.	1.2	10
12	Biomechanical characterization of SARS-CoV-2 spike RBD and human ACE2 protein-protein interaction. Biophysical Journal, 2021, 120, 1011-1019.	0.2	87
13	Structure, Dynamics, Receptor Binding, and Antibody Binding of the Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein in a Viral Membrane. Journal of Chemical Theory and Computation, 2021, 17, 2479-2487.	2.3	62
14	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Proteinâ€“Lipid Modulations in Archaeal Membranes. Journal of Physical Chemistry B, 2021, 125, 4714-4725.	1.2	10
15	Site-Specific Lipidation Enhances IFITM3 Membrane Interactions and Antiviral Activity. ACS Chemical Biology, 2021, 16, 844-856.	1.6	22
16	CHARMM-GUI Polymer Builder for Modeling and Simulation of Synthetic Polymers. Journal of Chemical Theory and Computation, 2021, 17, 2431-2443.	2.3	58
17	Additive CHARMM36 Force Field for Nonstandard Amino Acids. Journal of Chemical Theory and Computation, 2021, 17, 3554-3570.	2.3	39
18	Structural Insight into Phospholipid Transport by the MlaFEBD Complex from P. aeruginosa. Journal of Molecular Biology, 2021, 433, 166986.	2.0	24

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19	Conformationally flexible core-bearing detergents with a hydrophobic or hydrophilic pendant: Effect of pendant polarity on detergent conformation and membrane protein stability. Acta Biomaterialia, 2021, 128, 393-407.	4.1	15
20	CHARMM-GUI LBS Finder & Refiner for Ligand Binding Site Prediction and Refinement. Journal of Chemical Information and Modeling, 2021, 61, 3744-3751.	2.5	9
21	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. Journal of Chemical Information and Modeling, 2021, 61, 4145-4151.	2.5	24
22	CHARMM-GUI Membrane Builder for Lipid Nanoparticles with Ionizable Cationic Lipids and PEGylated Lipids. Journal of Chemical Information and Modeling, 2021, 61, 5192-5202.	2.5	25
23	Biophysical characterization of lynxâ€nicotinic receptor interactions using atomic force microscopy. FASEB BioAdvances, 2021, 3, 1034-1042.	1.3	2
24	Structural basis for the association of PLEKHA7 with membrane-embedded phosphatidylinositol lipids. Structure, 2021, 29, 1029-1039.e3.	1.6	18
25	Dynamic Interactions of Fully Glycosylated SARS-CoV-2 Spike Protein with Various Antibodies. Journal of Chemical Theory and Computation, 2021, 17, 6559-6569.	2.3	13
26	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. Journal of Chemical Information and Modeling, 2021, 61, 831-839.	2.5	59
27	Accurate simulation of surfaces and interfaces of ten FCC metals and steel using Lennardâ€“Jones potentials. Npj Computational Materials, 2021, 7, .	3.5	28
28	Developing initial conditions for simulations of asymmetric membranes: a practical recommendation. Biophysical Journal, 2021, 120, 5041-5059.	0.2	14
29	Systematic Assessment of Accessibility to the Surface of Staphylococcus aureus. ACS Chemical Biology, 2021, 16, 2527-2536.	1.6	15
30	CHARMM-GUI Ligand Designer for Template-Based Virtual Ligand Design in a Binding Site. Journal of Chemical Information and Modeling, 2021, 61, 5336-5342.	2.5	8
31	Differential Interactions between Human ACE2 and Spike RBD of SARS-CoV-2 Variants of Concern. Journal of Chemical Theory and Computation, 2021, 17, 7972-7979.	2.3	57
32	CHARMMâ€GUI DEER facilitator for spinâ€pair distance distribution calculations and preparation of restrainedâ€ensemble molecular dynamics simulations. Journal of Computational Chemistry, 2020, 41, 415-420.	1.5	19
33	Preferred conformations of lipooligosaccharides and oligosaccharides of Moraxella catarrhalis. Glycobiology, 2020, 30, 86-94.	1.3	6
34	GlyMDB: Glycan Microarray Database and analysis toolset. Bioinformatics, 2020, 36, 2438-2442.	1.8	14
35	Calcium and hydroxyapatite binding site of human vitronectin provides insights to abnormal deposit formation. Proceedings of the National Academy of Sciences of the United States of America, 2020, 117, 18504-18510.	3.3	11
36	CHARMM-GUI supports the Amber force fields. Journal of Chemical Physics, 2020, 153, 035103.	1.2	175

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37	CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations. Journal of Chemical Theory and Computation, 2020, 16, 7207-7218.	2.3	57
38	Conformational States of the Cytoprotective Protein Bcl-xL. Biophysical Journal, 2020, 119, 1324-1334.	0.2	10
39	Experimentally Guided Computational Methods Yield Highly Accurate Insights into Transmembrane Interactions within the T Cell Receptor Complex. Journal of Physical Chemistry B, 2020, 124, 10303-10310.	1.2	1
40	Modeling and Simulation of Bacterial Outer Membranes with Lipopolysaccharides and Enterobacterial Common Antigen. Journal of Physical Chemistry B, 2020, 124, 5948-5956.	1.2	26
41	Mutually constructive roles of Ail and LPS in Yersinia pestis serum survival. Molecular Microbiology, 2020, 114, 510-520.	1.2	19
42	Developing a Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein Model in a Viral Membrane. Journal of Physical Chemistry B, 2020, 124, 7128-7137.	1.2	240
43	Dynamics and Interactions of GPI-Linked lynx1 Protein with/without Nicotinic Acetylcholine Receptor in Membrane Bilayers. Journal of Physical Chemistry B, 2020, 124, 4017-4025.	1.2	7
44	Improving Protein-Ligand Docking Results with High-Throughput Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2020, 60, 2189-2198.	2.5	152
45	Cooperativity in Proteasome Core Particle Maturation. IScience, 2020, 23, 101090.	1.9	5
46	Molecular Simulations of Gram-Negative Bacterial Membranes Come of Age. Annual Review of Physical Chemistry, 2020, 71, 171-188.	4.8	44
47	Broadening Activity of Polymyxin by Quaternary Ammonium Grafting. ACS Infectious Diseases, 2020, 6, 1427-1435.	1.8	9
48	Escherichia coli O176 LPS structure and dynamics: A NMR spectroscopy and MD simulation study. Current Research in Structural Biology, 2020, 2, 79-88.	1.1	8
49	A mechano-reactive coarse-grained model of the blood-clotting agent von Willebrand factor. Journal of Chemical Physics, 2019, 151, 124905.	1.2	13
50	Ligand-Binding-Site Structure Refinement Using Molecular Dynamics with Restraints Derived from Predicted Binding Site Templates. Journal of Chemical Theory and Computation, 2019, 15, 6524-6535.	2.3	16
51	Quantitative Characterization of Proteinâ€“Lipid Interactions by Free Energy Simulation between Binary Bilayers. Journal of Chemical Theory and Computation, 2019, 15, 6491-6503.	2.3	7
52	CHARMM-GUIGlycan Modelerfor modeling and simulation of carbohydrates and glycoconjugates. Glycobiology, 2019, 29, 320-331.	1.3	222
53	CHARMMâ€GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. Journal of Computational Chemistry, 2019, 40, 893-899.	1.5	42
54	Modeling of Specific Lipopolysaccharide Binding Sites on a Gram-Negative Porin. Journal of Physical Chemistry B, 2019, 123, 5700-5708.	1.2	11

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55	Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation. Biophysical Journal, 2019, 116, 1095-1104.	0.2	27
56	Stalis : A Computational Method for Templateâ€Based Ab Initio Ligand Design. Journal of Computational Chemistry, 2019, 40, 1622-1632.	1.5	4
57	Uâ€shaped caveolinâ€1 conformations are tightly regulated by hydrogen bonds with lipids. Journal of Computational Chemistry, 2019, 40, 1570-1577.	1.5	8
58	Clustering and dynamics of crowded proteins near membranes and their influence on membrane bending. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 24562-24567.	3.3	52
59	Analysis of Lipid Order States and Domains in Lipid Bilayer Simulations. Journal of Chemical Theory and Computation, 2019, 15, 688-697.	2.3	12
60	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. Journal of Chemical Theory and Computation, 2019, 15, 775-786.	2.3	388
61	Structural Conservation and Effects of Alterations in T Cell Receptor Transmembrane Interfaces. Biophysical Journal, 2018, 114, 1030-1035.	0.2	8
62	Multiple Conformational States Contribute to the 3D Structure of a Glucan Decasaccharide: A Combined SAXS and MD Simulation Study. Journal of Physical Chemistry B, 2018, 122, 1169-1175.	1.2	9
63	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. Nature Chemical Biology, 2018, 14, 489-496.	3.9	39
64	Molecular Basis of Aqueous-like Activity of Lipase Treated with Glucose-Headed Surfactant in Organic Solvent. Journal of Physical Chemistry B, 2018, 122, 10659-10668.	1.2	3
65	Insight into Elongation Stages of Peptidoglycan Processing in Bacterial Cytoplasmic Membranes. Scientific Reports, 2018, 8, 17704.	1.6	6
66	Long-ranged Protein-glycan Interactions Stabilize von Willebrand Factor A2 Domain from Mechanical Unfolding. Scientific Reports, 2018, 8, 16017.	1.6	8
67	Structure of an EIIC sugar transporter trapped in an inward-facing conformation. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 5962-5967.	3.3	18
68	Augmenting the antinociceptive effects of nicotinic acetylcholine receptor activity through lynx1 modulation. PLoS ONE, 2018, 13, e0199643.	1.1	18
69	Synthetic Immunotherapeutics against Gram-negative Pathogens. Cell Chemical Biology, 2018, 25, 1185-1194.e5.	2.5	29
70	Simulation Study of Occk5 Functional Properties in Pseudomonas aeruginosa Outer Membranes. Journal of Physical Chemistry B, 2018, 122, 8185-8192.	1.2	12
71	Quantitative Characterization of Cholesterol Partitioning between Binary Bilayers. Journal of Chemical Theory and Computation, 2018, 14, 2829-2833.	2.3	14
72	Biophysical and functional characterization of Norrin signaling through Frizzled4. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, 8787-8792.	3.3	30

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73	Refinement of OprH-LPS Interactions by Molecular Simulations. Biophysical Journal, 2017, 112, 346-355.	0.2	50
74	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. Current Opinion in Structural Biology, 2017, 43, 131-140.	2.6	42
75	CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. Journal of Computational Chemistry, 2017, 38, 1879-1886.	1.5	311
76	Molecular Simulation and Biochemical Studies Support an Elevator-type Transport Mechanism inÂEIIC. Biophysical Journal, 2017, 112, 2249-2252.	0.2	7
77	Simulating Biomolecules: Festschrift to commemorate the 60th birthday of Charles L. Brooks III. Journal of Computational Chemistry, 2017, 38, 1111-1113.	1.5	0
78	G-LoSA for Prediction of Protein-Ligand Binding Sites and Structures. Methods in Molecular Biology, 2017, 1611, 97-108.	0.4	15
79	Conformational Dynamics of the Lipopolysaccharide from Escherichia coli O91 Revealed by Nuclear Magnetic Resonance Spectroscopy and Molecular Simulations. Biochemistry, 2017, 56, 3826-3839.	1.2	17
80	Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation. Biophysical Journal, 2017, 112, 1185-1197.	0.2	48
81	Gramicidin A Channel Formation Induces LocalÂLipid Redistribution II: A 3D Continuum Elastic Model. Biophysical Journal, 2017, 112, 1198-1213.	0.2	22
82	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. Journal of Physical Chemistry B, 2017, 121, 3718-3723.	1.2	24
83	Effects of N-Glycan Composition on Structure and Dynamics of IgG1 Fc and Their Implications for Antibody Engineering. Scientific Reports, 2017, 7, 12659.	1.6	31
84	Characterizing Residue-Bilayer Interactions Using Gramicidin A as a Scaffold and Tryptophan Substitutions as Probes. Journal of Chemical Theory and Computation, 2017, 13, 5054-5064.	2.3	14
85	Heterogeneity in nonâ€epitope loop sequence and outer membrane protein complexes alters antibody binding to the major porin protein PorB in serogroup B Neisseria meningitidis. Molecular Microbiology, 2017, 105, 934-953.	1.2	15
86	CHARMMâ€GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. Journal of Computational Chemistry, 2017, 38, 2354-2363.	1.5	150
87	Glycan Reader is improved to recognize most sugar types and chemical modifications in the Protein Data Bank. Bioinformatics, 2017, 33, 3051-3057.	1.8	94
88	Transmembrane features governing Fc receptor CD16A assembly with CD16A signaling adaptor molecules. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, E5645-E5654.	3.3	32
89	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	1.5	224
90	Asymmetric Cryo-EM Structure of Anthrax Toxin Protective Antigen Pore with Lethal Factor N-Terminal Domain. Toxins, 2017, 9, 298.	1.5	12

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91	Transmembrane motions of PglB induced by LLO are coupled with EL5 loop conformational changes necessary for OST activity. Glycobiology, 2017, 27, 734-742.	1.3	6
92	Preferred conformations ofN-glycan core pentasaccharide in solution and in glycoproteins. Glycobiology, 2016, 26, cwv083.	1.3	34
93	L-Met Activates Arabidopsis GLR Ca2+ Channels Upstream of ROS Production and Regulates Stomatal Movement. Cell Reports, 2016, 17, 2553-2561.	2.9	71
94	CHARMM-GUI Input Generator for NAMD, Gromacs, Amber, Openmm, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. Biophysical Journal, 2016, 110, 641a.	0.2	63
95	The Structure of a Sugar Transporter of the Glucose EIIC Superfamily Provides Insight into the Elevator Mechanism of Membrane Transport. Structure, 2016, 24, 956-964.	1.6	37
96	Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues. Biophysical Journal, 2016, 111, 1600-1603.	0.2	0
97	An extensive simulation study of lipid bilayer properties with different head groups, acyl chain lengths, and chain saturations. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 3093-3104.	1.4	51
98	A conserved Î±Î² transmembrane interface forms the core of a compact T-cell receptorâ€“CD3 structure within the membrane. Proceedings of the National Academy of Sciences of the United States of America, 2016, 113, E6649-E6658.	3.3	40
99	Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. Journal of Physical Chemistry B, 2016, 120, 11761-11772.	1.2	47
100	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. Biophysical Journal, 2016, 111, 1750-1760.	0.2	88
101	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. Biophysical Journal, 2016, 111, 1987-1999.	0.2	41
102	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. Biophysical Journal, 2016, 110, 2698-2709.	0.2	65
103	Molecular dynamics simulation strategies for proteinâ€“micelle complexes. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1566-1572.	1.4	19
104	Challenges in structural approaches to cell modeling. Journal of Molecular Biology, 2016, 428, 2943-2964.	2.0	51
105	Gâ€ŁoSA: An efficient computational tool for local structureâ€centric biological studies and drug design. Protein Science, 2016, 25, 865-876.	3.1	33
106	Converting One-Face Î±-Helix Mimetics into Amphiphilic Î±-Helix Mimetics as Potent Inhibitors of Proteinâ€“Protein Interactions. ACS Combinatorial Science, 2016, 18, 36-42.	3.8	15
107	CHARMM-GUI Input Generator for NAMD, GROMACS, AMBER, OpenMM, and CHARMM/OpenMM Simulations Using the CHARMM36 Additive Force Field. Journal of Chemical Theory and Computation, 2016, 12, 405-413.	2.3	2,567
108	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. Biophysical Journal, 2016, 110, 930-938.	0.2	64

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109	Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1635-1651.	1.4	111
110	How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?. Journal of Chemical Theory and Computation, 2015, 11, 3466-3477.	2.3	64
111	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. Glycobiology, 2015, 26, cwv101.	1.3	15
112	Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy. Journal of Chemical Theory and Computation, 2015, 11, 1255-1266.	2.3	13
113	Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes. Biophysical Journal, 2015, 108, 1954-1962.	0.2	11
114	GS-align for glycan structure alignment and similarity measurement. Bioinformatics, 2015, 31, 2653-2659.	1.8	11
115	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. Scientific Reports, 2015, 5, 8926.	1.6	187
116	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. Journal of Chemical Theory and Computation, 2015, 11, 4486-4494.	2.3	340
117	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. Biophysical Journal, 2015, 109, 2012-2022.	0.2	89
118	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. Biophysical Journal, 2015, 109, 2090-2100.	0.2	18
119	Transmembrane Complexes of DAP12 Crystallized in Lipid Membranes Provide Insights into Control of Oligomerization in Immunoreceptor Assembly. Cell Reports, 2015, 11, 1184-1192.	2.9	20
120	Lipopolysaccharide Membrane Building and Simulation. Methods in Molecular Biology, 2015, 1273, 391-406.	0.4	41
121	STâ€analyzer: A webâ€based user interface for simulation trajectory analysis. Journal of Computational Chemistry, 2014, 35, 957-963.	1.5	12
122	Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase. Biophysical Journal, 2014, 107, 1885-1895.	0.2	21
123	CHARMM-GUIMembrane Buildertoward realistic biological membrane simulations. Journal of Computational Chemistry, 2014, 35, 1997-2004.	1.5	1,802
124	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. Advances in Protein Chemistry and Structural Biology, 2014, 96, 235-265.	1.0	214
125	Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. Journal of Physical Chemistry B, 2014, 118, 4315-4325.	1.2	38
126	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2520-2529.	1.4	82

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127	Potential pharmacological chaperones targeting cancer-associated MCL-1 and Parkinson disease-associated Î±-synuclein. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11007-11012.	3.3	55
128	Theory of Adaptive Optimization for Umbrella Sampling. Journal of Chemical Theory and Computation, 2014, 10, 2719-2728.	2.3	21
129	CHARMM-GUI PACE CG Builder for Solution, Micelle, and Bilayer Coarse-Grained Simulations. Journal of Chemical Information and Modeling, 2014, 54, 1003-1009.	2.5	47
130	Multidimensional umbrella sampling and replicaâ€exchange molecular dynamics simulations for structure prediction of transmembrane helix dimers. Journal of Computational Chemistry, 2014, 35, 300-308.	1.5	32
131	Probing the U-Shaped Conformation of Caveolin-1 in a Bilayer. Biophysical Journal, 2014, 106, 1371-1380.	0.2	33
132	E.Âcoli Outer Membrane and Interactions with OmpLA. Biophysical Journal, 2014, 106, 2493-2502.	0.2	128
133	Assessing smectic liquid-crystal continuum models for elastic bilayer deformations. Chemistry and Physics of Lipids, 2013, 169, 19-26.	1.5	20
134	Molecular Dynamics and NMR Spectroscopy Studies of E.Âcoli Lipopolysaccharide Structure and Dynamics. Biophysical Journal, 2013, 105, 1444-1455.	0.2	153
135	Ligand Binding Site Detection by Local Structure Alignment and Its Performance Complementarity. Journal of Chemical Information and Modeling, 2013, 53, 2462-2470.	2.5	21
136	CHARMM-GUI Micelle Builder for Pure/Mixed Micelle and Protein/Micelle Complex Systems. Journal of Chemical Information and Modeling, 2013, 53, 2171-2180.	2.5	99
137	Two Dimensional Window Exchange Umbrella Sampling for Transmembrane Helix Assembly. Journal of Chemical Theory and Computation, 2013, 9, 13-17.	2.3	38
138	CHARMM-GUI Ligand Binder for Absolute Binding Free Energy Calculations and Its Application. Journal of Chemical Information and Modeling, 2013, 53, 267-277.	2.5	71
139	NMR-Based Simulation Studies of Pf1 Coat Protein in Explicit Membranes. Biophysical Journal, 2013, 105, 691-698.	0.2	18
140	Restricted N-glycan Conformational Space in the PDB and Its Implication in Glycan Structure Modeling. PLoS Computational Biology, 2013, 9, e1002946.	1.5	29
141	Glycan fragment database: a database of PDB-based glycan 3D structures. Nucleic Acids Research, 2012, 41, D470-D474.	6.5	49
142	Transmembrane Helix Assembly by Window Exchange Umbrella Sampling. Physical Review Letters, 2012, 108, 108102.	2.9	61
143	Identification of Ligand Templates using Local Structure Alignment for Structure-Based Drug Design. Journal of Chemical Information and Modeling, 2012, 52, 2784-2795.	2.5	25
144	Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains. Journal of Physical Chemistry B, 2012, 116, 9424-9431.	1.2	140

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145	NMR Observable-Based Structure Refinement of DAP12-NKG2C Activating Immunoreceptor Complex in Explicit Membranes. Biophysical Journal, 2012, 102, L27-L29.	0.2	25
146	Influence of Hydrophobic Mismatch on Structures and Dynamics of Gramicidin A and Lipid Bilayers. Biophysical Journal, 2012, 102, 1551-1560.	0.2	92
147	Application of Binding Free Energy Calculations to Prediction of Binding Modes and Affinities of MDM2 and MDMX Inhibitors. Journal of Chemical Information and Modeling, 2012, 52, 1821-1832.	2.5	41
148	Web interface for brownian dynamics simulation of ion transport and its applications to betaâ€barrel pores. Journal of Computational Chemistry, 2012, 33, 331-339.	1.5	43
149	Brownian Dynamics Simulations of Ion Transport through the VDAC. Biophysical Journal, 2011, 100, 611-619.	0.2	56
150	Molecular Dynamics Studies of Ion Permeation in VDAC. Biophysical Journal, 2011, 100, 602-610.	0.2	78
151	Solid-State NMR Ensemble Dynamics as a Mediator between Experiment and Simulation. Biophysical Journal, 2011, 100, 2922-2928.	0.2	17
152	Transmembrane Helix Orientation and Dynamics: Insights from Ensemble Dynamics with Solid-State NMR Observables. Biophysical Journal, 2011, 100, 2913-2921.	0.2	29
153	Transmembrane Signaling of Chemotaxis Receptor Tar: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2011, 100, 2955-2963.	0.2	33
154	Membrane Tension, Lipid Adaptation, Conformational Changes, and Energetics in MscL Gating. Biophysical Journal, 2011, 101, 671-679.	0.2	16
155	Orientation of Fluorescent Lipid Analogue BODIPY-PC to Probe Lipid Membrane Properties: Insights from Molecular Dynamics Simulations. Journal of Physical Chemistry B, 2011, 115, 6157-6165.	1.2	26
156	Novel Pyrrolopyrimidine-Based Î±-Helix Mimetics: Cell-Permeable Inhibitors of Proteinâ˜Protein Interactions. Journal of the American Chemical Society, 2011, 133, 676-679.	6.6	121
157	Glycan reader: Automated sugar identification and simulation preparation for carbohydrates and glycoproteins. Journal of Computational Chemistry, 2011, 32, 3135-3141.	1.5	172
158	Protegrinâ€1 orientation and physicochemical properties in membrane bilayers studied by potential of mean force calculations. Journal of Computational Chemistry, 2010, 31, 2859-2867.	1.5	20
159	A Repulsive Electrostatic Mechanism for Protein Export through the Type III Secretion Apparatus. Biophysical Journal, 2010, 98, 452-461.	0.2	18
160	Revisiting Hydrophobic Mismatch with Free Energy Simulation Studies of Transmembrane Helix Tilt and Rotation. Biophysical Journal, 2010, 99, 175-183.	0.2	106
161	Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. Journal of Physical Chemistry B, 2010, 114, 13342-13348.	1.2	109
162	Structural, NMR Spectroscopic, and Computational Investigation of Hemin Loading in the Hemophore HasAp from Pseudomonas aeruginosa. Journal of the American Chemical Society, 2010, 132, 9857-9872.	6.6	82

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163	NMR characterization of hydrophobic collapses in amyloidogenic unfolded states and their implications for amyloid formation. Biochemical and Biophysical Research Communications, 2010, 396, 800-805.	1.0	1
164	Betaâ€hairpin restraint potentials for calculations of potentials of mean force as a function of betaâ€hairpin tilt, rotation, and distance. Journal of Computational Chemistry, 2009, 30, 1334-1343.	1.5	8
165	Novel free energy calculations to explore mechanisms and energetics of membrane protein structure and function. Journal of Computational Chemistry, 2009, 30, 1622-1633.	1.5	20
166	Molecular dynamics studies on structure and dynamics of phospholamban monomer and pentamer in membranes. Proteins: Structure, Function and Bioinformatics, 2009, 76, 86-98.	1.5	22
167	CHARMM-GUI Membrane Builder for Mixed Bilayers and Its Application to Yeast Membranes. Biophysical Journal, 2009, 97, 50-58.	0.2	1,346
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