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## List of Publications by Year in descending order

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206  
papers

25,721  
citations

22153

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8396

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docs citations

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times ranked

19029  
citing authors

#	ARTICLE	IF	CITATIONS
1	Comparative Molecular Dynamics Simulation Studies of Realistic Eukaryotic, Prokaryotic, and Archaeal Membranes. <i>Journal of Chemical Information and Modeling</i> , 2022, 62, 1036-1051.	5.4	32
2	Structural basis of neuropeptide Y signaling through Y1 receptor. <i>Nature Communications</i> , 2022, 13, 853.	12.8	20
3	Foldable Detergents for Membrane Protein Study: Importance of Detergent Core Flexibility in Protein Stabilization. <i>Chemistry - A European Journal</i> , 2022, 28, .	3.3	13
4	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. <i>Journal of Chemical Theory and Computation</i> , 2022, 18, 479-493.	5.3	53
5	<scp>CHARMMâ€GUI</scp> Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. <i>Journal of Computational Chemistry</i> , 2022, 43, 359-375.	3.3	24
6	Molecular Condensate in a Membrane: A Tugging Game between Hydrophobicity and Polarity with Its Biological Significance. <i>Langmuir</i> , 2022, 38, 5955-5962.	3.5	1
7	Evolutionary balance between foldability and functionality of a glucose transporter. <i>Nature Chemical Biology</i> , 2022, 18, 713-723.	8.0	13
8	A systematic analysis of proteinâ€carbohydrate interactions in the Protein Data Bank. <i>Glycobiology</i> , 2021, 31, 126-136.	2.5	13
9	Structure, Dynamics, and Interactions of GPI-Anchored Human Glypican-1 with Heparan Sulfates in a Membrane. <i>Glycobiology</i> , 2021, 31, 593-602.	2.5	6
10	Ligand-Binding-Site Refinement to Generate Reliable Holo Protein Structure Conformations from Apo Structures. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 535-546.	5.4	19
11	Influences of <i>Vibrio cholerae</i> Lipid A Types on LPS Bilayer Properties. <i>Journal of Physical Chemistry B</i> , 2021, 125, 2105-2112.	2.6	10
12	Biomechanical characterization of SARS-CoV-2 spike RBD and human ACE2 protein-protein interaction. <i>Biophysical Journal</i> , 2021, 120, 1011-1019.	0.5	87
13	Structure, Dynamics, Receptor Binding, and Antibody Binding of the Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein in a Viral Membrane. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2479-2487.	5.3	62
14	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Proteinâ€Lipid Modulations in Archaeal Membranes. <i>Journal of Physical Chemistry B</i> , 2021, 125, 4714-4725.	2.6	10
15	Site-Specific Lipidation Enhances IFITM3 Membrane Interactions and Antiviral Activity. <i>ACS Chemical Biology</i> , 2021, 16, 844-856.	3.4	22
16	CHARMM-GUI Polymer Builder for Modeling and Simulation of Synthetic Polymers. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 2431-2443.	5.3	58
17	Additive CHARMM36 Force Field for Nonstandard Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3554-3570.	5.3	39
18	Structural Insight into Phospholipid Transport by the MlaFEBD Complex from <i>P. aeruginosa</i> . <i>Journal of Molecular Biology</i> , 2021, 433, 166986.	4.2	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. <i>Acta Biomaterialia</i> , 2021, 128, 393-407.	8.3	15
20	CHARMM-GUI <i>LBS Finder &amp; Refiner</i> for Ligand Binding Site Prediction and Refinement. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 3744-3751.	5.4	9
21	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 4145-4151.	5.4	24
22	CHARMM-GUI Membrane Builder for Lipid Nanoparticles with Ionizable Cationic Lipids and PEGylated Lipids. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5192-5202.	5.4	25
23	Biophysical characterization of nicotinic receptor interactions using atomic force microscopy. <i>FASEB BioAdvances</i> , 2021, 3, 1034-1042.	2.4	2
24	Structural basis for the association of PLEKHA7 with membrane-embedded phosphatidylinositol lipids. <i>Structure</i> , 2021, 29, 1029-1039.e3.	3.3	18
25	Dynamic Interactions of Fully Glycosylated SARS-CoV-2 Spike Protein with Various Antibodies. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 6559-6569.	5.3	13
26	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 831-839.	5.4	59
27	Accurate simulation of surfaces and interfaces of ten FCC metals and steel using Lennard-Jones potentials. <i>Npj Computational Materials</i> , 2021, 7, .	8.7	28
28	Developing initial conditions for simulations of asymmetric membranes: a practical recommendation. <i>Biophysical Journal</i> , 2021, 120, 5041-5059.	0.5	14
29	Systematic Assessment of Accessibility to the Surface of <i>Staphylococcus aureus</i> . <i>ACS Chemical Biology</i> , 2021, 16, 2527-2536.	3.4	15
30	CHARMM-GUI <i>Ligand Designer</i> for Template-Based Virtual Ligand Design in a Binding Site. <i>Journal of Chemical Information and Modeling</i> , 2021, 61, 5336-5342.	5.4	8
31	Differential Interactions between Human ACE2 and Spike RBD of SARS-CoV-2 Variants of Concern. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 7972-7979.	5.3	57
32	CHARMM-GUI DEER facilitator for spin-pair distance distribution calculations and preparation of restrained ensemble molecular dynamics simulations. <i>Journal of Computational Chemistry</i> , 2020, 41, 415-420.	3.3	19
33	Preferred conformations of lipooligosaccharides and oligosaccharides of <i>Moraxella catarrhalis</i> . <i>Glycobiology</i> , 2020, 30, 86-94.	2.5	6
34	GlyMDB: Glycan Microarray Database and analysis toolset. <i>Bioinformatics</i> , 2020, 36, 2438-2442.	4.1	14
35	Calcium and hydroxyapatite binding site of human vitronectin provides insights to abnormal deposit formation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2020, 117, 18504-18510.	7.1	11
36	CHARMM-GUI supports the Amber force fields. <i>Journal of Chemical Physics</i> , 2020, 153, 035103.	3.0	175

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37	CHARMM-GUI Free Energy Calculator for Absolute and Relative Ligand Solvation and Binding Free Energy Simulations. <i>Journal of Chemical Theory and Computation</i> , 2020, 16, 7207-7218.	5.3	57
38	Conformational States of the Cytoprotective Protein Bcl-xL. <i>Biophysical Journal</i> , 2020, 119, 1324-1334.	0.5	10
39	Experimentally Guided Computational Methods Yield Highly Accurate Insights into Transmembrane Interactions within the T Cell Receptor Complex. <i>Journal of Physical Chemistry B</i> , 2020, 124, 10303-10310.	2.6	1
40	Modeling and Simulation of Bacterial Outer Membranes with Lipopolysaccharides and Enterobacterial Common Antigen. <i>Journal of Physical Chemistry B</i> , 2020, 124, 5948-5956.	2.6	26
41	Mutually constructive roles of Ail and LPS in <i>Yersinia pestis</i> serum survival. <i>Molecular Microbiology</i> , 2020, 114, 510-520.	2.5	19
42	Developing a Fully Glycosylated Full-Length SARS-CoV-2 Spike Protein Model in a Viral Membrane. <i>Journal of Physical Chemistry B</i> , 2020, 124, 7128-7137.	2.6	240
43	Dynamics and Interactions of GPI-Linked lynx1 Protein with/without Nicotinic Acetylcholine Receptor in Membrane Bilayers. <i>Journal of Physical Chemistry B</i> , 2020, 124, 4017-4025.	2.6	7
44	Improving Protein-Ligand Docking Results with High-Throughput Molecular Dynamics Simulations. <i>Journal of Chemical Information and Modeling</i> , 2020, 60, 2189-2198.	5.4	152
45	Cooperativity in Proteasome Core Particle Maturation. <i>IScience</i> , 2020, 23, 101090.	4.1	5
46	Molecular Simulations of Gram-Negative Bacterial Membranes Come of Age. <i>Annual Review of Physical Chemistry</i> , 2020, 71, 171-188.	10.8	44
47	Broadening Activity of Polymyxin by Quaternary Ammonium Grafting. <i>ACS Infectious Diseases</i> , 2020, 6, 1427-1435.	3.8	9
48	Escherichia coli O176 LPS structure and dynamics: A NMR spectroscopy and MD simulation study. <i>Current Research in Structural Biology</i> , 2020, 2, 79-88.	2.2	8
49	A mechano-reactive coarse-grained model of the blood-clotting agent von Willebrand factor. <i>Journal of Chemical Physics</i> , 2019, 151, 124905.	3.0	13
50	Ligand-Binding-Site Structure Refinement Using Molecular Dynamics with Restraints Derived from Predicted Binding Site Templates. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6524-6535.	5.3	16
51	Quantitative Characterization of Protein-Lipid Interactions by Free Energy Simulation between Binary Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 6491-6503.	5.3	7
52	CHARMM-GUI Glycan Modeler for modeling and simulation of carbohydrates and glycoconjugates. <i>Glycobiology</i> , 2019, 29, 320-331.	2.5	222
53	CHARMM-GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. <i>Journal of Computational Chemistry</i> , 2019, 40, 893-899.	3.3	42
54	Modeling of Specific Lipopolysaccharide Binding Sites on a Gram-Negative Porin. <i>Journal of Physical Chemistry B</i> , 2019, 123, 5700-5708.	2.6	11

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55	Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation. <i>Biophysical Journal</i> , 2019, 116, 1095-1104.	0.5	27
56	Stalis : A Computational Method for Template-Based Ab Initio Ligand Design. <i>Journal of Computational Chemistry</i> , 2019, 40, 1622-1632.	3.3	4
57	U-shaped caveolin-1 conformations are tightly regulated by hydrogen bonds with lipids. <i>Journal of Computational Chemistry</i> , 2019, 40, 1570-1577.	3.3	8
58	Clustering and dynamics of crowded proteins near membranes and their influence on membrane bending. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2019, 116, 24562-24567.	7.1	52
59	Analysis of Lipid Order States and Domains in Lipid Bilayer Simulations. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 688-697.	5.3	12
60	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 775-786.	5.3	388
61	Structural Conservation and Effects of Alterations in T Cell Receptor Transmembrane Interfaces. <i>Biophysical Journal</i> , 2018, 114, 1030-1035.	0.5	8
62	Multiple Conformational States Contribute to the 3D Structure of a Glucan Decasaccharide: A Combined SAXS and MD Simulation Study. <i>Journal of Physical Chemistry B</i> , 2018, 122, 1169-1175.	2.6	9
63	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. <i>Nature Chemical Biology</i> , 2018, 14, 489-496.	8.0	39
64	Molecular Basis of Aqueous-like Activity of Lipase Treated with Glucose-Headed Surfactant in Organic Solvent. <i>Journal of Physical Chemistry B</i> , 2018, 122, 10659-10668.	2.6	3
65	Insight into Elongation Stages of Peptidoglycan Processing in Bacterial Cytoplasmic Membranes. <i>Scientific Reports</i> , 2018, 8, 17704.	3.3	6
66	Long-ranged Protein-glycan Interactions Stabilize von Willebrand Factor A2 Domain from Mechanical Unfolding. <i>Scientific Reports</i> , 2018, 8, 16017.	3.3	8
67	Structure of an EIIc sugar transporter trapped in an inward-facing conformation. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 5962-5967.	7.1	18
68	Augmenting the antinociceptive effects of nicotinic acetylcholine receptor activity through lynx1 modulation. <i>PLoS ONE</i> , 2018, 13, e0199643.	2.5	18
69	Synthetic Immunotherapeutics against Gram-negative Pathogens. <i>Cell Chemical Biology</i> , 2018, 25, 1185-1194.e5.	5.2	29
70	Simulation Study of Occk5 Functional Properties in <i>Pseudomonas aeruginosa</i> Outer Membranes. <i>Journal of Physical Chemistry B</i> , 2018, 122, 8185-8192.	2.6	12
71	Quantitative Characterization of Cholesterol Partitioning between Binary Bilayers. <i>Journal of Chemical Theory and Computation</i> , 2018, 14, 2829-2833.	5.3	14
72	Biophysical and functional characterization of Norrin signaling through Frizzled4. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2018, 115, 8787-8792.	7.1	30

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73	Refinement of OprH-LPS Interactions by Molecular Simulations. <i>Biophysical Journal</i> , 2017, 112, 346-355.	0.5	50
74	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. <i>Current Opinion in Structural Biology</i> , 2017, 43, 131-140.	5.7	42
75	CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. <i>Journal of Computational Chemistry</i> , 2017, 38, 1879-1886.	3.3	311
76	Molecular Simulation and Biochemical Studies Support an Elevator-type Transport Mechanism in $\Delta$ IC. <i>Biophysical Journal</i> , 2017, 112, 2249-2252.	0.5	7
77	Simulating Biomolecules: Festschrift to commemorate the 60th birthday of Charles L. Brooks III. <i>Journal of Computational Chemistry</i> , 2017, 38, 1111-1113.	3.3	0
78	G-LoSA for Prediction of Protein-Ligand Binding Sites and Structures. <i>Methods in Molecular Biology</i> , 2017, 1611, 97-108.	0.9	15
79	Conformational Dynamics of the Lipopolysaccharide from <i>Escherichia coli</i> O91 Revealed by Nuclear Magnetic Resonance Spectroscopy and Molecular Simulations. <i>Biochemistry</i> , 2017, 56, 3826-3839.	2.5	17
80	Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation. <i>Biophysical Journal</i> , 2017, 112, 1185-1197.	0.5	48
81	Gramicidin A Channel Formation Induces Local Lipid Redistribution II: A 3D Continuum Elastic Model. <i>Biophysical Journal</i> , 2017, 112, 1198-1213.	0.5	22
82	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. <i>Journal of Physical Chemistry B</i> , 2017, 121, 3718-3723.	2.6	24
83	Effects of N-Glycan Composition on Structure and Dynamics of IgG1 Fc and Their Implications for Antibody Engineering. <i>Scientific Reports</i> , 2017, 7, 12659.	3.3	31
84	Characterizing Residue-Bilayer Interactions Using Gramicidin A as a Scaffold and Tryptophan Substitutions as Probes. <i>Journal of Chemical Theory and Computation</i> , 2017, 13, 5054-5064.	5.3	14
85	Heterogeneity in non-epitope loop sequence and outer membrane protein complexes alters antibody binding to the major porin protein PorB in serogroup B <i>Neisseria meningitidis</i> . <i>Molecular Microbiology</i> , 2017, 105, 934-953.	2.5	15
86	CHARMM-GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. <i>Journal of Computational Chemistry</i> , 2017, 38, 2354-2363.	3.3	150
87	Glycan Reader is improved to recognize most sugar types and chemical modifications in the Protein Data Bank. <i>Bioinformatics</i> , 2017, 33, 3051-3057.	4.1	94
88	Transmembrane features governing Fc receptor CD16A assembly with CD16A signaling adaptor molecules. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2017, 114, E5645-E5654.	7.1	32
89	CHARMM-GUI 10 years for biomolecular modeling and simulation. <i>Journal of Computational Chemistry</i> , 2017, 38, 1114-1124.	3.3	224
90	Asymmetric Cryo-EM Structure of Anthrax Toxin Protective Antigen Pore with Lethal Factor N-Terminal Domain. <i>Toxins</i> , 2017, 9, 298.	3.4	12

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91	Transmembrane motions of PglB induced by LLO are coupled with EL5 loop conformational changes necessary for OST activity. <i>Glycobiology</i> , 2017, 27, 734-742.	2.5	6
92	Preferred conformations of N-glycan core pentasaccharide in solution and in glycoproteins. <i>Glycobiology</i> , 2016, 26, cwv083.	2.5	34
93	L-Met Activates Arabidopsis GLR Ca <sup>2+</sup> Channels Upstream of ROS Production and Regulates Stomatal Movement. <i>Cell Reports</i> , 2016, 17, 2553-2561.	6.4	71
94	CHARMM-GUI Input Generator for NAMD, Gromacs, Amber, Openmm, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. <i>Biophysical Journal</i> , 2016, 110, 641a.	0.5	63
95	The Structure of a Sugar Transporter of the Glucose EIC Superfamily Provides Insight into the Elevator Mechanism of Membrane Transport. <i>Structure</i> , 2016, 24, 956-964.	3.3	37
96	Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues. <i>Biophysical Journal</i> , 2016, 111, 1600-1603.	0.5	0
97	An extensive simulation study of lipid bilayer properties with different head groups, acyl chain lengths, and chain saturations. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 3093-3104.	2.6	51
98	A conserved $\alpha$ -helix transmembrane interface forms the core of a compact T-cell receptor-CD3 structure within the membrane. <i>Proceedings of the National Academy of Sciences of the United States of America</i> , 2016, 113, E6649-E6658.	7.1	40
99	Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. <i>Journal of Physical Chemistry B</i> , 2016, 120, 11761-11772.	2.6	47
100	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. <i>Biophysical Journal</i> , 2016, 111, 1750-1760.	0.5	88
101	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. <i>Biophysical Journal</i> , 2016, 111, 1987-1999.	0.5	41
102	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. <i>Biophysical Journal</i> , 2016, 110, 2698-2709.	0.5	65
103	Molecular dynamics simulation strategies for protein-micelle complexes. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 1566-1572.	2.6	19
104	Challenges in structural approaches to cell modeling. <i>Journal of Molecular Biology</i> , 2016, 428, 2943-2964.	4.2	51
105	LoSA: An efficient computational tool for local structure-centric biological studies and drug design. <i>Protein Science</i> , 2016, 25, 865-876.	7.6	33
106	Converting One-Face $\alpha$ -Helix Mimetics into Amphiphilic $\alpha$ -Helix Mimetics as Potent Inhibitors of Protein-Protein Interactions. <i>ACS Combinatorial Science</i> , 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. <i>Journal of Chemical Theory and Computation</i> , 2016, 12, 405-413.	5.3	2,567
108	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. <i>Biophysical Journal</i> , 2016, 110, 930-938.	0.5	64

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109	Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2016, 1858, 1635-1651.	2.6	111
110	How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 3466-3477.	5.3	64
111	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. <i>Glycobiology</i> , 2015, 26, cwv101.	2.5	15
112	Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 1255-1266.	5.3	13
113	Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes. <i>Biophysical Journal</i> , 2015, 108, 1954-1962.	0.5	11
114	GS-align for glycan structure alignment and similarity measurement. <i>Bioinformatics</i> , 2015, 31, 2653-2659.	4.1	11
115	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. <i>Scientific Reports</i> , 2015, 5, 8926.	3.3	187
116	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. <i>Journal of Chemical Theory and Computation</i> , 2015, 11, 4486-4494.	5.3	340
117	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. <i>Biophysical Journal</i> , 2015, 109, 2012-2022.	0.5	89
118	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. <i>Biophysical Journal</i> , 2015, 109, 2090-2100.	0.5	18
119	Transmembrane Complexes of DAP12 Crystallized in Lipid Membranes Provide Insights into Control of Oligomerization in Immunoreceptor Assembly. <i>Cell Reports</i> , 2015, 11, 1184-1192.	6.4	20
120	Lipopolysaccharide Membrane Building and Simulation. <i>Methods in Molecular Biology</i> , 2015, 1273, 391-406.	0.9	41
121	STAnalyzer: A web-based user interface for simulation trajectory analysis. <i>Journal of Computational Chemistry</i> , 2014, 35, 957-963.	3.3	12
122	Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase. <i>Biophysical Journal</i> , 2014, 107, 1885-1895.	0.5	21
123	CHARMM-GUI Membrane Builder toward realistic biological membrane simulations. <i>Journal of Computational Chemistry</i> , 2014, 35, 1997-2004.	3.3	1,802
124	CHARMM-GUI PDB Manipulator for Advanced Modeling and Simulations of Proteins Containing Nonstandard Residues. <i>Advances in Protein Chemistry and Structural Biology</i> , 2014, 96, 235-265.	2.3	214
125	Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. <i>Journal of Physical Chemistry B</i> , 2014, 118, 4315-4325.	2.6	38
126	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. <i>Biochimica Et Biophysica Acta - Biomembranes</i> , 2014, 1838, 2520-2529.	2.6	82

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127	Potential pharmacological chaperones targeting cancer-associated MCL-1 and Parkinson disease-associated $\alpha$ -synuclein. Proceedings of the National Academy of Sciences of the United States of America, 2014, 111, 11007-11012.	7.1	55
128	Theory of Adaptive Optimization for Umbrella Sampling. Journal of Chemical Theory and Computation, 2014, 10, 2719-2728.	5.3	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.	5.4	47
130	Multidimensional umbrella sampling and replica-exchange molecular dynamics simulations for structure prediction of transmembrane helix dimers. Journal of Computational Chemistry, 2014, 35, 300-308.	3.3	32
131	Probing the U-Shaped Conformation of Caveolin-1 in a Bilayer. Biophysical Journal, 2014, 106, 1371-1380.	0.5	33
132	E. Coli Outer Membrane and Interactions with OmpLA. Biophysical Journal, 2014, 106, 2493-2502.	0.5	128
133	Assessing smectic liquid-crystal continuum models for elastic bilayer deformations. Chemistry and Physics of Lipids, 2013, 169, 19-26.	3.2	20
134	Molecular Dynamics and NMR Spectroscopy Studies of E. Coli Lipopolysaccharide Structure and Dynamics. Biophysical Journal, 2013, 105, 1444-1455.	0.5	153
135	Ligand Binding Site Detection by Local Structure Alignment and Its Performance Complementarity. Journal of Chemical Information and Modeling, 2013, 53, 2462-2470.	5.4	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.	5.4	99
137	Two Dimensional Window Exchange Umbrella Sampling for Transmembrane Helix Assembly. Journal of Chemical Theory and Computation, 2013, 9, 13-17.	5.3	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.	5.4	71
139	NMR-Based Simulation Studies of Pf1 Coat Protein in Explicit Membranes. Biophysical Journal, 2013, 105, 691-698.	0.5	18
140	Restricted N-glycan Conformational Space in the PDB and Its Implication in Glycan Structure Modeling. PLoS Computational Biology, 2013, 9, e1002946.	3.2	29
141	Glycan fragment database: a database of PDB-based glycan 3D structures. Nucleic Acids Research, 2012, 41, D470-D474.	14.5	49
142	Transmembrane Helix Assembly by Window Exchange Umbrella Sampling. Physical Review Letters, 2012, 108, 108102.	7.8	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.	5.4	25
144	Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains. Journal of Physical Chemistry B, 2012, 116, 9424-9431.	2.6	140

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145	NMR Observable-Based Structure Refinement of DAP12-NKG2C Activating Immunoreceptor Complex in Explicit Membranes. <i>Biophysical Journal</i> , 2012, 102, L27-L29.	0.5	25
146	Influence of Hydrophobic Mismatch on Structures and Dynamics of Gramicidin A and Lipid Bilayers. <i>Biophysical Journal</i> , 2012, 102, 1551-1560.	0.5	92
147	Application of Binding Free Energy Calculations to Prediction of Binding Modes and Affinities of MDM2 and MDMX Inhibitors. <i>Journal of Chemical Information and Modeling</i> , 2012, 52, 1821-1832.	5.4	41
148	Web interface for brownian dynamics simulation of ion transport and its applications to beta-barrel pores. <i>Journal of Computational Chemistry</i> , 2012, 33, 331-339.	3.3	43
149	Brownian Dynamics Simulations of Ion Transport through the VDAC. <i>Biophysical Journal</i> , 2011, 100, 611-619.	0.5	56
150	Molecular Dynamics Studies of Ion Permeation in VDAC. <i>Biophysical Journal</i> , 2011, 100, 602-610.	0.5	78
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