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List of Publications by Year in descending order

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206 papers	25,721 citations	22153 59 h-index	8396 147 g-index
226 all docs	226 docs citations	226 times ranked	19029 citing authors

#	Article	IF	Citations
1	CHARMMâ€GUI: A webâ€based graphical user interface for CHARMM. Journal of Computational Chemistry, 2008, 29, 1859-1865.	3.3	5,402
2	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.	5.3	2,567
3	CHARMM-GUIMembrane Buildertoward realistic biological membrane simulations. Journal of Computational Chemistry, 2014, 35, 1997-2004.	3.3	1,802
4	CHARMM-GUI Membrane Builder for Mixed Bilayers and Its Application to Yeast Membranes. Biophysical Journal, 2009, 97, 50-58.	0.5	1,346
5	Automated Builder and Database of Protein/Membrane Complexes for Molecular Dynamics Simulations. PLoS ONE, 2007, 2, e880.	2.5	930
6	Generalized born model with a simple smoothing function. Journal of Computational Chemistry, 2003, 24, 1691-1702.	3.3	642
7	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. Journal of Computational Chemistry, 2004, 25, 265-284.	3.3	523
8	Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. Computer Physics Communications, 1998, 111, 59-75.	7.5	500
9	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. Journal of Chemical Theory and Computation, 2019, 15, 775-786.	5.3	388
10	An Implicit Membrane Generalized Born Theory for the Study of Structure, Stability, and Interactions of Membrane Proteins. Biophysical Journal, 2003, 85, 2900-2918.	0.5	384
11	Theoretical and computational models of biological ion channels. Quarterly Reviews of Biophysics, 2004, 37, 15-103.	5.7	362
12	Ion Permeation and Selectivity of OmpF Porin: A Theoretical Study Based on Molecular Dynamics, Brownian Dynamics, and Continuum Electrodiffusion Theory. Journal of Molecular Biology, 2002, 322, 851-869.	4.2	353
13	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. Journal of Chemical Theory and Computation, 2015, 11, 4486-4494.	5.3	340
14	Balancing Solvation and Intramolecular Interactions:Â Toward a Consistent Generalized Born Force Field. Journal of the American Chemical Society, 2006, 128, 3728-3736.	13.7	327
15	CHARMM-GUI ligand reader and modeler for CHARMM force field generation of small molecules. Journal of Computational Chemistry, 2017, 38, 1879-1886.	3.3	311
16	Ions and Counterions in a Biological Channel: A Molecular Dynamics Simulation of OmpF Porin from Escherichia coli in an Explicit Membrane with 1M KCl Aqueous Salt Solution. Journal of Molecular Biology, 2002, 319, 1177-1197.	4.2	252
17	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.	2.6	240
18	A Grand Canonical Monte Carloâ€“Brownian Dynamics Algorithm for Simulating Ion Channels. Biophysical Journal, 2000, 79, 788-801.	0.5	226

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19	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	3.3	224
20	Generalized solvent boundary potential for computer simulations. Journal of Chemical Physics, 2001, 114, 2924-2937.	3.0	223
21	CHARMM-GUIGlycan Modelerfor modeling and simulation of carbohydrates and glycoconjugates. Glycobiology, 2019, 29, 320-331.	2.5	222
22	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.	2.3	214
23	PBEQ-Solver for online visualization of electrostatic potential of biomolecules. Nucleic Acids Research, 2008, 36, W270-W275.	14.5	194
24	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. Scientific Reports, 2015, 5, 8926.	3.3	187
25	Ion Permeation through the Î±-Hemolysin Channel: Theoretical Studies Based on Brownian Dynamics and Poisson-Nernst-Plank Electrodiffusion Theory. Biophysical Journal, 2004, 87, 2299-2309.	0.5	179
26	CHARMM-GUI supports the Amber force fields. Journal of Chemical Physics, 2020, 153, 035103.	3.0	175
27	Glycan reader: Automated sugar identification and simulation preparation for carbohydrates and glycoproteins. Journal of Computational Chemistry, 2011, 32, 3135-3141.	3.3	172
28	Ion Channels, Permeation, and Electrostatics: Insight into the Function of KcsA. Biochemistry, 2000, 39, 13295-13306.	2.5	167
29	Interfacial folding and membrane insertion of designed peptides studied by molecular dynamics simulations. Proceedings of the National Academy of Sciences of the United States of America, 2005, 102, 6771-6776.	7.1	167
30	Molecular Dynamics and NMR Spectroscopy Studies of E.Âcoli Lipopolysaccharide Structure and Dynamics. Biophysical Journal, 2013, 105, 1444-1455.	0.5	153
31	Improving Protein-Ligand Docking Results with High-Throughput Molecular Dynamics Simulations. Journal of Chemical Information and Modeling, 2020, 60, 2189-2198.	5.4	152
32	CHARMMâ€GUI Martini Maker for modeling and simulation of complex bacterial membranes with lipopolysaccharides. Journal of Computational Chemistry, 2017, 38, 2354-2363.	3.3	150
33	Improving the CHARMM Force Field for Polyunsaturated Fatty Acid Chains. Journal of Physical Chemistry B, 2012, 116, 9424-9431.	2.6	140
34	Implicit solvation based on generalized Born theory in different dielectric environments. Journal of Chemical Physics, 2004, 120, 903-911.	3.0	136
35	E.Âcoli Outer Membrane and Interactions with OmpLA. Biophysical Journal, 2014, 106, 2493-2502.	0.5	128
36	Novel Pyrrolopyrimidine-Based Î±-Helix Mimetics: Cell-Permeable Inhibitors of Proteinâ˜Protein Interactions. Journal of the American Chemical Society, 2011, 133, 676-679.	13.7	121

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37	Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1635-1651.	2.6	111
38	Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. Journal of Physical Chemistry B, 2010, 114, 13342-13348.	2.6	109
39	Revisiting Hydrophobic Mismatch with Free Energy Simulation Studies of Transmembrane Helix Tilt and Rotation. Biophysical Journal, 2010, 99, 175-183.	0.5	106
40	Optimized atomic radii for protein continuum electrostatics solvation forces. Biophysical Chemistry, 1999, 78, 89-96.	2.8	99
41	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
42	Glycan Reader is improved to recognize most sugar types and chemical modifications in the Protein Data Bank. Bioinformatics, 2017, 33, 3051-3057.	4.1	94
43	Influence of Hydrophobic Mismatch on Structures and Dynamics of Gramicidin A and Lipid Bilayers. Biophysical Journal, 2012, 102, 1551-1560.	0.5	92
44	Imaging the Electrostatic Potential of Transmembrane Channels: Atomic Probe Microscopy of OmpF Porin. Biophysical Journal, 2002, 82, 1667-1676.	0.5	90
45	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. Biophysical Journal, 2015, 109, 2012-2022.	0.5	89
46	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. Biophysical Journal, 2016, 111, 1750-1760.	0.5	88
47	Biomechanical characterization of SARS-CoV-2 spike RBD and human ACE2 protein-protein interaction. Biophysical Journal, 2021, 120, 1011-1019.	0.5	87
48	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.	13.7	82
49	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 2520-2529.	2.6	82
50	Molecular Dynamics Studies of Ion Permeation in VDAC. Biophysical Journal, 2011, 100, 602-610.	0.5	78
51	Membrane Assembly of Simple Helix Homo-Oligomers Studied via Molecular Dynamics Simulations. Biophysical Journal, 2007, 92, 854-863.	0.5	75
52	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
53	L-Met Activates Arabidopsis GLR Ca2+ Channels Upstream of ROS Production and Regulates Stomatal Movement. Cell Reports, 2016, 17, 2553-2561.	6.4	71
54	Brownian dynamics simulations of ions channels: A general treatment of electrostatic reaction fields for molecular pores of arbitrary geometry. Journal of Chemical Physics, 2001, 115, 4850-4861.	3.0	69

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55	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. Journal of Computational Chemistry, 2005, 26, 1565-1578.	3.3	67
56	Differences in the Electrostatic Surfaces of the Type III Secretion Needle Proteins PrgI, BsaL, and MxiH. Journal of Molecular Biology, 2007, 371, 1304-1314.	4.2	66
57	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. Biophysical Journal, 2016, 110, 2698-2709.	0.5	65
58	De novo Folding of Membrane Proteins: An Exploration of the Structure and NMR Properties of the fd Coat Protein. Journal of Molecular Biology, 2004, 337, 513-519.	4.2	64
59	Generation and application of new rat monoclonal antibodies against synthetic FLAG and OLLAS tags for improved immunodetection. Journal of Immunological Methods, 2008, 331, 27-38.	1.4	64
60	How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?. Journal of Chemical Theory and Computation, 2015, 11, 3466-3477.	5.3	64
61	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. Biophysical Journal, 2016, 110, 930-938.	0.5	64
62	Peptide and Protein Folding and Conformational Equilibria: Theoretical Treatment of Electrostatics and Hydrogen Bonding with Implicit Solvent Models. Advances in Protein Chemistry, 2005, 72, 173-198.	4.4	63
63	CHARMM-GUI Input Generator for NAMD, Gromacs, Amber, Openmm, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. Biophysical Journal, 2016, 110, 641a.	0.5	63
64	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.	5.3	62
65	Transmembrane Helix Assembly by Window Exchange Umbrella Sampling. Physical Review Letters, 2012, 108, 108102.	7.8	61
66	Refinement of NMR Structures Using Implicit Solvent and Advanced Sampling Techniques. Journal of the American Chemical Society, 2004, 126, 16038-16047.	13.7	60
67	Transmembrane Helix Tilting: Insights from Calculating the Potential of Mean Force. Physical Review Letters, 2008, 100, 018103.	7.8	60
68	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. Journal of Chemical Information and Modeling, 2021, 61, 831-839.	5.4	59
69	CHARMM-GUI Polymer Builder for Modeling and Simulation of Synthetic Polymers. Journal of Chemical Theory and Computation, 2021, 17, 2431-2443.	5.3	58
70	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.	5.3	57
71	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.	5.3	57
72	Brownian Dynamics Simulations of Ion Transport through the VDAC. Biophysical Journal, 2011, 100, 611-619.	0.5	56

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73	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.	7.1	55
74	CHARMM-GUI Nanomaterial Modeler for Modeling and Simulation of Nanomaterial Systems. Journal of Chemical Theory and Computation, 2022, 18, 479-493.	5.3	53
75	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.	7.1	52
76	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.	2.6	51
77	Challenges in structural approaches to cell modeling. Journal of Molecular Biology, 2016, 428, 2943-2964.	4.2	51
78	Refinement of OprH-LPS Interactions by Molecular Simulations. Biophysical Journal, 2017, 112, 346-355.	0.5	50
79	Glycan fragment database: a database of PDB-based glycan 3D structures. Nucleic Acids Research, 2012, 41, D470-D474.	14.5	49
80	Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation. Biophysical Journal, 2017, 112, 1185-1197.	0.5	48
81	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
82	Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. Journal of Physical Chemistry B, 2016, 120, 11761-11772.	2.6	47
83	Molecular Simulations of Gram-Negative Bacterial Membranes Come of Age. Annual Review of Physical Chemistry, 2020, 71, 171-188.	10.8	44
84	Web interface for brownian dynamics simulation of ion transport and its applications to betaâ€barrel pores. Journal of Computational Chemistry, 2012, 33, 331-339.	3.3	43
85	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. Current Opinion in Structural Biology, 2017, 43, 131-140.	5.7	42
86	CHARMMâ€GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. Journal of Computational Chemistry, 2019, 40, 893-899.	3.3	42
87	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.	5.4	41
88	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. Biophysical Journal, 2016, 111, 1987-1999.	0.5	41
89	Lipopolysaccharide Membrane Building and Simulation. Methods in Molecular Biology, 2015, 1273, 391-406.	0.9	41
90	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.	7.1	40

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91	Implementation and application of helixâ€“helix distance and crossing angle restraint potentials. Journal of Computational Chemistry, 2007, 28, 669-680.	3.3	39
92	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. Nature Chemical Biology, 2018, 14, 489-496.	8.0	39
93	Additive CHARMM36 Force Field for Nonstandard Amino Acids. Journal of Chemical Theory and Computation, 2021, 17, 3554-3570.	5.3	39
94	Role of Hydrogen Bonding and Helixâ˜Lipid Interactions in Transmembrane Helix Association. Journal of the American Chemical Society, 2008, 130, 6456-6462.	13.7	38
95	Two Dimensional Window Exchange Umbrella Sampling for Transmembrane Helix Assembly. Journal of Chemical Theory and Computation, 2013, 9, 13-17.	5.3	38
96	Preferred Orientations of Phosphoinositides in Bilayers and Their Implications in Protein Recognition Mechanisms. Journal of Physical Chemistry B, 2014, 118, 4315-4325.	2.6	38
97	Electrostatic free energy calculations using the generalized solvent boundary potential method. Journal of Chemical Physics, 2002, 117, 7381-7388.	3.0	37
98	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.	3.3	37
99	Generation of native-like protein structures from limited NMR data, modern force fields and advanced conformational sampling. Journal of Biomolecular NMR, 2005, 31, 59-64.	2.8	36
100	Restraint potential and free energy decomposition formalism for helical tilting. Chemical Physics Letters, 2007, 441, 132-135.	2.6	34
101	Preferred conformations ofN-glycan core pentasaccharide in solution and in glycoproteins. Glycobiology, 2016, 26, cwv083.	2.5	34
102	Transmembrane Signaling of Chemotaxis Receptor Tar: Insights from Molecular Dynamics Simulation Studies. Biophysical Journal, 2011, 100, 2955-2963.	0.5	33
103	Probing the U-Shaped Conformation of Caveolin-1 in a Bilayer. Biophysical Journal, 2014, 106, 1371-1380.	0.5	33
104	Gâ€ŁoSA: An efficient computational tool for local structureâ€centric biological studies and drug design. Protein Science, 2016, 25, 865-876.	7.6	33
105	Multidimensional umbrella sampling and replicaâ€exchange molecular dynamics simulations for structure prediction of transmembrane helix dimers. Journal of Computational Chemistry, 2014, 35, 300-308.	3.3	32
106	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.	7.1	32
107	Comparative Molecular Dynamics Simulation Studies of Realistic Eukaryotic, Prokaryotic, and Archaeal Membranes. Journal of Chemical Information and Modeling, 2022, 62, 1036-1051.	5.4	32
108	Effects of N-Glycan Composition on Structure and Dynamics of IgG1 Fc and Their Implications for Antibody Engineering. Scientific Reports, 2017, 7, 12659.	3.3	31

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109	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.	7.1	30
110	Application of solid-state NMR restraint potentials in membrane protein modeling. Journal of Magnetic Resonance, 2008, 193, 68-76.	2.1	29
111	Transmembrane Helix Orientation and Dynamics: Insights from Ensemble Dynamics with Solid-State NMR Observables. Biophysical Journal, 2011, 100, 2913-2921.	0.5	29
112	Restricted N-glycan Conformational Space in the PDB and Its Implication in Glycan Structure Modeling. PLoS Computational Biology, 2013, 9, e1002946.	3.2	29
113	Synthetic Immunotherapeutics against Gram-negative Pathogens. Cell Chemical Biology, 2018, 25, 1185-1194.e5.	5.2	29
114	Proteinâ€“protein interactions in actinâ€“myosin binding and structural effects of R405Q mutation: A molecular dynamics study. Proteins: Structure, Function and Bioinformatics, 2006, 64, 156-166.	2.6	28
115	Accurate simulation of surfaces and interfaces of ten FCC metals and steel using Lennardâ€“Jones potentials. Npj Computational Materials, 2021, 7, .	8.7	28
116	Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation. Biophysical Journal, 2019, 116, 1095-1104.	0.5	27
117	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.	2.6	26
118	Modeling and Simulation of Bacterial Outer Membranes with Lipopolysaccharides and Enterobacterial Common Antigen. Journal of Physical Chemistry B, 2020, 124, 5948-5956.	2.6	26
119	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
120	NMR Observable-Based Structure Refinement of DAP12-NKG2C Activating Immunoreceptor Complex in Explicit Membranes. Biophysical Journal, 2012, 102, L27-L29.	0.5	25
121	CHARMM-GUI Membrane Builder for Lipid Nanoparticles with Ionizable Cationic Lipids and PEGylated Lipids. Journal of Chemical Information and Modeling, 2021, 61, 5192-5202.	5.4	25
122	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. Journal of Physical Chemistry B, 2017, 121, 3718-3723.	2.6	24
123	Structural Insight into Phospholipid Transport by the MlaFEBD Complex from P. aeruginosa. Journal of Molecular Biology, 2021, 433, 166986.	4.2	24
124	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. Journal of Chemical Information and Modeling, 2021, 61, 4145-4151.	5.4	24
125	<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.	3.3	24
126	Molecular dynamics studies on structure and dynamics of phospholamban monomer and pentamer in membranes. Proteins: Structure, Function and Bioinformatics, 2009, 76, 86-98.	2.6	22

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127	Gramicidin A Channel Formation Induces LocalÂLipid Redistribution II: A 3D Continuum Elastic Model. Biophysical Journal, 2017, 112, 1198-1213.	0.5	22
128	Site-Specific Lipidation Enhances IFITM3 Membrane Interactions and Antiviral Activity. ACS Chemical Biology, 2021, 16, 844-856.	3.4	22
129	All-atom molecular dynamics simulations of Synaptotagmin-SNARE-complexin complexes bridging a vesicle and a flat lipid bilayer. ELife, 0, 11, .	6.0	22
130	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
131	Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase. Biophysical Journal, 2014, 107, 1885-1895.	0.5	21
132	Theory of Adaptive Optimization for Umbrella Sampling. Journal of Chemical Theory and Computation, 2014, 10, 2719-2728.	5.3	21
133	Novel free energy calculations to explore mechanisms and energetics of membrane protein structure and function. Journal of Computational Chemistry, 2009, 30, 1622-1633.	3.3	20
134	Protegrinâ€1 orientation and physicochemical properties in membrane bilayers studied by potential of mean force calculations. Journal of Computational Chemistry, 2010, 31, 2859-2867.	3.3	20
135	Assessing smectic liquid-crystal continuum models for elastic bilayer deformations. Chemistry and Physics of Lipids, 2013, 169, 19-26.	3.2	20
136	Transmembrane Complexes of DAP12 Crystallized in Lipid Membranes Provide Insights into Control of Oligomerization in Immunoreceptor Assembly. Cell Reports, 2015, 11, 1184-1192.	6.4	20
137	Structural basis of neuropeptide Y signaling through Y1 receptor. Nature Communications, 2022, 13, 853.	12.8	20
138	Molecular dynamics simulation strategies for proteinâ€“micelle complexes. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1566-1572.	2.6	19
139	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.	3.3	19
140	Mutually constructive roles of Ail and LPS in Yersinia pestis serum survival. Molecular Microbiology, 2020, 114, 510-520.	2.5	19
141	Ligand-Binding-Site Refinement to Generate Reliable Holo Protein Structure Conformations from Apo Structures. Journal of Chemical Information and Modeling, 2021, 61, 535-546.	5.4	19
142	Comparative Molecular Dynamics Simulation Studies of Protegrin-1 Monomer and Dimer in Two Different Lipid Bilayers. Biophysical Journal, 2009, 97, 787-795.	0.5	18
143	A Repulsive Electrostatic Mechanism for Protein Export through the Type III Secretion Apparatus. Biophysical Journal, 2010, 98, 452-461.	0.5	18
144	NMR-Based Simulation Studies of Pf1 Coat Protein in Explicit Membranes. Biophysical Journal, 2013, 105, 691-698.	0.5	18

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145	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. Biophysical Journal, 2015, 109, 2090-2100.	0.5	18
146	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.	7.1	18
147	Augmenting the antinociceptive effects of nicotinic acetylcholine receptor activity through lynx1 modulation. PLoS ONE, 2018, 13, e0199643.	2.5	18
148	Structural basis for the association of PLEKHA7 with membrane-embedded phosphatidylinositol lipids. Structure, 2021, 29, 1029-1039.e3.	3.3	18
149	Solid-State NMR Ensemble Dynamics as a Mediator between Experiment and Simulation. Biophysical Journal, 2011, 100, 2922-2928.	0.5	17
150	Conformational Dynamics of the Lipopolysaccharide from Escherichia coli O91 Revealed by Nuclear Magnetic Resonance Spectroscopy and Molecular Simulations. Biochemistry, 2017, 56, 3826-3839.	2.5	17
151	Membrane Tension, Lipid Adaptation, Conformational Changes, and Energetics in MscL Gating. Biophysical Journal, 2011, 101, 671-679.	0.5	16
152	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.	5.3	16
153	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. Glycobiology, 2015, 26, cwv101.	2.5	15
154	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
155	G-LoSA for Prediction of Protein-Ligand Binding Sites and Structures. Methods in Molecular Biology, 2017, 1611, 97-108.	0.9	15
156	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.	2.5	15
157	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.	8.3	15
158	Systematic Assessment of Accessibility to the Surface of Staphylococcus aureus. ACS Chemical Biology, 2021, 16, 2527-2536.	3.4	15
159	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.	5.3	14
160	Quantitative Characterization of Cholesterol Partitioning between Binary Bilayers. Journal of Chemical Theory and Computation, 2018, 14, 2829-2833.	5.3	14
161	GlyMDB: Glycan Microarray Database and analysis toolset. Bioinformatics, 2020, 36, 2438-2442.	4.1	14
162	Developing initial conditions for simulations of asymmetric membranes: a practical recommendation. Biophysical Journal, 2021, 120, 5041-5059.	0.5	14

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163	Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy. Journal of Chemical Theory and Computation, 2015, 11, 1255-1266.	5.3	13
164	A mechano-reactive coarse-grained model of the blood-clotting agent von Willebrand factor. Journal of Chemical Physics, 2019, 151, 124905.	3.0	13
165	A systematic analysis of proteinâ€“carbohydrate interactions in the Protein Data Bank. Glycobiology, 2021, 31, 126-136.	2.5	13
166	Dynamic Interactions of Fully Glycosylated SARS-CoV-2 Spike Protein with Various Antibodies. Journal of Chemical Theory and Computation, 2021, 17, 6559-6569.	5.3	13
167	Foldable Detergents for Membrane Protein Study: Importance of Detergent Core Flexibility in Protein Stabilization. Chemistry - A European Journal, 2022, 28, .	3.3	13
168	Evolutionary balance between foldability and functionality of a glucose transporter. Nature Chemical Biology, 2022, 18, 713-723.	8.0	13
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