Wonpil Im

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

204 papers	16,508 citations	55 h-index	126 g-index
226 ext. papers	21,546 ext. citations	4.8 avg, IF	6.88 L-index

#	Paper	IF	Citations
204	Binding of Human ACE2 and RBD of Omicron Enhanced by Unique Interaction Patterns Among SARS-CoV-2 Variants of Concern. **2022**,		2
203	Structural basis of neuropeptide Y signaling through Y1 receptor.. *Nature Communications*, **2022**, 13, 853	17.4	1
202	CHARMM-GUI for Template-Based Virtual Ligand Design in a Binding Site. *Journal of Chemical Information and Modeling*, **2021**, 61, 5336-5342	6.1	1
201	Differential Interactions between Human ACE2 and Spike RBD of SARS-CoV-2 Variants of Concern. *Journal of Chemical Theory and Computation*, **2021**,	6.4	20
200	Developing initial conditions for simulations of asymmetric membranes: a practical recommendation. *Biophysical Journal*, **2021**, 120, 5041-5059	2.9	2
199	Systematic Assessment of Accessibility to the Surface of. *ACS Chemical Biology*, **2021**, 16, 2527-2536	4.9	0
198	Biomechanical characterization of SARS-CoV-2 spike RBD and human ACE2 protein-protein interaction. *Biophysical Journal*, **2021**, 120, 1011-1019	2.9	26
197	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	6.4	26
196	Location and Conformational Ensemble of Menaquinone and Menaquinol, and Protein-Lipid Modulations in Archaeal Membranes. *Journal of Physical Chemistry B*, **2021**, 125, 4714-4725	3.4	3
195	Site-Specific Lipidation Enhances IFITM3 Membrane Interactions and Antiviral Activity. *ACS Chemical Biology*, **2021**, 16, 844-856	4.9	7
194	CHARMM-GUI Polymer Builder for Modeling and Simulation of Synthetic Polymers. *Journal of Chemical Theory and Computation*, **2021**, 17, 2431-2443	6.4	12
193	Additive CHARMM36 Force Field for Nonstandard Amino Acids. *Journal of Chemical Theory and Computation*, **2021**, 17, 3554-3570	6.4	5
192	Structural Insight into Phospholipid Transport by the MlaFEBD Complex from P. aeruginosa. *Journal of Molecular Biology*, **2021**, 433, 166986	6.5	5
191	Differential Interactions Between Human ACE2 and Spike RBD of SARS-CoV-2 Variants of Concern **2021**,		16
190	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	10.8	4
189	A systematic analysis of protein-carbohydrate interactions in the Protein Data Bank. *Glycobiology*, **2021**, 31, 126-136	5.8	5
188	Structure, Dynamics, and Interactions of GPI-Anchored Human Glypican-1 with Heparan Sulfates in a Membrane. *Glycobiology*, **2021**, 31, 593-602	5.8	1

187	Ligand-Binding-Site Refinement to Generate Reliable Holo Protein Structure Conformations from Apo Structures. *Journal of Chemical Information and Modeling*, **2021**, 61, 535-546	6.1	7
186	Influences of Lipid A Types on LPS Bilayer Properties. *Journal of Physical Chemistry B*, **2021**, 125, 2105-2112	3.4	2
185	CHARMM-GUI for Ligand Binding Site Prediction and Refinement. *Journal of Chemical Information and Modeling*, **2021**, 61, 3744-3751	6.1	2
184	CHARMM-GUI Free Energy Calculator for Practical Ligand Binding Free Energy Simulations with AMBER. *Journal of Chemical Information and Modeling*, **2021**, 61, 4145-4151	6.1	4
183	CHARMM-GUI Membrane Builder for Lipid Nanoparticles with Ionizable Cationic Lipids and PEGylated Lipids. *Journal of Chemical Information and Modeling*, **2021**, 61, 5192-5202	6.1	2
182	Biophysical characterization of lynx-nicotinic receptor interactions using atomic force microscopy.. *FASEB BioAdvances*, **2021**, 3, 1034-1042	2.8	0
181	Structural basis for the association of PLEKHA7 with membrane-embedded phosphatidylinositol lipids. *Structure*, **2021**, 29, 1029-1039.e3	5.2	6
180	Dynamic Interactions of Fully Glycosylated SARS-CoV-2 Spike Protein with Various Antibodies. *Journal of Chemical Theory and Computation*, **2021**, 17, 6559-6569	6.4	2
179	CHARMM-GUI Supports Hydrogen Mass Repartitioning and Different Protonation States of Phosphates in Lipopolysaccharides. *Journal of Chemical Information and Modeling*, **2021**, 61, 831-839	6.1	10
178	Accurate simulation of surfaces and interfaces of ten FCC metals and steel using Lennard□Jones potentials. *Npj Computational Materials*, **2021**, 7,	10.9	4
177	S-palmitoylation and sterol interactions mediate antiviral specificity of IFITM isoforms. **2021**,		1
176	CHARMM-GUI Drude prepper for molecular dynamics simulation using the classical Drude polarizable force field. *Journal of Computational Chemistry*, **2021**,	3.5	4
175	Conformational States of the Cytoprotective Protein Bcl-xL. *Biophysical Journal*, **2020**, 119, 1324-1334	2.9	2
174	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	3.4	
173	Modeling and Simulation of Bacterial Outer Membranes with Lipopolysaccharides and Enterobacterial Common Antigen. *Journal of Physical Chemistry B*, **2020**, 124, 5948-5956	3.4	9
172	Mutually constructive roles of Ail and LPS in Yersinia pestis serum survival. *Molecular Microbiology*, **2020**, 114, 510-520	4.1	9
171	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	3.4	131
170	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	3.4	4

169	Improving Protein-Ligand Docking Results with High-Throughput Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 2189-2198	6.1	69
168	Cooperativity in Proteasome Core Particle Maturation. *IScience*, **2020**, 23, 101090	6.1	0
167	Molecular Simulations of Gram-Negative Bacterial Membranes Come of Age. *Annual Review of Physical Chemistry*, **2020**, 71, 171-188	15.7	22
166	Broadening Activity of Polymyxin by Quaternary Ammonium Grafting. *ACS Infectious Diseases*, **2020**, 6, 1427-1435	5.5	4
165	O176 LPS structure and dynamics: A NMR spectroscopy and MD simulation study. *Current Research in Structural Biology*, **2020**, 2, 79-88	2.8	5
164	Developing a Fully-glycosylated Full-length SARS-CoV-2 Spike Protein Model in a Viral Membrane **2020**,		4
163	Biomechanical Characterization of SARS-CoV-2 Spike RBD and Human ACE2 Protein-Protein Interaction **2020**,		6
162	Preferred conformations of lipooligosaccharides and oligosaccharides of Moraxella catarrhalis. *Glycobiology*, **2020**, 30, 86-94	5.8	4
161	GlyMDB: Glycan Microarray Database and analysis toolset. *Bioinformatics*, **2020**, 36, 2438-2442	7.2	6
160	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	11.5	3
159	CHARMM-GUI supports the Amber force fields. *Journal of Chemical Physics*, **2020**, 153, 035103	3.9	36
158	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	6.4	28
157	CHARMM-GUI DEER facilitator for spin-pair distance distribution calculations and preparation of restrained-ensemble molecular dynamics simulations. *Journal of Computational Chemistry*, **2020**, 41, 415-420	3.5	5
156	A mechano-reactive coarse-grained model of the blood-clotting agent von Willebrand factor. *Journal of Chemical Physics*, **2019**, 151, 124905	3.9	7
155	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	6.4	10
154	Quantitative Characterization of Protein-Lipid Interactions by Free Energy Simulation between Binary Bilayers. *Journal of Chemical Theory and Computation*, **2019**, 15, 6491-6503	6.4	2
153	CHARMM-GUI Glycan Modeler for modeling and simulation of carbohydrates and glycoconjugates. *Glycobiology*, **2019**, 29, 320-331	5.8	101
152	CHARMM-GUI Nanodisc Builder for modeling and simulation of various nanodisc systems. *Journal of Computational Chemistry*, **2019**, 40, 893-899	3.5	27

151	Modeling of Specific Lipopolysaccharide Binding Sites on a Gram-Negative Porin. *Journal of Physical Chemistry B*, **2019**, 123, 5700-5708	3.4	5
150	Physical Properties of Bacterial Outer Membrane Models: Neutron Reflectometry & Molecular Simulation. *Biophysical Journal*, **2019**, 116, 1095-1104	2.9	16
149	Stalis: A Computational Method for Template-Based Ab Initio Ligand Design. *Journal of Computational Chemistry*, **2019**, 40, 1622-1632	3.5	3
148	U-shaped caveolin-1 conformations are tightly regulated by hydrogen bonds with lipids. *Journal of Computational Chemistry*, **2019**, 40, 1570-1577	3.5	3
147	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	11.5	21
146	Analysis of Lipid Order States and Domains in Lipid Bilayer Simulations. *Journal of Chemical Theory and Computation*, **2019**, 15, 688-697	6.4	8
145	CHARMM-GUI Membrane Builder for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. *Journal of Chemical Theory and Computation*, **2019**, 15, 775-786	6.4	152
144	Structural Conservation and Effects of Alterations in T Cell Receptor Transmembrane Interfaces. *Biophysical Journal*, **2018**, 114, 1030-1035	2.9	6
143	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	3.4	8
142	Unfolding of a ClC chloride transporter retains memory of its evolutionary history. *Nature Chemical Biology*, **2018**, 14, 489-496	11.7	22
141	Simulation Study of Occk5 Functional Properties in Pseudomonas aeruginosa Outer Membranes. *Journal of Physical Chemistry B*, **2018**, 122, 8185-8192	3.4	9
140	Quantitative Characterization of Cholesterol Partitioning between Binary Bilayers. *Journal of Chemical Theory and Computation*, **2018**, 14, 2829-2833	6.4	5
139	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	11.5	20
138	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	3.4	3
137	Insight into Elongation Stages of Peptidoglycan Processing in Bacterial Cytoplasmic Membranes. *Scientific Reports*, **2018**, 8, 17704	4.9	4
136	Long-ranged Protein-glycan Interactions Stabilize von Willebrand Factor A2 Domain from Mechanical Unfolding. *Scientific Reports*, **2018**, 8, 16017	4.9	7
135	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	11.5	13
134	Augmenting the antinociceptive effects of nicotinic acetylcholine receptor activity through lynx1 modulation. *PLoS ONE*, **2018**, 13, e0199643	3.7	12

133	Synthetic Immunotherapeutics against Gram-negative Pathogens. *Cell Chemical Biology*, **2018**, 25, 1185-1194.e5	8.2	14
132	Refinement of OprH-LPS Interactions by Molecular Simulations. *Biophysical Journal*, **2017**, 112, 346-355	2.9	32
131	Modeling and simulation of bacterial outer membranes and interactions with membrane proteins. *Current Opinion in Structural Biology*, **2017**, 43, 131-140	8.1	30
130	Molecular Simulation and Biochemical Studies Support an Elevator-type Transport Mechanism in EIIC. *Biophysical Journal*, **2017**, 112, 2249-2252	2.9	4
129	Simulating Biomolecules: Festschrift to commemorate the 60th birthday of Charles L. Brooks III. *Journal of Computational Chemistry*, **2017**, 38, 1111-1113	3.5	
128	G-LoSA for Prediction of Protein-Ligand Binding Sites and Structures. *Methods in Molecular Biology*, **2017**, 1611, 97-108	1.4	10
127	Conformational Dynamics of the Lipopolysaccharide from Escherichia coli O91 Revealed by Nuclear Magnetic Resonance Spectroscopy and Molecular Simulations. *Biochemistry*, **2017**, 56, 3826-3839	3.2	16
126	Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation. *Biophysical Journal*, **2017**, 112, 1185-1197	2.9	31
125	Gramicidin A Channel Formation Induces Local Lipid Redistribution II: A 3D Continuum Elastic Model. *Biophysical Journal*, **2017**, 112, 1198-1213	2.9	15
124	CHARMM-GUI MDFF/xMDFF Utilizer for Molecular Dynamics Flexible Fitting Simulations in Various Environments. *Journal of Physical Chemistry B*, **2017**, 121, 3718-3723	3.4	13
123	Effects of N-Glycan Composition on Structure and Dynamics of IgG1 Fc and Their Implications for Antibody Engineering. *Scientific Reports*, **2017**, 7, 12659	4.9	19
122	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	6.4	11
121	Heterogeneity in non-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	4.1	10
120	Glycan Reader is improved to recognize most sugar types and chemical modifications in the Protein Data Bank. *Bioinformatics*, **2017**, 33, 3051-3057	7.2	59
119	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	11.5	20
118	CHARMM-GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, **2017**, 38, 1114-1124	3.5	119
117	Asymmetric Cryo-EM Structure of Anthrax Toxin Protective Antigen Pore with Lethal Factor N-Terminal Domain. *Toxins*, **2017**, 9,	4.9	9
116	Transmembrane motions of PglB induced by LLO are coupled with EL5 loop conformational changes necessary for OST activity. *Glycobiology*, **2017**, 27, 734-742	5.8	5

115	Preferred conformations of N-glycan core pentasaccharide in solution and in glycoproteins. *Glycobiology*, **2016**, 26, 19-29	5.8	26
114	Protein Dynamics and Ion Traffic in Bacterioferritin Function: A Molecular Dynamics Simulation Study on wild-type and Mutant Pseudomonas Aeruginosa BfrB **2016**, 1118-1129		
113	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	3.8	32
112	A conserved transmembrane interface forms the core of a compact T-cell receptor-CD3 structure within the membrane. *Proceedings of the National Academy of Sciences of the United States of America*, **2016**, 113, E6649-E6658	11.5	30
111	Influence of Cholesterol on Phospholipid Bilayer Structure and Dynamics. *Journal of Physical Chemistry B*, **2016**, 120, 11761-11772	3.4	36
110	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. *Biophysical Journal*, **2016**, 111, 1750-1760	2.9	60
109	Influence of Ganglioside GM1 Concentration on Lipid Clustering and Membrane Properties and Curvature. *Biophysical Journal*, **2016**, 111, 1987-1999	2.9	29
108	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. *Biophysical Journal*, **2016**, 110, 2698-2709	2.9	52
107	Molecular dynamics simulation strategies for protein-micelle complexes. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1566-72	3.8	14
106	Challenges in structural approaches to cell modeling. *Journal of Molecular Biology*, **2016**, 428, 2943-64	6.5	36
105	G-LoSA: An efficient computational tool for local structure-centric biological studies and drug design. *Protein Science*, **2016**, 25, 865-76	6.3	19
104	Converting One-Face Helix Mimetics into Amphiphilic Helix Mimetics as Potent Inhibitors of Protein-Protein Interactions. *ACS Combinatorial Science*, **2016**, 18, 36-42	3.9	10
103	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, 405-13	6.4	1303
102	Dynamics and Interactions of OmpF and LPS: Influence on Pore Accessibility and Ion Permeability. *Biophysical Journal*, **2016**, 110, 930-8	2.9	54
101	Molecular dynamics simulations of biological membranes and membrane proteins using enhanced conformational sampling algorithms. *Biochimica Et Biophysica Acta - Biomembranes*, **2016**, 1858, 1635-51	3.8	88
100	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. *Glycobiology*, **2016**, 26, 251-60	5.8	13
99	L-Met Activates Arabidopsis GLR Ca Channels Upstream of ROS Production and Regulates Stomatal Movement. *Cell Reports*, **2016**, 17, 2553-2561	10.6	45
98	CHARMM-GUI Input Generator for NAMD, Gromacs, Amber, Openmm, and CHARMM/OpenMM Simulations using the CHARMM36 Additive Force Field. *Biophysical Journal*, **2016**, 110, 641a	2.9	21

97	The Structure of a Sugar Transporter of the Glucose EIIC Superfamily Provides Insight into the Elevator Mechanism of Membrane Transport. *Structure*, **2016**, 24, 956-64	5.2	31
96	Effects of Spin-Labels on Membrane Burial Depth of MARCKS-ED Residues. *Biophysical Journal*, **2016**, 111, 1600-1603	2.9	
95	Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes. *Biophysical Journal*, **2015**, 108, 1954-62	2.9	9
94	GS-align for glycan structure alignment and similarity measurement. *Bioinformatics*, **2015**, 31, 2653-9	7.2	9
93	Effects of N-glycosylation on protein conformation and dynamics: Protein Data Bank analysis and molecular dynamics simulation study. *Scientific Reports*, **2015**, 5, 8926	4.9	122
92	CHARMM-GUI Martini Maker for Coarse-Grained Simulations with the Martini Force Field. *Journal of Chemical Theory and Computation*, **2015**, 11, 4486-94	6.4	181
91	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophysical Journal*, **2015**, 109, 2012-22	2.9	60
90	Insight into Early-Stage Unfolding of GPI-Anchored Human Prion Protein. *Biophysical Journal*, **2015**, 109, 2090-100	2.9	14
89	Transmembrane Complexes of DAP12 Crystallized in Lipid Membranes Provide Insights into Control of Oligomerization in Immunoreceptor Assembly. *Cell Reports*, **2015**, 11, 1184-92	10.6	18
88	How Tolerant are Membrane Simulations with Mismatch in Area per Lipid between Leaflets?. *Journal of Chemical Theory and Computation*, **2015**, 11, 3466-77	6.4	44
87	Potential Application of Alchemical Free Energy Simulations to Discriminate GPCR Ligand Efficacy. *Journal of Chemical Theory and Computation*, **2015**, 11, 1255-66	6.4	8
86	Lipopolysaccharide membrane building and simulation. *Methods in Molecular Biology*, **2015**, 1273, 391-406	1.4	31
85	ST-analyzer: a web-based user interface for simulation trajectory analysis. *Journal of Computational Chemistry*, **2014**, 35, 957-63	3.5	11
84	Lipid-linked oligosaccharides in membranes sample conformations that facilitate binding to oligosaccharyltransferase. *Biophysical Journal*, **2014**, 107, 1885-1895	2.9	17
83	CHARMM-GUI Membrane Builder toward realistic biological membrane simulations. *Journal of Computational Chemistry*, **2014**, 35, 1997-2004	3.5	1004
82	CHARMM-GUI PDB manipulator for advanced modeling and simulations of proteins containing nonstandard residues. *Advances in Protein Chemistry and Structural Biology*, **2014**, 96, 235-65	5.3	96
81	Preferred orientations of phosphoinositides in bilayers and their implications in protein recognition mechanisms. *Journal of Physical Chemistry B*, **2014**, 118, 4315-25	3.4	21
80	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 2520-9	3.8	63

79	Potential pharmacological chaperones targeting cancer-associated MCL-1 and Parkinson disease-associated □synuclein. *Proceedings of the National Academy of Sciences of the United States of America*, **2014**, 111, 11007-12	11.5	51
78	Theory of Adaptive Optimization for Umbrella Sampling. *Journal of Chemical Theory and Computation*, **2014**, 10, 2719-2728	6.4	16
77	CHARMM-GUI PACE CG Builder for solution, micelle, and bilayer coarse-grained simulations. *Journal of Chemical Information and Modeling*, **2014**, 54, 1003-9	6.1	33
76	Multidimensional umbrella sampling and replica-exchange molecular dynamics simulations for structure prediction of transmembrane helix dimers. *Journal of Computational Chemistry*, **2014**, 35, 300-8	3.5	26
75	Probing the U-shaped conformation of caveolin-1 in a bilayer. *Biophysical Journal*, **2014**, 106, 1371-80	2.9	28
74	E. coli outer membrane and interactions with OmpLA. *Biophysical Journal*, **2014**, 106, 2493-502	2.9	97
73	Assessing smectic liquid-crystal continuum models for elastic bilayer deformations. *Chemistry and Physics of Lipids*, **2013**, 169, 19-26	3.7	16
72	Molecular dynamics and NMR spectroscopy studies of E. coli lipopolysaccharide structure and dynamics. *Biophysical Journal*, **2013**, 105, 1444-55	2.9	125
71	Ligand binding site detection by local structure alignment and its performance complementarity. *Journal of Chemical Information and Modeling*, **2013**, 53, 2462-70	6.1	17
70	CHARMM-GUI micelle builder for pure/mixed micelle and protein/micelle complex systems. *Journal of Chemical Information and Modeling*, **2013**, 53, 2171-80	6.1	61
69	Two Dimensional Window Exchange Umbrella Sampling for Transmembrane Helix Assembly. *Journal of Chemical Theory and Computation*, **2013**, 9, 13-17	6.4	33
68	CHARMM-GUI Ligand Binder for absolute binding free energy calculations and its application. *Journal of Chemical Information and Modeling*, **2013**, 53, 267-77	6.1	51
67	NMR-based simulation studies of Pf1 coat protein in explicit membranes. *Biophysical Journal*, **2013**, 105, 691-8	2.9	18
66	Restricted N-glycan conformational space in the PDB and its implication in glycan structure modeling. *PLoS Computational Biology*, **2013**, 9, e1002946	5	22
65	Glycan fragment database: a database of PDB-based glycan 3D structures. *Nucleic Acids Research*, **2013**, 41, D470-4	20.1	41
64	Web interface for Brownian dynamics simulation of ion transport and its applications to beta-barrel pores. *Journal of Computational Chemistry*, **2012**, 33, 331-9	3.5	38
63	Identification of ligand templates using local structure alignment for structure-based drug design. *Journal of Chemical Information and Modeling*, **2012**, 52, 2784-95	6.1	23
62	Improving the CHARMM force field for polyunsaturated fatty acid chains. *Journal of Physical Chemistry B*, **2012**, 116, 9424-31	3.4	102

61	NMR observable-based structure refinement of DAP12-NKG2C activating immunoreceptor complex in explicit membranes. *Biophysical Journal*, **2012**, 102, L27-9	2.9	23
60	Influence of hydrophobic mismatch on structures and dynamics of gramicidin a and lipid bilayers. *Biophysical Journal*, **2012**, 102, 1551-60	2.9	78
59	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, 1821-32	6.1	27
58	Transmembrane helix assembly by window exchange umbrella sampling. *Physical Review Letters*, **2012**, 108, 108102	7.4	51
57	Brownian dynamics simulations of ion transport through the VDAC. *Biophysical Journal*, **2011**, 100, 611-619	2.9	49
56	Molecular dynamics studies of ion permeation in VDAC. *Biophysical Journal*, **2011**, 100, 602-610	2.9	68
55	Solid-state NMR ensemble dynamics as a mediator between experiment and simulation. *Biophysical Journal*, **2011**, 100, 2922-8	2.9	17
54	Transmembrane helix orientation and dynamics: insights from ensemble dynamics with solid-state NMR observables. *Biophysical Journal*, **2011**, 100, 2913-21	2.9	28
53	Transmembrane signaling of chemotaxis receptor tar: insights from molecular dynamics simulation studies. *Biophysical Journal*, **2011**, 100, 2955-63	2.9	32
52	Membrane tension, lipid adaptation, conformational changes, and energetics in MscL gating. *Biophysical Journal*, **2011**, 101, 671-9	2.9	14
51	Orientation of fluorescent lipid analogue BODIPY-PC to probe lipid membrane properties: insights from molecular dynamics simulations. *Journal of Physical Chemistry B*, **2011**, 115, 6157-65	3.4	24
50	Novel pyrrolopyrimidine-based α-helix mimetics: cell-permeable inhibitors of protein–protein interactions. *Journal of the American Chemical Society*, **2011**, 133, 676-9	16.4	110
49	Glycan Reader: automated sugar identification and simulation preparation for carbohydrates and glycoproteins. *Journal of Computational Chemistry*, **2011**, 32, 3135-41	3.5	118
48	A repulsive electrostatic mechanism for protein export through the type III secretion apparatus. *Biophysical Journal*, **2010**, 98, 452-61	2.9	16
47	Revisiting hydrophobic mismatch with free energy simulation studies of transmembrane helix tilt and rotation. *Biophysical Journal*, **2010**, 99, 175-83	2.9	91
46	Cholesterol flip-flop: insights from free energy simulation studies. *Journal of Physical Chemistry B*, **2010**, 114, 13342-8	3.4	97
45	Structural, NMR spectroscopic, and computational investigation of hemin loading in the hemophore HasAp from Pseudomonas aeruginosa. *Journal of the American Chemical Society*, **2010**, 132, 9857-72	16.4	58
44	NMR characterization of hydrophobic collapses in amyloidogenic unfolded states and their implications for amyloid formation. *Biochemical and Biophysical Research Communications*, **2010**, 396, 800-5	3.4	1

43	Protegrin-1 orientation and physicochemical properties in membrane bilayers studied by potential of mean force calculations. *Journal of Computational Chemistry*, **2010**, 31, 2859-67	3.5	19
42	Beta-hairpin restraint potentials for calculations of potentials of mean force as a function of beta-hairpin tilt, rotation, and distance. *Journal of Computational Chemistry*, **2009**, 30, 1334-43	3.5	8
41	Novel free energy calculations to explore mechanisms and energetics of membrane protein structure and function. *Journal of Computational Chemistry*, **2009**, 30, 1622-33	3.5	19
40	Molecular dynamics studies on structure and dynamics of phospholamban monomer and pentamer in membranes. *Proteins: Structure, Function and Bioinformatics*, **2009**, 76, 86-98	4.2	19
39	CHARMM-GUI Membrane Builder for mixed bilayers and its application to yeast membranes. *Biophysical Journal*, **2009**, 97, 50-8	2.9	891
38	Comparative molecular dynamics simulation studies of protegrin-1 monomer and dimer in two different lipid bilayers. *Biophysical Journal*, **2009**, 97, 787-95	2.9	18
37	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	2.5	48
36	Role of hydrogen bonding and helix-lipid interactions in transmembrane helix association. *Journal of the American Chemical Society*, **2008**, 130, 6456-62	16.4	37
35	PBEQ-Solver for online visualization of electrostatic potential of biomolecules. *Nucleic Acids Research*, **2008**, 36, W270-5	20.1	163
34	Transmembrane helix tilting: insights from calculating the potential of mean force. *Physical Review Letters*, **2008**, 100, 018103	7.4	56
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