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List of Publications by Citations

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	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
203	CHARMM-GUI Membrane Builder toward realistic biological membrane simulations. *Journal of Computational Chemistry*, **2014**, 35, 1997-2004	3.5	1004
202	CHARMM-GUI Membrane Builder for mixed bilayers and its application to yeast membranes. *Biophysical Journal*, **2009**, 97, 50-8	2.9	891
201	Automated builder and database of protein/membrane complexes for molecular dynamics simulations. *PLoS ONE*, **2007**, 2, e880	3.7	616
200	Generalized born model with a simple smoothing function. *Journal of Computational Chemistry*, **2003**, 24, 1691-702	3.5	578
199	Performance comparison of generalized born and Poisson methods in the calculation of electrostatic solvation energies for protein structures. *Journal of Computational Chemistry*, **2004**, 25, 265-84	3.5	465
198	Continuum solvation model: Computation of electrostatic forces from numerical solutions to the Poisson-Boltzmann equation. *Computer Physics Communications*, **1998**, 111, 59-75	4.2	459
197	An implicit membrane generalized born theory for the study of structure, stability, and interactions of membrane proteins. *Biophysical Journal*, **2003**, 85, 2900-18	2.9	346
196	Theoretical and computational models of biological ion channels. *Quarterly Reviews of Biophysics*, **2004**, 37, 15-103	7	321
195	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, 851-69	6.5	312
194	Balancing solvation and intramolecular interactions: toward a consistent generalized Born force field. *Journal of the American Chemical Society*, **2006**, 128, 3728-36	16.4	290
193	Ions and counterions in a biological channel: a molecular dynamics simulation of OmpF porin from Escherichia coli in an explicit membrane with 1 M KCl aqueous salt solution. *Journal of Molecular Biology*, **2002**, 319, 1177-97	6.5	230
192	Generalized solvent boundary potential for computer simulations. *Journal of Chemical Physics*, **2001**, 114, 2924-2937	3.9	206
191	A Grand Canonical Monte Carlo-Brownian dynamics algorithm for simulating ion channels. *Biophysical Journal*, **2000**, 79, 788-801	2.9	192
190	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
189	PBEQ-Solver for online visualization of electrostatic potential of biomolecules. *Nucleic Acids Research*, **2008**, 36, W270-5	20.1	163
188	Ion permeation through the alpha-hemolysin channel: theoretical studies based on Brownian dynamics and Poisson-Nernst-Plank electrodiffusion theory. *Biophysical Journal*, **2004**, 87, 2299-309	2.9	163

187	Ion channels, permeation, and electrostatics: insight into the function of KcsA. *Biochemistry*, **2000**, 39, 13295-306	3.2	158
186	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, 6771-6	11.5	157
185	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
184	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
183	Molecular dynamics and NMR spectroscopy studies of E. coli lipopolysaccharide structure and dynamics. *Biophysical Journal*, **2013**, 105, 1444-55	2.9	125
182	Implicit solvation based on generalized Born theory in different dielectric environments. *Journal of Chemical Physics*, **2004**, 120, 903-11	3.9	124
181	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
180	CHARMM-GUI 10 years for biomolecular modeling and simulation. *Journal of Computational Chemistry*, **2017**, 38, 1114-1124	3.5	119
179	Glycan Reader: automated sugar identification and simulation preparation for carbohydrates and glycoproteins. *Journal of Computational Chemistry*, **2011**, 32, 3135-41	3.5	118
178	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
177	Improving the CHARMM force field for polyunsaturated fatty acid chains. *Journal of Physical Chemistry B*, **2012**, 116, 9424-31	3.4	102
176	CHARMM-GUI Glycan Modeler for modeling and simulation of carbohydrates and glycoconjugates. *Glycobiology*, **2019**, 29, 320-331	5.8	101
175	E. coli outer membrane and interactions with OmpLA. *Biophysical Journal*, **2014**, 106, 2493-502	2.9	97
174	Cholesterol flip-flop: insights from free energy simulation studies. *Journal of Physical Chemistry B*, **2010**, 114, 13342-8	3.4	97
173	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
172	Optimized atomic radii for protein continuum electrostatics solvation forces. *Biophysical Chemistry*, **1999**, 78, 89-96	3.5	94
171	Revisiting hydrophobic mismatch with free energy simulation studies of transmembrane helix tilt and rotation. *Biophysical Journal*, **2010**, 99, 175-83	2.9	91
170	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

169	Imaging the electrostatic potential of transmembrane channels: atomic probe microscopy of OmpF porin. *Biophysical Journal*, **2002**, 82, 1667-76	2.9	79
168	Influence of hydrophobic mismatch on structures and dynamics of gramicidin a and lipid bilayers. *Biophysical Journal*, **2012**, 102, 1551-60	2.9	78
167	Membrane assembly of simple helix homo-oligomers studied via molecular dynamics simulations. *Biophysical Journal*, **2007**, 92, 854-63	2.9	74
166	Improving Protein-Ligand Docking Results with High-Throughput Molecular Dynamics Simulations. *Journal of Chemical Information and Modeling*, **2020**, 60, 2189-2198	6.1	69
165	Molecular dynamics studies of ion permeation in VDAC. *Biophysical Journal*, **2011**, 100, 602-610	2.9	68
164	A systematic molecular dynamics simulation study of temperature dependent bilayer structural properties. *Biochimica Et Biophysica Acta - Biomembranes*, **2014**, 1838, 2520-9	3.8	63
163	Application of torsion angle molecular dynamics for efficient sampling of protein conformations. *Journal of Computational Chemistry*, **2005**, 26, 1565-78	3.5	63
162	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
161	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. *Biophysical Journal*, **2015**, 109, 2012-22	2.9	60
160	Bilayer Properties of Lipid A from Various Gram-Negative Bacteria. *Biophysical Journal*, **2016**, 111, 1750-1760	2.9	60
159	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
158	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
157	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, 513-9	6.5	58
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155	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	3.9	58
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153	Differences in the electrostatic surfaces of the type III secretion needle proteins PrgI, BsaL, and MxiH. *Journal of Molecular Biology*, **2007**, 371, 1304-14	6.5	55
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150	BamA POTRA Domain Interacts with a Native Lipid Membrane Surface. *Biophysical Journal*, **2016**, 110, 2698-2709	2.9	52
149	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
148	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
147	Transmembrane helix assembly by window exchange umbrella sampling. *Physical Review Letters*, **2012**, 108, 108102	7.4	51
146	Brownian dynamics simulations of ion transport through the VDAC. *Biophysical Journal*, **2011**, 100, 611-619	3.9	49
145	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
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132	Two Dimensional Window Exchange Umbrella Sampling for Transmembrane Helix Assembly. *Journal of Chemical Theory and Computation*, **2013**, 9, 13-17	6.4	33
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128	Gramicidin A Channel Formation Induces Local Lipid Redistribution I: Experiment and Simulation. *Biophysical Journal*, **2017**, 112, 1185-1197	2.9	31
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