Sunhwan Jo

List of Publications by Year
in descending order

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45 papers	14,662 citations	186265 28 h-index	233421 45 g-index
45 all docs	45 docs citations	45 times ranked	13040 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	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
7	CHARMMâ€GUI 10 years for biomolecular modeling and simulation. Journal of Computational Chemistry, 2017, 38, 1114-1124.	3.3	224
8	CHARMM-GUIGlycan Modelerfor modeling and simulation of carbohydrates and glycoconjugates. Glycobiology, 2019, 29, 320-331.	2.5	222
9	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
10	Glycan reader: Automated sugar identification and simulation preparation for carbohydrates and glycoproteins. Journal of Computational Chemistry, 2011, 32, 3135-3141.	3.3	172
11	Molecular Dynamics and NMR Spectroscopy Studies of E.Âcoli Lipopolysaccharide Structure and Dynamics. Biophysical Journal, 2013, 105, 1444-1455.	0.5	153
12	Constant-pH Molecular Dynamics Simulations for Large Biomolecular Systems. Journal of Chemical Theory and Computation, 2017, 13, 5933-5944.	5.3	139
13	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
14	Exploring the Conformational Transitions of Biomolecular Systems Using a Simple Two-State Anisotropic Network Model. PLoS Computational Biology, 2014, 10, e1003521.	3.2	112
15	Cholesterol Flip-Flop: Insights from Free Energy Simulation Studies. Journal of Physical Chemistry B, 2010, 114, 13342-13348.	2.6	109
16	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
17	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
18	A generic implementation of replica exchange with solute tempering (REST2) algorithm in NAMD for complex biophysical simulations. Computer Physics Communications, 2015, 197, 304-311.	7.5	54

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19	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
20	Optimization and Evaluation of Site-Identification by Ligand Competitive Saturation (SILCS) as a Tool for Target-Based Ligand Optimization. Journal of Chemical Information and Modeling, 2019, 59, 3018-3035.	5.4	47
21	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
22	Molecular Dynamics Simulations of the Cx26 Hemichannel: Insights into Voltage-Dependent Loop-Gating. Biophysical Journal, 2012, 102, 1341-1351.	0.5	35
23	Preferred conformations ofN-glycan core pentasaccharide in solution and in glycoproteins. Glycobiology, 2016, 26, cwv083.	2.5	34
24	Identification and characterization of fragment binding sites for allosteric ligand design using the site identification by ligand competitive saturation hotspots approach (SILCS-Hotspots). Biochimica Et Biophysica Acta - General Subjects, 2020, 1864, 129519.	2.4	34
25	Reduced Free Energy Perturbation/Hamiltonian Replica Exchange Molecular Dynamics Method with Unbiased Alchemical Thermodynamic Axis. Journal of Physical Chemistry B, 2018, 122, 9435-9442.	2.6	33
26	String Method for Proteinâ€“Protein Binding Free-Energy Calculations. Journal of Chemical Theory and Computation, 2019, 15, 5829-5844.	5.3	33
27	Transmembrane Helix Orientation and Dynamics: Insights from Ensemble Dynamics with Solid-State NMR Observables. Biophysical Journal, 2011, 100, 2913-2921.	0.5	29
28	Restricted N-glycan Conformational Space in the PDB and Its Implication in Glycan Structure Modeling. PLoS Computational Biology, 2013, 9, e1002946.	3.2	29
29	The Salmonella Type III Secretion System Inner Rod Protein PrgJ Is Partially Folded. Journal of Biological Chemistry, 2012, 287, 25303-25311.	3.4	28
30	Lipid-Linked Oligosaccharides in Membranes Sample Conformations That Facilitate Binding to Oligosaccharyltransferase. Biophysical Journal, 2014, 107, 1885-1895.	0.5	21
31	Exploring proteinâ€protein interactions using the siteâ€identification by ligand competitive saturation methodology. Proteins: Structure, Function and Bioinformatics, 2019, 87, 289-301.	2.6	21
32	Computational Characterization of Antibodyâ€“Excipient Interactions for Rational Excipient Selection Using the Site Identification by Ligand Competitive Saturation-Biologics Approach. Molecular Pharmaceutics, 2020, 17, 4323-4333.	4.6	20
33	NMR-Based Simulation Studies of Pf1 Coat Protein in Explicit Membranes. Biophysical Journal, 2013, 105, 691-698.	0.5	18
34	Rapid and accurate estimation of proteinâ€“ligand relative binding affinities using site-identification by ligand competitive saturation. Chemical Science, 2021, 12, 8844-8858.	7.4	18
35	Solid-State NMR Ensemble Dynamics as a Mediator between Experiment and Simulation. Biophysical Journal, 2011, 100, 2922-2928.	0.5	17
36	Determination of Ionic Hydration Free Energies with Grand Canonical Monte Carlo/Molecular Dynamics Simulations in Explicit Water. Journal of Chemical Theory and Computation, 2018, 14, 5290-5302.	5.3	17

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37	Roles of glycans in interactions between gp120 and HIV broadly neutralizing antibodies. Glycobiology, 2015, 26, cwv101.	2.5	15
38	Leveraging the Information from Markov State Models To Improve the Convergence of Umbrella Sampling Simulations. Journal of Physical Chemistry B, 2016, 120, 8733-8742.	2.6	14
39	STâ€analyzer: A webâ€based user interface for simulation trajectory analysis. Journal of Computational Chemistry, 2014, 35, 957-963.	3.3	12
40	Solid-State NMR-Restrained Ensemble Dynamics of a Membrane Protein in Explicit Membranes. Biophysical Journal, 2015, 108, 1954-1962.	0.5	11
41	Efficient Determination of Relative Entropy Using Combined Temperature and Hamiltonian Replica-Exchange Molecular Dynamics. Journal of Chemical Theory and Computation, 2015, 11, 2234-2244.	5.3	11
42	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.	2.6	9
43	Toward Biotherapeutics Formulation Composition Engineering using Site-Identification by Ligand Competitive Saturation (SILCS). Journal of Pharmaceutical Sciences, 2021, 110, 1103-1110.	3.3	9
44	Application of site-identification by ligand competitive saturation in computer-aided drug design. New Journal of Chemistry, 2022, 46, 919-932.	2.8	8
45	Simple Synthesis of a Heterocyclophane Exhibiting Antiâ€câ€Met Activity by Acting as a Hatch Blocking Access to the Active Site**. Chemistry - A European Journal, 2021, 27, 1648-1654.	3.3	1