

Jumin Lee

List of Publications by Year in descending order

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31
papers

7,223
citations

331670

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414414

32
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docs citations

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times ranked

7941
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	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
3	<sc>CHARMM-GUI</sc> 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
4	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
5	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
6	Additive CHARMM36 Force Field for Nonstandard Amino Acids. <i>Journal of Chemical Theory and Computation</i> , 2021, 17, 3554-3570.	5.3	39
7	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
8	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
9	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
10	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
11	Preferred conformations of lipooligosaccharides and oligosaccharides of <i>Moraxella catarrhalis</i> . <i>Glycobiology</i> , 2020, 30, 86-94.	2.5	6
12	CHARMM-GUI supports the Amber force fields. <i>Journal of Chemical Physics</i> , 2020, 153, 035103.	3.0	175
13	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
14	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
15	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
16	CHARMM-GUI Glycan Modeler for modeling and simulation of carbohydrates and glycoconjugates. <i>Glycobiology</i> , 2019, 29, 320-331.	2.5	222
17	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
18	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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19	CHARMM-GUI <i>Membrane Builder</i> for Complex Biological Membrane Simulations with Glycolipids and Lipoglycans. <i>Journal of Chemical Theory and Computation</i> , 2019, 15, 775-786.	5.3	388
20	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
21	Molecular Simulation and Biochemical Studies Support an Elevator-type Transport Mechanism in EIIIC. <i>Biophysical Journal</i> , 2017, 112, 2249-2252.	0.5	7
22	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
23	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
24	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
25	CHARMM-GUI 10 years for biomolecular modeling and simulation. <i>Journal of Computational Chemistry</i> , 2017, 38, 1114-1124.	3.3	224
26	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
27	The Structure of a Sugar Transporter of the Glucose EIIIC Superfamily Provides Insight into the Elevator Mechanism of Membrane Transport. <i>Structure</i> , 2016, 24, 956-964.	3.3	37
28	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
29	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
30	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
31	CHARMM-GUI <i>Membrane Builder</i> toward realistic biological membrane simulations. <i>Journal of Computational Chemistry</i> , 2014, 35, 1997-2004.	3.3	1,802