Josh V Vermaas

List of Publications by Year
in descending order

44 papers	1,765 citations	236612 25 h-index	329751 37 g-index
49 all docs	49 docs citations	49 times ranked	2481 citing authors

#	Article	IF	Citations
1	Mechanism of lignin inhibition of enzymatic biomass deconstruction. Biotechnology for Biofuels, 2015, 8, 217.	6.2	195
2	Supercomputer-Based Ensemble Docking Drug Discovery Pipeline with Application to Covid-19. Journal of Chemical Information and Modeling, 2020, 60, 5832-5852.	2.5	134
3	ChAdOx1 interacts with CAR and PF4 with implications for thrombosis with thrombocytopenia syndrome. Science Advances, 2021, 7, eabl8213.	4.7	112
4	Passive membrane transport of lignin-related compounds. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 23117-23123.	3.3	94
5	CHARMM-GUI HMMM Builder for Membrane Simulations with the Highly Mobile Membrane-Mimetic Model. Biophysical Journal, 2015, 109, 2012-2022.	0.2	89
6	Effects of Lytic Polysaccharide Monooxygenase Oxidation on Cellulose Structure and Binding of Oxidized Cellulose Oligomers to Cellulases. Journal of Physical Chemistry B, 2015, 119, 6129-6143.	1.2	87
7	Advances in Multiscale Modeling of Lignocellulosic Biomass. ACS Sustainable Chemistry and Engineering, 2020, 8, 3512-3531.	3.2	79
8	TopoGromacs: Automated Topology Conversion from CHARMM to GROMACS within VMD. Journal of Chemical Information and Modeling, 2016, 56, 1112-1116.	2.5	63
9	Systematic parameterization of lignin for the CHARMM force field. Green Chemistry, 2019, 21, 109-122.	4.6	51
10	Partitioning of Amino Acids into a Model Membrane: Capturing the Interface. Journal of Physical Chemistry B, 2014, 118, 1481-1492.	1.2	48
11	Molecular Lignin Solubility and Structure in Organic Solvents. ACS Sustainable Chemistry and Engineering, 2020, 8, 17839-17850.	3.2	48
12	Conformational heterogeneity of Î± -synuclein in membrane. Biochimica Et Biophysica Acta - Biomembranes, 2014, 1838, 3107-3117.	1.4	47
13	Automated Transformation of Lignin Topologies into Atomic Structures with LigninBuilder. ACS Sustainable Chemistry and Engineering, 2019, 7, 3443-3453.	3.2	47
14	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease. Chemical Science, 2021, 12, 1513-1527.	3.7	47
15	Atomic-level description of proteinâ€“lipid interactions using an accelerated membrane model. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 1573-1583.	1.4	40
16	The dissociation mechanism of processive cellulases. Proceedings of the National Academy of Sciences of the United States of America, 2019, 116, 23061-23067.	3.3	40
17	Differential Membrane Binding Mechanics of Synaptotagmin Isoforms Observed in Atomic Detail. Biochemistry, 2017, 56, 281-293.	1.2	39
18	The cellular membrane as a mediator for small molecule interaction with membrane proteins. Biochimica Et Biophysica Acta - Biomembranes, 2016, 1858, 2290-2304.	1.4	37

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19	A Microscopic View of Phospholipid Insertion into Biological Membranes. Journal of Physical Chemistry B, 2014, 118, 1754-1764.	1.2	36
20	A Quantitative Molecular Atlas for Interactions Between Lignin and Cellulose. ACS Sustainable Chemistry and Engineering, 2019, 7, 19570-19583.	3.2	36
21	GPU-Accelerated Drug Discovery with Docking on the Summit Supercomputer. , 2020, , .		36
22	Mesoscale Reactionâ€“Diffusion Phenomena Governing Ligninâ€First Biomass Fractionation. ChemSusChem, 2020, 13, 4495-4509.	3.6	35
23	Efficient Exploration of Membrane-Associated Phenomena at Atomic Resolution. Journal of Membrane Biology, 2015, 248, 563-582.	1.0	33
24	Lignin-KMC: A Toolkit for Simulating Lignin Biosynthesis. ACS Sustainable Chemistry and Engineering, 2019, 7, 18313-18322.	3.2	33
25	Electrostatic lock in the transport cycle of the multidrug resistance transporter EmrE. Proceedings of the National Academy of Sciences of the United States of America, 2018, 115, E7502-E7511.	3.3	32
26	Activity and Thermostability of GH5 Endoglucanase Chimeras from Mesophilic and Thermophilic Parents. Applied and Environmental Microbiology, 2019, 85, .	1.4	28
27	High-throughput virtual laboratory for drug discovery using massive datasets. International Journal of High Performance Computing Applications, 2021, 35, 452-468.	2.4	24
28	Membrane Permeability of Fatty Acyl Compounds Studied via Molecular Simulation. Journal of Physical Chemistry B, 2017, 121, 11311-11324.	1.2	23
29	Membrane Permeability of Terpenoids Explored with Molecular Simulation. Journal of Physical Chemistry B, 2018, 122, 10349-10361.	1.2	21
30	Extension of the Highly Mobile Membrane Mimetic to Transmembrane Systems through Customized in Silico Solvents. Journal of Physical Chemistry B, 2017, 121, 3764-3776.	1.2	19
31	Supercomputing Pipelines Search for Therapeutics Against COVID-19. Computing in Science and Engineering, 2021, 23, 7-16.	1.2	19
32	Beyond the Boltzmann factor for corrections to scaling in ferromagnetic materials and critical fluids. European Physical Journal B, 2009, 71, 1-6.	0.6	17
33	Assembly and Analysis of Cell-Scale Membrane Envelopes. Journal of Chemical Information and Modeling, 2022, 62, 602-617.	2.5	17
34	Data-guided Multi-Map variables for ensemble refinement of molecular movies. Journal of Chemical Physics, 2020, 153, 214102.	1.2	12
35	Redox Potential Tuning through Differential Quinone Binding in the Photosynthetic Reaction Center of Rhodobacter sphaeroides. Biochemistry, 2015, 54, 2104-2116.	1.2	11
36	Exploring cryo-electron microscopy with molecular dynamics. Biochemical Society Transactions, 2022, 50, 569-581.	1.6	10

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37	Q-Band Electron-Nuclear Double Resonance Reveals Out-of-Plane Hydrogen Bonds Stabilize an Anionic Ubisemiquinone in Cytochrome bo3 from Escherichia coli. Biochemistry, 2016, 55, 5714-5725.	1.2	9
38	Microscopic Characterization of Membrane Transporter Function by In Silico Modeling and Simulation. Methods in Enzymology, 2016, 578, 373-428.	0.4	8
39	Characterization of 2- and 3-Methoxy in Ubiquinone Binding and Redox Tuning within the Photosynthetic Reaction Center of Rhodobacter Sphaeroides. Biophysical Journal, 2014, 106, 370a.	0.2	0
40	Advances in Atomic-Level Simulations of Large-Scale Functional Motions of Membrane Transporters. Biophysical Journal, 2015, 108, 371a.	0.2	0
41	Chapter 7. Computational Characterization of Molecular Mechanisms of Membrane Transporter Function. RSC Theoretical and Computational Chemistry Series, 2016, , 197-236.	0.7	0
42	Plant terpenoid permeability through biological membranes explored via molecular simulations. Biophysical Journal, 2022, 121, 72a.	0.2	0
43	Lipid specificity of the membrane binding signal protein PLAFP. Biophysical Journal, 2022, 121, 433a-434a.	0.2	0
44	Correlating the transport cycle of small multidrug resistance transporters. Biophysical Journal, 2022, 121, 393a-394a.	0.2	0