

Roland Schulz

List of Publications by Year in descending order

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Version: 2024-02-01

14
papers

21,341
citations

840119

11
h-index

1125271

13
g-index

14
all docs

14
docs citations

14
times ranked

27504
citing authors

#	ARTICLE	IF	CITATIONS
1	GROMACS: High performance molecular simulations through multi-level parallelism from laptops to supercomputers. <i>SoftwareX</i> , 2015, 1-2, 19-25.	1.2	14,414
2	GROMACS 4.5: a high-throughput and highly parallel open source molecular simulation toolkit. <i>Bioinformatics</i> , 2013, 29, 845-854.	1.8	6,072
3	Common processes drive the thermochemical pretreatment of lignocellulosic biomass. <i>Green Chemistry</i> , 2014, 16, 63-68.	4.6	198
4	Mechanism of lignin inhibition of enzymatic biomass deconstruction. <i>Biotechnology for Biofuels</i> , 2015, 8, 217.	6.2	195
5	Simulation Analysis of the Temperature Dependence of Lignin Structure and Dynamics. <i>Journal of the American Chemical Society</i> , 2011, 133, 20277-20287.	6.6	126
6	Scaling of Multimillion-Atom Biological Molecular Dynamics Simulation on a Petascale Supercomputer. <i>Journal of Chemical Theory and Computation</i> , 2009, 5, 2798-2808.	2.3	94
7	Solvent-Driven Preferential Association of Lignin with Regions of Crystalline Cellulose in Molecular Dynamics Simulation. <i>Biomacromolecules</i> , 2013, 14, 3390-3398.	2.6	68
8	Hydration Control of the Mechanical and Dynamical Properties of Cellulose. <i>Biomacromolecules</i> , 2014, 15, 4152-4159.	2.6	44
9	<i>Bacillus subtilis</i> Lipid Extract, A Branched-Chain Fatty Acid Model Membrane. <i>Journal of Physical Chemistry Letters</i> , 2017, 8, 4214-4217.	2.1	42
10	Taskâ€parallel message passing interface implementation of Autodock4 for docking of very large databases of compounds using highâ€performance superâ€computers. <i>Journal of Computational Chemistry</i> , 2011, 32, 1202-1209.	1.5	39
11	Initial Recognition of a Cellodextrin Chain in the Cellulose-Binding Tunnel May Affect Cellobiohydrolase Directional Specificity. <i>Biophysical Journal</i> , 2013, 104, 904-912.	0.2	33
12	Instantaneous Normal Modes and the Protein Glass Transition. <i>Biophysical Journal</i> , 2009, 96, 476-484.	0.2	12
13	Enabling grandâ€canonical Monte Carlo: Extending the flexibility of GROMACS through the GromPy python interface module. <i>Journal of Computational Chemistry</i> , 2012, 33, 1207-1214.	1.5	4
14	Molecular Simulation in the Energy Biosciences. <i>RSC Biomolecular Sciences</i> , 2012, , 87-114.	0.4	0