Shuzhe Wang

List of Publications by Year
in descending order

11 papers	241 citations	1307594 7 h-index	1372567 10 g-index
11 all docs	11 docs citations	11 times ranked	290 citing authors

#	Article	IF	Citations
1	Improving Conformer Generation for Small Rings and Macrocycles Based on Distance Geometry and Experimental Torsional-Angle Preferences. Journal of Chemical Information and Modeling, 2020, 60, 2044-2058.	5.4	82
2	Rationalization of the Membrane Permeability Differences in a Series of Analogue Cyclic Decapeptides. Journal of Chemical Information and Modeling, 2019, 59, 294-308.	5.4	55
3	Combining Machine Learning and Molecular Dynamics to Predict P-Glycoprotein Substrates. Journal of Chemical Information and Modeling, 2020, 60, 4730-4749.	5.4	30
4	Effect of Flexibility, Lipophilicity, and the Location of Polar Residues on the Passive Membrane Permeability of a Series of Cyclic Decapeptides. Journal of Medicinal Chemistry, 2021, 64, 12761-12773.	6.4	22
5	Use of molecular dynamics fingerprints (MDFPs) in SAMPL6 octanolâ€“water log P blind challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 393-403.	2.9	19
6	Evaluation of nine condensed-phase force fields of the GROMOS, CHARMM, OPLS, AMBER, and OpenFF families against experimental cross-solvation free energies. Physical Chemistry Chemical Physics, 2021, 23, 13055-13074.	2.8	9
7	Volume-scaled common nearest neighbor clustering algorithm with free-energy hierarchy. Journal of Chemical Physics, 2021, 154, 084106.	3.0	8
8	Incorporating NOE-Derived Distances in Conformer Generation of Cyclic Peptides with Distance Geometry. Journal of Chemical Information and Modeling, 2022, , .	5.4	7
9	Machine Learning with and for Molecular Dynamics Simulations. Chimia, 2019, 73, 1024.	0.6	5
10	Passing the Barrier â€“ How Computer Simulations Can Help to Understand and Improve the Passive Membrane Permeability of Cyclic Peptides. Chimia, 2021, 75, 518-521.	0.6	4
11	Simulation Studies on the Lipid Interaction and Conformation of Novel Drug-Delivery Pseudopeptidic Polymers. Journal of Physical Chemistry B, 2017, 121, 9113-9125.	2.6	0