Yue Shi

List of Publications by Year
in descending order

12	858	1039406 9	1372195 10
papers	citations	h-index	g-index

14	14	14	1285
all docs	docs citations	times ranked	citing authors

#	Article	IF	Citations
1	Molecular Dynamics Studies of Modular Polyketide Synthase Ketoreductase Stereospecificity. Biochemistry, 2015, 54, 2346-2359.	1.2	15
2	Temperature Dependence of the Complexation Mechanism of Celecoxib and Hydroxyl-Î²-cyclodextrin in Aqueous Solution. Pharmaceutics, 2014, 6, 467-480.	2.0	9
3	Reversible Covalent Inhibition of eEFâ€2K by Carbonitriles. ChemBioChem, 2014, 15, 2435-2442.	1.3	23
4	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. Journal of Chemical Theory and Computation, 2013, 9, 4046-4063.	2.3	524
5	Probing the Effect of Conformational Constraints on Binding. , 2012, , .		0
6	Manipulating JNK Signaling with (â^')-Zuonin A. ACS Chemical Biology, 2012, 7, 1873-1883.	1.6	20
7	From in Silico Discovery to Intracellular Activity: Targeting JNKâ€“Protein Interactions with Small Molecules. ACS Medicinal Chemistry Letters, 2012, 3, 721-725.	1.3	25
8	Probing the Effect of Conformational Constraint on Phosphorylated Ligand Binding to an SH2 Domain Using Polarizable Force Field Simulations. Journal of Physical Chemistry B, 2012, 116, 1716-1727.	1.2	42
9	The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. Journal of Chemical Theory and Computation, 2012, 8, 1721-1736.	2.3	77
10	Multipole electrostatics in hydration free energy calculations. Journal of Computational Chemistry, 2011, 32, 967-977.	1.5	69
11	Trypsin-ligand binding free energy calculation with AMOEBA. , 2009, 2009, 2328-31.		9
12	Molecular Simulation of Equilibrium Solubility and Diffusion of Water in Polymer Electrolyte Membranes. , 2009, , .		0