

# Yue Shi

## List of Publications by Year in descending order

Source: <https://exaly.com/author-pdf/12109964/publications.pdf>

Version: 2024-02-01

12  
papers

858  
citations

1039406

9  
h-index

1372195

10  
g-index

14  
all docs

14  
docs citations

14  
times ranked

1285  
citing authors

#	ARTICLE	IF	CITATIONS
1	Polarizable Atomic Multipole-Based AMOEBA Force Field for Proteins. <i>Journal of Chemical Theory and Computation</i> , 2013, 9, 4046-4063.	2.3	524
2	The Structure, Thermodynamics, and Solubility of Organic Crystals from Simulation with a Polarizable Force Field. <i>Journal of Chemical Theory and Computation</i> , 2012, 8, 1721-1736.	2.3	77
3	Multipole electrostatics in hydration free energy calculations. <i>Journal of Computational Chemistry</i> , 2011, 32, 967-977.	1.5	69
4	Probing the Effect of Conformational Constraint on Phosphorylated Ligand Binding to an SH2 Domain Using Polarizable Force Field Simulations. <i>Journal of Physical Chemistry B</i> , 2012, 116, 1716-1727.	1.2	42
5	From in Silico Discovery to Intracellular Activity: Targeting JNK-Protein Interactions with Small Molecules. <i>ACS Medicinal Chemistry Letters</i> , 2012, 3, 721-725.	1.3	25
6	Reversible Covalent Inhibition of eEF2K by Carbonitriles. <i>ChemBioChem</i> , 2014, 15, 2435-2442.	1.3	23
7	Manipulating JNK Signaling with (âˆ“)-Zuonin A. <i>ACS Chemical Biology</i> , 2012, 7, 1873-1883.	1.6	20
8	Molecular Dynamics Studies of Modular Polyketide Synthase Ketoreductase Stereospecificity. <i>Biochemistry</i> , 2015, 54, 2346-2359.	1.2	15
9	Trypsin-ligand binding free energy calculation with AMOEBA. , 2009, 2009, 2328-31.		9
10	Temperature Dependence of the Complexation Mechanism of Celecoxib and Hydroxyl-Î²-cyclodextrin in Aqueous Solution. <i>Pharmaceutics</i> , 2014, 6, 467-480.	2.0	9
11	Molecular Simulation of Equilibrium Solubility and Diffusion of Water in Polymer Electrolyte Membranes. , 2009, , .		0
12	Probing the Effect of Conformational Constraints on Binding. , 2012, , .		0