

Yujie Wu

List of Publications by Year in Descending Order

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The third column is the impact factor (IF) of the journal, and the fourth column is the number of citations of the article.

20
papers

3,637
citations

17
h-index

21
g-index

21
ext. papers

4,171
ext. citations

4.1
avg. IF

4.96
L-index

#	Paper	IF	Citations
20	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. <i>Journal of Chemical Information and Modeling</i> , 2019 , 59, 3955-3967	6.1	15
19	Accurate Calculation of Relative Binding Free Energies between Ligands with Different Net Charges. <i>Journal of Chemical Theory and Computation</i> , 2018 , 14, 6346-6358	6.4	45
18	Accurate and Reliable Prediction of the Binding Affinities of Macrocycles to Their Protein Targets. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 6290-6300	6.4	29
17	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. <i>Journal of Chemical Theory and Computation</i> , 2017 , 13, 42-54	6.4	68
16	Accurate and reliable prediction of relative ligand binding potency in prospective drug discovery by way of a modern free-energy calculation protocol and force field. <i>Journal of the American Chemical Society</i> , 2015 , 137, 2695-703	16.4	633
15	Lead optimization mapper: automating free energy calculations for lead optimization. <i>Journal of Computer-Aided Molecular Design</i> , 2013 , 27, 755-70	4.2	76
14	Modeling Local Structural Rearrangements Using FEP/REST: Application to Relative Binding Affinity Predictions of CDK2 Inhibitors. <i>Journal of Chemical Theory and Computation</i> , 2013 , 9, 1282-93	6.4	128
13	Prediction of Absolute Solvation Free Energies using Molecular Dynamics Free Energy Perturbation and the OPLS Force Field. <i>Journal of Chemical Theory and Computation</i> , 2010 , 6, 1509-19	6.4	959
12	An improved multistate empirical valence bond model for aqueous proton solvation and transport. <i>Journal of Physical Chemistry B</i> , 2008 , 112, 467-82	3.4	203
11	Charge delocalization in proton channels, I: the aquaporin channels and proton blockage. <i>Biophysical Journal</i> , 2007 , 92, 46-60	2.9	106
10	Charge delocalization in proton channels, II: the synthetic LS2 channel and proton selectivity. <i>Biophysical Journal</i> , 2007 , 92, 61-9	2.9	54
9	Proton transport behavior through the influenza A M2 channel: insights from molecular simulation. <i>Biophysical Journal</i> , 2007 , 93, 3470-9	2.9	98
8	Proton solvation and transport in aqueous and biomolecular systems: insights from computer simulations. <i>Journal of Physical Chemistry B</i> , 2007 , 111, 4300-14	3.4	260
7	Origins of proton transport behavior from selectivity domain mutations of the aquaporin-1 channel. <i>Biophysical Journal</i> , 2006 , 90, L73-5	2.9	68
6	Flexible simple point-charge water model with improved liquid-state properties. <i>Journal of Chemical Physics</i> , 2006 , 124, 024503	3.9	742
5	A computational study of the closed and open states of the influenza a M2 proton channel. <i>Biophysical Journal</i> , 2005 , 89, 2402-11	2.9	41
4	Computer Simulations of Proton Transport Through the M2 Channel of the Influenza A Virus 2005 , 131-145		

3	Computational studies of proton transport through the M2 channel. <i>FEBS Letters</i> , 2003 , 552, 23-7	3.8	17
2	A computer simulation study of the hydrated proton in a synthetic proton channel. <i>Biophysical Journal</i> , 2003 , 85, 864-75	2.9	61
1	A mutant subtilisin E with enhanced thermostability. <i>World Journal of Microbiology and Biotechnology</i> , 2000 , 16, 249-251	4.4	9