Yujie Wu

List of Publications by Citations

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	Prediction of Absolute Solvation Free Energies using Molecular Dynamics Free Energy Perturbation and the OPLS Force Field. *Journal of Chemical Theory and Computation*, **2010**, 6, 1509-19	6.4	959
19	Flexible simple point-charge water model with improved liquid-state properties. *Journal of Chemical Physics*, **2006**, 124, 024503	3.9	742
18	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. *Journal of the American Chemical Society*, **2015**, 137, 2695-703	16.4	633
17	Proton solvation and transport in aqueous and biomolecular systems: insights from computer simulations. *Journal of Physical Chemistry B*, **2007**, 111, 4300-14	3.4	260
16	An improved multistate empirical valence bond model for aqueous proton solvation and transport. *Journal of Physical Chemistry B*, **2008**, 112, 467-82	3.4	203
15	Modeling Local Structural Rearrangements Using FEP/REST: Application to Relative Binding Affinity Predictions of CDK2 Inhibitors. *Journal of Chemical Theory and Computation*, **2013**, 9, 1282-93	6.4	128
14	Charge delocalization in proton channels, I: the aquaporin channels and proton blockage. *Biophysical Journal*, **2007**, 92, 46-60	2.9	106
13	Proton transport behavior through the influenza A M2 channel: insights from molecular simulation. *Biophysical Journal*, **2007**, 93, 3470-9	2.9	98
12	Lead optimization mapper: automating free energy calculations for lead optimization. *Journal of Computer-Aided Molecular Design*, **2013**, 27, 755-70	4.2	76
11	Accurate Modeling of Scaffold Hopping Transformations in Drug Discovery. *Journal of Chemical Theory and Computation*, **2017**, 13, 42-54	6.4	68
10	Origins of proton transport behavior from selectivity domain mutations of the aquaporin-1 channel. *Biophysical Journal*, **2006**, 90, L73-5	2.9	68
9	A computer simulation study of the hydrated proton in a synthetic proton channel. *Biophysical Journal*, **2003**, 85, 864-75	2.9	61
8	Charge delocalization in proton channels, II: the synthetic LS2 channel and proton selectivity. *Biophysical Journal*, **2007**, 92, 61-9	2.9	54
7	Accurate Calculation of Relative Binding Free Energies between Ligands with Different Net Charges. *Journal of Chemical Theory and Computation*, **2018**, 14, 6346-6358	6.4	45
6	A computational study of the closed and open states of the influenza a M2 proton channel. *Biophysical Journal*, **2005**, 89, 2402-11	2.9	41
5	Accurate and Reliable Prediction of the Binding Affinities of Macrocycles to Their Protein Targets. *Journal of Chemical Theory and Computation*, **2017**, 13, 6290-6300	6.4	29
4	Computational studies of proton transport through the M2 channel. *FEBS Letters*, **2003**, 552, 23-7	3.8	17

List of Publications

3	Toward Atomistic Modeling of Irreversible Covalent Inhibitor Binding Kinetics. *Journal of Chemical Information and Modeling*, **2019**, 59, 3955-3967	6.1	15
2	A mutant subtilisin E with enhanced thermostability. *World Journal of Microbiology and Biotechnology*, **2000**, 16, 249-251	4.4	9
1	Computer Simulations of Proton Transport Through the M2 Channel of the Influenza A Virus **2005**, 131-145		