Caitlin C Bannan

List of Publications by Citations

11 papers	323 citations	7 h-index	17 g-index
23 ext. papers	418 ext. citations	5.3 avg, IF	3.38 L-index

#	Paper	IF	Citations
11	Calculating Partition Coefficients of Small Molecules in Octanol/Water and Cyclohexane/Water. *Journal of Chemical Theory and Computation*, **2016**, 12, 4015-24	6.4	104
10	Blind prediction of cyclohexane-water distribution coefficients from the SAMPL5 challenge. *Journal of Computer-Aided Molecular Design*, **2016**, 30, 927-944	4.2	80
9	Escaping Atom Types in Force Fields Using Direct Chemical Perception. *Journal of Chemical Theory and Computation*, **2018**, 14, 6076-6092	6.4	62
8	Toward Learned Chemical Perception of Force Field Typing Rules. *Journal of Chemical Theory and Computation*, **2019**, 15, 402-423	6.4	23
7	SAMPL6 challenge results from [Formula: see text] predictions based on a general Gaussian process model. *Journal of Computer-Aided Molecular Design*, **2018**, 32, 1165-1177	4.2	17
6	Development and Benchmarking of Open Force Field v1.0.0-the Parsley Small-Molecule Force Field. *Journal of Chemical Theory and Computation*, **2021**, 17, 6262-6280	6.4	12
5	Open Force Field Consortium: Escaping atom types using direct chemical perception with SMIRNOFF v0.1		11
4	Improving small molecule force fields by identifying and characterizing small molecules with inconsistent parameters. *Journal of Computer-Aided Molecular Design*, **2021**, 35, 271-284	4.2	6
3	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field		3
2	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field		2
1	Development and Benchmarking of Open Force Field v1.0.0, the Parsley Small Molecule Force Field		2