

Caitlin C Bannan

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.

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