Callum J Dickson

List of Publications by Year in Descending Order

14 papers	1,276 citations	13 h-index	17 g-index
17 ext. papers	1,620 ext. citations	5.8 avg, IF	4.45 L-index

#	Paper	IF	Citations
14	Inhibitor binding influences the protonation states of histidines in SARS-CoV-2 main protease.. *Chemical Science*, **2021**, 12, 1513-1527	9.4	29
13	Revealing Molecular Determinants of hERG Blocker and Activator Binding. *Journal of Chemical Information and Modeling*, **2020**, 60, 192-203	6.1	20
12	Hidden bias in the DUD-E dataset leads to misleading performance of deep learning in structure-based virtual screening. *PLoS ONE*, **2019**, 14, e0220113	3.7	68
11	Using Membrane Partitioning Simulations To Predict Permeability of Forty-Nine Drug-Like Molecules. *Journal of Chemical Information and Modeling*, **2019**, 59, 236-244	6.1	15
10	Calculating Kinetic Rates and Membrane Permeability from Biased Simulations. *Journal of Physical Chemistry B*, **2018**, 122, 11571-11578	3.4	15
9	Structure-Kinetic Relationships of Passive Membrane Permeation from Multiscale Modeling. *Journal of the American Chemical Society*, **2017**, 139, 442-452	16.4	78
8	Contributions of the membrane dipole potential to the function of voltage-gated cation channels and modulation by small molecule potentiators. *Biochimica Et Biophysica Acta - Biomembranes*, **2017** , 1859, 177-194	3.8	18
7	Uncoupling the Structure-Activity Relationships of Adrenergic Receptor Ligands from Membrane Binding. *Journal of Medicinal Chemistry*, **2016**, 59, 5780-9	8.3	17
6	Simulation of lipid bilayer self-assembly using all-atom lipid force fields. *Physical Chemistry Chemical Physics*, **2016**, 18, 10573-84	3.6	32
5	Imaging plasma membrane phase behaviour in live cells using a thiophene-based molecular rotor. *Chemical Communications*, **2016**, 52, 13269-13272	5.8	29
4	Imaging phase separation in model lipid membranes through the use of BODIPY based molecular rotors. *Physical Chemistry Chemical Physics*, **2015**, 17, 18393-402	3.6	66
3	Lipid14: The Amber Lipid Force Field. *Journal of Chemical Theory and Computation*, **2014**, 10, 865-879	6.4	725
2	GAFFlipid: a General Amber Force Field for the accurate molecular dynamics simulation of phospholipid. *Soft Matter*, **2012**, 8, 9617	3.6	151
1	Further evaluation of quantum chemical methods for the prediction of non-specific binding of positron emission tomography tracers. *Physical Chemistry Chemical Physics*, **2011**, 13, 21552-7	3.6	7