Michael R Jones

List of Publications by Year
in descending order

11 papers	137 citations	1307366 7 h-index	1372474 10 g-index
11 all docs	11 docs citations	11 times ranked	168 citing authors

#	Article	IF	Citations
1	Obtaining QM/MM binding free energies in the SAMPL8 drugs of abuse challenge: indirect approaches. Journal of Computer-Aided Molecular Design, 2022, 36, 263-277.	1.3	4
2	A replica exchange umbrella sampling (REUS) approach to predict hostâ€“guest binding free energies in SAMPL8 challenge. Journal of Computer-Aided Molecular Design, 2021, 35, 667-677.	1.3	5
3	Quantum chemical predictions of waterâ€“octanol partition coefficients applied to the SAMPL6 logP blind challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 485-493.	1.3	13
4	Multi-phase Boltzmann weighting: accounting for local inhomogeneity in molecular simulations of waterâ€“octanol partition coefficients in the SAMPL6 challenge. Journal of Computer-Aided Molecular Design, 2020, 34, 471-483.	1.3	7
5	SAMPL6 logP challenge: machine learning and quantum mechanical approaches. Journal of Computer-Aided Molecular Design, 2020, 34, 495-510.	1.3	11
6	Impact of intracellular ionic strength on dimer binding in the NF-kB Inducing kinase. Journal of Structural Biology, 2018, 202, 183-190.	1.3	0
7	SAMPL6 hostâ€“guest challenge: binding free energies via a multistep approach. Journal of Computer-Aided Molecular Design, 2018, 32, 1097-1115.	1.3	16
8	Prediction of CB[8] hostâ€“guest binding free energies in SAMPL6 using the double-decoupling method. Journal of Computer-Aided Molecular Design, 2018, 32, 1059-1073.	1.3	13
9	Absolute and relative pKa predictions via a DFT approach applied to the SAMPL6 blind challenge. Journal of Computer-Aided Molecular Design, 2018, 32, 1179-1189.	1.3	25
10	Partition coefficients for the SAMPL5 challenge using transfer free energies. Journal of Computer-Aided Molecular Design, 2016, 30, 1129-1138.	1.3	19
11	Calculating distribution coefficients based on multi-scale free energy simulations: an evaluation of MM and QM/MM explicit solvent simulations of water-cyclohexane transfer in the SAMPL5 challenge. Journal of Computer-Aided Molecular Design, 2016, 30, 989-1006.	1.3	24