Eliot Boulanger

List of Publications by Year
in descending order

9 papers	392 citations	1040056 9 h-index	1474206 9 g-index
9 all docs	9 docs citations	9 times ranked	606 citing authors

#	Article	IF	Citations
1	QM/MM methods for free energies and photochemistry. Current Opinion in Structural Biology, 2018, 49, 72-76.	5.7	43
2	Optimized Lennard-Jones Parameters for Druglike Small Molecules. Journal of Chemical Theory and Computation, 2018, 14, 3121-3131.	5.3	44
3	Importance of MM Polarization in QM/MM Studies of Enzymatic Reactions: Assessment of the QM/MM Drude Oscillator Model. Journal of Chemical Theory and Computation, 2017, 13, 2954-2961.	5.3	34
4	Chemical substitutions in the selectivity filter of potassium channels do not rule out constricted-like conformations for C-type inactivation. Proceedings of the National Academy of Sciences of the United States of America, 2017, 114, 11145-11150.	7.1	29
5	Hybrid Quantum Mechanics/Molecular Mechanics/Coarse Grained Modeling: A Triple-Resolution Approach for Biomolecular Systems. Journal of Chemical Theory and Computation, 2015, 11, 1809-1818.	5.3	39
6	Toward QM/MM Simulation of Enzymatic Reactions with the Drude Oscillator Polarizable Force Field. Journal of Chemical Theory and Computation, 2014, 10, 1795-1809.	5.3	40
7	Quantum mechanics/molecular mechanics dual Hamiltonian free energy perturbation. Journal of Chemical Physics, 2013, 139, 064105.	3.0	39
8	A microiterative intrinsic reaction coordinate method for large QM/MM systems. Physical Chemistry Chemical Physics, 2013, 15, 14188.	2.8	10
9	Solvent Boundary Potentials for Hybrid QM/MM Computations Using Classical Drude Oscillators: A Fully Polarizable Model. Journal of Chemical Theory and Computation, 2012, 8, 4527-4538.	5.3	114