

Supporting Information for: Sticking to (First) Principles: Quantum Molecular Dynamics and Bayesian Probabilistic Methods to Simulate Aquatic Pollutant Absorption Spectra

1. Experimental molar absorption spectra ('solute'.csv)
2. Example GAMESS MD and TD-DFT inputs (md.inp, td.inp)
3. maintained Python and Matlab scripts can be obtained from the the Eustis Lab Github page http://github.com/eustislab/md_scripts.