Absorption and emission properties of aqueous tryptophan from TD-DFT calculations

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Tryptophan is an essential amino acid consisting of an amino group, a carboxylic acid group, and an indole side chain. Our goal is predicting fluorescent properties of Trp. We use Gaussian and time-dependent density functional theory to optimize the first and second excited states starting from a ground-state optimized conformation. Our first goal has been to determine an accurate and time-efficient functional and basis set with which to perform further calculations. With this method we can calculate excited-state structures, as well as oscillator strengths, dipole moments, and excitation energies of each excited state. Plots of excitation energy vs. optimization step number help to determine the validity of Gaussian's optimization, as several functionals often get confused about which excited state it is following. Then we analyze these structures and data to determine the fluorescence trends of Trp. We use analogous calculations with a conformation of Trp that has been optimized with water molecules to model Trp in its aqueous environment.