Estrogen hormones are commonly found in surface waters as harmful pollutants. Fluorescence can be used to detect these pollutants and photolysis can be used to treat them. Photolysis may reduce the harmful effects of the estrogens by breaking them down. In order to better understand the breakdown of estrone into its photolysis product lumiestrone, the structures and excited states in several solvents were analyzed with Gaussian; absorption and fluorescence energies were also computed. Experimental solvent trends were reproduced and the stabilization of the first excited state points to possible reasons for the different photolysis behavior of the molecules. Lumiestrone had lower energy structures compared to estrone. Results varied based on the presence, hydrogen bonding ability, and polarity of the solvent.