Abstract

Semiempirical (AM1, PM3, and ZINDO) and \textit{ab initio} (HF/6-31G* and B3LYP/6-31G*) quantum chemical calculations have been combined with several popular continuum solvent models (SM2, SM5.4, SM5.42, PCM, and CPCM) and explicit salvation to study the effects of substituents and different solvents on the structures and electronic absorption spectra of aminocoumarin dyes. The implications of the results for the fluorescent properties and proposed nonradiative decay routes in aminocoumarin dyes will be discussed.