

Photophysical Properties of New Psoralen-Adenine Derivatives

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The model compounds, MOPCH2OCnAd (n=2, 3, 5, 6, 8, and 10) in which 5 position of 8-methoxypsoralen (8-MOP) is linked by various lengths of polymethylene bridge to N⁹ of adenine. UV absorption spectra are identical with the sum of MOPCH₂OC3 and adenine absorption spectra. Solvent effects on the UV absorption and fluorescence emission spectra indicate that the lowest excited singlet state is the $(\pi \to \pi^{\prime})$ state. The spectral characteristics of the fluorescence of MOPCH₂OCnAd are strongly dependent upon the nature of the solvents. The fluorescence emission spectra in polar aprotic solvents are broad and structureless due to the excimer formation through the folded conformation accelerated by hydrophobic $\pi - \pi$ stacking interaction. Increasing polarity of the protic solvents leads to higher population of unfolded conformation stabilized through favorable solvation and H-bonding, and consequently to an increase in the fluorescence intensity, fluorescence lifetime, and a shift of fluorescence maximum to longer wavelengths. The decay characteristics of the fluorescence in polar protic solvents shows two exponential decays with the lifetimes of 0.6-0.8 and 1.6-1.9 ns in 5% ethanol/water, while MOPCH₂OC3 shows 0.5 and 1.7 ns fluorescence lifetimes. The long-lived component of fluorescence can be attributed to the relaxed species (i.e., the species for which the solvent reorientation (or relaxation) has occurred), while the short-lived components can be associated with the unrelaxed, or only partially relaxed, species.