TIME-RESOLVED FLUORESCENCE OF TRYPTOPHANYL DIPEPTIDES FROM MOLECULAR DYNAMICS

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Time-resolved information on the effect of a peptide-bonded amino acid on the spectroscopy of tryptophan was obtained using molecular dynamics. The computational method (molecular dynamics + INDO/S) was applied to several tryptophan-containing dipeptides. The presence of the additional amino acid on the indole ring has the effect of altering the $S_0 - S_2$ charge transfer characteristic of the indoles. Furthermore, the nature of the second amino acid plays a role in the evolution of the fluorescence following excitation. The red shifts in fluorescence wavelength following photoexcitation were calculated for several dipeptides in water. Of the dipeptides studied so far, the range of observed red shifts varies from a low of 1800 cm$^{-1}$ for tryptophanylserine, to a high of 2800 cm$^{-1}$ for glycyltryptophan. The time scales of the shifts are sensitive to the nature of the second amino acid. The polarity of the side chain correlates largely with the dipole moment induced in the indole ring, but this does not appear to correlate with the observed red shift in the different dipeptides. The broadening of the spectra caused by the conformational changes of the second amino acid increases as a function of its size and polarity.