

Inhibition of Photoisomerization in Green Fluorescent Protein

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Abstract:

The Green Fluorescent Proteins are a powerful and popular tool in cellular and molecular biology. Its p-hydroxybenzylidene-imidazolinone fluorophore forms autocatalytically after folding, eliminating the need for exogenous dyes. Synthetic models of these fluorophores show absorbance similar to those of the protein, but do not fluoresce in liquid solution. We examine a model of the GFP fluorophore via the tools of ab initio quantum chemistry and characterize relevant features of the excited state surface. We find that isomerization of the double-bonded bridge of the fluorophore is favored in the excited state and can lead to radiationless de-excitation of the molecule. Isomerization is accompanied by significant redistribution of electronic charge, which can interact unfavorably with the protein environment.