

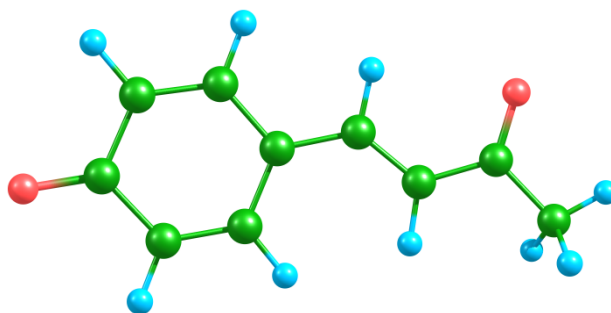
Probing the effect of the environment on the excited state dynamics of biological chromophores by *ab initio* quantum chemistry.

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The key step in activation of many photoreceptors is photoisomerization of a conjugated chromophore inside the protein matrix. To reveal the atomistic details of the photo-isomerization process we use computer simulations. In our work, we use the multi-configurational self-consistent field (CASSCF also with multi-configurational perturbation theory) level of *ab initio* theory to model electronic structure of biological chromophores in gas phase and solution. We characterize reactant, product and intersection geometries as well as the minimum energy pathways that connect these structures. We also compute absorption spectra of these structures, with which we assign measured time-resolved photon-absorption spectra. To understand also the factors controlling the isomerization, we incorporate the effect of the environment (i.e. solvent) at different levels of sophistication, including continuum models, forcefields (MM), Effective Fragment potentials (EFP) and *ab initio*, as well as combination of these. Finally, to explore the role of dynamics, we compare minimum energy pathways to molecular dynamics trajectories. New results on the deactivation of the photoactive yellow protein chromophore in different solvents as well as the explanation for the large difference in the photochemistry of the chromophore in these solvents that were observed experimentally by Changenet-Barret and co-workers [1] will be reported.



- [1] Changenet-Barret, P., Lacomat, F., Plaza, P., J. Photochem. Photobiol. A: Chem., 234:177–181, 2012.