Computational insight in double-bond isomerization of ionic chromophores in photosensory proteins

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Abstract:

Double-bond isomerization is a reaction that is widely employed in light activation of biological photoreceptor proteins. Such proteins commonly bind their chromophores in an ionized (protonated or deprotonated) state. Using computational-chemistry methods, we elucidate if there is a specific chemical mechanism allowing control of double bond isomerization of an ionic chromophore by interactions with the receptor protein. Common features of two prominent examples will be considered, double bond isomerization of the retinal protonated Schiff base in bacteriorhodopsin and of deprotonated p-coumaric methylthioester in photoactive yellow protein.