

Secondary structural changes in phytochromes

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Phytochromes are a major family of red-light photosensor receptors, which are found in higher plants, bacteria, algae and fungi.[1] These biliprotein photoreceptors control diverse cellular functions. For example, in plants they regulate seed germination, stem extension, flowering time and other several light effects.[2]

The phytochrome photoreceptors are divided into two main groups that have antagonistic photobiological properties; the so-called canonical phytochromes and the bathyphytochromes. While the former are thermally stable in the parent Pr (red absorbing) state, the latter exhibit a dark-adapted Pfr (far-red absorbing) state. The co-factor that senses light consists of tetra-pyrrole rings connected by three methylene bridges, that is buried inside the GAF domain of the phytochrome, whereas the photo-sensory domain of the phytochrome is built out of PAS-GAF-PHY domains. It is known that, an incident red light could cause a flip of ring-D around the methylene bridge. This isomerization induces secondary structural changes (figure:1) in the PHY domain of the phytochrome.[3;4]

In our theoretical studies, we employ MD-simulations to understand and explain these important rearrangements at an atomic level and their role in the signalling processes by phytochromes.

Figure:1: left: Cph1-phytochrome in Pr form, right: PaBphP-phytochrome in Pfr form.

References:

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- [2] Lars-Oliver Essen, Jo Mailliet, and Jon Hughes. The structure of a complete phytochrome sensory module in the pr ground state. *Journal of Computational Chemistry*, 30(10), 2008.
- [3] Xiaojing Yang, Zhong Ren, Jane Kuk, and Keith Moffat. Temperature-scan cryocrystallography reveals reaction intermediates in bacteriophytochrome. *Nature*, 479:428-433, November 2011.
- [4] Heikki Takala, Alexander Bjoerling, Oskar Berntsson, Heli Lehtivuori, Stephan Niebling, Maria Hoerke, Irina Kosheleva, Robert Henning, Andreas Menzel, Janne A. Ihalainen, and Sebastian Westenhoff. Signal amplification and transductions in phytochrome photoreceptors. *Nature*, (509):245-248, May 2014.

figure 1

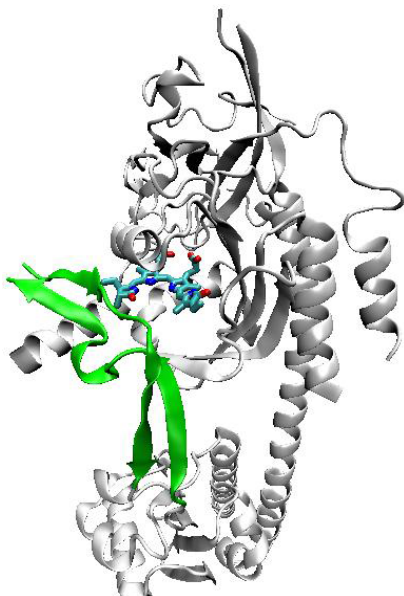


figure 2

