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An integral approach toward elucidating the molecular mechanism of the biological photoreceptor phytochrome

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Phytochromes are ubiquitous modular photoreceptors in plants, bacteria, and fungi that use light as a source of information to control a variety of physiological processes. Upon light absorption by the chromophore, a linear methine-bridged tetrapyrrole, the photosensor module can switch between two stable states, denoted according to their absorption maxima as Pr (red-absorbing) and Pfr (far-red absorbing). The photoinduced transformations are initiated by the E/Z photoisomerization of the methine bridge between the pyrrole rings C and D, followed by a structural relaxation of the chromophore and its immediate surroundings. The last step of the reaction cascade to the photoactivated state involves a secondary structure change of the so-called tongue region which constitutes a link between the photosensor and the output module, usually a histidine kinase, to initiate the downstream signaling processes. In addition to the photoinduced bidirectional reaction pathways there are quasi-unidirectional thermal decay routes back to the stable dark states that are Pr and Pfr in prototypical and bathy phytochromes. Despite achievements in determining the 3D structures of the stable parent states, the mechanism of the underlying molecular reaction steps are yet not known. Here, we present the results of an integral methodological approach including protein crystallography, vibrational spectroscopies and advanced theoretical methods. Within joint efforts of four research groups we have focused on the bacterial bathy phytochrome Agp2. On the basis of the 3D structures of the parent state Pfr and the functional intermediate Meta-F and guided by molecular dynamics simulations and quantum mechanics – molecular mechanics hybrid methods, the results from a comprehensive static and time resolved resonance Raman and IR spectroscopic characterization were analysed and combined to provide a plausible description of the nature, sequence and dynamics of the elementary reaction steps of the photoinduced and thermal processes in phytochromes.

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