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Unraveling origin of spectral tuning in phytochrome photoreceptor proteins enables rational design of the near-infrared absorbing molecular tools

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Near-infrared absorbing molecular tools are in high demand for *in vivo* imaging and control of biological processes. Such tools can be engineered on the basis of phytochrome photoreceptor proteins which play a central role in red/far-red light reception in various organisms. Phytochromes can photoswitch between two thermally stable red-absorbing (Pr) and far-red-absorbing (Pfr) forms, although the molecular mechanism inducing the spectral tuning in phytochromes was unknown yet. We performed computational studies and identified molecular origin of the red spectral shift in the Pfr state. Quantum-chemical calculations demonstrated that interactions between the ring D of the tetrapyrrole chromophore and conserved aspartate lead to a change in the tetrapyrrole electronic structure, which translates to the red shift of the absorption maximum. The MD simulations demonstrated that these interactions can form only after other structural changes take place in the protein ensuring a coupling of the phytochrome spectral and conformational switching. Our study provides understanding of how hydrogen bonding controls phytochrome optical properties and enables rational design of phytochromes and other tetrapyrrole binding proteins as optogenetic tools and fluorescent proteins operating in the far-red spectral region.

Biography

Egle Maximowitsch has completed her Bachelor's Degree in Biochemistry at Vilnius University, Lithuania in 2013 and Master's Degree in Molecular Biosciences at Heidelberg University, Germany in 2015. Since 2015, she is a PhD student in Computational Photobiology at Max Planck Institute for Medical Research in Heidelberg, Germany.

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