

Time-resolved solution X-ray scattering of photoactive proteins

Sebastian Westenhoff¹

¹Department of Chemistry and Molecular Biology, University of Gothenburg,
westenho@chem.gu.se

Photoactive enzymes modulate their activity according to light conditions. We have studied a series of photosensitive proteins, with the goal to identify their structural changes when they are photoswitched. I will present these results. The structural changes range from refolding and quaternary rearrangements in phytochromes, a coiled-coil transition in a light-gated histidine kinase, and redox-driven rearrangements in cryptochromes.

In order to obtain structural information in solution, we have used time-resolved solution X-ray scattering. I provide an overview over the technique and discuss how it can be used to provide specific information on structural changes in solution. In particular, I will present how model-free structural parameters can be extracted and how more detailed structural models can be generated and validated against the difference scattering data. We have also investigated some of the proteins with NMR spectroscopy, infrared spectroscopy, and crystallography. I will discuss the scope and limitations of time-resolved X-ray solution scattering against this background.

References

1. O. Berntsson, R. P. Diensthuber, M. R. Panman, A. Björling, A. J. Hughes, L. Henry, S. Niebling, G. Newby, M. Liebi, A. Menzel, R. Henning, I. Kosheleva, A. Möglich, and S. Westenhoff, "Time-Resolved X-Ray Solution Scattering Reveals the Structural Photoactivation of a Light-Oxygen-Voltage Photoreceptor," **Structure**, vol. 25, no. 6, p. 933–938.e3, Jun. 2017.
2. O. Berntsson, R. P. Diensthuber, M. R. Panman, A. Björling, E. Gustavsson, M. Hoernke, A. J. Hughes, L. Henry, S. Niebling, H. Takala, J. A. Ihalainen, G. Newby, S. Kerruth, J. Heberle, M. Liebi, A. Menzel, R. Henning, I. Kosheleva, A. Möglich, and S. Westenhoff, "Sequential conformational transitions and α -helical supercoiling regulate a sensor histidine kinase," **Nat. Comm.**, vol. 8, no. 1, p. 284, Aug. 2017.
3. A. Björling, O. Berntsson, H. Lehtivuori, H. Takala, A. J. Hughes, M. Panman, M. Hoernke, S. Niebling, L. Henry, R. Henning, I. Kosheleva, V. Chukharev, N. V. Tkachenko, A. Menzel, G. Newby, D. Khakhulin, M. Wulff, J. A. Ihalainen, and S. Westenhoff, "Structural photoactivation of a full-length bacterial phytochrome," **Sci. Adv.**, vol. 2, no. 8, p. e1600920, Aug. 2016.
4. A. Björling, S. Niebling, M. Marcellini, D. Van Der Spoel, and S. Westenhoff, "Deciphering solution scattering data with experimentally guided molecular dynamics simulations," **J. Chem. Theory Comput.**, vol. 11, no. 2, pp. 780–787, Jan. 2015.
5. H. Takala, A. Björling, O. Berntsson, H. Lehtivuori, S. Niebling, M. Hoernke, I. Kosheleva, R. Henning, A. Menzel, J. A. Ihalainen, and S. Westenhoff, "Signal amplification and transduction in phytochrome photosensors," **Nature**, vol. 509, no. 7499, pp. 245–248, 2014.
6. J. A. Ihalainen, E. Gustavsson, L. Schroeder, S. Donnini, H. Lehtivuori, L. Isaksson, C. Thöing, V. Modi, O. Berntsson, B. Stucki-Buchli, A. Liukkonen, H. Häkkänen, E. Kalenius, S. Westenhoff, and T. Kottke, "Chromophore-Protein Interplay during the Phytochrome Photocycle Revealed by Step-Scan FTIR Spectroscopy," **JACS**, vol. 140, no. 39, pp. 12396–12404, 2018.