Experimental report

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Proposal: 8-04-828 **Council:** 4/2018

Title: Light-induced dynamics changes of a LOV photoreceptor measured using kinetic quasi-elastic and elastic incoherent neutron scattering

Research area: Biology

This proposal is a new proposal

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Samples: photoreceptor

Instrument	Requested days	Allocated days	From	To
IN13	6	6	25/09/2018	01/10/2018
IN16B	6	5	21/09/2018	26/09/2018

Abstract:

Members of the LOV protein family are blue-light photoreceptors employing LOV domains as photosensory modules, controlling a number of cellular responses like phototropism, chloroplast movement, stomatal opening, regulation of circadian rhythms, photo-induced growth patterns and pigment synthesis. LOV domains are structurally well-conserved that typically bind a flavin chromophore. Upon light absorption, they undergo a covalent bond formation between the C4a atom of the flavin ring and the sulfur of the neighboring cysteine residue. The photocycle is thermally reversible and in the dark, the FMN-cysteinyl adduct decays to the ground state on a timescale of seconds to days. In this proposal we suggest to investigate changes of molecular dynamics through the dark recovery process of the photoreceptor PpSB1-LOV by experiments on IN16B and IN13. PpSB1-LOV has a dark recovery time of 39 h that enables kinetic QENS and EINS experiments. The aim of the experiments is to identify, if changes in molecular dynamics are directly linked to local rearrangements around the chromophore. Potentially we would also be able to identify transient intermediates that show different dynamics

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We have measured the dynamics of the photoreceptor SB1 using kinetic elastic scans on IN13 and kinetic quasi-elastic scattering (QENS) on IN16B. The SB1 photoreceptor was first illuminated with blue light and neutron scattering was then measured as a function of time while the protein changed from the light-excited state towards the dark-adapted ground state. The known dark recovery time of SB1 from UV/vis spectroscopy is around 40h. A representative QENS spectrum of SB1 in the dark-adapted ground state after D2O subtraction is shown in figure 1. The data was fitted with two Lorentzians accounting for slow global protein diffusion and fast internal dynamics. An elastic peak was observed as well, which is most likely due to the contribution of the empty sample holder.

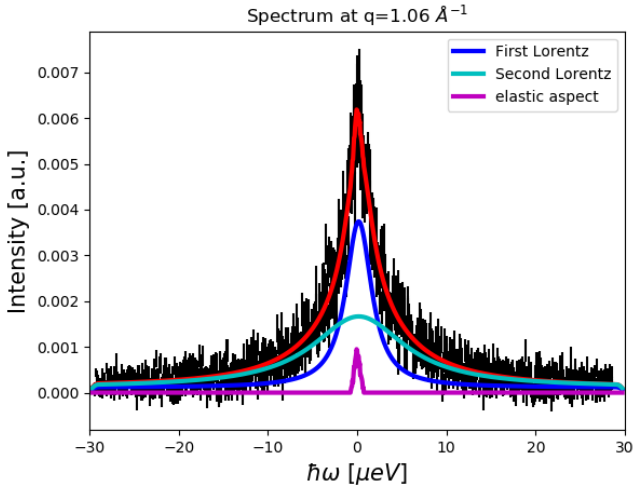

Figure 1: Representative QENS spectrum of SB1 in the dark state measured on IN16B.

Mean square displacements were calculated from the recorded QENS data and are shown in figure 2. The red line is a fit according to $MSD(t) = A \cdot e^{-\frac{t}{\tau}} + c$.

The obtained relaxation time is from the IN16B QENS data is $\tau = 11.4 \pm 4.7\ h$. This is a bit surprising result as the dark relaxation time obtained from UV/vis is 40h.

However, that observation would indicate that local changes around the chromophore and dynamical changes in the protein are decoupled and at least one intermediate is populated during the light to dark transition that has different dynamic behavior than the light-excited state. Its dynamics are, however, similar to the fully dark adapted ground state.

The IN13 data are currently still under evaluation.

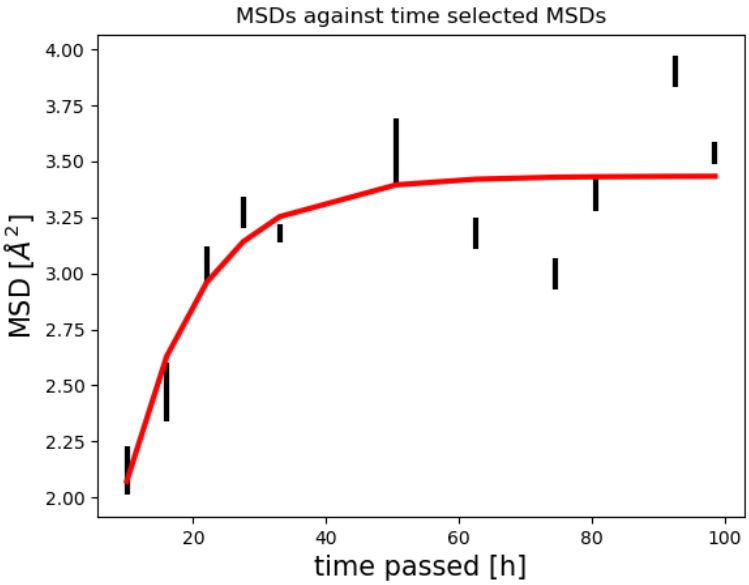

Figure 2: Mean square displacement of SB1 after illumination of the protein as a function of time.