Contribution ID: **85** Type: **Talk**

Ternary complex formation and photoactivation of a photoenzyme results in altered protein structure and dynamics

Tuesday, 10 December 2019 15:40 (25 minutes)

The interplay between protein dynamics and catalysis remains a fundamental question in enzymology. Here, we investigate the ns-timescale dynamics (1) and solution structures (2) of a light-dependent NADPH: protochlorophyllide oxidoreductase (LPOR), a photoenzyme crucial for chlorophyll synthesis. Due to the lack of an LPOR structure, the global structural and dynamic consequences of LPOR/Pchlide/NADPH ternary complex formation remained elusive up to now. By employing quasielastic neutron scattering (QENS) we show that the formation of the ternary holoprotein complex as well as photoactivation lead to progressive rigidification of the protein. Molecular dynamics (MD) simulations, in good agreement with the experimental QENS results, suggests that the increased flexibility observed for the apoprotein stems from structural fluctuations of the NADPH and Pchlide substrate binding sites of the enzyme. In addition, we investigated structural properties of the apo and holoproteins using MD simulations, multi-wavelength analytical ultracentrifugation (MWA-AUC) and small angle X-ray scattering (SAXS) experiments to build a consensus model of the LPOR apoprotein and the substrate/cofactor/LPOR ternary complex. Our findings advance the structural and dynamic understanding of LPORs and provide a first link between protein dynamics and catalysis for this enzyme class.

1. Stadler et al. J. Phys. Chem. B, 2019, 123, 34, 7372-7384
2. Schneidewind et al. Communications Biology, accepted

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Session Classification: Soft Matter

Track Classification: Soft Matter