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Detecting and Identifying Solution-structural Change in Photoactive Proteins

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Akademisk avhandling för filosofie doktorsexamen i naturvetenskap, som med tillstånd från Naturvetenskapliga fakulteten kommer att offentligt försvaras fredagen den 18:e december 2015 kl 13:00 i Carl Kylberg, Institutionen för kemi och molekylärbiologi, Medicinaregatan 7B, Göteborg.

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Abstract

Conformational dynamics allow proteins to fulfil their biological roles, yet the understanding of these molecular machines is largely limited to structural snapshots. Time-resolved X-ray scattering provides a possible way of uncovering such dynamics, but hinges on the ability to trigger reactions, and most critically on the ability to interpret the resulting data. This thesis explores how such experiments can be carried out and analysed.

First, a computational tool for the interpretation of time-resolved X-ray scattering data is presented and tested. It is found that the method works for systems which undergo concerted domain movements, but fails for those where the structure changes in more subtle ways. The method is a potential starting point for systematic, molecular dynamics based interpretation schemes, and provides the most general and unbiased scheme yet.

Further, the time-resolved X-ray scattering technique is applied to the phytochrome family of light-sensing proteins. The results establish a comprehensive mechanism of signal transduction in a particular member of the family. A comparative study shows that this mechanism is also found in several other protein relatives, implying that a core structural apparatus has been conserved and reused for various purposes during evolution.

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