Macromolecular Structure Phasing through UV-radiation Damage

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The continuously increasing demand for synchrotron beam time, both from academic and industrial users, is a direct outcome of the exponential growth of protein crystallography. Fully automated procedures at every level at all synchrotrons are being implemented, allowing the screening of a profusion of sample crystals for more and more projects. However, the sample recognition and centering in the X-ray beam represents one of the major obstacles to achieving such automation. Several independent algorithms have been developed to achieve crystal recognition and centering. UV-based crystal centering takes advantage of the properties of UV-light that specifically reacts with aromatic residues present in proteins or with DNA base pairs. Although very efficient for visualizing protein crystals, a well-known side effect of illuminating biological samples with strong UV-sources resides in the damages induced on the exposed crystals. While these damages can affect the inner structure of the irradiated samples, the structural alterations generated can be extracted and provide new phasing information for solving macromolecular structures, also known as UV radiation induced phasing (UV-RIP). Based on the resulting investigation, a consensus methodology for practical use of UV-RIP at the Photon Factory is proposed.