MS16 Time-resolved diffraction and scattering techniques

MS16-02

Time-resolved serial synchrotron crystallography for the functional characterization of proteins

P. Mehrabi [1], E. Schulz [1]

[1]Universität Hamburg - Hamburg (Germany)

Abstract

Functional characterization of proteins requires insights into the interplay between structure and dynamics. Classical approaches to X-ray crystallography via populating intermediate states by mutation or chemical trapping only provide static time-averaged data sets. Acquiring dynamic data is thus highly important. This leads to dynamic models which better represent the true behaviour of the system. However, elucidating models of protein dynamics that are related to functional characteristics is often rife with difficulty, as enzyme systems are highly complex, and require structural data as a function of time where key insights can be obtained by visualizing the wide range of both internal motions and interactions with the solvent environment. Considering this, serial time-resolved approaches are powerful tools to elucidate time-dependent structures. To this end we have combined and established novel fixed target approaches which enable unique data collection strategies, such as the “Hit And REturn” (HARE) approach. As well as novel reaction initiation strategies with the use of piezo droplet injectors. The “Liquid Application Method for time-resolved Analysis” (LAMA) method simplifying reaction initiation for systems that are not naturally amenable to light activation. Building upon and advancing these current technologies with the use of environmental control of both temperature and humidity and further advances in sample handling and data acquisition strategies are enabling us to delve further into the regulatory mechanisms of allostery and water networks for proteins, inevitably providing insights into fundamental enzymology.