MS01 - Micro & nano crystals in MX

Chairs: Dr. Helen Ginn, Dr. Thomas White

MS01-P01

Theory and methods in phasing of microcrystals of biological macromolecules

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During the last decade, crystallography of microcrystals has become the method of choice for a large number of projects in structural biology. Still today, attempts to collect data from microcrystals of 5–20 μm at their longest dimension, require a dedicated strategy and multi-crystal data collection. While most of the crystal structures can be solved by molecular replacement, in many cases still experimental phasing from microcrystals is needed.

De novo determination of macromolecular structures requires accurate measurement of structure factors and thereby estimation of the phases from the crystals of the given specimen. The anomalous signal from naturally occurring (S, P, Ca, etc) or incorporated (Se, Hg, etc) anomalous scatterers, can be harnessed with a Single-wavelength Anomalous Dispersion (SAD) experiment. Today, the properties of new synchrotron and XFEL sources, or new long-wavelength tunable beamlines for microcrystals [1,2], optimization of the X-ray scanning routines, data collection and processing flows [3], new algorithms for data merging [4], allow to collect, in just few hours, a full data set with anomalous signal by merging data from more than hundred micro crystals collected thus enabling X-ray diffraction data collection and phasing in microcrystallography (Fig. 1) [5]. Moreover, by conducting an extensive survey of 115 PDB sulphur SAD depositions and testing the statistical distribution that these represented, a useful predictor for aiding experimental success using sulphur SAD was developed [6]. So, we will present the current state-of-art of theory and methods in our hands for data collection and phasing in microcrystallography of biological macromolecules.

Keywords: microcrystals, phasing, long wavelength

MS01-P02

Retinal isomerization in bacteriorhodopsin captured by a femtosecond X-ray laser

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Ultrafast isomerization of retinal is the primary step in photoresponsive biological functions including vision in humans and ion-transport across bacterial membranes. We studied the sub-picosecond structural dynamics of retinal isomerization in the light-driven proton pump bacteriorhodopsin using an X-ray laser. A series of structural snapshots with near-atomic spatial and temporal resolution in the femtosecond regime show how the excited all-trans retinal samples conformational states within the protein binding pocket prior to passing through a twisted geometry and emerging in the 13-cis conformation. Our findings suggest ultrafast collective motions of aspartic acid residues and functional water molecules in the proximity of the retinal Schiff base as a key ingredient for this stereo-selective and effcient photochemical reaction.

References:

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Nango, E. et al. (2016). Science, 354, 1552-1557.
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