DANDRITE
Danish Research Institute of Translational Neuroscience
Nordic EMBL Partnership for Molecular Medicine

AARHUS UNIVERSITY
DEPARTMENT OF MOLECULAR BIOLOGY AND GENETICS

DANDRITE Topical Seminar / MBG Focus Talk

Monday 14th March 2016, from 11:30 – 12:30

Conference room 303, building 3130, 3rd floor
Aarhus University, Dept. Molecular Biology and Genetics,
Gustav Wieds Vej 10C, 8000 Aarhus C

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Instrument Scientist - Neutron Macromolecular Crystallography
European Spallation Source ERIC
Lund, Sweden

NMX – A Macromolecular Diffractometer at the European Spallation

Neutron crystallography is the most unambiguous way of determining the hydrogen positions in biological macromolecules, but it remains experimentally very challenging due to the low brightness of the existing neutron sources and the small number of dedicated neutron instruments. The European Spallation Source (ESS) is a European project to build the world's brightest neutron source in Lund, Sweden. One of the first instruments planned at this facility is the NMX macromolecular diffractometer. The NMX instrument is a time-of-flight (TOF) quasi-Laue diffractometer optimised for small samples and large unit cells in order to locate the hydrogen atoms relevant for the function macromolecules.

The ESS long pulse source with its highly brilliant neutron moderator is ideally suited for a macromolecular diffractometer. We estimate that a macromolecular diffractometer at the ESS could be used to collect data from crystals of ~200 µm dimension in some days, which represents an order of magnitude improvement over currently available sources. More importantly it broadens the range of systems that can be investigated to many biologically very interesting molecules, including membrane proteins such as proton pumps.

One of the limiting factors with current neutron instruments is that the fixed detector geometry only allows a maximal unit cell edge of ~150 Å to be resolved without a compromise in the diffraction resolution (d_{min}). The NMX detectors will be mounted on robotic arms, allowing larger unit cells to be resolved by increasing the crystal-to-detector distance. This incurs an increase in the data collection time, but reflections to the same d_{min} can still be observed by moving the detectors. Many of the scientifically most interesting systems, such as proton pumping membrane proteins, crystallise in large unit cells, so being able to resolve a large unit cell edge is a unique advantage. The combination of a neutron flux higher than leading high flux reactor instruments, such as LADI-III, together with the ability to resolve large unit cells and the ability to separate signal from background by time-of-flight leads to world-leading performance particularly with the experimentally most challenging systems. This would transform neutron crystallography into a technique that could answer a significantly larger number of hydrogen related questions in biomolecular science than before.

Host:
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