

MBG FOCUS TALK

Hosted by Ditlev Brodersen, Dept. Molecular Biology and Genetics, Aarhus University

Wednesday 5th March 2025 from 10:00-11:00
In faculty club meeting room (1870-816)



Aaron Finke

Instrument Data Scientist

Data Management and Software Centre, European Spallation Source

Adjunct Associate Professor

Dept. Molecular Biology and Genetics, Aarhus University

(More) Neutrons for Biology: The NMX Instrument at the European Spallation Source

Neutron protein crystallography (NPX) is a technique that is rapidly expanding, with the majority of structures being published in the last decade. A complementary technique to X-ray crystallography and CryoEM in the truest sense, NPX is primarily used to locate the positions of hydrogen atoms in proteins, which is not possible with X-ray methods, nor indeed CryoEM, due to the negligible scattering of hydrogen atoms by X-rays and electrons. NPX also is a radiation-damage free technique, in contrast to X-ray and electron techniques.

Given that proton transfer is the predominant enzyme-catalyzed reaction, appearing in over half of catalytic mechanisms, one would expect NPX to be far more utilized than it currently is. There are less than 300 neutron structures in the PDB. Why is this? The main reason: neutron sources are weak, especially compared to modern synchrotron X-ray sources. Thus, the crystal sizes currently required for NPX are very large— 500 μm at a minimum. Additionally, sample deuteration is sometimes required, to reduce background scatter from the incoherent scattering of neutrons by protons.

The upcoming NMX instrument at the European Spallation Source (ESS) in Lund, Sweden aims to overcome the issues currently hindering NPX from being a more popular method. Slated to become the world's most powerful source for neutrons for research, ESS will provide NMX with a neutron flux up to an order of magnitude higher than the current, greatly cutting down the size requirement of crystal samples. In addition, a new detector technology with flexible geometry will enable, along with the higher flux, assessment of protein crystals with larger unit cell lengths, up to 300 \AA .

In this talk I will discuss in more detail the potential and current limitations of NPX, how the NMX instrument aims to revolutionize NPX, the current timeframe for ESS operation, and how interested users can get involved.