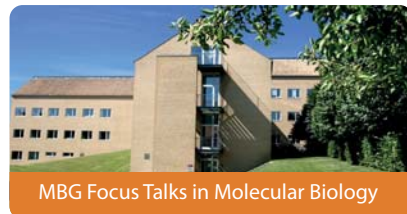


MBG FOCUS TALK

hosted by Section for Structural Biology



Tuesday 29th May 2018 from 10:30-11:00

MBG conference room (3130-303), Gustav Wieds Vej 10C, 8000 Aarhus

By Esko Oksanen, PhD ,Instrument Scientist

European Spallation Source ERIC, Lund, Sweden

Neutron macromolecular crystallography at ESS – where are we today?

The European Spallation Source (ESS) – that is under construction in Lund, Sweden – will be the most powerful neutron source in the world. The long-pulse design of ESS is particularly well-suited for macromolecular crystallography and the NMX instrument is expected to allow data collection from orders of magnitude smaller crystals than on existing neutron sources in a fraction of the time needed today. However even with the power of the ESS the growth of large crystals remains the most significant bottleneck for neutron structure determination, but few crystallographers are expert in the specialist methods for maximising crystal size. Therefore the ESS will provide a support platform for crystal growth optimisation available to the users even before first neutrons. The questions addressed by neutron crystallography typically concern hydrogen atoms, the chemistry of which is quite complex. Computational chemistry methods can be crucial in interpreting the data, so we are also developing methods to combine quantum chemical calculations with crystallographic refinement.

Host: Prof. Poul Nissen