

ACA 2008 Workshop

WK.02 Neutron Macromolecular Crystallography from Expression to Refinement

Organizers: Leighton Coates, coatesl@ornl.gov

Paul Langan, langan_paul@lanl.gov

Workshop Fee: \$60 for Students, \$100 all others

Abstract

Neutron protein crystallography is in a period of expansion at the moment, the number of instruments suitable for data collection will quadruple within the coming years. Two new beamlines based at ORNL are envisioned to start operations in 2009 opening up new capacity and experimental possibilities within the field. This full day workshop has two main objectives 1) Introduce current and future users to the new experimental possibilities that will be enabled by improved instrumentation operating at the most powerful neutron sources in the world. 2) Introduce newly released structure refinement tools that will drastically reduce the knowledge barrier required to conduct a neutron study. This software has many novel features that make it unique from any other protein refinement software in existence. Expert tuition by the software authors will enable users to make the most of this newly released software. **Description** A one day workshop on neutron macromolecular crystallography is proposed for the Saturday preceding the ACA 2008 meeting in Knoxville. The workshop will include an introduction to the field which will be pitched to be understandable to beginners and experts alike. The morning part of the workshop will concentrate on advances in molecular biology techniques and instrumentation to help lower the crystal size requirement for a neutron diffraction study. This was identified as the major bottleneck in neutron protein crystallography during a workshop held at the 2006 ACA meeting in Hawaii. Topaz, a single crystal diffractometer based at the SNS will begin operations.

8.25 Welcome (Leighton Coates, ORNL)

8.30 Introduction and Protein Perdeuteration (Kevin Weiss or Hugh O'Neil, ORNL)

9.15 Optimal Protein Crystallization Techniques (Nobuo Niimura, Ibaraki)

9.50 Hydrogen deuterium exchange patterns (Chris Dealwis, Case Western)

10.30 Coffee Break

11.00 Structural highlight- Joint Refinement of DFPase (Julian Chen, Frankfurt)

11.30 New Neutron Beamlines (Christina Hoffman, ORNL)

12.00 LADI III and D lab (Forsyth, Blakeley or Teixeira, ILL)

12.30 Lunch

1.30 Tutorial Overview (Paul Langan, LANL)

1.35 nCNS (Marat Mustyakimov, LANL)

3.00 Coffee Break

3.30 phenix.refine (Pavel Afonine, LBNL)

5.00 Wrap up and discussion