

Workshops Schedule

April 9, 2015

Please note each workshop will run in the morning and be repeated in the afternoon so attendees can participate in two workshops.

7:30 AM Registration opens at 7:30 AM in the APS Atrium

8:30 AM Morning Workshop Sessions

10:00 AM Coffee

10:30 AM Morning Workshop Sessions - continued

12:00 PM Lunch at Guest House

1:30 PM Afternoon Workshop Sessions

3:00 PM Coffee

3:30 PM Afternoon Workshop Sessions - continued

5:00 PM Workshops end

6:00 PM Dinner at Guest House

7:30 PM Welcome Reception and Registration at Guest House

9:00 PM Registration Closes

Workshop Abstracts

Beamline Tours and Innovative Micro-crystallography Tools

Hosts: **Michael Becker** and **Surajit Banerjee**

Location: Bldg. 436, Sector 23 (GM/CA@APS) and Sector 24 (NE-CAT)

Description: Staff at APS Sector 23 (GM/CA@APS) and Sector 24 (NE-CAT) will host beamline tours, with particular emphasis on demonstrating tools that enable micro-crystallography on challenging macromolecular crystals, such as with membrane-protein crystals grown in mesophase. These will include hardware features, such as mini-beam collimators and a laser system for Second Order Nonlinear Imaging of Chiral Crystals (SONICC), and software features for different scanning techniques – diffraction based centering, raster and vector data collection along with the automated data processing pipeline, RAPD (Rapid Automated Processing of Data).

Lipidic Cubic Phase and Serial Crystallography

Host: **Vadim Cherezov** and **Wei Liu**

Location: Bldg 401 A1100

Description: Serial crystallography, in which data are collected from many small crystals intersecting with X-ray beam at random orientations, has recently demonstrated a great success at X-ray free-electron lasers as well as at third generation synchrotron sources. Lipidic Cubic Phase (LCP) is a membrane-mimetic material that supports membrane protein crystallization and makes an ideal matrix for delivery of membrane and soluble protein crystals for data collection by serial crystallography. The workshop will focus on sample preparation in LCP and will address other questions related to serial crystallography.

Round table on expression/purification

Host: **James Love**

Location: Bldg 401 Auditorium

Description: The major bottleneck in working with membrane proteins remains expression and purification of 'good quality', functionally active material for structural and other studies. Technologies have advanced to make more and more targets tractable and this round table will focus, in a very informal manner, on what methods are working in different labs together with useful troubleshooting and money saving tips.

(Workshops continued)

Data analysis for membrane proteins

Host: **James Holton**

Location: Bldg. 401 E1100

The central problem of membrane protein crystallography is that you generally can't get good enough data from just one crystal. This is not a new problem in crystallography (in fact, it is the oldest), but it has definitely been recalcitrant to automation. The large combinatorial explosion of possible ways to merge data from more than a dozen or so crystals is mostly to blame, but the phenomenon of non-isomorphism is particularly exacerbating. Fortunately, in recent years, several critical algorithmic advances have been made, mostly in the arena of XFEL data processing, but the gap between 3rd and 4th generation sources is now being bridged. Automated procedures are on the horizon, but in the meantime a simple re-visiting of the fundamental principles laid down by the pioneers of crystallography can go a long way to getting your particular project organized and streamlined to make the best use of the crystals that you've got. We will review these principles, and showcase the latest software for addressing the problems of multi-crystal crystallography.

Protein Science at the Advanced Protein Characterization Facility

Host: **Andrzej Joachimiak**

Location: Bldg. 446

The APCF is a new facility recently added to the structural biology portfolio at the Argonne National Laboratory. The physical co-location of APCF with the Advanced Photon Source allows for rapid structural characterization of proteins, and is a unique feature at US light sources.

The APCF utilizes high-throughput methods and has expanded capacity to clone genes, express, produce and crystallize proteins and other macromolecules. Crystals are grown at nanoliter scale from hundreds of conditions and are delivered to APS beamlines where data are collected and three-dimensional structures are often determined in near real time. The biochemical functions of proteins can be deciphered through a combination of structural and bioinformatics data and can be experimentally validated by functional assays.

The workshop will include an introduction to the facility and a tour of the APCF laboratories. Presentations will include several examples of important drug targets and their complexes with ligands, and protein-protein and protein-DNA complexes. Strategies for engineering and optimization of proteins used in our structural and biochemical studies will be discussed.