The CBMS Workbench 2022 - Cycle 3

AGENDA

September 27 - 29, 2022

The times shown are in EDT US Eastern Daylight Saving.

Time conversion Link: https://www.worldtimebuddy.com/

September 27 - Tuesday

Solution Scattering at LIX

09:00 Welcome

09:15 Lecture: Getting to know LIX
   Lin Yang (BNL - CBMS)

10:15 Video Demonstration: The LIX beamline: sample preparation and data collection
   The LIX Team (BNL – CBMS)

10:45 Break and Q&A

11:00 Lecture: SAXS Overview
   Shirish Chondakar (BNL - CBMS)

11:45 Break and Q&A

Joint Session

12:15 Lecture: Overview of the CBMS Program
   Sean McSweeney (BNL - CBMS)

   Christopher Gisriel (Yale University)
   Chris Gisriel is a postdoctoral associate in lab of Gary Brudvig in Yale University’s Department of Chemistry. He received his PhD in Biochemistry at Arizona State University. Chris is an expert in structural biology of photosynthetic membrane protein complexes, having
published structure using a number of techniques including traditional X-ray crystallography, free electron laser crystallography, and single-particle cryo-electron microscopy. Chris is the recipient of various awards, most recently the NIH Pathway to Independence K99 award.

13:10 Lecture: User Access, Training and Outreach: Do’s and Don’ts
Vivian Stojanoff (BNL - CBMS)

13:30 Break

**Macromolecular Crystallography at A/FMX**

13:40 Lecture: Getting to know the MX beam lines

14:10 Lecture: The Data collection Software and the LSDC user interface

14:40 Break and Q&A

15:00 Tutorial: Phenix
Pavel Afonine (Lawrence Berkeley National Laboratory)
Pavel Afonine was born in Russia, raised in Mongolia, and schooled in Western Europe. He received his doctor's degree (PhD) in computational structural biology in 2003 (Henri Poincaré University, France). As research scientist fellow at Lawrence Berkeley National Laboratory (USA), he has been working on diffraction and cryo-EM methods development for the past 19 years. He is one of the key developers of Phenix software suite. Pavel is co-founded Quantum Refinement (Q|R) project of which he is still an active member. A recipient of several prizes Pavel is an avid enthusiast of teaching crystallography, cryo-EM and computing.

17:30 Adjourn

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**September 28 - Wednesday**

**Solution Scattering at LIX**

09:00 Lecture: SAXS/WAXS Data Analysis and Modeling
James Byrnes (BNL - CBMS)

09:45 Lecture: How to submit data to the SASBDB
Shirish Chodankar (BNL - CBMS)
10:10 Break
10:20 Lecture: *In-line SEC and sample preparation*  
    James Byrnes (BNL - CBMS)
10:50 Lecture: *Overview to mail-in measurements at LiX - Mail-in protocol*  
    Lin Yang (BNL - CBMS)

11:30 Break

**Joint Session**

12:00 Lecture: Water Networks Repopulate Protein–Ligand Interfaces with Temperature  
    Marcus Fischer (St. Jude Children’s Research Hospital)
    Marcus Fischer discovered his passion for structural biology during his undergraduate studies in the beautiful Hanseatic city of Lübeck (Germany). During his B.Sc. & M.Sc. studies he conducted research projects in Montpellier (France), Shanghai (China), and Toronto (Canada). He received a Ph.D. in Structural Biology and Chemistry from the University of York (UK) where he worked with Rod Hubbard on fragment-based ligand discovery. During his postdoc with Brian Shoichet, he spent time both in San Francisco (USA), and Toronto (Canada) where he used model proteins to isolate important terms for computational ligand discovery, especially protein flexibility and solvation. He began his independent career at St. Jude in 2017 where his lab is “Exploring the protein conformational landscape for ligand discovery” with a focus on using multi-temperature crystallography

12:40 Lecture: TBD  
    Dale Kreitler

**Macromolecular Crystallography at A/FMX**

09:00 - 17:00 Data Collection by Users (AMX & FMX) - Remote Data Collection by users  
    AMX and FMX team

09:00 - 17:00 Data Collection by Users (FMX) - Remote Data Collection by users  
    FMX team

*Only those who have completed BNL credentials and have completed the connection test will be able to connect to the beam line computers. Those participants only following the MX Workbench will be scheduled in the Morning.*
13:30 - 14:30 Demonstration: Data collection on AMX & FMX

15:30 - 18:00 Participants with credentials following both workbenches will be able to access to collect on provide samples on their own or collect on provided samples

13:30 - 17:00 Data Collection at LIX on participant samples

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**September 29 - Thursday**

*Molecular Crystallography at A/FMX*

09:00 Tutorial: Crystallographic statistics - what do they mean? Kay Diederichs (Universität Konstanz)

09:55 Tutorial: XDS usage - introduction and demonstration Kay Diederichs (Universität Konstanz)

10:45 Break

11:00 Lecture/Tutorial: Auto Proc after midnight Kevin Battaile (NYSBC)

12:00 Break

**Solution Scattering at LIX**

12:30 Tutorial: Introduction to data analysis using the program RAW Kushol Gupta (University of Pennsylvania)

14:30 Lecture: *Data Processing Details* Lin Yang (BNL - CBMS)

15:30 - 17:00 Data Collection at LIX on participant samples