Workshop Schedule

Workshop 2: Applications of Small Angle Scattering to Structural Biology: An Introduction

Organizers: Kushol Gupta, Michal Hammel, Jesse Hopkins

Sunday, July 7, 2024 @ 8:00 AM - 5:30 PM MT

Kindly be aware that the provided schedule is provisional and may be subject to adjustments.

Time	Topic
8:00 AM	**Registration and software installation help; Speaker introduction**
8:15 AM	**BioSAS overview** **Greg Hura (ALS)** *What is SAS and why is it useful?*
8:45 AM	**Basic data reduction and model-independent analysis** **Jesse Hopkins (BioCAT, APS)** *Overview of basic data reduction and model independent analysis, including: Guinier analysis, molecular weight determination, Porod and Kratky plots and flexibility, indirect Fourier transforms and the P(r) function*
10:00AM	**Coffee break**
10:15 AM	**Tutorial 1: Basic data reduction and model-independent analysis** **Jesse Hopkins (BioCAT, APS)** *Hands-on tutorial in how to do basic data reduction and model-independent data analysis*
11:45 AM	**Lunch (provided)**
12:00 PM	**Working Lunch: Introduction to Small Angle Neutron Scattering** **Sai Venkatesh Pingali (ORNL)** *Introduction to SANS, and how it differs from SAXS*
12:30 PM	**Working Lunch: Laboratory Source SAXS** **Andreas Keilbach (Anton Paar)** *Capabilities and opportunities of laboratory source BioSAXS*
12:45 PM	**Sample preparation and complementary biophysical methods for sample assessment** **Kushol Gupta (University of Pennsylvania)** *Best practices for sample purification and preparation for SAS, including the importance of characterization with complementary biophysical methods including static and dynamic light scattering.*
1:45 PM	**SEC-SAXS** **Steve Meisburger (MacCHESS, CHESS)**

	An introduction to experiment and analysis for size exclusion chromatography coupled to SAXS (SEC-SAXS)
2:15 PM	**Tutorial 2: SEC-SAXS data analysis** **Jesse Hopkins (BioCAT, APS) and Steve Meisburger (MacCHESS, CHESS)** *Hands-on tutorial in how to analyze SEC-SAXS data, including buffer subtraction, selecting useful peak regions and an introduction to deconvolution approaches*
2:45 PM	**Coffee break**
3:00 PM	**Model-dependent analysis of SAS data** **Michal Hammel (ALS)** *Calculating scattering profiles from atomic models, atomistic modeling and ensemble modeling. Includes use of AlphaFold predicted structures to model SAS data.*
3:30PM	**Tutorial 3: Atomistic modelling** **Michal Hammel (ALS)** *How to calculate, evaluate, and display atomistic ensemble model using FoXS, MultiFOXS, FoXSDock, and BILBOMD*
4:00 PM	***Ab initio* reconstruction of shape from scattering data** **Thomas Grant (University at Buffalo)** *Calculate, evaluate, and display bead models (DAMMIF/N) and electron density models (DENSS)*
4:30 PM	**Tutorial 4: *Ab initio* reconstruction of shape from scattering data** **Thomas Grant (University at Buffalo)** *Calculate, evaluate, and display bead models (DAMMIF/N) and electron density models (DENSS)*
5:00 PM	**Publishing SAS data** **Thomas Weiss (SSRL)** *Best practices for data presentation, validation, and supporting information*
5:30 PM	**Conclusion**