Workshop Schedule

Workshop 1: Advanced Structure Refinement with Olex2 & NoSpherA2

Organizers: Michael Bodensteiner & Florian Kleemiss
Sunday, July 7, 2024 @ 9:00 AM MT

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

Start	End	Topic
9:00 AM	10:00 AM	Introduction / Workflow in Olex2
10:00 AM	10:15 AM	Coffee Break
10:15 AM	12:00 PM	Handling disorder / Solvent Masking / Fragment DB
12:00 PM	1:00 PM	Lunch on your own
1:00 PM	3:00 PM	Non-spherical refinement using NoSpherA2
3:00 PM	3:15 PM	Coffee Break
3:15 PM	4:00 PM	Olex2 magic tricks with and customizing of Olex2
4:00 PM	5:00 PM	Participants' structural problemsn / Q&A
5:00 PM	5:15 PM	Closing

Participants will be asked to install the necessary software on their personal laptops prior to the workshop. This software includes the primary package Olex2 and users' personal copies of ORCA or pySCF for use in NoSpherA2. Recommended other programs: SHELX. We provide assistance, if necessary, before the workshop from 830-900 am.