Workshop #3: Structure refinement and disorder modelling with Olex2 and NoSpherA2

Date/Time	Friday, July 7, 2023 @ 8:00 AM ET		Registration Fees (registration fee includes catering during coffee and lunch break)
Location	Essex AB		Regular: $180 Per Person Retired: $180 Per Person PostDoc: $120 Per Person Student: $120 Per Person Corporate: $180 Per Person
Max Capacity	50		
Main Contact	Florian Kleemiss		

Announcements

Welcome to our newest ACA Fellows!

Description

Olex2 has become one of the most widely used software for working with single-crystal diffraction data. There are many features that make dealing even with complicated structures very easy. For example, setting up complicated disorder models, the introduction of constraints & restraints and the use of well-documented solvent masks. One of the newest and most revolutionary features is the introduction of non-spherical form factors in the refinement at the click of a button: Non-Spherical Atoms in Olex2 NoSpherA2.

SPONSORED BY:

In this workshop, we will introduce the features that establish a robust routine workflow for the expert refinement of difficult structures. This includes – but is not limited to – treatment of solvent molecules, disorder, fragment-based model building and the generation of publication-quality material directly after the refinement. We will also introduce the workflow implementation of NoSpherA2 and discuss the advantages of this sophisticated refinement technique, which include the significant improvement of the model quality, often allowing for the reliable refinement of hydrogen atom positions from X-ray data.

The workshop will be based on a watch-and-repeat model, where examples are shown on stage. Participants are then encouraged to try the features on their computers, first using provided examples and ultimately with their data

Schedule*

Time	Instructor/Topic
8:30 AM - 8:45 AM ET	Florian Kleemiss | Introduction / Outline
8:45 AM - 9:30 AM ET	Ilia Guzei • Workflow in Olex2 – Solving and refining sucrose • File Editing / Refinement options
9:30 AM - 10:00 AM ET	Michael Bodensteiner | Refining conformational disorder
10:00 AM - 10:30 AM ET	Coffee Break
10:30 AM - 11:00 AM ET	Ilia Guzei | Refinement of disorder across a symmetry element
11:00 AM - 11:30 AM ET	Florian Kleemiss | Use of solvent masks (BYPASS)
11:30 AM - 12:00 PM ET	Michael Bodensteiner | Producing a publishable CIF and CheckCIF
12:00 PM - 1:00 PM ET	Lunch (included)
1:00 PM - 1:30 PM ET	Ilia Guzei | Using FragmentDB for "known suspects"
1:30 PM - 3:00 PM ET	Florian Kleemiss • NoSpherA2 – How it works • Refinement of exemplary structures using NoSpherA2
3:00 PM - 3:30 PM ET	Coffee Break
3:30 PM - 4:00 PM ET	Florian Kleemiss | Visualizations and diagrams with Olex2
4:00 PM - 6:30 PM ET	• Participants' examples and Q&A • Group discussion of results/ progress/ survey

Instructors

Michael Bodensteiner

OlexSys Ltd.

Ilia Guzei

Chemistry, UW Madison

Florian Kleemiss

University of Regensburg

Back to top ⌃

Three Minute Thesis Sponsors

Anton Paar

Opening Reception Sponsor

BIORTUS

Special Sponsors

Rigaku

ALTOS

YSIG Lunch Sponsor

AIP

Diamond Level Sponsors [$5,000+]

Rigaku

BIORTUS

ThermoFisher SCIENTIFIC

Ruby Level Sponsors [$2,500-$4,999]

Anton Paar

nano soft

NEW ENGLAND BioLabs Inc. — be INSPIRED drive DISCOVERY stay GENUINE

Genentech
A Member of the Roche Group

MiTeGen
www.mitegen.com

AIP

MERCK
INVENTING FOR LIFE

SHUIMU

NSF's ChemMatCARS UCHICAGO

BRUKER

Emerald Level Sponsors [$1,000-$2,499]

STRUCTURA BIOTECHNOLOGY

Poly Crystallography, Inc.

Structural Dynamics

DECTRIS
detecting the future

TESCAN
PERFORMANCE IN NANOSPACE

WYATT TECHNOLOGY

Nanome

SEISMIC THERAPEUTIC

xenocs
Exploring the very small

ALTOS

REFEYN

Sapphire Level Sponsors [$1-$999]

GATAN AMETEK

HELIX BIOSTRUCTURES

NIS
NANOIMAGING SERVICES

sptlabtech & quantifoil

WYATT TECHNOLOGY

diamond

American Crystallographic Association, Inc.

About Us | Join | Privacy Policy