



Rigaku



## 3D-ED Workshop ICIQ Tarragona

Monday 23rd of October

**14:00** *Welcome*

**14:30 – 18:00: Introduction into Electron Diffraction, origins of 3D-ED**

14:30 – 15:15 Introduction into Electron Diffraction, Origins of 3D-ED (Tatiana Gorelik)

15:15 – 16:00 Visit of the laboratory

16:00 - 16:30 Coffee break

16:30 – 17:15 Measurement strategies (Sergi Plana)

17:15 – 18:00 Trouble shooting software/hardware (Workshop team)

Tuesday 24th of October

**9:00 - 13:00: Measurement software, sample preparation and measurement strategy**

9:00 – 9:30 Electron diffractometers for crystallographers (Paul Klar)

9:30 – 10:00 Sample preparation I (Tatiana Gorelik)

10:00 – 10:30 Sample preparation II (Jakub Wojciechowski, Christian Schürmann).

10:30 – 11:00 Coffee break

11:00 – 12:00 Selecting samples and instrument settings (Christian Schürmann)

12:00 – 13:00 Non-standard measurement: beam sensitive, cryo-preparation (Christian Schürmann, Jakub Wojciechowski)

13:00 – 14:00 Lunch

**14:00 - 17:30: Kinematical refinement and software.**

14:00 – 14:45 Introduction to CrysAlisPro and standard data processing (Mathias Meyer)

14:45 – 15:30 Data processing challenges / Merging data (Jordi Benet)

15:30 - 16:00 Coffee Break

16:00 – 17:00 Olex (Horst Puschmann)

17:00 – 17:30 Nosferat2 (Oleg Dolomanov)



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## Wednesday 25th of October

### **9:00 - 13:00: Dynamical Refinement and Software, Absolute Structure Determination**

9:00 – 9:30 Introduction to multiple scattering (Sergi Plana)

9:30 – 10:00 Introduction to dynamical refinement and absolute structure determination (applications) (Paul Klar)

10:00 – 10:30 Absolute structure determination at pharmaceutical compounds (Jordi Benet)

10:30 – 11:00 Coffee break

11:00 – 13:00 Demonstration + tutorial: Structure determination using Jana2020 (Paul Klar)

13:00 – 14:00 Lunch

### **14:00 - 17:30: Measurements hands on and data processing (Workshop team)**

Three groups: Sample preparation  
Measurement  
Software

15:30 - 16:00 Coffee Break

Three groups: Sample preparation  
Measurement  
Software

## Thursday 26th of October

### **9:00 - 13:00: Hands on cryo-preparation and low temperature (Workshop team)**

Three groups: Sample preparation  
Measurement  
Software

12:15 – 13:00 Final discussion and closing (Workshop team)