Workshop presentation

The Cambridge Structural Database (CSD), curated by the Cambridge Crystallographic Data Centre (CCDC) is a reference in crystallochemistry, and lies at the interface of chemistry and structural biology. In addition to a very comprehensive database of over one million organic and metal-organic crystal structures, the CCDC develops and curates the CSD Software, which harnesses the wealth of information in the database to help scientists gain new insights in their structures.

The *Société Chimique de France, section Bretagne-Pays de Loire*, proposes in close collaboration with the French network for professional crystallographers ЯÉCIPROCS and the CCDC a presentation and practical training of the tools available in the CSD.

A short lecture (1,5 hours) is proposed between 10h and 11h30 to give an overview of the possibilities of the CSD for everyone - student, post-doc or staff - working with small-molecule structures (ligands, complexes, polymeric). The afternoon session (13h30-17h) is a practical training for those with activated CSD licenses. If you do not know who is the CSD referent in your laboratory, please contact directly the trainer who will give you the name of your CSD referent. The CSD software needs to be installed and activated on your laptop before the start of the afternoon session.

Both morning and afternoon session will be held in English.

Practical Information

- Date: 05/07/2023 10h30-17h
- Organisers: Thierry Roisnel, Carmelo Prestipino, Marie Dallon (ISCR, Rennes) & Elzbieta Trzop (IPR, Rennes)
- Trainer: Arie van der Lee (IEM, Montpellier) - CSD ambassador for France
- Participation fees: free
- Registration : https://cdifx.univ-rennes1.fr/CSD_Rennes2023_register.html
- Registration deadline : friday June 23th
- Location: Institut des Sciences Chimiques de Rennes, Campus de Beaulieu, Rennes
- web site: https://cdifx.univ-rennes1.fr/CSD_Rennes2023.html

Program

- Crystallographic data bases and how to access them in France
- The Cambridge Structural Database (CSD) - overview
- Deposit and retrieve structures at the CSD - why and how?
- WebCSD and CSD Enterprise
- Tools provided by the CSD for the analysis of structural data

  - Basic tools:
    * Mercury - visualisation and geometric measurements (bonds, angles, torsion angles), publication-ready structural drawings
    * Conquest - comparison with analogous structures, structure search with literature data.
  - More advanced tools:
    * CSD Materials - analysis of intra- and inter-molecular interactions
    * CSD Materials - analysis of packing of molecular structures
    * CSD Mogul - validation of intramolecular geometric features

- Some capita selecta