Taller sobre *Cambridge Structural Database (CSD)* y sus herramientas

Consejo Superior de Investigaciones Científicas
Madrid (21- 23 septiembre 2016)

Taller impartido por el **Cambridge Crystallographic Data Centre** (CCDC), organizado por el **CSIC**, en su condición de *National Affiliated Center* del CSD System en España, con la colaboración del **Grupo Especializado de Cristalografía y Crecimiento Cristalino (GE3C)** de la Real Sociedad Española de Química (RSEQ) y de la **Factoría de Cristalización (FIS2015-71928-REDC).** Con patrocinio de la empresa **BRUKER**.

Se celebrarán dos sesiones idénticas, de día y medio cada una, en el CSIC, en la sede de la **Unidad de Recursos de Información Científica para la Investigación** (C/ Joaquín Costa, 22. 28002 Madrid)

Organización:

CSIC
Consejo Superior de Investigaciones Científicas

www.ccdc.cam.ac.uk

Co-organización:

GE3C

factoría de CRISTALIZACIÓN

Patrocinio:

BRUKER

The Cambridge Crystallographic Data Centre (CCDC) is dedicated to supporting structural chemistry research by rigorously compiling the Cambridge Structural Database (CSD), the world's only comprehensive and fully curated database of over 800,000 experimentally determined organic and metal-organic crystal structures. This unparalleled resource to the scientific community and its knowledge-based applications for conformational assessment, intermolecular interaction analysis, crystal engineering and formulation studies continue to guide structural chemistry research in over 1,200 academic institutions worldwide and all of the world's top pharmaceutical companies.

These two workshops will include sessions on:

CSD Introduction

- Introduction to the CCDC, the CSD and CCDC software

CSD-Community

- Structure deposition using the new data deposition services
- Structure access using the new CSD web interface
- Datasets, data citations, discoverability and DOIs
- High resolution visualisation of structures using Mercury
- 3D printing through Mercury

CSD-Materials

- Introduction to Conquest and Mercury
- Investigating and analyzing intermolecular interactions
- Understanding polymorph stability using 3D interaction mapping
- Comparing and understanding a polymorph family
- Knowledge based co-crystal design
- Programmatic access to the CSD using the Python API

CSD-Discovery

- Applications of the CSD System in drug discovery
- Introduction to Mogul (a knowledge-based library of molecular geometry)
- Investigation of conformational preference on activity, using ConQuest, Mercury and Mogul
- Analysis of ligand geometry in a protein-ligand crystal structure

Taller 1:

Miércoles 21/09/2016: 9:00 a 17:30

9.00-9.30	Registro
9.30-10.00	CSD Introduction
10.00-11.00	CSD-Community – Part 1
11.00-11.30	Pausa
11.30-13.00	CSD-Community – Part 2
13.00-14.00	Almuerzo
14.00-15.30	CSD-Materials – Part 1
15.30-16.00	Pausa
16.00-17.30	CSD-Materials – Part 2

Jueves 22/09/2016: 9:00 a 12:00

9.00-10.30	CSD-Discovery – Part 1
10.30-11.00	Pausa
11.00-12.00	CSD-Discovery – Part 2
12.00	End of Workshop

Taller 2:

Jueves 22/09/2016: 13:00 a 17:00

13.00-13.30	Registro
13.30-14.00	CSD Introduction
14.00-15.00	CSD-Community – Part 1
15.00-15.30	Pausa
15.30-17.00	CSD-Community – Part 2

Viernes 23/09/2016: 9:00 a 17:00

9.00-10.30	CSD-Materials – Part 1
10.30-11.00	Pausa
11.00-12.30	CSD-Materials – Part 2
12.30-13.30	Almuerzo
13.30-15.00	CSD-Discovery – Part 1
15.00-15.30	Pausa
15.30-17.00	CSD-Discovery – Part 2
17.00	End of Workshop

Se recomienda a los asistentes llevar al taller sus ordenadores portátiles, con la base CSD instalada.

Localización:

Consejo Superior de Investigaciones Científicas

Unidad de Recursos de Información Científica para la Investigación
C/ Joaquín Costa, 22. 28002 Madrid

2ª planta. Sala 215

Persona de contacto: Mercedes Baquero (mbaquero@bib.csic.es)