CSD

CSD-System

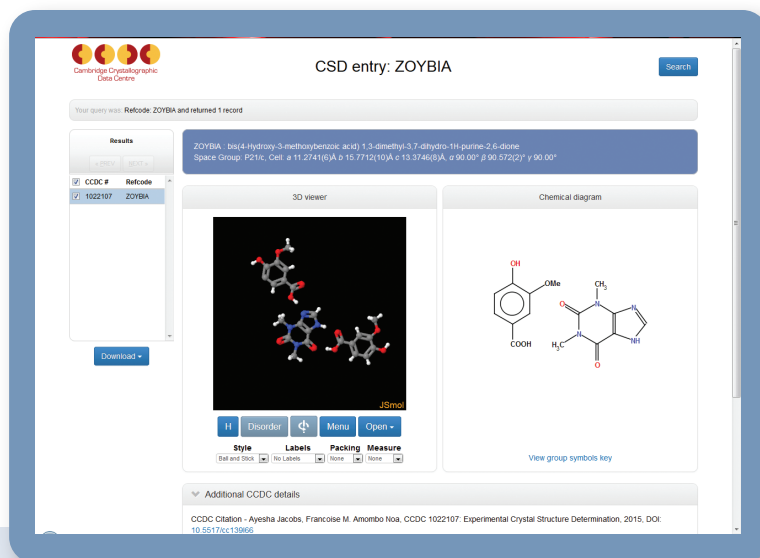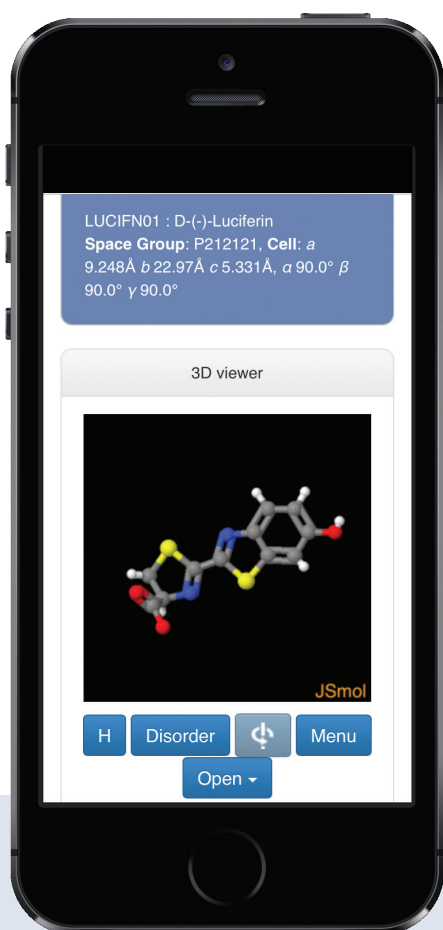Unlock value from crystal structure information in the CSD

The **Cambridge Structural Database** (CSD) is the world's most comprehensive and up-to-date knowledge base of crystal structure data, curated using CSD-derived knowledge and by expert scientific editors, and comprising over 775,000 structures and associated chemical data. The **Cambridge Crystallographic Data Centre** (CCDC) enhances the CSD's value to research scientists worldwide by providing state-of the art visualisation and analysis software to exploit this collection of all known small molecule crystal structures. CSD data supports chemistry research worldwide with over 1,200 user sites and 8,000 publication citations, and you can access the CSD on the desktop, via the web and through scripting APIs.

The **CSD-System** suite comprises the **Cambridge Structural Database** (CSD) with desktop and web-based access (**WebCSD**), 3D searching, advanced visualisation and structural geometry analysis, intermolecular interaction analysis, conformation analysis, and support for tailored application building (**CSD Python API**).

Find

WebCSD offers cross-platform web-based structure lookup for the research community. You can easily access, visualise and analyse crystal structure data to support your research, education, or peer review, and you will experience a consistent user interface, whatever your device.

Intuitive access to comprehensive, high quality, and up-to-date structure data for desktop or mobile devices at **www.ccdc.cam.ac.uk/getstructures**

LUCIFN01 : D-(-)-Luciferin
Space Group: P212121, **Cell**: *a* 9.248Å *b* 22.97Å *c* 5.331Å, *α* 90.0° *β* 90.0° *γ* 90.0°

3D viewer

JSmol

H | Disorder | φ | Menu

Open ▾

CSD entry: ZOYBIA

Cambridge Crystallographic Data Centre

Search

Your query was: Refcode: ZOYBIA and returned 1 record

ZOYBIA : bis(4-Hydroxy-3-methoxybenzoic acid) 1,3-dimethyl-3,7-dihydro-1H-purine-2,6-dione
Space Group: P21/c, Cell: *a* 11.2741(6)Å *b* 15.7712(10)Å *c* 13.3746(8)Å, *α* 90.00° *β* 90.572(2)° *γ* 90.00°

Results

CCDC # | Refcode
1022107 | ZOYBIA

Download ▾

3D viewer

Chemical diagram

JSmol

H | Disorder | φ | Menu | Open ▾

Style | Labels | Packing | Measure
Ball and Stick | No Labels | None | None

View group symbols key

Additional CCDC details

CCDC Citation - Ayesha Jacobs, Francoise M. Amombo Noa, CCDC 1022107: Experimental Crystal Structure Determination, 2015, DOI: 10.5517/cc139l66

Search

With **ConQuest**, it's easy to answer very specific structure questions on your desktop using highly flexible 3D searching of the CSD and local in-house databases. You can quickly identify the most relevant structures across the CSD based on a wide range of properties, including chemical constraints such as cyclicity, and use interaction and structure-property knowledge gained to drive design decisions.
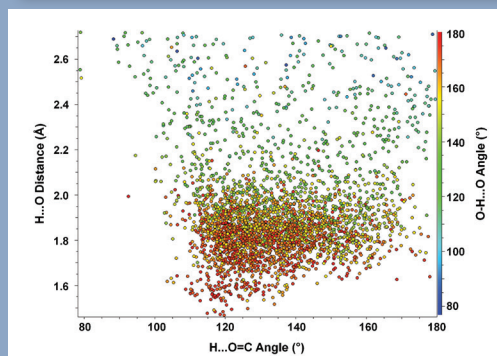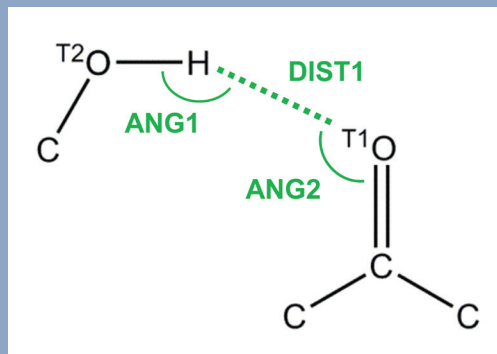

Powerful searching options – example shows searching constrained by Dist1 with results displayed as a scatterplot, and an example hit
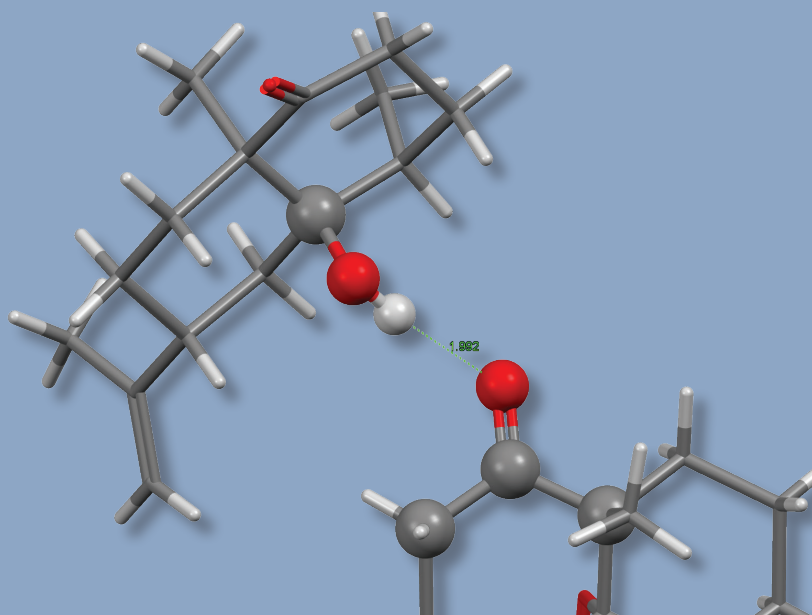
Visualise

Mercury, the CSD visualisation and analysis application, provides rapid, high quality structure representations for effective scientific communication. A wide variety of representations are available including molecular conformations, crystal structures, crystallographic planes and simulated morphologies; and you can easily incorporate images and videos into papers, presentations, and teaching materials.

One-click generation of high quality structure representations for effective scientific communication, including POV-rendering, videos and even 3D printing (including plinth)
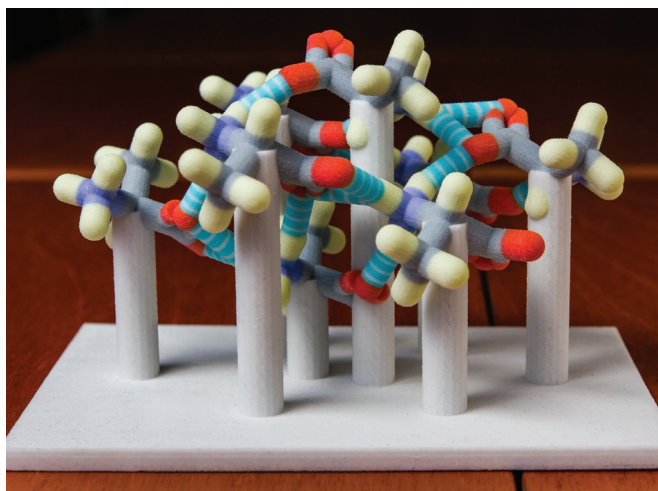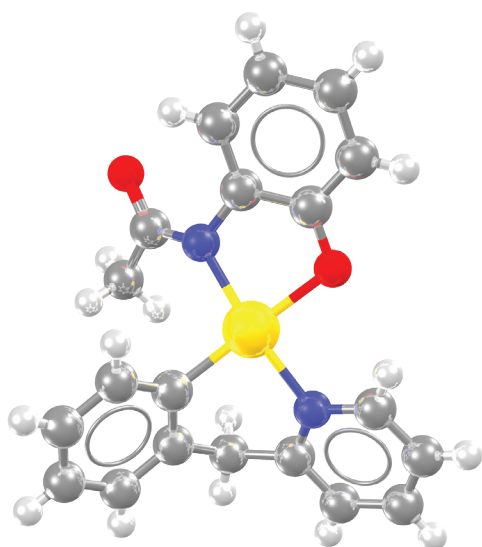
Conformations

By combining millions of chemically classified bond lengths, angles, torsion angles, and ring conformations in the CSD, **Mogul** provides precise information on preferred molecular geometries. Interactive plots enable you to rapidly validate the complete geometry of a given query structure and identify any unusual features.

Rapid conformation assessment – example shows analysis of the highlighted torsion angle in the crystal structure of meloxicam (CSD refcode: ENICOU). The orientation of the thiazole ring in the structure is consistent with the distribution of angles for similar torsions in the CSD.
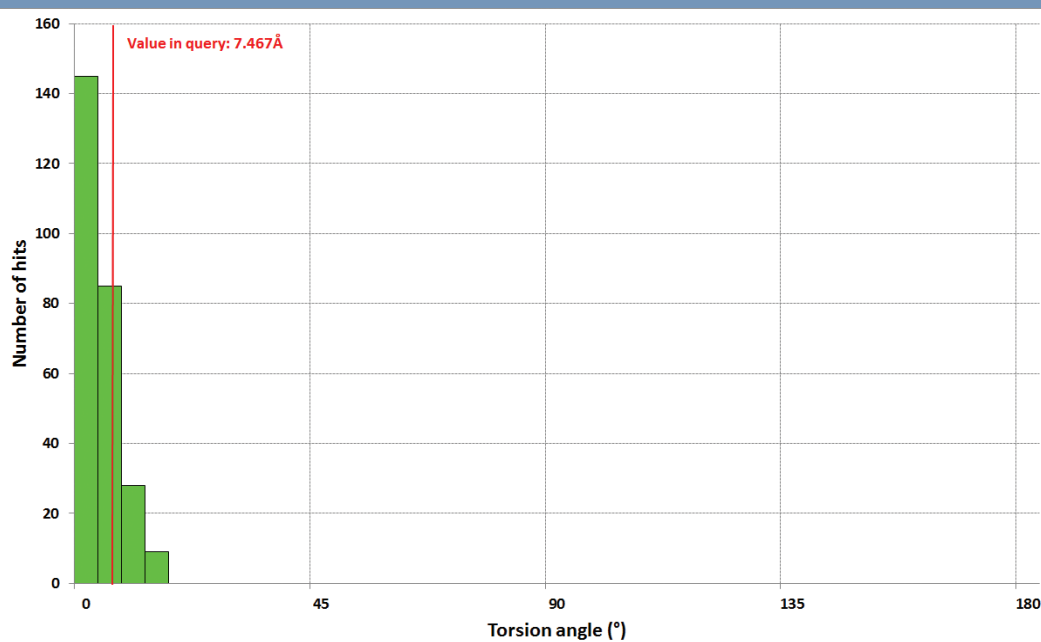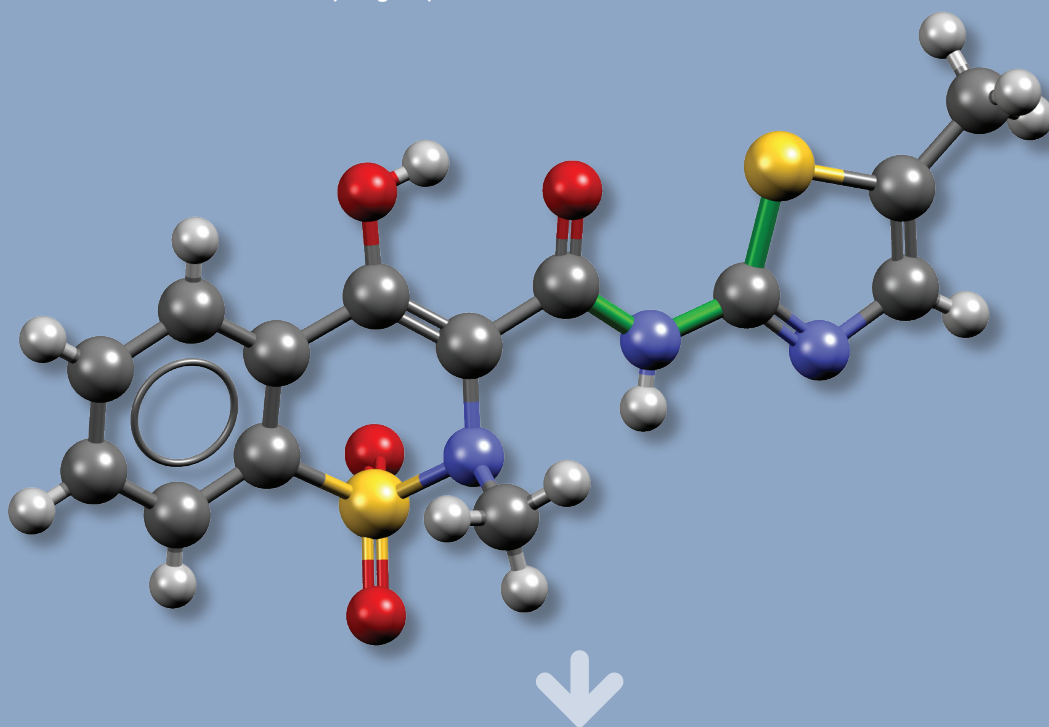
Interactions

IsoStar uses the wealth of interaction information available in the CSD and in the Protein Data Bank (PDB) to show the probability and characteristics of interactions between specific pairs of chemical functional groups. You can easily explore the intermolecular interaction distribution for your functional group of interest and assess the most likely interaction geometry based on experimental evidence. In drug discovery, this information can be used to identify and understand isosteric replacement, for example carboxylic acid and tetrazole display the same characteristic interaction patterns.

Analysis of carbonyl-OH and amide-NH interactions in the CSD showing scatterplot and contour surface
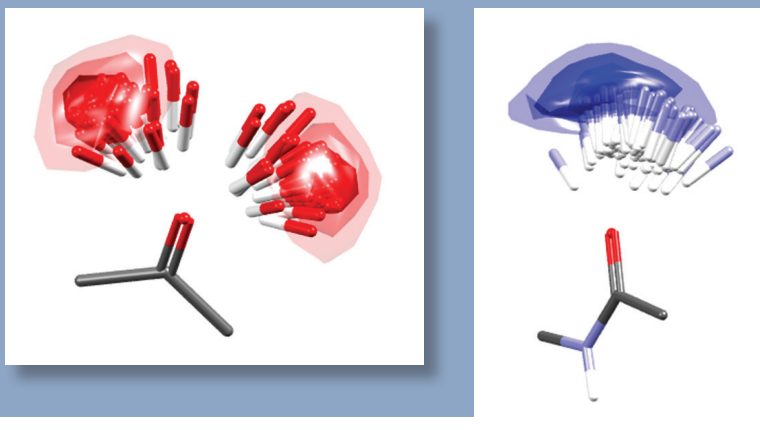
Connect

The **CSD Python API** (Application Programming Interface) enables you to create tailored scripts using the whole spectrum of CSD functionality to answer your targeted research questions, or integrate access to crystal data and CSD functions seamlessly into 3rd party software. Functions include:

- Reading and writing of molecules, crystals and entries
- Search capabilities (including substructure, similarity, text/numeric & reduced cell)
- Geometry analysis
- Interaction analysis
- Molecular & crystallographic descriptor calculation
- 2D diagram generation

Batch mode execution is supported as well as the ability to run scripts from within Mercury. You can construct and share protocols that exploit crystal data and analysis functions to support collaboration across diverse and distributed research environments.

> *"Being able to construct and combine detailed searches of structural and publication data allows for some very creative research projects. In using the API I was able to create complex searches that were easily exchangeable among different classes of compounds. I would not have been able to complete my research without it."*

Amy Sarjeant (Research Assistant Professor, Northwestern University, USA)

Construct and combine detailed search and analysis functionality to produce tailored scripting workflows

Who can benefit from using CSD-System?

- Chemists in academia and industry wanting to discover, access and visualise crystal structures easily to support their research.

- Crystallographers and modellers wanting to mine, visualise and analyse crystal structure data.

- Medicinal chemists and modellers wanting to optimise geometry and interactions as part of their ligand design process.

- Depositors, reviewers and publishers wanting to access crystallographic data and for the data to be readily accessible to other researchers, discoverable and reusable.

- Educators wanting to use crystal structure data to enhance the learning experience for their students.

What's new for CSD-System visualisation?

- Fast and convenient generation of high quality graphics using POV-Ray rendering.

- Easy movie generation.

- One-click output of model files for 3D printing.

What's in the new CSD Python API?

- Access to the complete range of CSD functions, enabling users to embed crystallographic data analysis in tailored scripts.

- Ability to integrate crystal data and CSD functions into 3rd party software.

- Batch mode execution.

THE CAMBRIDGE
CRYSTALLOGRAPHIC
DATA CENTRE

CSD
50
1965 ~ 2015