The Cambridge Structural Database 2016

What's New?

Welcome to the new CSD-System. We wanted to do something spectacular for our user communities worldwide to mark the 50th anniversary of the Cambridge Structural Database, and we have. This release marks the biggest change in the delivery of the CSD since it first appeared in computerized form.

For the first time, we have brought together the CCDC's entire range of structure-based analysis, visualization and communication tools to create CSD-Enterprise – our new, complete offering, delivered by default to every academic researcher, educator and student. There is huge emphasis on communication, allowing studies across groups and disciplines, automating complex analysis processes, visualizing systems and gathering results for sharing, collaboration, presentation and publication.

Here is the new CSD product line up:

For all academic users and for commercial organizations, including our Research Partners:

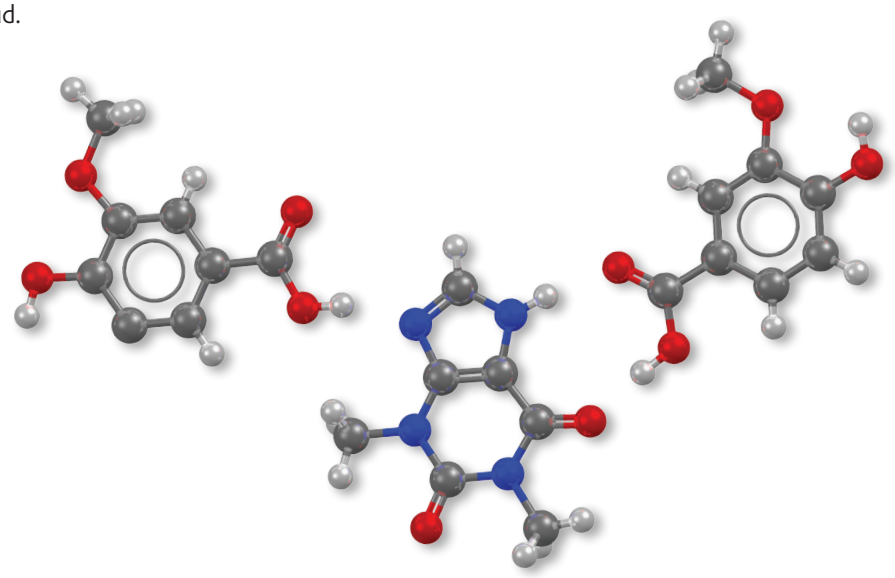
- **CSD-Enterprise** - Our complete set of solutions. ALL academic users of the core CSD-System or our protein-ligand docking application, GOLD, will now receive everything, with no upgrade required. CSD-Enterprise is also available to cross-discipline research groups in industry.

For commercial users:

- **CSD-System** - The essential CSD database and analysis tools for all scientists who need comprehensive and validated structural chemistry data
- **CSD-Discovery** - Our specialist set of solutions for users in discovery chemistry operations
- **CSD-Materials** - Our specialist set of solutions for users studying the structure and properties of crystalline materials

Of course, there's a lot of new data and exciting new functionality with this release, too, and that's all described below. We've added more entries to the CSD than ever before and included new capabilities to support and communicate your research, from complete Python Application Programming Interface access to all CSD functionality through to 3D printing support.

Thank you for your continuing support of the CCDC and the CSD – a unique resource for structural chemistry of which our whole community can be proud.



The 750,000th entry in the CSD (refcode: ZOYBIA, DOI:10.5517/cc139166)

CSD-Enterprise – Access the CSD and all CCDC application software

The new system for all academic users and for eligible industrial sites

For the first time, ALL academic users have access to ALL of the CCDC software with the launch of CSD-Enterprise. If you are a user in an educational institution, you can now use the Cambridge Structural Database (CSD) and as many CCDC-released software products as you want. **CSD-Enterprise includes everything in the CSD-System, CSD-Discovery and CSD-Materials**, described below.

The CSD - The world's essential database of crystal structures

The Cambridge Structural Database (CSD) is the world's comprehensive and up-to-date database of crystal structures, fully validated and ready to use. This year's new release breaks all records! At more than 785,000 entries, the 2016 CSD release (CSD version 5.37) adds almost 70,000 new entries – the biggest annual increase ever. Containing important and unique structures not available anywhere else, the CSD is used by scientists worldwide and provides the complete crystal structure database for chemists working with any organic and metal-organic compounds. This year, the CSD features more than 4,000 new entries published directly through the CSD. The 2016 release includes targeted enhancements to over 50,000 existing CSD entries, improving the consistency and discoverability of structures in the database. New data is constantly added to the CSD and the first update will already mean you will immediately have access to more than 800,000 entries.

CSD-System – Find, analyse and communicate crystal structures

For all academic users through CSD-Enterprise and for existing commercial users

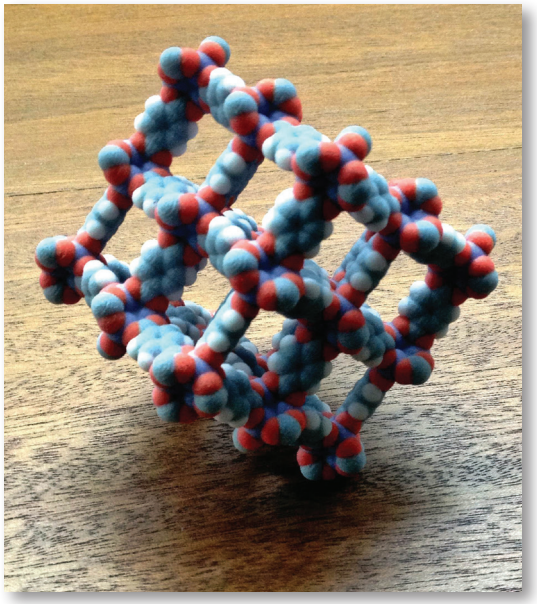
The CSD-System brings you the essential crystallographic and structural chemistry capabilities to deliver knowledge from the CSD: powerful 2D/3D search, extensive geometry analysis tools, inter- and intramolecular interaction analysis, high impact graphics and new Application Programming Interface (API) connectivity.

The exciting new CSD Python API means you can now access almost all capabilities of the CSD-System programmatically. You can:

- Create your own specialist analysis applications using any CSD-driven functions, configuring CSD-based analysis for your research needs
- Publish your own custom menus in Mercury to support collaboration and teaching
- Share your custom CSD Python API functions with others as a member of the worldwide CSD user community and benefit from their routines, all through the user forum on the CCDC website
- Access functionality from pipelining tools or your own web pages

Enhancements to Mercury for analysis and visualization include the ability to:

- Produce new, high-impact graphics renderings, for publications and displays
- Output files for 3D printing
- Produce movies, to demonstrate dynamic processes
- Identify and assign chiral centres *(R* or *S)*



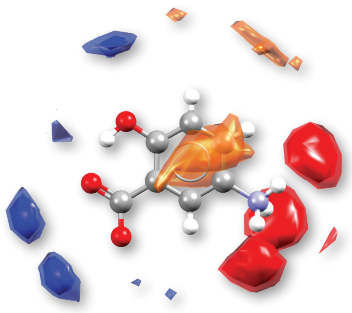
3D printed model of a metal organic framework (refcode: SAHYIK, DOI:10.5517/cc8md6g) created using Mercury

CSD-Discovery – Discover new molecules

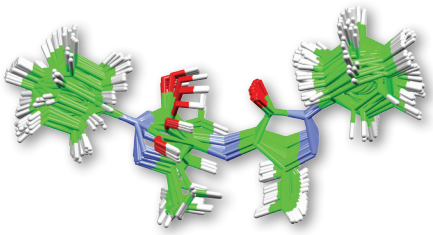
New for all academic users through CSD-Enterprise and for commercial users upgrading to CSD-Discovery or CSD-Enterprise. CSD-Discovery incorporates the CSD-System, SuperStar, GOLD, Relibase and new functionality.

CSD-Discovery provides in one place all the tools you need for discovering new molecules:

- Create, or download from our portal, CSD-driven analyses and workflows. Publish them to your own menu in Mercury with the new CSD Python API
- Understand your structures and explore ligand geometry with confidence using two powerful new CSD data-driven features:
  - Conformer Generator - the only one of its kind driven directly from all the latest validated experimental data in the CSD, rather than force field estimations
  - Ligand Overlay - applying the CSD to identify common binding modes, interactions and geometries of structurally diverse ligands
- Validate your receptor-bound ligand geometry using the same CSD routines in place at the Protein Data Bank, adding confidence to your publications and submissions
- Search, analyse and visualize protein-ligand structures using SuperStar and Relibase. Identify receptor site similarity based on structure, even when there is a low, or no sequence match.
- Perform protein-ligand docking experiments and virtual screening using GOLD, now also fully supported for Mac platforms, enabling interoperability with the CSD-System, within CSD-Discovery



Full interaction map for the anti-inflammatory mesalazine (refcode: SAQJAV01, DOI:10.5517/ccy7cxf)



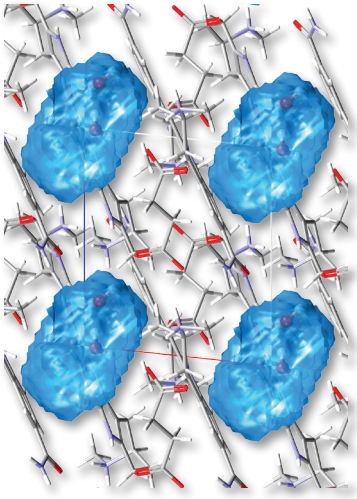
Ensemble of conformations generated by the CSD-driven conformer generator (refcode: CEPMOA, DOI:10.5517/cc8y29k)

CSD-Materials – Engineer new materials

New for all academic users and for industrial users upgrading to CSD-Materials or CSD-Enterprise. CSD-Materials incorporates the CSD-System, CSD Solid Form Module, DASH and new functionality.

CSD-Materials helps you explore exciting new materials through analysing intra- and intermolecular interactions within the lattice, helping you to understand your material's behaviours and refine its properties:

- Create, or download from our portal, CSD-driven analyses and workflows. Publish them to your own menu in Mercury with the new CSD Python API
- Communicate your results with new high impact graphics and 3D printing support, highlighting lattice void spaces and channels
- Discover preferred intra- and intermolecular interactions and engineer changes to satisfy these requirements
- Interpret crystal packing and compare with CSD data using powerful packing feature, similarity and motif searches, and hydrogen bond propensity analysis
- Understand the effects of hydration on your lattice with the new hydrate analyser
- Explore the structures of potential co-crystals using the new molecular complementarity tool
- Explore solid state molecular geometry using the new CSD-driven Conformer Generator – unique because all results are generated from all the latest experimental data in the CSD
- Solve your powder crystal structure using CSD data with DASH



Crystal packing displaying space occupied by water molecules (refcode: MEXSEP, DOI:10.5517/cc10ck42)

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