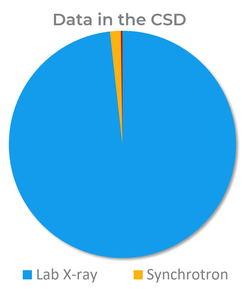
From Structure to Publication: How to Utilise Your FAIRE License

CCDC
advancing structural science

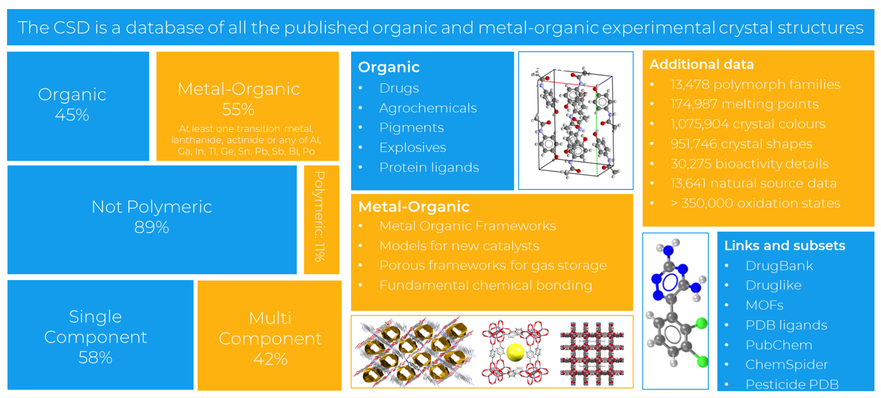
FAIRE and the Cambridge Structural Database

The Frank H. Allen International Research and Education programme (FAIRE)[1] provides a campus-wide Academic CSD-Enterprise license, free of charge, to researchers in parts of the world with demonstrable need. Your FAIRE license gives you access to the Cambridge Structural Database (CSD) and CSD Software. The CSD is a curated database of over 1.25 million small molecule organic and metal-organic experimental crystal structures.[2] Data is curated in house, validated and stored in a standardised format so that the structures are searchable, reusable and easily findable.



The CSD contains a wealth of structural information from drugs, pigments, and protein ligands, to metal organic frameworks, large clusters, and catalyst structures. These structures are enriched with bibliographic information, 2D structural diagrams, and experimental details, as well as physical and chemical properties. This can be invaluable for your research whether it is experimental or computational.

CSD Software is included with your license, giving you access to the desktop software ConQuest and Mercury, which provide you with all the core functionality you need to search the CSD and analyse crystal structures. If you work in life sciences, then you can explore GOLD and CSD-CrossMiner to perform protein-ligand docking and pharmacophore searching. As a companion to CSD desktop software, WebCSD provides you with flexible online searching capability. CSD-Python API is also provided which allows you to harness these programs' functionality programmatically.

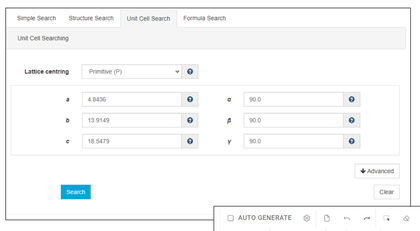


Find out how you can use the CSD data and CSD software to enhance the analysis of multiple aspects of your structures to enrich your publications.

Here we use CSD entry UNOYEE[3] to demonstrate how you could perform crystal structure analysis using CSD Software for a publication in a journal such as *Acta Crystallographica E*.

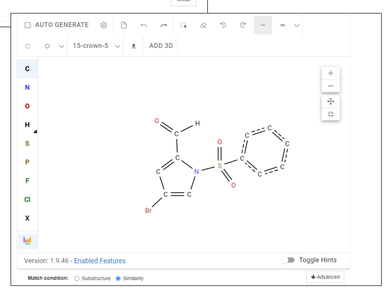
Is my compound novel?

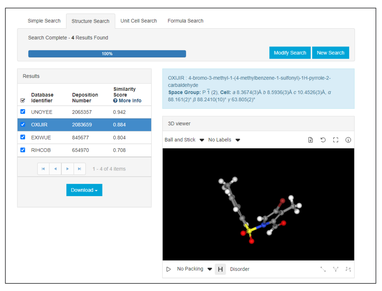
The first thing you will want to know is if your structure is novel. Has it been published before? Are there many similar compounds? You can use ConQuest and WebCSD to check this.

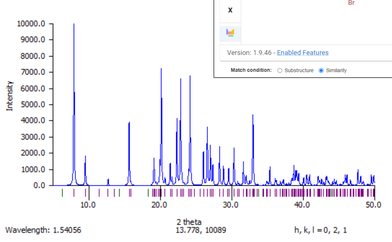


Screen the CSD for unit cell hits as you collect your data using WebCSD. You can also use CellCheckCSD during data collection.

Find comparable structures using substructure or similarity searching with WebCSD.



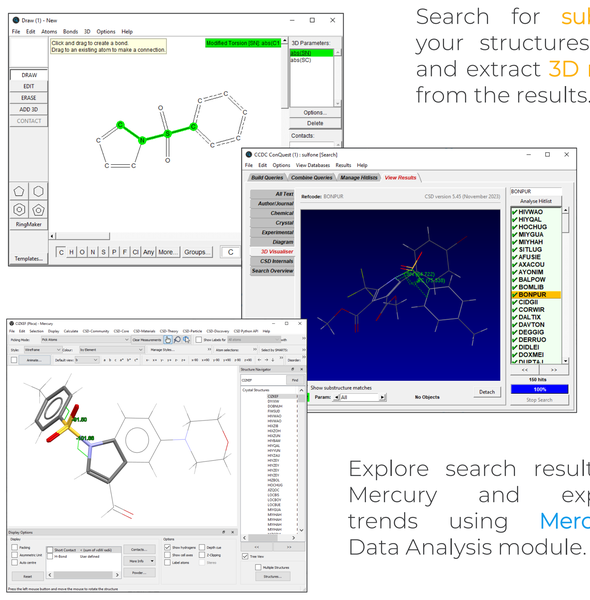




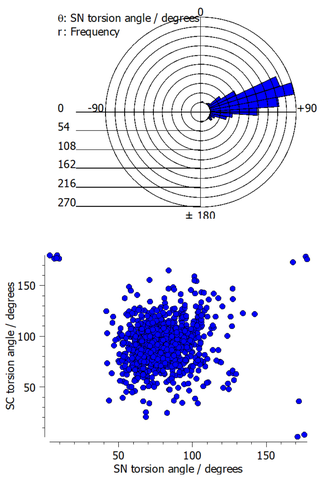
Compare experimental powder patterns with simulated powder patterns from CSD structures or your own single crystal structures using Mercury.

Database surveys and analysis

Search the CSD for structures related to yours using ConQuest. Identify relevant literature from bibliographic records, discover chemical, physical and biological properties, and explore 3D structure.



Search for substructures of your structures in ConQuest and extract 3D measurements from the results.

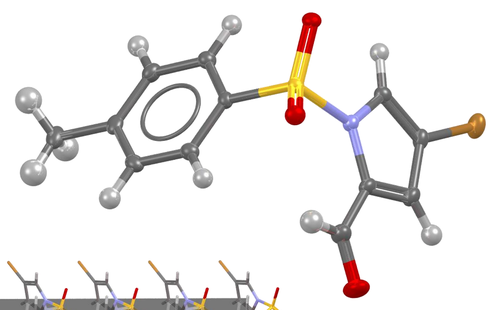


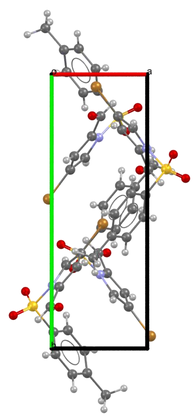
Explore search results in Mercury and explore trends using Mercury's Data Analysis module.

Create plots or export data for analysis in other software.

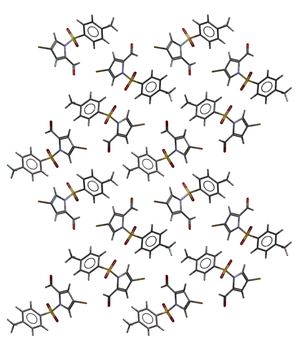
Structure visualisation

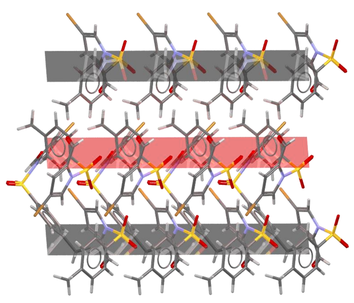
Structures can be visualised in Mercury. Different styles are available and customisable allowing you to make publication quality images.





View unit cell contents and packing diagrams.

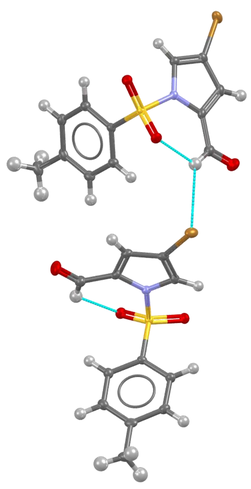


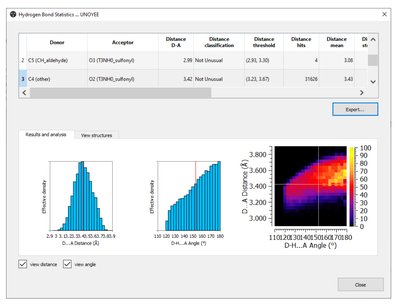


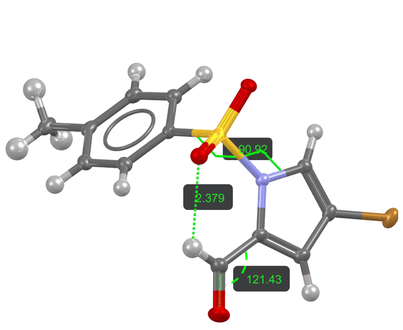
View slices of the crystal structure.

Structure analysis

Analyse your structures in Mercury to uncover intermolecular and intramolecular interactions.



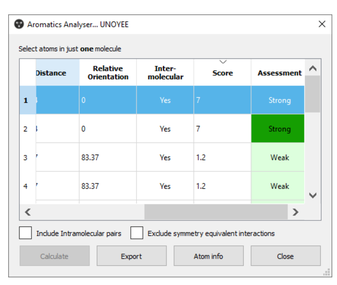


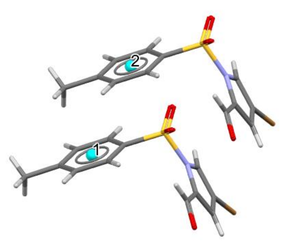


Automatic Hydrogen Bond Statistics calculations.

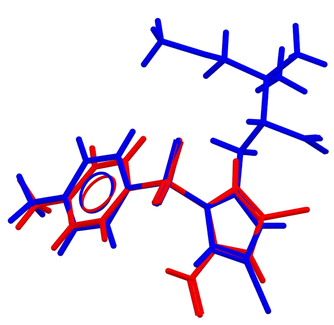
Measure and visualise distances, angles and torsions..

Explore hydrogen bond networks with customisable hydrogen bond definitions.

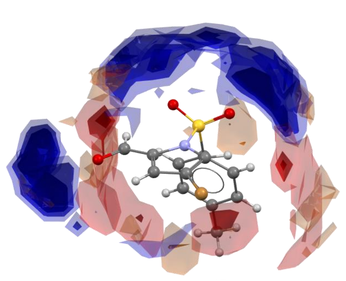




Uncover and evaluate aromatic interactions with Aromatics Analyser.



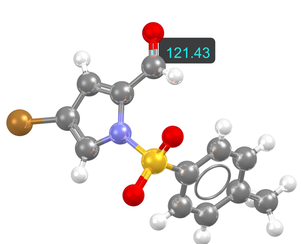
Assess conformational and structural similarities with similar molecules using Structure/Molecule Overlay.

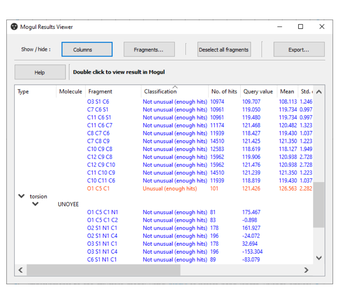


Predict and assess intermolecular interactions with a range of functional groups using Full Interaction Maps.

Structure validation

Check for unusual geometric features which might point to interesting chemistry or suggest improvements to the structural model using Mogul to assess bond length, valence angles, torsion angles and rings.





Don't forget to cite the CSD and acknowledge the FAIRE programme in any publications that use the CSD Portfolio. Find more information on how to cite the CSD in our FAQ's here: https://ccdc-info.com/3yBbTXt

1. https://www.ccdc.cam.ac.uk/community/ccdc-for-the-community/faire-grants/
2. C. R. Groom, I. J. Bruno, M. P. Lightfoot and S. C. Ward, The Cambridge Structural Database, *Acta Cryst. B*, 2016, **72**, 171
3. C. J. Kingsbury, H. C. Sample and M. O. Senge, *Acta Cryst. E.*, 2021, **77**, 341

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