Cambridge Structural Database: The Comprehensive Repository of Validated and Curated Small Molecule Organic and Metal-organic Crystal Structures

Established in 1965 with historical structures dating back to the 1920s, the Cambridge Structural Database (CSD) now contains over 1.1M accurate 3D structures with data from X-ray and neutron diffraction analyses and additional curation from the CCDC. The database is used by researchers across the pharmaceutical, agrochemical, and fine chemicals industries to predict and guide future discoveries.

Fully discoverable and accessible, the CSD is an essential trusted scientific resource giving big-data insights using powerful algorithms for molecular analysis. A CoreTrustSeal certified data repository.

Organic crystal structures include:

- Drugs and pharmaceuticals
- Agrochemicals
- Pigments
- Explosives
- Protein ligands.

Metal-Organic crystal structures include:

- Metal Organic Frameworks (MOFs)
- Models for new catalysts
- Porous frameworks for gas storage
- Fundamental chemical bonding.

Features

Validated chemical representation

Fully discoverable and trusted, the experimental data is further curated to include data from additional sources - for example common names, bioactivity, natural source, cross-reference to other enantiomers or racemates or polymorphs. This additional data allows easy grouping further enhancing discoverability and value as a knowledge base. Disordered structures are clearly represented owing to CCDC curation.

Fully empirical

Real world data brings trusted data insights and science to life for teaching.

Greater than the sum of its parts

The data from a collection of 1.1M structures can be compared, analysed and grouped to show common themes, trends and guides for further analysis and experimentation. Almost infinitely more valuable than the individual structures in isolation.

Interoperable and re-usable

All electronically deposited structures have their own DOI which helps for FAIR principles of interoperability and re-use of data.

Search and extract knowledge

CCDC software enables scientists to work with the CSD structural data to extract new insights. This includes public and proprietary, experimental and predicted data.

Target searches to structures of interest

Pre-calculated subsets of the CSD for specialist areas of chemistry that allow researchers to target searches to structures of interest.