Harness knowledge-based science

CSD-Core

For all users of CSD-Core, CSD-Materials, CSD-Discovery or CSD-Enterprise

For structural chemists, the components in CSD-Core provide the ability to:

- Search based on text, numeric data or structural features
- Visualise and analyse crystal structures
- Assess intramolecular and intermolecular geometries
- Build carefully tailored workflows for automation of research

Web-based structure search & retrieval
Access, visualise and analyse crystal structure data using WebCSD to support your research, education or peer review. Includes searching by structure, unit cell and text/numeric queries.

Sophisticated & flexible searching
Build specific and detailed search queries using ConQuest to drive your research using highly flexible text/numeric and 3D structural search options. Quickly identify structures based on a wide range of properties.

Tailored research & connectivity
Create tailored scripts using the CSD Python API and all the CSD functionality to answer your targeted research questions. Integrate access to crystal data and CSD functions seamlessly with 3rd party software.

Knowledge base of molecular geometries
Harness the millions of chemically classified bond lengths, angles, torsion angles, and ring conformations in the CSD using Mogul to obtain precise information on preferred molecular geometries.

Knowledge base of intermolecular interactions
Use IsoStar and the wealth of structural information available in the CSD to investigate the frequency and characteristics of intermolecular interactions between pairs of chemical functional groups.

High quality visualisation & analysis
View, explore and analyse molecules, crystal structures and simulated particles using Mercury. Generate high quality graphics using polyhedral representations for the metal-organic coordination centres. Produce high resolution graphics, videos and 3D printable models. Visualise macromolecules in Hermes.
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In response to feedback from users and a desire to further develop our systems in the future in new directions, we have now finished rewriting our search engine in C++. The original search engine behind ConQuest was written in the 1970s and was tied to a specific database format (ASER). Since the development of Mercury, we’ve been writing new, reusable chemistry algorithms in C++ which have been slowly replacing the older parts of the CCDC code base and this has now fully replaced the old code.

The development of CSD searching since 1970

1970: 1st reference book to search

1978: 1st electronic structure search

1991: 1st graphical search interface

2018: Complete C++ search engine

The rewriting of ConQuest’s fundamental search engine means that:

- Many complex 2D substructure searches are now much faster
- Nearly all types of search are significantly faster than the previous version
- Element and formula searches are more effective
- Many text searches now give more accurate results, especially author searches which now properly handle international name conventions

During 2020, targeted improvements have also been made to WebCSD based on user feedback including:

- Ability to expand the 3D visualiser to full screen
- New formula searching option
- Beta release of CSD-Sketcher - dedicated sketcher for searching