CCDC
advancing structural science

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
- Visualize and analyse crystal structures
- Assess intra- and inter-molecular geometries
- Build tailored workflows for automated, repeatable analyses

108,392 new structures have been added to the CSD in the last 2 years

Web-Based Structure Search & Retrieval

Access, visualize 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.

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.

High-Quality Visualization & 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. Visualize macromolecules in Hermes.

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.

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.

CSD-Core: Harness Knowledge-Based Science

CSD-Core allows you to search, visualize, and analyse crystal structure data, to compare your findings to the world's published data.

With CSD-Core you get full access to the Cambridge Structural Database (CSD), the world's repository for experimentally determined small-molecule organic and metal-organic crystal structures. It is continually updated with more than 50,000 structures added each year. Each structure undergoes automated checks and manual curation by scientific editors to enrich the data.

The tools within CSD-Core allow you to derive big-data insights from the CSD and apply these to the design and development of new molecular materials.

Case Studies:

Training machine learning models: here authors used data from the CSD to train machine learning models and explain how functional groups impact H_2 uptake to help design metal-organic frameworks (MOFs) for hydrogen storage tanks.
R. Maria Giappa et al, Int. J. Hydrog., 2021. 46, 54, 27612-27621

Identify and develop semiconductors: here scientists identified semiconductors in the CSD and analysed these to predict the optimal (hole) mobility achievable. This helped to prioritize experimental work and develop a scalable tool to discover semiconductors.
T. Nematiaram et al, Adv. Funt. Mater., 2020, 30, 30, 2001906

Optimization of MOFs: here researchers screened mixed-matrix membrane structures from the CSD including MOFs to evaluate them for volatile organic compound (VOC) recovery. They ultimately identified and optimized a two-stage process which reduced operating costs and energy consumption while recovering high-purity reusable propane.
C. Song et al, J. Clean. Prod., 2021, 321, 129049

CSD-Core Capabilities:

- 3D display and manipulation of structures
- High resolution graphics and movie generation
- 3D printing file output
- PXRD pattern simulation and comparison
- Molecule and structure editing
- Plotting and charting
- Descriptive statistics
- Interactive visualization
- Filtering and categorization
- Reporting
- Bond length assessment
- Valence angle assessment
- Torsion angle assessment
- Ring geometry assessment
- Fragment interaction maps
- Retrieve via bibliographic information, DOI, CSD identifiers or compound name
- Search by chemical formula, cell parameters, 2D/3D substructure, similarity and more
- Integration to Pipeline Pilot and KNIME component collections