

What is the CSD?

The Cambridge Structural Database (CSD) is a collection of >800,000 small-molecule **organic and organometallic crystal structures** that can be visualised and downloaded using a host of software applications, including:

WebCSD	A browser-based interface to the CSD data
ConQuest	For searching and retrieving CSD data
Mercury	A range of 3D structure visualisation tools

Where are the crystal structures from?

The 3D crystal structures which make up the CSD are derived from the **published literature** and **directly deposited data**. Each structure is validated and cross-checked by experts to ensure the CSD remains a **highly curated database**.

The 6 most featured journals are:

<i>Inorg. Chem.</i>	<i>Organometallics</i>
<i>Dalton & J. Chem. Soc., Dalton Trans.</i>	<i>J. Am. Chem. Soc.</i>
<i>Acta Crystallogr., Sect E</i>	<i>Acta Crystallogr., Sect C</i>

WebCSD - access the CSD in your web browser

WebCSD allows **searching and visualisation** of the CSD **within a web browser**. 3D structures can be exported in *.cif, *.sdf or *.mol2 format.

Search by:

- Structure / substructure
- Reduced cell
- Structural similarity
- Bibliographic information, compound name

Access the CSD via the
Physical Sciences Data-science Service

at www.psd.ac.uk

email: info@psds.ac.uk

ConQuest

The ConQuest application allows the user to search the CSD by:

- **Compound name**, formula, bibliographic information
- **Compound structure** / substructure with chemical constraints (charge, cyclicality)
- **3D molecular constraints**, conformational preferences
- Non-bonded contacts, **intermolecular interactions**

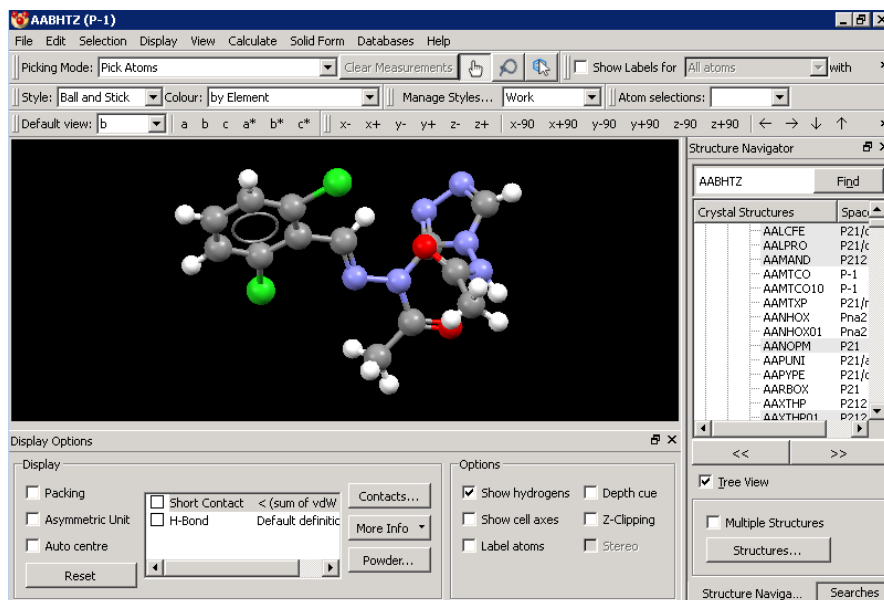
For advanced 3D visualisation, **export the hit list to Mercury**.

Mercury

The Mercury application is used for **advanced 3D visualisation** and export of crystal structures. **Distances, angles and dihedrals** can be measured.

Many properties can be calculated, including:

- **Packing**
- **Contacts**
- **Powder pattern**
- **Intermolecular potentials**



How do I access the CSD?

Access to the browser-based **WebCSD** is authenticated by **IP address**. If working off-campus a PSDS username and password will be issued. The applications **ConQuest** and **Mercury** (and others) are accessed via a **Remote Desktop Connection**. Signup for this at www.psd.ac.uk.

The CSD is developed by the Cambridge Crystallographic Data Centre (CCDC), and is provided to the UK academic community via the **PSDS at www.psd.ac.uk**. The Physical Sciences Data-science Service is funded by the EPSRC.

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