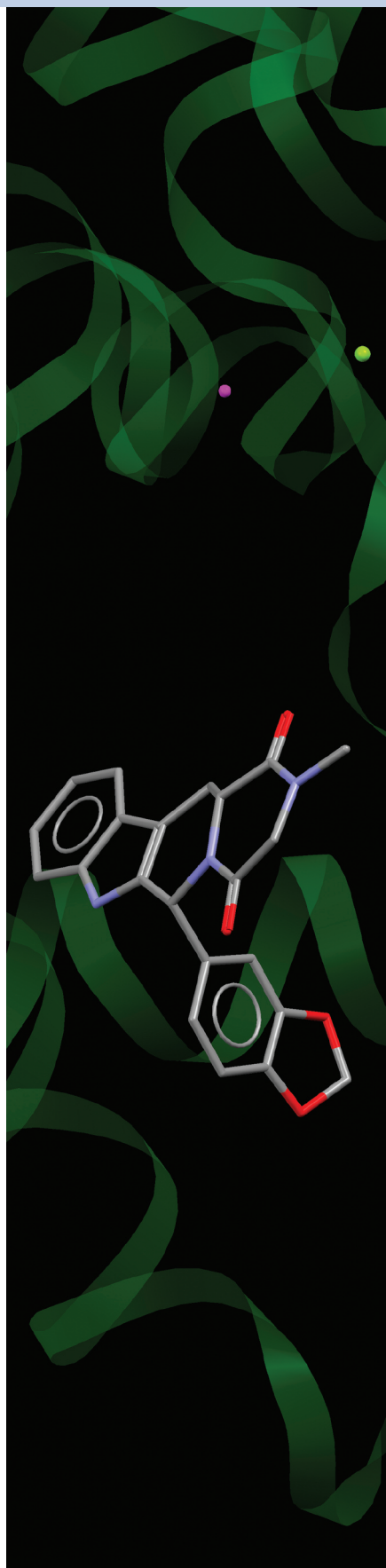


# The CCDC Product Range

## Knowledge and Discovery from Experimental Crystal Structures



### Cambridge Structural Database System (CSDS)

(featuring: Cambridge Structural Database, PreQuest, ConQuest, Mogul, IsoStar, Mercury, Vista and WebCSD)

Access the world's repository of validated crystal structure data for organic and metal-organic compounds and download regular web updates. Build proprietary in-house databases. Search and visualise crystal structures. Analyse molecular dimensions, conformational preferences, pharmacophoric patterns and intermolecular interactions. Instantly retrieve information on molecular geometries and intermolecular interactions using knowledge-based libraries derived from the CSD and the PDB. Access the CSD online via WebCSD.

### Materials Module of Mercury\*

Visualise, analyse and explore molecular structures and extended packing networks. Search sets of structures for specific interaction motifs or general packing features and compare geometries; identify regions of structural similarity in different crystal structures that share a local packing feature; compare packing patterns of structures and quantify similarity between polymorphs, hydrates and solvates.

### Relibase+

Search, retrieve and analyse protein-ligand complexes from both the PDB and proprietary databases. Investigate protein-ligand interactions. Compare ligand binding modes and identify ligand-induced conformational changes. Explore crystal packing effects, access detailed information on the water structure and secondary structure in entries and detect unexpected similarities amongst binding sites with low sequence homology. Construct complex queries using a dedicated scripting environment.

### GOLD Suite

(featuring Hermes, GOLD and GoldMine)

Access GOLD through the 3D visualiser provided (Hermes); interactively set-up accurate and reliable protein-ligand dockings using either an expert interface or an easy to use wizard. Use Hermes to inspect docking results. Comprehensively post-process and filter docking results by defining and calculating descriptors that characterise favourable binding features. Create GoldMine databases of single or multiple sets of docking data (e.g. from different docking runs); filter ligands using Boolean logic to obtain a list of poses that satisfy a selection of criteria.

### SuperStar\*

Predict protein-ligand interactions. Generate maps of interaction hotspots in protein binding sites or around small molecules, using experimental information about intermolecular interactions from both the CSD and the PDB. Derive pharmacophore points and use in CSDS searches or QSAR studies.

### DASH

Solve crystal structures using a globally optimised fit of models to indexed powder diffraction data, either from synchrotron or monochromatic laboratory X-ray sources.

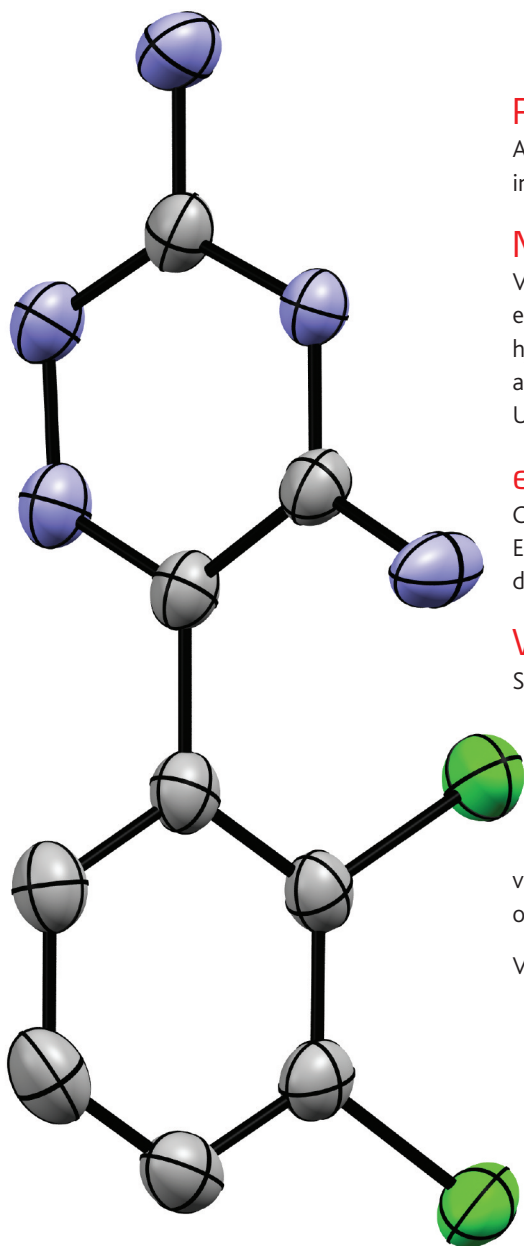
Utilise experimental torsion angle data from the CSD to aid structure solution.

Visualise and analyse candidate solutions. Perform Rietveld refinement using interfaces to external programs or the internal rigid-body refinement module.

\*Available to CSDS subscribers as additional modules.

# The CCDC Product Range

## Free Services



### Relibase

Access a subset of Relibase+ functionality for free on the web (academic users only, for internal research, development or teaching purposes only).

### Mercury

Visualise crystal structures in a variety of representation modes (including displacement ellipsoids) and explore crystal packing. Build networks of intermolecular contacts, including hydrogen bonds and short-range non-bonded interactions. Measure geometric parameters and export images for publication. Supports most common file formats, including CIFs. Users of the CSD System have access to additional functionality.

### enCIFer

Check, edit and visualise CIFs. Locate and correct syntax and format violations. Edit CIFs with enCIFer to preserve format-compliant files for deposition with journals and databases or for storage in laboratory archives.

### WebCite

Search hundreds of classified references and synopses of research applications of CCDC products published worldwide.

### Education Resources

Employ real crystal structure data in your teaching course by making use of the free 500-structure CSD teaching subset and teaching exercises. Work with real measured data; visualise and manipulate molecules in 3D; see first-hand how molecules interact with each other, other molecules and ions.

Visit [www.ccdc.cam.ac.uk/free\\_services](http://www.ccdc.cam.ac.uk/free_services) for further details.

## The Cambridge Crystallographic Data Centre

CCDC products are firmly based on scientific quality and relevance. We collaborate and publish widely, and several of our products arose from these collaborations.

Our products are widely used in industry and academia, particularly in structural chemistry, rational molecular design and pharmaceutical materials development.

Originating in 1965 in the Chemistry Department of the University of Cambridge, the CCDC is now an independent non-profit company situated on the University's Chemistry Campus.

