# CSD-System

Harness knowledge-based science

Overview

For structural chemists, the components in CSD-System 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
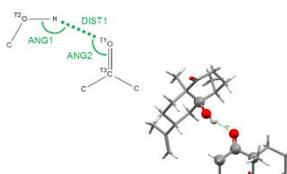
CSD-System components
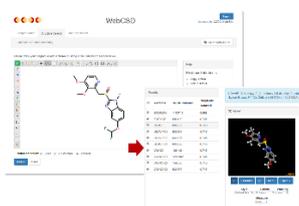
Web-based structure search & retrieval

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.
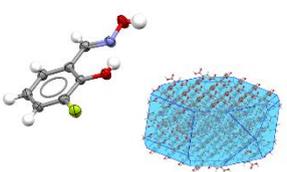
High quality visualisation & analysis

View, explore and analyse molecules, crystal structures and simulated particles using Mercury. Generate high resolution graphics, videos and 3D printable models to communicate your science.
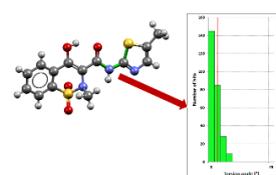
Knowledge base of molecular geometries

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

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.

Case studies

(a) Investigation of the geometric preferences of aminofuranoside rings

Understanding the structural chemistry around rings, including common conformations and possible transition pathways, can be aided by analysis of crystal structures in the CSD. The geometry of aminofuranoside rings, key units in nucleic acids, has been investigated in this way by Murray-Rust and Motherwell.[1] In this case, each of the five internal torsion angles of the ring can be defined in a substructure search query using ConQuest – the results of this search, including torsion angle parameters per hit can be analysed in Mercury's Data Analysis functionality.

Using principal component analysis (PCA) within Mercury, we can reduce the number of parameters for this geometry down to just two variables which capture the variance of the original five parameters. Plotting these principal components, we see two main clusters that indicate the common C2'-endo and C3'-endo conformations of the ring. Outliers indicate possible pathways for ring deformation, such as the O1'-endo conformation illustrated, which is stabilised here by an intramolecular hydrogen-bond.

[1] P. Murray-Rust & W.D. S. Motherwell, Acta Cryst. (1978) B34, 2534-2546.
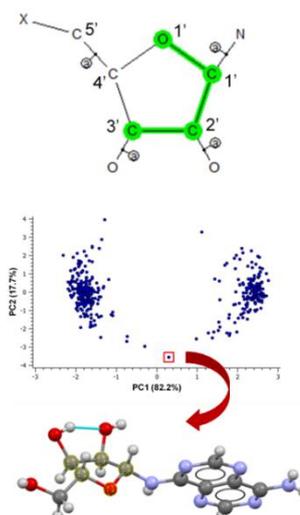
(b) Analysis of the interaction patterns of tetrazolate & carboxylate groups

Bioisosterism is a concept that is well understood in medicinal chemistry whereby one functional group can roughly mimic the size and properties of another functional group to produce similar biological properties. Many of these bioisosteric transformations are discovered through trial and error, but it is possible to use knowledge of the interaction properties of the groups to improve our understanding of the process.

Once such known bioisosteric pair is that of the carboxylate and tetrazolate functional groups. Allen and co-workers[2] illustrated how use of the 3D interaction data and theoretical calculation information in IsoStar can clearly explain why these two functional groups behave in a similar way despite their structural differences.

[2] F. H. Allen, C. R. Groom, J. W. Liebeschuetz, D. A. Bardwell, T. S. G. Olsson & P. A. Wood, J. Chem. Inf. Model. (2012) 52, 857-866.
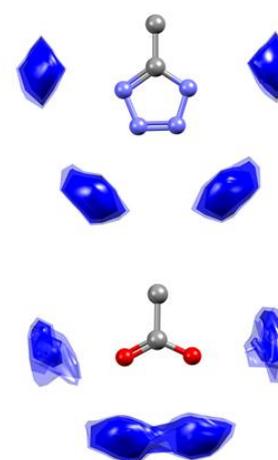
How to find out more?

Visit the CSD-System page on the CCDC website to learn more about the various components within CSD-System and to discover what's new in the functionality in the latest CSD release.

https://www.ccdc.cam.ac.uk/solutions/csd-system/