



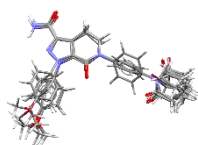
Overview

For solid-state scientists, the components in CSD-Materials provide solid form informatics capabilities, allowing you to understand and design materials. The functionality includes sophisticated analysis & prediction of molecular geometry, intermolecular interactions and crystal packing.

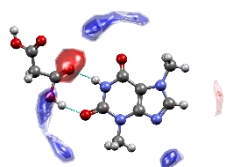


CSD-Materials components

Generation of molecular conformations

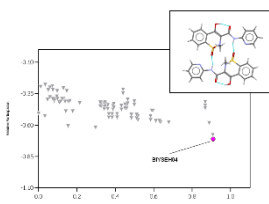


Rapidly generate plausible molecular conformations by using the wealth of information available in the Cambridge Structural Database. Aids the prediction of crystal packing and co-crystal design.



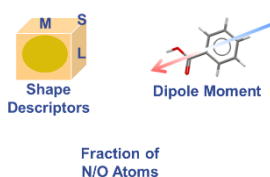
Prediction of intermolecular interactions in the solid-state

Determine the most likely geometries of intermolecular interactions using the knowledge in the CSD. Quickly evaluate the interactions in existing structures compared to the CSD and predict the interactions in new structures.



Assessment of the likelihood of hydrogen-bonding patterns

Enumerate all the possible hydrogen-bonding patterns available for a molecule (or molecules) and the relative likelihood of each. Predict the most likely hydrogen-bonding outcome and the risk of polymorphism for the system.

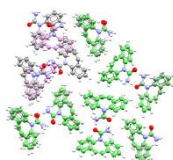


Prediction of co-crystallisation based on molecular descriptors

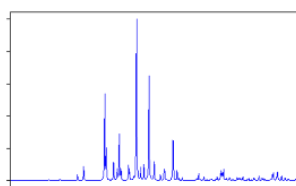
Quickly screen a wide range of possible co-formers for a given target based on molecule descriptors. Results will show which co-formers are very **unlikely** to form co-crystals with the target, reducing the number of experiments needed.

Fraction of N/O Atoms

Analysis of packing similarity, patterns and motifs



Analyse and compare packing patterns using the flexible motif, packing feature and packing similarity components. Quickly determine the similarity between solid forms as well as the recurring and robust packing features within the forms.



Crystal structure solution from powder diffraction data

Determine crystal structures from powder diffraction patterns using the simulated annealing algorithms in DASH. Solve structures faster using the 3D structural knowledge contained within the CSD.

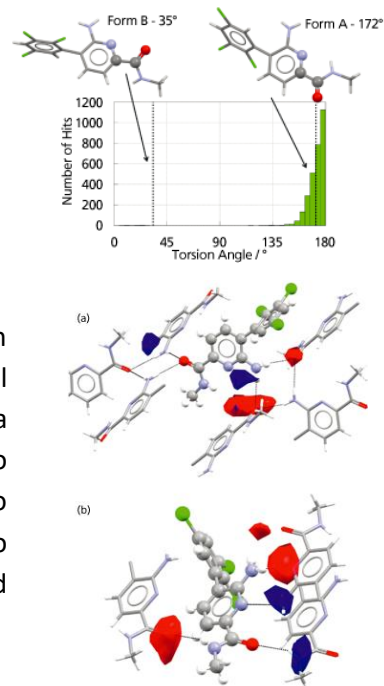
Case studies

(a) Conformational polymorphism of a pain candidate drug

A pain candidate drug that was under active development by Pfizer was identified to crystallise as two polymorphs – Form A and the stable Form B. The two forms are distinguished by both different molecule conformations and different hydrogen-bonding. Structural informatics was used to understand the polymorphism and the relative stability of these forms.

Form B was observed to have a less likely molecular conformation than form A when analysed compared to data in the CSD. Analysis of the full interaction maps in the two forms shows that form B, however, exhibits a set of intermolecular interactions with more likely geometries compared to form A. In this case, form B adopts a less likely molecular conformation to achieve a more stable hydrogen bond network. Informatics was used to provide rationalisation and reassurance around the stability of the two solid forms.

¹N. Feeder, E. Pidcock, R. Docherty et al., *J. Pharm. Pharmacol.* (2015) 67, 857-868.

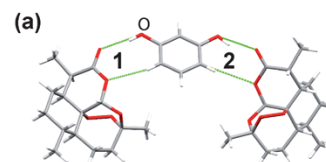
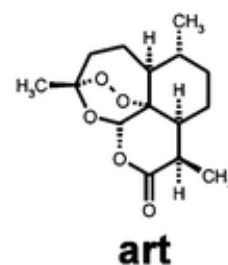


(b) Finding new co-crystal forms of artemisinin

The antimalarial drug artemisinin (art) has been studied previously to try to determine new solid forms, with potentially improved physicochemical properties, without success. A research group at the University of Cambridge carried out another extensive experimental screen to find co-crystals using 74 potential co-formers whilst also making knowledge-based predictions.

Two new co-crystal solid forms were discovered for artemisinin from the 74 sets of experiments (a success rate of just 2.7%). Analysis of molecular descriptors based on the CSD showed that 33 of the 74 co-formers (44%) were not worth trying in the first place though due to incompatible molecular properties. This knowledge would have reduced the number of experiments by nearly a half and almost doubled the success rate (4.9%).

²S. Karki, L. Fábíán et al., *CrystEngComm* (2010) 12, 4038-4041.



How to find out more?



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

<https://www.ccdc.cam.ac.uk/solutions/csd-materials/>

info@ccdc.cam.ac.uk
www.ccdc.cam.ac.uk
UK: +44 1223 336408

Doc no. 107CSDM18



The Cambridge Crystallographic
Data Centre