

# Materials Module in Mercury CSD

## Find, Identify and Analyse Crystal Packing Motifs

Mercury CSD [1] is a program for visualising, analysing and exploring molecular structures and extended packing networks (see [http://www.ccdc.cam.ac.uk/products/csd\\_system/mercury\\_csd/](http://www.ccdc.cam.ac.uk/products/csd_system/mercury_csd/)). The rational design of the solid-state forms of drugs has become a topic of major interest and this has prompted the development of a new unit of functionality for Mercury CSD, in collaboration with the Pfizer Institute. The new functionality is called the *Materials* Module [2].

The Cambridge Structural Database (CSD) [3] is the definitive database of experimentally-determined small molecule organic and organometallic crystal structures and contains valuable information about how molecules pack and interact in the crystalline state. Using the highly customisable searches available in Mercury's *Materials* module, you can:

- search sets of structures for specific interaction motifs or general packing features and compare geometries (Fig. 1)
- identify regions of structural similarity in different crystal structures that share a local packing feature (Fig. 2)
- compare packing patterns of structures and quantify similarity between polymorphs, hydrates and solvates (Fig. 3) i.e. by probing similarities and differences between different crystal forms

These motif searches and analyses are applicable to such problems as:

- co-crystal design
- counter-ion selection
- polymorph prediction
- crystal engineering studies

Searches may be carried out on the entire CSD, or on currently loaded files, ConQuest hitlists, refile lists or lists of structures e.g. generated by a polymorph prediction program.

The *Materials* module is an add-on component of the CSD System ([http://www.ccdc.cam.ac.uk/products/csd\\_system/](http://www.ccdc.cam.ac.uk/products/csd_system/)):

- Academic institutions: *FREE* access with CSD System release.
- Industrial organisations contact: [materialsmercury@ccdc.cam.ac.uk](mailto:materialsmercury@ccdc.cam.ac.uk) for further information.

### Other CCDC products and services related to Mercury CSD:

- Cambridge Structural Database System
- DASH – software for structure solution from powder diffraction data
- SuperStar – predicting interaction hotspots in protein binding sites and around small molecules

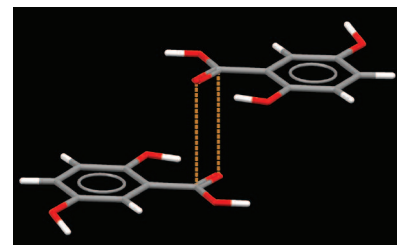


Fig.1: A carbonyl-carbonyl stacking interaction found using Mercury's motif search functionality. The compound is CSD entry BESKAL which has anti-arthritis properties.

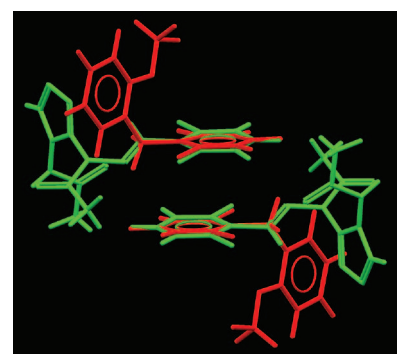


Fig.2: Results of a packing similarity search for the pi-stacking interaction in the unit cell of AABHTZ (green). The interaction is matched in CBPEBM with RMS 0.16Å.

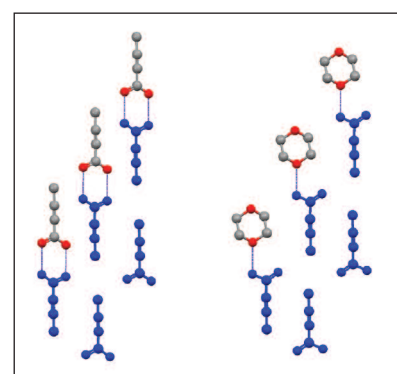


Fig.3: Region of common packing found by a packing similarity search. The reference structure is TETROL (left) and the hit structure (right) is XAKGEW.

### References:

[1] C. F. Macrae, P. R. Edgington, P. McCabe, E. Pidcock, G. P. Shields, R. Taylor, M. Towler and J. van de Streek, *J. Appl. Cryst.*, **39**, 453-457, 2006

[2] C. F. Macrae, I. J. Bruno, J. A. Chisholm, P. R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. van de Streek, P. A Wood, *J. Appl. Cryst.*, in press

[3] F. H. Allen, *Acta Cryst.*, **B58**, 380-388, 2002

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## More Detail

### Motif Searching

Choose functional groups to be involved in motifs and allow Mercury to generate all possible interactions between the functional groups. As the search for motifs proceeds a frequency of occurrence for each motif is calculated and displayed (Fig.4).

#### Presentation of results:

Motifs are highlighted and options for highlighting are fully customisable. Structures that contain the motif(s) are listed for selection either by motif (all structures that contain the motif are grouped) or by structure (all motifs found within the structure are given). Motifs can be logically combined to probe interaction geometries further.

#### Motif searching allows you to:

Search for extended functional group interactions quickly and easily and assess the geometric possibilities on the likelihood of occurrence.

### Packing Feature Searching

Select a packing feature of interest by choosing as many or as few constituent atoms as desired. Atoms can be selected from multiple molecules. Set the level of geometric similarity required for matched structures (Fig.5).

#### Presentation of results:

The packing feature structure is overlaid with matching structures and atoms that constitute the packing feature are highlighted. The RMS deviation for each matching structure is calculated with respect to the target packing feature.

#### Packing feature searches allow you to:

Flexibly search for any arrangement of atoms or groups in 3D space using a crystal structure as a template and to easily find the most closely matched structures.

### Crystal Packing Similarity

Select a crystal structure and search for similar packing arrangements in structures containing that molecule. Options to control the level of similarity are available (Fig.6).

#### Presentation of results:

The similarly packed areas of the two compared structures are displayed and an RMS deviation is calculated for each pair of structures. Structures can be grouped on the level of similarity.

#### Crystal packing similarity searches allow you to:

Easily find groups of similar structures amongst families of polymorphs and search a dataset for any multi-component system for which there is a crystal structure of one of the components available.

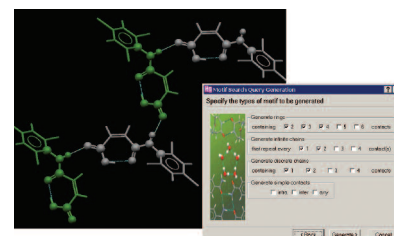


Fig.4: Example of a carboxylic acid-amide infinite chain motif generated using the *Materials* Module of Mercury. Inset shows the dialog used to select motif geometries.

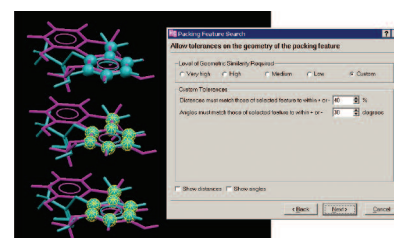


Fig.5: Results of a packing feature search using AWONUV as the search template (shown in pink). The matching structure is overlaid automatically and highlighted in a customisable way. The similarity between the matched structure and the template structure is controlled using the dialog shown.

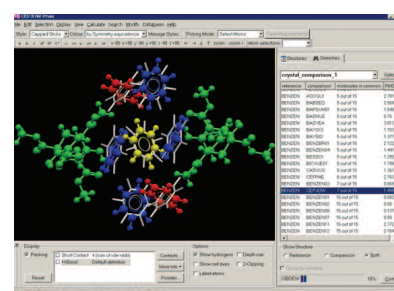


Fig.6: Results of a packing similarity search performed using benzene. All benzene solvates present in the dataset have been found. The benzene solvate shown (CEPJOW) is overlaid with the structure of benzene (shown in grey).