Analysis of Polymorphic Forms - Understanding and Quantifying Packing Similarity

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The identification, control and characterisation of polymorphic forms is of clear importance in the pharmaceutical industry. As the physicochemical properties of crystals can be highly dependant on the molecular packing pattern, an understanding of the similarities and differences between structures at the molecular level is crucial. Various methods currently exist for comparing crystal forms [1-3], with powder pattern comparison being the natural method of choice for identifying polymorphs during crystallization experiments.

We present the results of analysis carried out using the new Materials module of Mercury CSD [4], which has been used to study the packing patterns of polymorphs, hydrates and solvates. One of the new features allows comparison of the geometry of molecular clusters within different polymorphic forms (functionality derived from the COMPACK program [5]). The analysis of packing patterns in this way not only quantifies the similarity between the structures, but also identifies the specific regions in structures that are similar.

Further new features in Mercury allow searching of the Cambridge Structural Database (CSD) for specific interaction motifs or more general packing features as well as comparison of the geometries of these features. It is hoped that such analysis and understanding will help foster rational approaches to the control and discovery of crystal forms.

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