Automating the Identification of Packing Motifs; dSNAP

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With the explosion in high quality structural determinations in the area of small molecule crystallography, the problem of efficient and meaningful mining of the data in, for example, the Cambridge Structural Database (CSD) [1] is very relevant for structural chemists. The available databases represent an enormously powerful resource, but faced with more than 300,000 structures, such as are found in the CSD, the attempt to extract meaningful chemical information can be daunting.

The application of the recently developed program *dSNAP* to inter-molecular interactions and packing motifs is described through some novel examples. Similarity matching within *dSNAP* allows clustering of geometric data extracted from the CSD, which is found to be sensitive to small but significant geometry variations. This method relies solely on the extracted geometric information and is therefore independent of any chemical bias. However, the final interpretation of the different clusters in a chemically sensible way is still the sole responsibility of the structural chemist.

The method is illustrated by several examples, both simple and complex.

[1] Allen F.H., *Acta Crystallogr.*, 2002, **B58**, 380-388.

Keywords: database mining, cluster analysis, intermolecular packing