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## dSNAP: New Software for Analysing The Results Of Cambridge Data Base Searches

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Cambridge Structural Database (CSD) searches can produce thousands of 'hits' especially if a simple fragment is used, and as a result, processing and interpreting the results becomes a considerable task, and one in which it is easy to make mistakes. Cluster analysis using dendrograms, metric multidimensional scaling and suitable visualization tools can reduce the workload to a few hours with minimal user intervention, and thus minimal user bias. The real beauty of the method is in its interactivity and scalability: it allows you to go from an overview of the entire dataset and easily spot any outliers or errors, to the ability to 'drill down' within a cluster, looking at more and more detailed differences between different fragments in a statistically rigorous way. The formalism and the associated program are also invaluable in crystal engineering and structure prediction environments since it can readily identify the basic motifs in a structure and how they pack in the unit cell. The computer program we have developed to do this is dSNAP [1]. It is available free of charge from the web site http://www.chem.gla.ac.uk/snap.

[1] G. Barr, W. Dong, C. J. Gilmore, A. Parkin and C. C. Wilson,. *J. Appl. Cryst.* 2005, 38, 833-841.

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## New Software for Identifying Hydrogen Bond Motifs

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New software has been developed to efficiently search crystal structures to find the relative frequency of occurrence of various types of hydrogen bond motif. This software, which is built using the 'mercury' visualiser program [1], provides the ability to automatically generate sets of motif search queries for specific functional groups. For example, one can search for all possible hydrogen bond ring motifs that span four molecules that form between a carboxylic acid group and a water molecule. There may be very many motifs possible and the automatic generation step ensures that a comprehensive set of motifs are searched for and avoids the need to sketch search queries manually. Motif searching is performed using the search algorithm '3DSearch' [2]. We show how the graphical interface provides easy navigation of search results. Motifs can be sorted by frequency of occurrence to quickly identify the most and least common motifs as well as those motifs that are possible but are not observed. One can quickly view all motifs found in a given structure and view all structures that contain a specific motif, say the most frequently observed motif, or a specific combination of motifs. The search and visualisation of such motifs helps determine how certain functional groups can interact in the crystal. The identification of particular stable synthons has clear benefit for crystal engineering work as well as helping to assess polymorph stability and, for the area of co-crystal growth, helping decide potential co-crystal formers.

[1] Bruno, I. J., Cole, J. C., Edgington, P. R., Kessler, M. K., Macrae, C. F., McCabe, P., Pearson, J. & Taylor, R. (2002). *Acta Cryst*. B58, 389-397.

[2] Chisholm, J. A., Motherwell, S. (2004). *J. Appl. Cryst*. 37, 331-334.