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Crystallographic searches for weak interactions: The limitations of data mining

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The oldest and most successful application of data mining in chemistry is without a doubt the use of crystallographic databases. The common practice is to draw conclusions from the frequency of contacts observed in crystals to the relevance of the underlying non-covalent interactions. While this strategy has provided a wealth of information on structural data for stronger interactions it can be misleading in the search of weak interactions. This is illustrated by controversies about the hydrogen bond acceptor quality of organic fluorine, which culminated in the statement by Dunitz *et al.*, that "Organic Fluorine Hardly Ever Accepts Hydrogen Bonds", based on their finding of only 0.6% relevant hits in the CSD. The problem is that weak acceptors such as fluorine are introduced in thousands of compounds for very different reasons and then rarely can compete with other non-covalent interactions which can dominate in a given structure. Proposals to limit such situations in crystallographic searches will be presented, including complementary methods to measure related interaction energies in solution.

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