Microsymposium

MS67.006

Covalent Assistance to Supramolecular Synthesis

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The similarity of crystal engineering to organic synthesis has been noted by Desiraju and many concepts and strategies have been successfully transferred. We aim to combine the two fields of research into one new concept called "Covalent Assistance to Supramolecular Synthesis". The supramolecular reagent isonicotinic acid hydrazide (isoniazid) is a promising molecule in the supramolecular synthesis of multi-component molecular complexes (Lemmerer at al., 2010). Due to the covalent reaction of the carbohydrazide functional group with simple ketones and aldehydes, the hydrogen bonding functionality of isoniazid can be modified, where two of the hydrogen bond donors are replaced with hydrogen bonding "inert" hydrocarbons (Lemmerer et al., 2011). The "modifiers" bonded to the isoniazid then give a measure of control of the outcome of the supramolecular synthesis with various carboxylic acids depending on the identity and steric size of the modifier used. The steric size itself can be used to shield or to "mask" the remaining hydrogen bonding functionality of isoniazid such that common homomeric and heteromeric interactions are prevented from taking place.

[1] Lemmerer, A., Bernstein, J. & Kahlenberg V. (2010). CrystEngComm 12, 2856-2864., [2] Lemmerer, A., Bernstein, J. & Kahlenberg V. (2011). CrystEngComm 13, 5692-5708.

