## **Robotic Adventures in Crystallisation Space**

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An automated parallel crystallisation screen has been applied to the systematic recrystallisation of the thiazide diuretic hydrochlorothiazide. The work is carried out as part of the collaborative project "Control and Prediction of the Organic Solid-State" funded under the auspices of the UK Research Councils Basic Technology Programme. The screening approach provides accurate control of key crystallisation parameters, namely: solvent identity; temperature; agitation and rate of evaporation. Polycrystalline samples are characterised using a multi-sample X-ray powder diffractometer equipped with foil transmission geometry, CuKa1 radiation and a linear PSD [1]. The instrument is highly effective where there is a requirement to analyse 20 - 30 recrystallised samples per day, with an emphasis on obtaining the high-quality data that are important in pattern recognition (using e.g. PolySNAP [2]) and imperative in indexing. The results of multivariate analysis of the solvent properties and physical forms produced in the screen is presented along with the crystal structures of the novel forms with a view to identifying the factors underlying the formation of polymorphs and solvates of hydrochlorothiazide.

[1] Florence A.J., Baumgartner B., Weston C., Shankland N., Kennedy A.R., Shankland K., David W.I.F., *Int. J. Pharm.*, 2003, **92**, 1930. [2] Barr G., Dong W., Gilmore C., *J. Appl. Cryst.*, 2004, **37**, 658-664.

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