

## Poster Presentation

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### *Utilising Crystallographic Data to Better Design Solid Forms*

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Understanding crystalline forms in the pharmaceutical industry is very essential as the majority of small molecule drugs are delivered to patients in a crystalline state. Chemical and physical solid-state properties of an active pharmaceutical ingredient (API) such as stability, solubility, reactivity and bioavailability can be influenced by the formation of salts, anhydrous forms, hydrates, solvates, polymorphs and cocrystals. It is clear therefore, that an insight into molecular arrangements including existing interactions is required for effective drug development. The status quo to obtain experimental three-dimensional solid-state information is by x-ray structure analysis. One clear advantage of this method is its wide spread use due to the relative ease of use in a standard analytical laboratory and cost (compared for example to neutron diffraction). The Cambridge Structural Database (CSD) [1] consolidates the information of hundreds and thousands of determined crystal structures and offers plenty of opportunities to investigate solid-state properties more in detail. In order to exploit the readily available knowledge, a variety of informatics tools such as Full Interaction Maps (FIMS) [2] or Hydrogen Bond Propensity (HBP) [3] calculations were developed within the Crystal Form Consortium (<http://cfc.ccdc.cam.ac.uk>), a collaboration of people from leading industrial companies and experts from the CCDC. We will present how the CSD knowledge in combination with informatics tools can support effective drug development in a pharmaceutical environment.

[1] F.H. Allen, *Acta Cryst. B*58, 2002, 380-388., [2] P.A. Wood, T.S.G. Olsson, J.C. Cole, S.J. Cottrell, N. Feeder, P.T.A. Galek, C.R. Groom, E. Pidcock, *CrystEngComm*, 2013, 15, 65-72., [3] P.T.A. Galek, L. Fábrián, W.D.S. Motherwell, F.H. Allen, N. Feeder, *Acta Cryst. B*63, 2007, 768-782.

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