

Can predicted solid form landscapes provide insight into structure-property correlations?

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Crystal structure prediction (CSP) has emerged in recent years as a powerful technique to complement and augment experimental studies of organic solid forms. While the ultimate goal of CSP is often to predict the thermodynamically stable form of a given system from only the chemical diagram, hundreds or even thousands of plausible crystal structures are generated along the way. This landscape of potential solid forms contains a wealth of information on possible packing arrangements and intermolecular interactions, all of which can be used to infer the characteristic properties of the material in question.

Understanding the link between the crystal structure and the physical and mechanical properties of a material is crucial to all stages of pharmaceutical development. At the CCDC we are developing approaches to predict the properties of drug molecules based on novel analyses of their crystal structures. While application of these methods offers valuable insights into the potential downstream behaviour of drug candidates during formulation, when applied across a range of plausible crystal structures these tools can provide an unprecedented perspective on the characteristic behaviour of a molecule. Will a drug always form poor tablets or is there an as yet undiscovered packing arrangement that has the desired properties to compress well? This approach of interrogating the entire solid form landscape may provide answers to such questions.

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