Crystallography in a pharmaceutical environment: can computational modelling help?

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On the way from molecule to medicine crystallization of the active pharmaceutical ingredient (API) often forms a key part of the road. Molecules can crystallize in different solid forms which will have different properties, *e.g.* solubility, dissolution rate and mechanical properties. Therefore solid form selection and control is an important aspect of drug development of small molecules. Crystal Structure Prediction (CSP) forms an *in silico* contribution to solid form selection. Based on the 2D molecular diagram as input, the output of a CSP forms a set of crystal structures and their relative stability ranking. This is an assessment of the crystal structure landscape orthogonal to experimental solid form screening. Within this presentation an introduction to CSP and its usage within a pharmaceutical context will be given. Three characteristic cases will be discussed and an outlook towards possible property modelling in the future will be given.