Utilizing Data-Driven Tools to Investigate the Relative Stability of Solid Forms

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Pharmaceutically active drug molecules often exhibit competing polymorphs which differ in terms of crystal packing on account of their differing intermolecular interactions. Because these polymorphs may also differ in terms of mechanical stability, solubility, and bioavailability, it is of utmost importance to identify the possibility of alternative forms.
The Cambridge Structural Database (CSD) is comprised of over 1 million molecular crystal structures. We have mined the intermolecular interactions present in these structures to gain insights into their typical properties. In this talk, we will discuss how we utilize these tools to evaluate the relative stability of solid forms. We will discuss recent updates to our aromatics analyzer, hydrogen bond propensity, and hydrogen bond statistics tools, along with how these tools are used to evaluate the stability of solid forms.