The Prediction, Observation, and Analysis of a New Form of Cannabidiol

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Cannabidiol (CBD) is a phytocannabinoid which has become increasingly important as an active pharmaceutical ingredient (API), and is commonly isolated and used in its well-known and stable crystalline form (Form 1). However, the crystal structures of a series of CBD analogues, containing a different number of carbon atoms in the alkyl sidechain at C-5', shows that CBD Form 1 is an outlier in a group demonstrating homologous isomorphism.
This indicated the potential existence of an uncharacterised isomorphic CBD polymorph (Form 2).
High throughput crystallisation techniques, namely the ENaCt protocol, were used in combination with CBD homologue seeding to search for the presence of this predicted Form 2 of CBD. Optical analysis of the resultant crystals suggested the presence of a new form due to block like crystals rather than the needles associated with Form 1. Single Crystal X- Ray Diffraction (SCXRD) analysis of these crystals of CBD resulted in a structural model with packing that fits with the isomorphic series. This experiment represents the first example of directed polymorph discovery using high throughput ENaCt techniques.

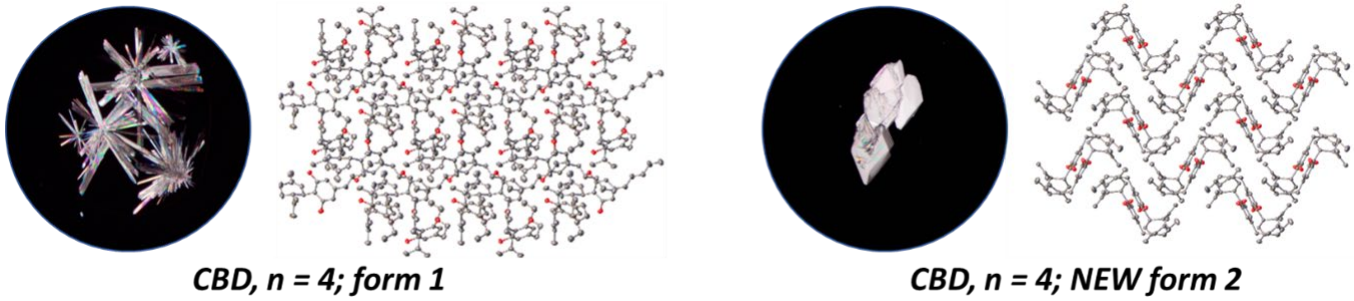

Figure 1