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Structural characterization, from synchrotron powder X-ray diffraction data of solid forms of Apremilast, a case of rich isostructural solvatomorphism

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Active Pharmaceutical Ingredients (APIs) can exist in different crystalline forms,
demanding a thorough investigation of their solid form landscape during drug discovery. Solvate formation is a common occurrence and in some cases, solvates can serve as intermediates in the production of the optimal form for further development. More challenging is to understand the reason for the formation of isostructural solvates, where the same host incorporates different solvent molecules. Although single crystal X-ray diffraction is the gold standard technique for determining crystal structures, its main limitation lies in the requirement of a single crystal of suitable size, quality and stability which is not always feasible. In the present case, we are studying the rich isostructural solvatomorphic API Apremilast which has been reported to exist in many isostructural solvates. Additional new solvates and cocrystals of Apremilast are reported here and synchrotron diffraction data of some forms, for which a good quality single crystal has not been obtained, have been recorded on Alba's high resolution MSPD line. These data should be good enough to deal with the structure solution from powders, by using
direct space methodologies of these very similar isostructural forms.

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