XRD in the Screening and Characterization of Pharmaceutical Cocrystals

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X-ray crystallography and crystal engineering play a crucial role in pharmaceutical development. The emphasis in these studies is to modify the physicochemical and pharmacokinetic properties of drugs as well as their solid crystalline forms for improved solubility, better stability and enhanced bioavailability. That the optimal crystalline form of a particular drug, e.g. polymorph, salt, cocrystal, solvate, hydrate, etc., is possible to derive by a combination of synthon-based design and high-throughput crystal form screen has resulted in the improvement of oral formulation for drugs. Apart from solubility and bioavailability, other properties which have been tuned for pharmaceuticals are permeability, half-life, color stability, cross reactivity for multi-drug compositions, tableting, compaction, etc. The engineering of multi-component cocrystals (ternary) offers the potential to arm multiple drug payloads in the same pharmaceutical composition. Powder X-ray diffraction (PXRD) and Structure determination from powder data (SDPD) are powerful techniques in pharmaceutical solid form development.

Representative case studies

1) Eutectics as Improved Pharmaceutical Materials. *Chem. Commun.* 2014, 906-923.
2) Multicomponent ternary cocrystals of the sulfonamide group with pyridine-amides and lactams. *Chem. Comm.*, **51**, 15578-15581 (2015).
3) Polymorphism, isostructurality and physicochemical properties of glibenclamide salts. *CrystEngComm*, **19**, 918-929 (2017).
4) Acemetacin cocrystal structures by powder X-ray diffraction, *IUCrJ*, 4, 206-214 (2017).
5) Epalrestat-Cytosine Cocrystal and Salt Structures: Attempt to Control E,Z --> Z,Z Isomerization. *Cryst. Growth Des.*, 2017, in press