Poster Presentation

MS075.P06

Cocrystals/salts of Furosemide : Interesting case of colour cocrystal polymorphism

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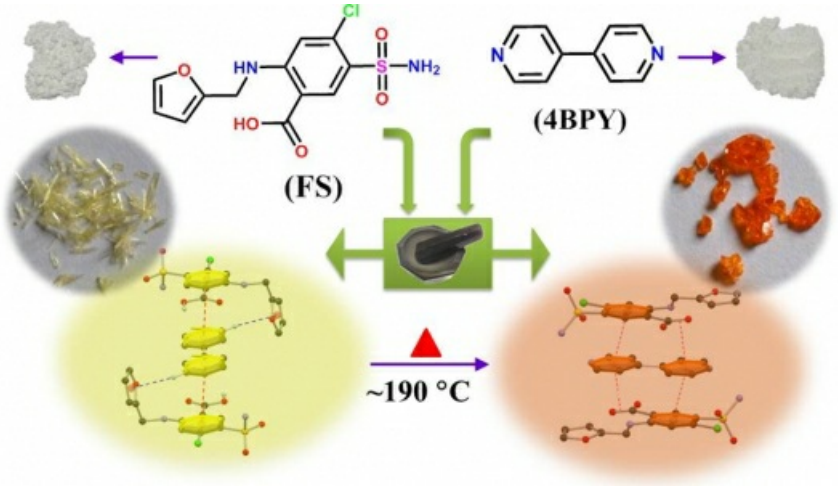
Developing cocrystals/salts of active pharmaceutical ingredients (APIs) has gained tremendous research interest in recent years owing to their potential to improve pharmaceutically relevant properties, like solubility, bioavailability, stability, hygroscopicity, crystallinity, etc.without affecting therapeutic efficacy. However, like single component crystals, cocrystals are also prone to display polymorphism owing to conformation tuning thereby exhibiting different physicochemical properties, e.g. Furosemide, a loop diuretic drug. We are interested in further investigating the polymorphic behaviour of Furosemide cocrystals/salts in order to gain more insight into the conformation tuning of Furosemide that eventually manifested into its cocrystal polymorphism. Interstingly cocrystals/salts of Furosemide with pyridines like 4,4'-bipyridine and its analogue produced colour cocrystal polymoprhs, yellow and orange.1 The single crystal structure analysis of polymorphs revealed the formation of sandwich motif through π- stacking interactions with variable geometries comprising two molecules of FS and one molecule of pyridine. The significant color difference between the polymorphs is attributed to the different level of conjugation generated by dissimilar π- stacking patterns between the two components. Investigation on the origin of the color difference using DFT calculations revealed the decrease in the HOMO−LUMO gap for orange crystals compared to yellow crystals.

[1] Sangtani, E. et al. (2015) Cryst .Growth Des., 15, 5858–5872.



Keywords: Color cocrystal polymorphism, Stacking interactions, Sandwich assembly