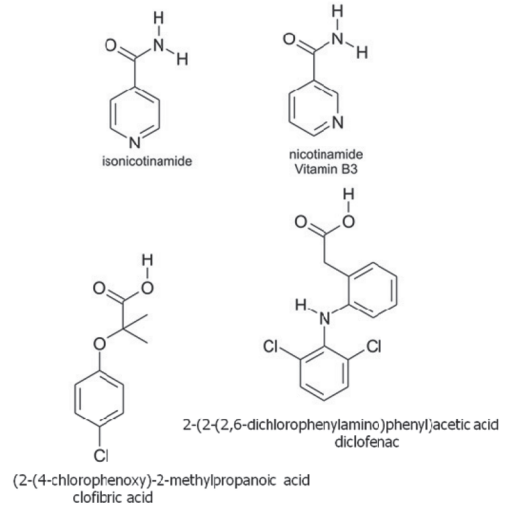
MS25-P1 **Pharmaceutical Co-crystals with Isonicotinamide.**
Nikoletta B. Báthori,[a] Andreas Lemmerer,[b] Gerhard A. Venter, [b] Susan A. Bourne [b] and Mino R. Caira[b] [a]*Department of Chemistry, Cape Peninsula University of Technology, Cape Town, South Africa.* [b] *Department of Chemistry, University of Cape Town, Rondebosch, South Africa.*
E-mail: bathorin@cput.ac.za

The design and synthesis of stable solid-state structures based on noncovalent interactions is comprised in the field of supramolecular chemistry. Active pharmaceutical ingredients (APIs) represent one group of materials to which this approach has been applied. One problem encountered is unsatisfactory bioavailability, limited by the solubility of the final drug compound, and further development is spent on improving its solubility without decreasing its performance or stability. Recently, this challenge has been met by crystallizing the API with other solid compounds forming a pharmaceutical cocrystal.

In this work, the cocrystals of industrially significant pharmaceutical compounds, the Vitamin B group member nicotinamide, the antihyperlipidemic drug clofibric acid, and the nonsteroidal anti-inflammatory drug diclofenac, are synthesized with the popular cocrystal former isonicotinamide and characterized by thermal analysis and single crystal X-ray diffraction. A survey of relevant structures in the Cambridge Structural Database of isonicotinamide and nicotinamide co-crystals is given for completeness, and the co-crystal former ability of isonicotinamide and nicotinamide was investigated by performing density functional theory calculations.



[1] Báthori, N. B., Lemmerer, A., Venter, G. A., Bourne, S. A., Caira, M. R. (2011). *Crystal Growth & Design,* 11, 75-87.

Keywords: crystal engineering, cocrystals; pharmaceutics

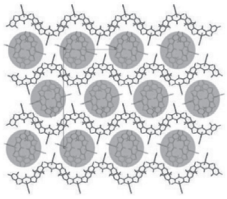
MS25-P2 **Cocrystal constructed of one component?**
Petra Bombicz,[a] Petra Smie,[b] Ewald Sattler, [b] [a]*Dept. Struct. Chem., Inst. of Org. Chem., Research Centre for Natural Sciences, Hungarian Academy of Sciences, Hungary,* [b]*Institute für Anorganische Chemie, Karlsruher Institut für Technologie, Germany*
E-mail: bombicz.petra@ttk.mta.hu

The United States Food and Drug Administration (FDA) released a draft guidance in December 2011 on regulatory classification of pharmaceutical cocrystals. It addressed two matters of topical interest to the crystal engineering communities: the proposed definition and classification of cocrystals. A session of the Indo-U.S. Bilateral Meeting titled The Evolving Role of Solid State Chemistry in Pharmaceutical Science held in India February 2012 was devoted to discussion of the FDA guidance draft. It converged to the definition [1]: *cocrystals are solids that are crystalline single phase materials composed of two or more different molecular and/or ionic compounds generally in a stoichiometric ratio*.

The discussion "What is a cocrystal" [2] goes back longer in the history. It seems cocrystal wins among the alternate expressions. Spelling - hyphenation - is still in question. The nature of constituents creates difficulties in classification, there is an overlap between salts, cocrystals and hydrates [1]. Dunitz states [3] "co-crystal encompasses molecular compounds, molecular complexes, solvates, inclusion compounds, channel compounds, clathrates, and possibly a few other types of multi-component crystals."

There is agreement in one point of the definitions can be found in the literature: cocrystals are multicomponent crystals. The question is that in what sense. Multicomponent means necessarily that the constituents are chemically different? Or can we call a crystal multicomponent if it contains one chemical molecule but crystallographically distinguishable molecules (Z'>=2) with well distinguishable functions in the crystal structure? What matters, the chemistry or the functionality in the definition of the cocrystal?

The crystal of the $(MeB\text{-}PMes)_3$ molecule is a chemically single component crystal. There are two crystallographically independent molecules in the asymmetric unit: they have clearly distinguishable different functions in the crystal. One molecule - the 'host' - takes part in the construction of the framework of the crystal. This framework forms empty channels which is filled with the other molecule - the 'guest'. There are C-H...pi type intermolecular interactions only in the crystal structure. Two of them assist the formation of the framework. One of them supports the channel filling column. The weakest hydrogen bond occurs between the framework and the filler.



Can we say it is a cocrystal? Do we need to extend the definition of the cocrystal that they are composed of two or more *chemically or functionally* different compounds?

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[1] Aitipamula S. et al., (2012) Cryst. Growth Des. 12, 2147-2152. and references therein
[2] Bond A.D., (2007) CrystEngComm, 9, 833-834. and references therein. [3] Dunitz J.D., (2003) CrystEngComm 5, 506.

Keywords: cocrystal; multicomponent crystal; functionality