Poster

Diversity and Similarity in Isonicotinamide Two-Component Phases with Alkyl Carboxylic Acids: Focus on Solvates

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Active pharmaceutical ingredients (APIs) can form different crystalline solid forms [1]. These include single component solid forms (polymorphs) and different types of two and multi component systems such as solvates, co-crystals etc. Solvates and co-crystals usually have physicochemical properties different from those of the pure API. These properties have an impact on the drug dosage form and the manufacturing route [2]. Therefore, crystal engineering opens new opportunities to obtain APIs with better physicochemical properties [3,4].

In the research we present an investigation of solvate formation of isonicotinamide (INA) with linear monocarboxylic acids and several other solvents. The obtained phase structures were determined using SCXRD and PXRD and characterized using thermal analysis, but their crystal structures were analyzed using theoretical calculations.

Four new INA solvates were obtained and crystallographic analysis of in total eight solvates were performed. Similar hydrogen bond patterns can be observed in all eight solvates. Based on the hydrogen bond motif present almost all solvates can be divided in two distinct types: type A (containing tetramer formed from two solvent molecules and INA dimer) and type B (containing trimer formed from a solvent:INA dimer and an additional solvent molecule), except for the formamide solvate which does not belong to any of these types.

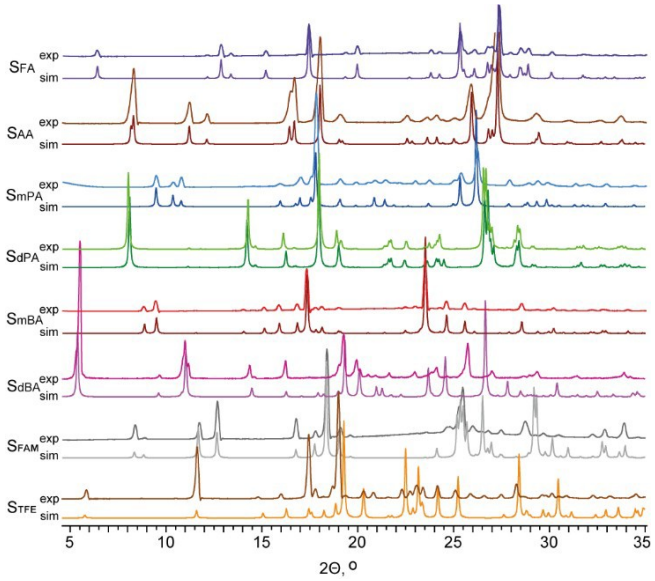

Figure 1. Experimental and simulated PXRD patterns (obtained from crystal structures) of INA solvates.

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This research was funded by "Strengthening of the capacity of doctoral studies at the University of Latvia within the framework of the new doctoral model", identification No. 8.2.2.0/20/I/006.