Poster

Crystalline forms of vitamin B7 - an example of a crystal engineer's nightmare

A.**M Dąbrowska[1], W. Kołodziejczyk[1], N. Piechalak[1], I.D. Madura[1]**

[1]Facutlty of Chemistry, Warsaw University of Technology, 00-664 Warsaw, Poland, Noakowskiego 3

izabela.madura@pw.edu.pl

The endeavour to enhance the solubility and stability of essential drugs or vitamins in pharmaceutical and cosmetic contexts has prompted the search for advanced methods in the field of crystal engineering. A lot of valuable research and developed methodologies have recently appeared in this topic, now also supported by machine learning algorithms, but the complexity of crystallization processes, especially for multicomponent systems, is still a challenge in efficient design and obtaining the desired systems.[1-4]

This study aimed to design and synthesize multicomponent systems focusing on biotin (vitamin B7 or H). The motivation behind this research stemmed from the considerable challenges associated with the poor water solubility of biotin, which led us to explore this system using a crystal engineering strategy to mitigate these limitations.

Initially, cocrystal design software was utilized to conceptualize these multicomponent systems. Molecular complementarity analysis, facilitated by the Cambridge Structural Database (CSD) exploration [5] and the Full Interaction Maps and Co-crystal Design modules from the Mercury program [6] aided in the selection of suitable components. Emphasis was placed on fostering hydrogen bond complementarity between vitamin molecules and chosen coformers or inducing the salt formation to optimize solubility and stability.

Subsequently, the designed systems were synthesized employing mechanochemical techniques such as neat griding, liquid-assisted griding, and suspension crystallization. These environmentally conscientious methods, known for their minimal solvent usage, underwent meticulous optimization to ensure successful synthesis. Powder X-ray diffraction measurements served for the comprehensive analysis of the synthesized samples.

Experimental findings yielded notable insights, including observations of polymorphic transformations and the emergence of new phases, particularly evident in systems featuring biotin and silver nitrate. Regrettably, the majority of samples manifested only as physical mixtures of substrates. Despite encountered challenges, this study underscores the necessity for further research endeavours, potentially exploring alternative synthesis and characterization methodologies, as well as the construction of accurate phase diagrams.

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The Nchem4 grant program of the WUT Scientific Council for Chemical Sciences is kindly acknowledged.