Microsymposium

Designed crystallization via sublimation

<u>Sudarshan Mahapatra</u>¹, Ramanaiah Chennuru¹ ¹Dr. Reddy's, Hyderabad, India E-mail: smahapatra@drreddys.com

Crystal structure determination of organic compounds is essential to understand structure-property correlation and is of specific importance in the pharmaceutical industries. In particular, the structure determination is unambiguously carried out using data obtained from a single crystal. One of the essentials for a successful structure determination is the requirement of a good quality single crystal or a single phase polycrystalline sample of the given material. Often crystals are formed with the incorporation of the solvent in the lattice during crystallization. In order to obtain crystal structures of anhydrous compounds, a novel approach is required where intervention of solvent can be entirely eliminated. There are a large number of methods to synthesize single crystals of a required compound like for example slow evaporation, vapour diffusion, solvent diffusion, sublimation, convection, and zone melting. Out of these techniques, slow solvent evaporation from a solution is frequently adopted to grow single crystals of organics, and this leads to the incorporation of the solvent in the crystal structure. On the other hand sublimation technique is found to be less explored towards single crystal generation and discovery of novel polymorphs. Designing of apparatus for single crystal growth assisting anhydrous crystal structure determination of different pharmaceutical compounds and generation of polymorphs will be a part of the discussion and presentation.

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Keywords: polymorph, sublimation and crystallization