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An efficient coformers selection for co-crystals screening of active pharmaceutical ingredients

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A ccording to commonly accepted definition a cocrystal is a homogeneous crystalline solid that consists of stoichiometric amounts of discrete neutral molecular species, which are solids under ambient conditions. These kind of dispersions differ from other solutions as for example eutectic or monotectic systems by molecular complex formation and congruent melting. The change of physico-chemical properties of co-crystals with respect of the co-formers is especially useful and important in the case of active pharmaceutical ingredients (API). There are many examples in the literature of significant improving of API behaviors both *in vivo* and *in vitro*. The advantages of cocrystallization for pharmaceutical industry are not only related to bioavailability enhancement but also to the increase of stability, hygroscopicity decrease, mechanical properties and intellectual property issues. Unfortunately predicting of the ability of co-crystal formation of an API with other co-formers is non-trivial and not straightforward task. That is whys two alternatives are proposed. Experimental part relies on fastening of co-crystal screening by utilization of orientation samples on glass surfaces as efficient, robust, fast and cost-preserving approach. On the other hand the QSPR approach was used for distinguishing of pairs of co-formers forming co-crystals from ones exhibiting simple eutectic behavior.



Fig.1. Histograms distinguishing properties of pairs forming cocrystals (left) from simple eutectic mixtures (right) based on heat of formation.

Biography

Piotr Cysewski received Profesor of Chemistry honour in 2013. He is the Director of Department of Physical Chemistry, Medical College of Bydgoszcz. He has published more than 60 papers in reputed journals in domain of theoretical and computational chemistry. Nowadays his activity is concerned with experimental and theopreica screeing of co-crystals of active pharmaceutica ingredients.

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