In the jungle, the mighty jungle, 
the crystals grow tonight!

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The process of crystal formation can sometimes be described as a walk through a dense jungle with no clear trail or map to guide you. Unexpected effects and unanticipated formation of “fancy crystals” are observed and this makes the life as scientist within a pharmaceutical industry very exciting! To get orientated in this “jungle” it is necessary to explore a broad experimental space to achieve the goal of identifying the form of an active pharmaceutical ingredient (API) with the most favorable properties for drug development.

Using a High Throughput Crystallization Approach (µL-scale) the crystallization conditions can be defined. A large number of different crystallization conditions may be tested and up to 384 experiments can be performed within one run using 96-well plate formats (4 plates). Different solvents and solvent mixtures in combination with a variety of counter ions (for ionisable drugs) and/or cocystal formers lead to a quick overview of the crystallization behavior of the API. This screening tool may be utilized for polymorph screening as well as for salt- and co-crystal-screening. All solid forms resulting out of this HT-screen (approx. 3mg/well) need to be analyzed by e.g. X-ray powder diffraction to check whether the compound crystallized or not. Furthermore, in order to characterize the resulting crystalline forms and to draw conclusions from the large amount of data (more than 100 patterns from a single experiment), a specific software tool is needed to handle and maintain an overview of the resulting “data jungle”. A case study will be presented to get a bit better orientation in the mighty jungle of crystal formation.

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