

Fast Polymorph Screening and Data Analysis by a new High Throughput X- ray Powder Diffraction Instrument: Example of an Active Pharmaceutical Ingredient which has the Tendency to Form Solvates

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Characterization and monitoring of solid state properties of the active ingredients and excipients are fundamental elements of the pharmaceutical development since batch to batch inconsistency can cause crucial problems in the manufacturing of the pharmaceutical dosage form, the quality of the formulation, the bioavailability and drug stability. The application of systematic procedures and an increase number of experiments combined with high resolution analytical equipment increase the probability to elucidate the relevant polymorphic and pseudo-polymorphic forms in pharmaceutical development. On the other hand, handling procedures during polymorphic screening can force physical transformation especially for solvates or hydrates and should be considered.

In the present communication, a new X-ray powder diffraction instrument working in transmission mode, with a 96 well plate sample holder is described for polymorph screening of a pharmaceutical compound which has the tendency to form solvates. For the polymorphism screening and analytical examination the same sample holder was applied without any manual sample handling.

The experimental details, analytical characterization and polymorphism and pseudo-polymorphism characterization will be demonstrated. The final characterization was completed by the determination of single crystal X-ray structures and their computational analysis. This was of great value for the identification and interpretation of the new crystalline forms and for the analysis of crucial causes and reasons for certain properties.

Based on the obtained results a controlled chemical and pharmaceutical manufacturing process could be achieved.