

## **MINIMIZING THE EFFECTS OF PREFERRED ORIENTATION IN X-RAY POWDER DIFFRACTION**

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X-ray powder diffraction (XRPD) is a fundamental tool in solid-state chemistry and particularly in the characterization and study of pharmaceutical solids. The technique is extremely useful in the identification of crystalline and amorphous phases and can be used for analyses of pure active pharmaceutical ingredients (API) or solids obtained from various drug product formulations such as tablets, capsules, creams, or suspensions. In increasing numbers of cases XRPD has been used to quantify solid-state compositions (including polymorphs, hydrates, solvates) as well as to calculate and determine crystal structures of API compounds. However, the use of XRPD for quantification and structure determination requires quality data with a high level of accuracy in both diffraction pattern peak positions and relative peak intensities. While accuracy of peak positions can be easily obtained using standard quality XRPD instrumentation, accuracy of peak intensities has largely depended on sample quality, particle size, preferred orientation (PO), and sample preparation/presentation.

In the following we present a novel (patent pending) XRPD holder to easily and significantly reduce PO due to morphology, sample preparation, and particle statistics (due to particle size effects). The device is an adaptation of a standard PANalytical transmission holder that significantly reduces/eliminates the effects of PO in samples and thereby improves the accuracy of diffraction pattern peak intensities essential for quantitative analyses and structure solutions.

Details of the device are presented and supporting diffraction patterns for significant data quality improvement are shown. Specifically, data collected for Gabapentin crystals using several different configurations and sample holders are presented and compared to the new holder.