

AUTOMATION OF XRPD DATA ACQUISITION AND PATTERN ANALYSIS

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When x-ray powder diffraction is used as a primary analytical technique in polymorph screening or salt selection, many patterns must be collected, analyzed, and sorted. The author will discuss SSCI's approach to automation of these tasks, including specially designed crystallizers and sample holders and automation of XRPD pattern matching. SSCI's new pattern matching software automatically sorts patterns into forms and mixtures. It has user interface tools that allow the scientist to view all results and change classification parameters and/or manually reclassify assignments if necessary. The program also provides sophisticated user tools for post-algorithm processing that are useful for viewing and analyzing subtle differences among patterns.