

USING ANALYTICAL DATA MANAGEMENT SYSTEMS TO ACCELERATE SALT AND POLYMORPH SCREENING

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Salt and polymorph screening are critical steps that occur between the late discovery and early development phases. These steps have far-reaching effects on the ultimate efficacy, patent protection, ease of manufacturing, and profitability of the final drug. A delicate balance must be maintained between speed and risks in deciding which form to develop. The decision process surrounding preformulation is quite complex, involving large quantities of chemical data from disparate sources that need to be evaluated--in a coordinated way--across multiple criteria. With the advent of high throughput XPRD and Raman data acquisition, preformulation scientists are being asked to explore even greater numbers of potentially developable forms than before. However, the data evaluation and final decision must still be made in the same amount of time (or faster).

In this work, we discuss the acceleration of the preformulation process through the use of modern software systems. Some data systems can read, process, store, retrieve, visualize, and report a wide variety of data type--XRD, Raman, HPLC, NMR, TGA, DSC, chemical structures, properties, and images—but too often this wide-based information is maintained in a passive form only. Not only is it possible to bring live information from different sources together in a homogeneous system, but it is also possible to allow interactive and automatic manipulations within the analytical data management system itself. Time savings of 20% to 80% have been achieved at various points in the workflow. Outline of such a system being implemented at a Pharmaceutical Company will be given.