

4371 Application of Raman Spectroscopy in High-Throughput Salt and Polymorph Screening

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With the development of an automated sample preparation platform such as CRISSY (Zinsser Analytic), the bottleneck of a comprehensive solid state screening has shifted from sample preparation to characterization.

Raman spectroscopy has been proven to be a valuable tool in solid state characterization. However, the diverse structures of APIs subjected to the screening present a serious challenge to an unequivocal identification of salts and polymorphs formed. Selected APIs were studied to provide more insight to the fast analysis by Raman spectroscopy. In addition, the effect of sample quality was investigated. The experimental results of this study, aided by the data examination that employed chemometric analysis techniques, helped us to better understand both the usefulness and the limitations of Raman spectroscopy applied in the high-throughput screening workflow.