

# INTEGRATED HYPERSPECTRAL IMAGING FOR COMPREHENSIVE MATERIALS CHARACTERIZATION

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The demands placed on analysis and characterization methods are on the rise as the complexity and sophistication of pharmaceutical products increases - qualitative and quantitative, macroscopic and microscopic, physical and chemical, a myriad of characteristics and properties. Since there is no single magic bullet technology to satisfy all these requirements, multiple technologies must be employed to achieve the best results. Hyperspectral imaging is a recent favorite in meeting these demands. Hyperspectral imaging records a large number of spatially resolved, full range, high quality spectra of a sample, and to generate spatial and spectral information. While a single spectroscopic technique offers one level of information on the sample, such as a specific polymorph or elemental distribution of an active ingredient, having both types of information in one data set offers much a deeper and more comprehensive understanding of the characteristics of the sample than when only one spectral dataset is used. The extent of information in hyperspectral imaging varies, depending on the spectroscopy selected. For example, elemental imaging using EDXRF provides elemental information at 10  $\mu\text{m}$  or greater spatial resolution. Raman hyperspectral imaging provides molecular information at the 1  $\mu\text{m}$  or smaller spatial resolution. While basic hyperspectral imaging utilizes just the combination of spectral and spatial information within one hyperspectral imaging mode, combining information from multiple hyperspectral imaging technologies offers a quantum step in the sample characterization. The integration of 2 hyperspectral datasets significantly increases the knowledge content of the combined data. However, the volume of this combined dataset tends to discourage merging data sets from multiple hyperspectral imaging technologies and processing it as one comprehensive result for the sample.

While chemometrics has been employed to mine data from various hyperspectral imaging technologies, the norm is to analyze data from each hyperspectral dataset and then compare the two individual sets after the fact, instead of processing the combined datasets. The merits of applying chemometrics to the combined data is not well established, even though the main objectives of chemometrics analysis is to regress a high volume level of raw data into a low volume level of representative data. This paper takes the first step to explore, determine and demonstrate the potential merit of the combination and integration of multiple hyperspectral imaging technologies processed with chemometrics. EDXRF maps (elemental analysis, relatively low spatial resolution and deep penetration) and Raman maps (molecular analysis, relatively high spatial resolution and shallow penetration) are recorded from selected samples, and then processed to establish correlations and complementary features.