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Is PXRD the gold standard in high throughput experiments?

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In high throughput crystallisation experiments designed to search for polymorphs, solvates, co-crystals *etc*., it is usual to consider powder X-ray diffraction (PXRD) data as the primary source of information for classifying the results, and most software used in this environment is designed to use such data [1]. In fact it is repeatedly referred to as the 'gold standard'. However, PXRD data has difficulties with preferred orientation, sample distribution, crystallinity *etc*., which is not the case for Raman spectroscopy provided that sufficient of the sample is irradiated. Recently new instruments have appeared (*e.g.* from Bruker-AXS) that combine PXRD with Raman techniques, and we have used this instrument to assess the viability of Raman spectroscopy in a high throughput environment.

Although the differences in Raman spectra are often not as pronounced as those in PXRD, we have found that the same techniques we have used to match powder patterns work well with Raman data providing the data have been properly smoothed and the background subtracted. This method uses the full measured spectrum not only the peaks, with option of using gradient data by itself or in conjunction with the spectrum. We will present pharmaceutical examples where the Raman data outperforms that of the PXRD data.

[1] Barr, G., Dong, W. &Gilmore, C.J. *J. Appl. Cryst.* (2004). 37, 658-664.