CHEMOMETRICS IN METHOD VALIDATION - WHY?

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Chemometrics is a tool that many scientists are reluctant or afraid to use; why? Is it because it is considered a "black box" difficult to use? It is certainly a useful and powerful tool worth discovering.

Many analytical methods (e.g. HPLC, GC-MS, ICP-MS) seem to be validated. However, are we sure that the best working conditions were identified and applied? Was the method properly optimised? A lot of time and money is spent applying the classical approaches described in the literature. "Design of Experiments" (DoE) may reduce the number of attempts and samples to be analysed while providing additional information related to interactions between the various experimental parameters investigated. Unfortunately, this information is not readily available in traditional approaches. Such an optimised method may proceed to the validation study. Several examples of DoE applications will be presented in the poster, related to Asymmetric Field Flow Fractionation (nanotechnology), GC x GC-MS, Raman and Supercritical fluids.

In the case of spectroscopic methods (e.g. Raman, infrared) where spectra are acquired, a multivariate approach may be appropriate to use the wealth of data available through the whole wavelength range (instead of a single/fixed wavelength). An example of Raman will be presented.

Even when the optimised method is validated, chemometrics is to be applied for multi-dimensional analytical methods, such as GCxGC-MS, to assess and correct for potential co-elution effects.

By now you know that chemometrics is useful; just give it a try.