

Multivariate data analysis of NMR data - beyond PCA and PLS

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In recent decades rapid spectroscopic measurements have revolutionized quality control in practically all areas of primary food and feed production. Near-infrared spectroscopy has been implemented for monitoring quality of millions of samples of cereals, milk and meat with unprecedented precision and speed. The key to this success is the extraordinary synergy that lies in the merging of spectroscopy and the new data technology called chemometrics. More recently, the integrated technology has received the FDA blessing in the so-called PAT (Process Analytical Technology) concept for internal quality control in the pharmaceutical industry.

A breakthrough in the use of quantitative NMR spectroscopy has been under way for more than 15 years in pharmaceutical research. In 1999, the concept of **metabonomics** was introduced by Nicholson's group at Imperial College (UK) (Nicholson, Lindon & Holmes, 1999) and defined as "quantitative NMR measurements of the multiparametric metabolic response from living organisms to pathophysiological stimuli or genetic modification". The impetus for combining NMR spectroscopy with multivariate data analysis in metabonomics was clearly the tremendously complex metabolic system in body fluids. Quantitative NMR analysis of intact food systems is very similar to the analysis of body fluids and offers similar challenges. Over the years a number of more advanced and dedicated chemometric algorithms have been developed around specific NIR applications and this talk will discuss some of these methods and their potential application to NMR data for the benefit of metabolome and quality control applications.