Title:

High resolution NMR analysis of complex mixtures

Authors & affiliations:

Adrian J. Charlton
Central Science Laboratory
Department for Environment, Food & Rural Affairs, Sand Hutton, York, YO41 1LZ, UK.

Introduction

Advances in analytical techniques and reduced computation times have facilitated the rapid characterisation of complex chemical and biochemical systems. Resolution and sensitivity enhancements have ensured a key role for high-resolution liquid state nuclear magnetic resonance (NMR) spectroscopy for the determination of compositional variation in complex matrices. A range of studies utilising cold-probe NMR and advanced data exploration techniques have illustrated the applicability of these techniques to issues facing the food and agricultural sectors.

Methods

Data analysis tools have been developed to facilitate the use of diverse NMR experimentation for the deconvolution of complex mixtures [1-3]. Artificial intelligence methods have been used to extract specific information from multivariate datasets, whilst further mathematical manipulations have been used to reduce data complexity and improve data quality. These methods have largely been applied to NMR "profiles" to elucidate trends in large datasets, rapidly pinpointing resonances for subsequent investigation using multidimensional NMR techniques.

Results and Discussion

Rapid determination of biomarkers of disease [4], product origin [5] and contamination [6] has illustrated the capability of modern data analysis techniques in combination with advanced NMR systems. Characterisation of biological systems has also been performed in support of genetic improvement and for the detection and characterisation of the effects of genetic modification [7]. These application-focussed studies have led to the development of the fundamental knowledge base that underpins food and agricultural sciences. Examples include the determination of the effect on the pea metabolome of biotic and abiotic stressors, including the interaction between genetic and environmental factors and their relation to product composition and quality.

[1] Davis, R.A. *et al.* **2006** *Chemometr. Intell. Lab.* 81, 50-59. **[2]** Davis, R.A., *et al.* **2007** *Chemometr. Intell. Lab.* 85, 144-154. **[3]** Poulding, S.M. *et al.* **2007** *J. Mag. Res.*189 190-199 **[4]** Charlton, A.J. *et al.* **2006** *Res. Vet. Sci.* 80, 275-280. **[5]** Charlton, A.J. *et al.* (2002) *J. Agri. Food Chem.* 50, 3098-3103. **[6]** Charlton A.J. *et al.* **2006** *J. Environ. Monitor*. 8, 1106-1110. **[7]** Charlton, A.J. *et al.* **2004** *Plant Biotech. J.* 2, 27-35.