21 Mixtures Analysis of Complex Samples

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The quantitative determination of mixtures components is very suitable to NMR analysis. Building on the success of qNMR, mixtures analysis does, however, create quite significant new problems. These may be dependent on the sample, givien that these cover a huge range, with differing complexities.

We have briefly described an approach to the problem that can be applied when part or all of one multiplet can be clearly seen for each component [1,2]. Building on a quick and powerful Global Spectrum peak Deconvolution (GSD), the method has at its heart the capability for users to define their "solutions" with total flexibility. This approach can be easily applied to relatively simple cases such as edible oils, Aloe vera, and beer analysis. Red wine analysis is much more complex, but the technique has a validated application here as well, identifying >50 components. [3]

We have developed a workflow that is equally suitable to operation via the User Interface, in Batch Mode, or as a "listener", performing analyses as they become available.

We now have further developed this proven functionality with the addition of 2 significant new capabilities. A simple structure database can be used to store information on important compounds, metadata, experimental spectra, and representations of the spin systems. We then provide an interactive way to quantify a mixture component in a way that can use the simulated spectrum. In that way, multiplets are correctly calculated, and the data becomes field-strength independent.

Identification of multiplets can be performed using a novel method: the multiplet is treated as a shape for which mathematical polynomials are calculated to high orders. The experimental spectrum is searched for peak line combinations that best match the descriptors.

We will explain this new approach and show its utility with mixtures analysis and application to real analysis problems of varying complexity.

1. M Bernstein, C Cobas, S Dominguez, M Pérez, A Barba, and J Edwards, "Extending and Facilitating Simple Mixtures Analysis", ENC, 2014, Boston, USA
2. M Bernstein, C Cobas, M Pérez, S Domínguez, C Peng, and A Barba Sánchez, "A Versatile Software Tool for Mixtures Analysis", SMASH, 2013, Santiago de Compostela, Spain
3. Susanne Klein, Heidger Institute, personal communication.