Overview: An automated approach to complex mixture analysis using Nuclear Magnetic Resonance (NMR) spectroscopy was developed for the Mestrelab platform and small molecule quantitation was performed on a series of Aloe vera raw materials and Aloe vera containing products utilizing nicotineamide as the internal concentration standard. The analysis automatically generates a comprehensive report of the three active components, degradation products, additives, and adulterants of commercial Aloe vera. Individual species are quantified using areas derived from Global Spectrum Deconvolution (GSD) analysis, which is insensitive to peak overlap and poor baseline. The strongest area for a mixture component can be flexibly connected into the desired concentration units using a flexible formula editor. The workflow is automated for high throughput analysis, but still allows visual inspection and editing of each sample to account for peak movements. The quantitative values derived from this rapid, straight-forward automated analysis allows decisions to be made on the purchase of materials by users as well as implementation of a controlled process strategy in the manufacture of the materials.

A complete NMR analysis of a number of beer varieties was also performed with a special emphasis on sour beers produced by wild fermentation. In this analysis the same sample was analyzed with the usual qNMR analysis performed to provide ethanol, bentonite, ethyl acetate, lactic acid, succinic acid, citric acid and malic acids concentrations along with glucose. The spectra and the NMR results are used as the basis for principal component analysis that will allow targeted and non-targeted identification of beer types and variations of intermediates in the brewing process.

For the beer process analysis in our laboratory the metabolite quantification were calculated on a concentration (mg/L) basis and samples were prepared by diluting 1 mL of the sample with 10 mL of D2O before analysis with 400 MHz NMR. The experiments were performed in a quantitative manner on a Varian Mercury 400-MHz NMR spectrometer operating at 200.12 MHz equipped with a 5 mm probe. Aloe samples were prepared using a Varian Mercury 400-MHz NMR spectrometer operated at 200.12 MHz and equipped with a 5 mm probe. Samples and the nicotineamide internal standard was weighed to within 0.1 mg. Aloe sample: g/ml calculations were obtained on a weight basis.

Spectrum analysis used Mestra 6.2.0 and the qNMR plug-in.

References: