

High-Throughput Push-Button NMR in Fruit Juice Quality Control Using Statistics and Quantification



NMR was successfully applied as a push button mixture analysis technique for quality control in the fruit juice industry. A wide range of quality assurance parameters are accessible in one single experiment resulting in a substantial reduction in analysis cost per sample and new insight into the product quality.

In recent years, NMR has seen a rapid expansion into the field of mixture analysis and screening applications as driven by metabolic screening and fingerprinting. Enabled by high throughput automation technology and the improved workflow on the NMR spectrometers NMR mixture analysis has now become a push button routine in fruit juice screening for quality control. This product is now named Bruker-SGF-Profiling.

Experimental conditions

^1H NMR experiments on juice samples (centrifuged where needed) adjusted in pH were acquired on a Bruker AVANCE™ NanoBay, operating in a flow injection mode (120 μl active volume) at 400 MHz. Spectra were recorded at 300 K. 1D- ^1H -NMR spectra of the resulting samples were acquired using the NOESY 1D (1) pulse sequence together with a rapid 2D-J-resolved for compound identification. The complete measurement procedure was performed under full automation. The data analysis was performed using the AMIX software package. AMIX identified and quantified relevant chemical entities and performed the spectral segmentation (bucketing). Embedded MATLAB routines for statistical data analysis comprised the discriminant analysis and SIMCA modelling. A spectral database of authentic juices was acquired and is constantly updated to allow optimal data analysis.

Results

Information on the major juice quality parameters were delivered in form of quantification of organic compounds, detection of redilution of direct juices with concentrate, fruit type purity and control of geographical origin. Statistical analysis was used to predict concentrations of single molecules, e.g. the concentrations of D-glucose in apple juice. It was possible to predict the glucose/fructose ratio, a parameter used in fruit juice industry for quality assessment. NMR provided the classification of juice sample towards the geographical origin (Figure 1). The mixture of different juices, e.g. adding low cost mandarin juice to high price orange juice was detected to less than 10%. The quantification of Vitamin C in various juices was realized and is shown in Figure 2.

Conclusions

NMR will play an important role in mixture analysis for fruit juice quality control. The main advantage of NMR is that a single NMR sample measurement can answer many questions. Similar analysis by traditional methods requires several independent measurements all of which may not be readily avail-

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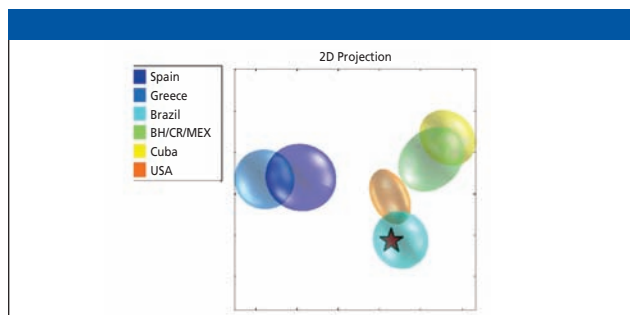


Figure 1: Classification of a new sample (asterisk) into the geographic origin models for orange juice having on average 35 authentic samples per region for model building.

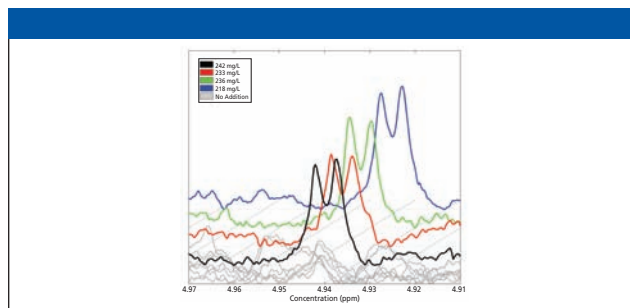


Figure 2: Automatic quantification of Vitamin C added to fruit juices.

able. The cost per sample is reduced substantially and allows the testing of a much larger set of samples thereby improving consumer security.

The methodology described for fruit juice quality control is only one example of a new field of NMR applications for statistical and quantitative analysis on mixture spectra. This approach has already been successfully used in metabonomics NMR on bodyfluids, tissue and cell extracts in toxicity and drug efficacy screening, medical or disease screening and population health and lifestyle screening.

Acknowledgement

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References

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