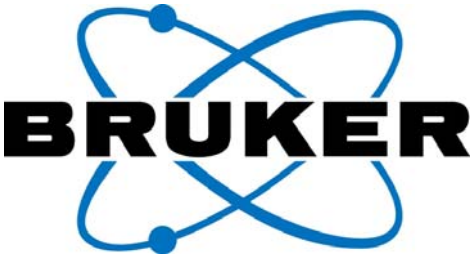
November 3, 2011 (13:15-14:15)



VENDOR SEMINAR:

BRUKER – INNOVATION AND TRADITION IN FOOD ANALYSIS

A new complete solution for automated, comprehensive ESI-(Q-)TOF full scan accurate mass screening of pesticides in food with high confidence

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Fast and comprehensive full scan accurate mass screening for hundreds of pesticides simultaneously has meanwhile found its way into routine use taking advantage of the high number of possible targets and additionally allowing for unknown evaluation and retrospective analysis. The screening procedure relies on full scan accurate mass data and a target compound database, which basically only needs the information about name (identifier in the result table) and sum formula (accurate mass information) of a target. However, the use of comprehensive databases containing hundreds or even thousands of sum formula/name entries only is anything else than advisable. In the case of pesticide screening in food low signal intensities in highly complex matrix samples have to be evaluated to achieve the required reporting levels, thus leading to a meaningless high number of false positive results. Inclusion of additional information and knowledge therefore is essential to obtain reliable results. The screening solution presented here makes use of multiple levels of confirmation and result rating for maximum confidence in the results. Examples for the workflow and system performance will be given.

Matrix matched standards reveal matrix MRM interferences and minimise false results in pesticide residue analysis of grains and pulses

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GCMS based analysis of pesticide residues in grains often results in enhanced response and the degree of enhancement is dependent on the type of grain. Some grain matrices cause matrix interference leading to false positives and false negatives, particularly when published MRMs are used without validation.

In this presentation, pesticide and matrix combinations will be shown that demonstrate the failure to accurately monitor particular pesticides in that matrix. The ideal combination of pesticide and matrix where the matrix background shows no interferences, and the combination where the matrix causes false positives or significant limitations in limits of detection and quantification will be discussed and illustrated. In extreme cases the matrix may completely supress the detection of some pesticides due to irreversible binding by matrix components. Published MRMs should be used only after they have been validated to be free from matrix interference in the matrix system under study.

Using GC-QQQ-MS, this approach has been tested in wheat, barley, oats, chick peas, canola and soybeans after a modified QuEChERS extractuion. Some examples of "problem pesticides" in each matrix will be presented.

Use and Qualification of TXRF for Trace Element Analysis of Dietary Supplements and Nutrients

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Total reflection X-ray fluorescence (TXRF) analysis has proven its capabilities in many different fields. The major advantages of the method are that it allows simultaneous multi-element detection and quantification down to the ppb range, using a highly sensitive spectrometer as the unique Bruker S2 PICOFOX is. Additionally, TXRF analysis shows no matrix effects, requires minimal sample amounts and almost no preparation effort.

The first part of the presentation focuses on the use of TXRF as a tool for investigating product adulteration issues during the food production processes as well as for qualifying phytochemical standards used in the dietary supplement industry. Real-world examples of how TXRF is used to solve quality issues with phytochemical reference standards, identify unknowns and analyze limited sample amounts will be covered.

The second part describes the analysis of liquid nutritional products (LNP). LNP are nutritionally supplemented for patients who are recovering from illness, injury or surgery and for people at risk of malnutrition. Mineral analysis is of crucial importance for product compliance and quality control. Here, TXRF spectroscopy is clearly identified as a suitable and rapid method for the multi-element quantification including macro and micro-nutrients.

NMR-Based Food Quality Screening

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Based on the metabolomics approach, 1H-Nuclear Magnetic Resonance (1H-NMR) screening has rapidly expanded in recent years in the area of food quality control. Indeed, 1H-NMR screening is a fast, multiparametric method, requiring only a small amount of sample and minimal sample preparation.

1H-NMR is a global, non-targeted approach allowing the acquisition of spectral fingerprints. The reliability and reproducibility of 1H-NMR, makes it a technique of choice for profiling of samples, by allowing the creation of statistical models based on authentic reference samples.

This non-targeted method allows the evaluation of numerous parameters linked to quality and authenticity, in only one measurement. Quantification of multiple relevant compounds, as well as classification and verification of the samples is done within minutes. This allows not only to assess the authenticity of the samples but also to detect unknown frauds that would not be detected by conventional targeted approaches.

The full automation of the measurement, including automated data analysis report generation, allows high-throughput analysis and consequently low costs per measurement. A further advantage is that the direct quantification with NMR does not require the use of internal standards.

The achievements of NMR-based screening of fruit juices and the different parameters evaluated will be discussed in detail. Validation results of the method will also be shown. In particular, comparison of NMR quantification results to official methods as well as results of proficiency testing with FAPAS® will be discussed.

Based on the experience on fruit juices, similar screening methods are under development for other food products like wine, edible oil and honey.

In conclusion, NMR is a very cost and time effective method for the simultaneous evaluation of many quality parameters in food.