A challenging story of GC-TOF MS: technology milestones and two amazing decades of its application in food analysis

November 3, 2015 (Tuesday)
12:30 to 13:30

Although the basics of Time of flight mass spectrometers (TOF MS) were established in 30s of 20th century, due to the lack of fast electronic the renewal of this technology was postponed to early 90s of last century. At this time the enormously fast, but extremely sensitive, first commercially available GC-TOF MS were introduced to the market. The nature of TOF MS technology, such as fast and sensitive acquisition of unskewed MS spectra, was followed by implementation advanced mathematical algorithms of data mining – automated peak find, deconvolution and scripting.
The potential of marketed fast GC-TOF MS instruments equipped with ion source not requiring its cleaning was later on extended by their combination with comprehensive gas chromatography (GCxGC).
The increased nowadays demands for analytical instrumentation can be summarized as: "One run covering all analyst's requirements, such as target and non-target screening, qualitative and quantitative capabilities along with easy and fast hardware-software handling and reasonable data file sizes". Such requirements were kept in mind within the GC-HRT instrument development employing the multi-reflection TOF MS analyzer (so called Flight Folded Path, FFP™). The GC-HRT routinely achieving mass resolution more than 50.000 FWHM and mass accuracy lower than 1ppm was recently upgraded with the GCxGC option extending its capabilities to the edge of possible – significantly enhanced separation combined with ultra-high resolution and ultimate mass accuracy.

Register and join the fantastic selection of TOF MS applications in food analysis presented by great scientists and excellent speakers in the same time.

Workshop program:

I. Black pepper authenticity testing based on SPME-GC-TOF MS

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Black pepper is valuable commodity on worldwide market and may become a subject of fraud. Cases of adulteration of ground black pepper with cheaper plant materials or mislabeling have been encountered. Smart approaches for the testing of black pepper authenticity are needed to disclose such practices and protect consumers. One of conceivable authentication strategies is profiling of black pepper volatiles.
The evaluated set of samples in our study consisted of 16 ground black peppers and in addition to these samples, other materials derived from pepper (oleoresin, spent – residual material of oleoresin production, pepper peels), that can be under certain conditions used for adulteration, were delivered by spice trading company. Beside of these samples, twelve more pepper samples were collected in retail markets in the Czech Republic.
In this study, black pepper volatile profiles were obtained using head-space solid-phase microextraction coupled to gas chromatography - mass spectrometry. Time of flight mass analyzer equipped with

automated deconvolution & peak find algorithm was used for primary data acquisition (TruTOF, LECO, USA). Using the Statistical Compare feature of the ChromaTof software by LECO, compounds were aligned in all off measured samples and after the normalization of their areas, the statistical analysis was performed in Simca software (Ulmetrics).
All the samples, both labeled as authentic pepper by our commercial partner and those from retail market grouped together using principal component analysis. Other 3 samples separated clearly. For one of "suspect" samples, organic solvents used for oleoresin isolation were the most decisive compounds. Other separated samples showed similar profiles of volatiles to those of pepper related materials mentioned above

II. Two-dimensional gas chromatography with time-of-flight mass spectrometric detection for determination of prohibited substances in food supplements

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In recent years a number of food supplements promising positive health effects, improving body shape and/or enhancing strong and endurance etc. have been introduced to the worldwide market. Food supplements include wide range of products containing various ingredients like herbs, herb extracts, vitamins, minerals, amino acids, proteins etc., however some of them can be contaminated by prohibited substances. Based on our 10 years experiences a number of compounds like anabolic steroids, tetrahydrocannabinol (THC) or even prescription drugs coming from cross-contamination or intentional manufacturer use can be found in these products.
To detect and identify unknown compounds in samples, non-target screening procedures based on full mass spectra measurement represent a feasible solution. For compounds that can be analysed by GC, two-dimensional gas chromatography with time-of-flight mass spectrometric detection (GCxGC-TOF) shows a method of choice. Enhanced sensitivity and chromatographic resolution resulting from separation of sample in two capillary columns with different polarities as well as unique identification of compounds due to the collection of full mass spectra are well known characteristics of this sophisticated technique.
Theoretical aspects together with practical examples and results of non-target screening of samples collected from Czech market during official control demonstrating potential of GCxGC-TOF will be presented.

III. Unknown off-flavor in plastic products of daily use – can HR TOF MS help to discover it?

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Odor emissions from plastic materials employed for production of various articles of daily use may represent a serious problem resulting in customers'´ complaints and, consequently, producers´ losses of market position. The identification of such ´smelly´ compounds and explanation of their release is a real laboratory challenge; since in many cases, they are present at (ultra)trace level, nevertheless have a very low odor threshold.

Non target screening of headspace volatiles employing solid phase microextraction coupled to gas chromatography / mass spectrometry (SPME-GC/MS) is a technique of choice. For this purpose, instrument equipped with high resolution time of flight mass analyzer (HR TOF) is the most suitable, since it enables acquisition of full high resolution spectral information, deconvolution of components occurring in complex mixtures. Identification / confirmation is then based spectral similarity, mass accuracy of detected ions and their isotopic pattern.

In a particular, two case studies will be presented:

i) Identification of compound causing musty odor in plastic inhaler

ii) Identification of compound causing "chemical"´ smell of plastic kettle.

IV. Application of GCxGC-HR TOF MS in food and food-related matrices

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Nowaday demands in the food analysis (but also other matrices) require highest level of confidence at trace and even ultra-trace levels. High resolution instruments are successfully delivering such information and easily enabling the confirmation of analyte's identity. The difficulties can be observed, when non-target analysis is required in complex matrices, such as tea extracts.

The experience of analysts across the globe has proven that the two-dimensional comprehensive GC separation (GCxGC) along with reliably fast MS detection can solve the "complex matrix" issues. A hyphenation of GC and HR TOF MS is then the logical combination for delivering the right results.

Within this contribution the examples of advantages of GCxGC-HR TOF MS on real-life sample examinations will be demonstrated.

V. „Let the Robot do it“
Automated Sample Preparation for Food Analysis-related matrices

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When it comes to determining chemical compounds in food or beverages, a laboratory must have dependable analytical tools and capabilities. Food toxins, environmental pollutants in food, flavor interaction, compound adulteration or odor threshold,- what do all these things have in common? - The need for analytical precision, dynamic range and sensitivity. GERSTEL is a recognized expert in these areas.
Our expertise in automated sample preparation and in LC/MS and GC/MS analysis makes GERSTEL your source of solutions in the food and beverage industry as well as in the field of health and food safety.
From an application focused on individual tasks such as liquid/liquid extraction to vortexing or sample weighing to a more complete sample preparation protocol, for example automation of QuEChERS, GERSTEL welcomes you to discuss the possibility for automation.
The complete GERSTEL product portfolio is specifically designed to meet your demand for high throughput and to enable modularity which might be necessary for new challenges in your analytical laboratory. GERSTEL offers a range of tools and techniques that are designed to meet customized challenges in the field of health and food safety laboratories.
Let us know how you do it