November 2, 2011 (13:15-14:15)

VENDOR SEMINAR:

RAPID SCREENING FOR FOOD ADULTERATION AND QUALITY BY DART MS

Ambient mass spectrometry employing a DART ion source for metabolomic fingerprinting/profiling: A powerful tool for beer origin recognition

Tomas Cajka, Katerina Riddellova, Monika Tomaniova, Jana Hajslova

Institute of Chemical Technology, Prague, Faculty of Food and Biochemical Technology, Department of Food Chemistry and Analysis, Technicka 3, 166 28 Prague 6, Czech Republic
e-mail: tomas.cajka@vscht.cz

Ambient mass spectrometry (MS) is a rapidly growing area representing an attractive alternative to conventional analytical approaches. Recently introduced ionization techniques, such as direct analysis in real time (DART), desorption electrospray ionization (DESI), or atmospheric pressure solids analysis probe (ASAP), allow direct examination of various types of samples in the open atmosphere and at ground potential. Little or no sample treatment prior to analysis is required. Additionally, time-consuming separation of sample components, which is usually employed by chromatographic methods, can be omitted with ambient MS.

In this presentation, the potential of DART–MS strategy to distinguish beers according to the brand origin will be demonstrated. In a first step, the DART–MS instrumental conditions were optimized to obtain the broadest possible representation of ionizable compounds occurring in beer samples (direct measurement, no sample preparation). In the next step, metabolomic fingerprints/profiles (mass spectra) of a large set of different beer brands (Trappist and non-Trappist specialty beers) were acquired. In the final phase, the experimental data were analyzed using partial least squares discriminant analysis (PLS-DA), linear discriminant analysis (LDA), and artificial neural networks with multilayer perceptrons (ANN-MLP) with the aim of distinguishing (i) the beers labeled as Rochefort 8; (ii) a group consisting of Rochefort 6, 8, 10 beers; and (iii) Trappist beers. The data generated by this emerging technique were also compared to those obtained by a “gold standard” represented by solid-phase microextraction (SPME) coupled to GC–TOFMS used for the analysis of beer volatiles.

Acknowledgement: The financial support by the European Commission through the 6th Framework Programme (contract no FP6-FOOD-2004-006942 – TRACE) and the Ministry of Education, Youth and Sports of the Czech Republic (MSM 6046137305) is gratefully acknowledged.

DART mass spectrometry and its coupling with planar chromatography: Identification of flavonoids and phenolic compounds in propolis

Elena S.Chernetsova[1,2], Gertrud E. Morlock[1,3]

1. Institute of Food Chemistry, University of Hohenheim, Garbenstrasse 28, 70599 Stuttgart, Germany
2. On leave from Russian Research Center “Kurchatov Institute”, Akademika Kurchatova sq. 1, 123182 Moscow, Russia, and People’s Friendship University of Russia, Miklukho-Maklaya st. 6, 117198 Moscow, Russia
3. Institute of Nutritional Science, Justus-Liebig-University of Giessen, Heinrich-Buff-Ring 26, 35392 Giessen, Germany

Propolis is a complex product of bees, which has been used in folk medicine for hundreds of years. As flavonoids and phenolic compounds are of primary interest due to their biological activity and positive action on

human health, their pattern was investigated in the propolis samples. For the initial screening and identification of marker compounds in the still unknown chemical profile of German propolis sorts, high-performance thin-layer chromatography (HPTLC) was used, and the differentiation between different types of propolis and the assignment of the origin of the propolis samples was performed. Hyphenated techniques, including post-chromatographic derivatization and different couplings of planar chromatography with mass spectrometry, were used for the identification of the components from the characteristic zones of marker compounds on the plate. The following possibilities of using DART-MS for flavonoids and phenolic marker compounds identification were studied:

1) DART-MS coupled with HPTLC *online* (analysis directly from the HPTLC plate) or *offline* (by means of collecting of the extracts from HPTLC zones and further analysis of these extracts), confirmation or identification of propolis components;
2) DART-MS with a benchtop Orbitrap mass analyser, identification of components in selected propolis extracts analysed as liquid samples, as dried spots on a carrier (HPTLC plate), or as extracts from the marker zones of HPTLC plate.

The respective results will be presented and discussed.

Acknowledgements: We are grateful to Irina Scholl for performing the HPTLC experiments during her diploma thesis, to Annette Schroeder and Nadine Kunz (Apicultural State Institute, Stuttgart, Germany) for providing the propolis samples, and to Maciej Bromirski and Olaf Scheibner (Thermo Fisher Scientific, Bremen, Germany) for assistance in analyzing samples using benchtop Orbitrap (Exactive). This work was financially supported by the program Erasmus Mundus Action 2 “IAMONET-RU“.

Ultra-Fast DART Screening to the Rescue: Detecting Adulteration of Dietary Supplements and Identifying Residual Pesticides using Direct Analysis in Real Time (DART) High-Resolution Accurate Mass Analysis

Elizabeth Crawford and Brian Musselman

IonSense, Inc., 999 Broadway, Suite 404, Saugus, Massachusetts, 01906 USA

www.ionsense.com

Herbal supplements ranging from weight loss supplements to natural antioxidant and nutrient supplements are current targets for adulteration and fraud. The need for fast and accurate characterization of herbal supplements, which generally contain complex mixtures of molecules, is growing as the counterfeiting of natural products is becoming more common. Pesticide detection in these consumer products and on the surfaces of fruits and vegetables is also of concern and a rapid screening technique is also needed.

DART mass spectrometry is used as a quick and efficient means of characterization of herbal supplements; to quickly screen and qualify both national and international herbal products for quality and contamination. The next generation DART ionization source, the ID-CUBE™ provides a low cost, simple method of screening with the sample analysis time of 10 seconds per sample. Liquid or solid samples are simply placed on the OpenSpot™ Sample Card; the card is place in the source and heated, producing ions via DART. The operation of this ionization source has been significantly simplified and miniaturized from the current generation DART-SVP ion source making it of greater interest as a tool in a mobile lab setting at border and importation agencies.

Rapid screening of pesticides present in herbal supplements and on the surfaces of fruits and vegetables has also been facilitated by using DART coupled with the high-resolution accurate mass Thermo Exactive mass spectrometer. This screening technique is demonstrated for both gross and residual levels of adulterants and pesticides in consumer commodities.

Evaluating Porous Materials for Sampling Pesticides from Surfaces using Direct Analysis in Real Time (DART)-Mass Spectrometry

Elizabeth Crawford and Brian Musselman

IonSense, Inc., 999 Broadway, Suite 404, Saugus, Massachusetts, 01906 USA

www.ionsense.com

Rapid screening of pesticides present on the surface of fruits and vegetables has been facilitated by using direct analysis in real time (DART) open air high resolution accurate mass mass spectrometry. These experiments focus on the use of various materials to collect pesticides from large objects including plants and produce commodities by using a vacuum-assisted sampling approach. Evaluation of the efficiency of various polymeric foams, cotton swabs and wire mesh for capture of analytes with and without the use of solvents will also be examined. Suitability of different materials as both sampling and desorption ionization support will be reported.

These experiments build on the original pesticide screening experiments where polyethylene foam was used as both the collection and desorption substrate. Small fruits and nuts were examined for pesticides using "Transmission-mode" DART-MS analysis[1].

1. Edison, S., et al., Rapid Commun. Mass Spectrom., 2011, 25, 127-139