

November 6, 2013 (13:15-14:15)



VENDOR SEMINAR:

ENHANCING THE VALUE OF DIRECT ANALYSIS IN REAL TIME (DART)-MS BY LEVERAGING SORBENT TECHNOLOGIES

Deploying DART in Analytical Workflows

Facundo Fernandez

Georgia Institute of Technology, Atlanta, Georgia, USA

DART is the most popular of the plasma-based ambient mass spectrometry ionization techniques, allowing for direct analysis of a variety of solid, liquid and gaseous samples without sample preparation. It can be used both in quantitative and qualitative experiments, and can provide the information necessary for identifying unknowns when coupled to high resolution accurate mass MS instruments. In this presentation we will provide examples on how DART is being used in a multi-technique tiered approach to detecting falsified medicines. Examples will include counterfeit contraceptives, antimalarials and antimicrobials. Tips and tricks necessary for optimum DART operation will be provided, and a comparison with other ambient techniques, such as DESI, discussed.

Low-level Pesticide Screening and Monitoring Wine Spoilage: Rapid Sample Concentration for Quantitative Analysis by DART Mass Spectrometry

Elizabeth Crawford^{1,2}, Paola Domizio^{3,4}, Brian Musselman¹, C. M. Lucy Joseph³, Linda F. Bisson³, Bart C. Weimer⁵ and Richard Jeannotte^{5,6}

¹ IonSense, Inc, 999 Broadway Suite 404, Saugus, MA 01906, USA

² Department of Food Analysis and Nutrition, Institute of Chemical Technology, Prague, Technická 3, 16628 Prague 6, Czech Republic

³ Department of Viticulture & Enology, University of California-Davis, Davis, CA 95616, USA

⁴ Dipartimento di Gestione Sistemi Agrari, Alimentari e Forestali (GESAAF), Università degli Studi di Firenze, 50144 Firenze, Italy

⁵ Department of Health and Reproduction, School of Veterinary Medicine, University of California-Davis, Davis, CA 95616, USA

⁶ Facultad de Ciencias, Universidad de Tarapacá, Arica, Chile

Pesticide screening and food spoilage monitoring are two important areas in food safety analysis. Rapid and sensitive screening methods ensure timely identification of emerging issues and increased safety for the public, as well as improved production conditions for manufacturers. A major source of wine spoilage worldwide is caused by the yeast *Brettanomyces bruxellensis*, which is responsible for significant economic loss in the wine and beer industries. Wines exhibiting a "Brett" character generally include medicinal and barnyard odors that are attributed to two volatile phenols, 4-ethylphenol (4-EP) and 4-ethylguaiacol (4-EG). When 4-EP and 4-EG are at levels less than 400 µg/L they contribute positively to the sensory complexity of the wine giving it a spicy, smoky and leather aroma. However, when levels are greater than 620 µg/L, the "Brett" character may be too strong and the wine contains off-flavor notes and is often no longer marketable.

A Direct Analysis in Real Time (DART) ambient ionization source was coupled to a high resolution accurate mass (HRAM) quadrupole mass spectrometer for full scan pesticide screening and

quantitative targeted MS/MS analysis of 4-EP and 4-EG markers in wine spoilage. Both analyses employed a rapid unattended sample concentration step using Twister stir bar sorptive extraction (SBSE) prior to ambient desorption ionization. The detection limits were in the very low ppb range for the targeted wine analyses and demonstrated an increased detection for a range of pesticides. Sample analysis time using the DART ionization approach was 3 minutes or less per sample to thermally desorb the analytes directly from the Twister sorptive stir bar surface. Rapid monitoring methods enhance consumer safety, protect the integrity of the product and allow the manufacturers to take control to prevent economic losses.

Leveraging Solid Phase Microextraction devices for removal of carbohydrates as a means of improving the quality of DART-MS results

Brian Musselman, Robert Goguen and Joseph Lapointe

IonSense, Inc., Saugus, Massachusetts, USA

Determination of composition and quality of herbal supplements are time consuming due to the nature of the active components and complexity of the sample matrix. In our work with DART-MS we observed that the presence of carbohydrates limits the utility of the method by creating a matrix effect where significant ion current is detected as the protonated sugars. In order to reduce the effect of those sugars on the results we have incorporate solid phase micro-extraction (SPME) of supplement extracts as a simple sample prep method for eliminating the sugar matrix effect. Flexible and rugged sorbent coated wire solid phase extraction devices (Supelco LC-Probe devices) have been evaluated for use in this application. The sorbent coated wires were utilized for both sample extraction and as a support for direct surface desorption ionization facilitating rapid analysis.

Results using this new direct analysis from sorbent coated wire method with supplements and foodstuffs will be described. Post-SPME Derivatization of samples to permit detection of thermally labile compounds such as polyols will also be discussed with results from recent analysis of teas and supplements.