

# 2023 NACRW Vendor Seminars

**V-1 Monday, July 24, 2023**

**7:15-8:15 am**

**WATERS CORP.**

**Location: Grand Ballroom A-D, 2<sup>nd</sup> floor**

## **Pesticides, Natural Toxins, and PFAS – Hot Topic Updates for Trace Contaminant Workflows**

*Emily Rose Britton, PhD, Principal Marketing Manager for Food & Natural Products, **Waters Corporation***

*Gordon Fujimoto, PhD, Chemical Analysis Group Leader, Americas MS Application Lab, **Waters Corporation***

Testing labs play an important role in the supply chain – they are essential in keeping the food supply safe, and yet consumers are often unaware of their existence! News coverage and rising concerns about contaminated food and water supplies have pulled back the curtain and shed light on the critical value of testing labs. Testing demand is on the rise, and new regulations and safety threats pose an opportunity for laboratories. So, what's your contaminant of choice? Pesticides, natural toxins, PFAS, all of the above? Join the Waters vendor seminar to hear about workflow and technology innovations for trace contaminant testing and a recent interlaboratory study and performance evaluation for the detection of PFAS in fish using LC-MS/MS.

## From PFAS to ergot alkaloids: residue testing working beyond pesticides

### Analysis of ergot alkaloids in a variety of simple and complex matrices by liquid chromatography-tandem quadrupole mass spectrometry

*Julie Brunkhorst<sup>1</sup>, Emilee Easter<sup>1</sup>, Kristen Moseley<sup>1</sup>, Kendra Adams<sup>2</sup>*

<sup>1</sup> *Trilogy Analytical Laboratory*

<sup>2</sup> *SCIEX*

Ergot alkaloids are mycotoxins produced by fungi most commonly associated with rye, wheat, barley and oats. On January 1st of 2022, the EU published maximum levels of ergot sclerotia and ergot alkaloids at the new maximum of 0.2-0.5 g/kg. To support import/export compliance a method was developed to quantitate ergot alkaloids in rye, wheat, barley, oats, finished feeds, feed ingredients and other matrices. The method developed utilizes liquid chromatography coupled with tandem quadrupole mass spectrometry and includes ergometrine, ergosine, ergotamine, ergocornine, ergocryptine, ergocristine, and ergovaline, as well as their corresponding -inine isomers.

## From the tap to our home: the analysis of perfluoroalkyl and polyfluoroalkyl substances (PFAS) across their lifecycle

*Holly Lee<sup>1</sup>, Jianru Stahl-Zeng<sup>1</sup>, Karl Oetjen<sup>1</sup>, and Craig Butt<sup>1</sup>*

<sup>1</sup> *SCIEX*

Recent detections of perfluoroalkyl and polyfluoroalkyl substances (PFAS) in apparel, cosmetics and food contact materials have elevated PFAS from an environmental issue into a public health concern given the potential toxicological impact of long-term exposure. As such, the fate of PFAS from use to disposal must be holistically considered by investigating these chemicals across their entire life cycle. We will present workflows for the quantitation and identification of PFAS in food, firefighting foams and cosmetics – products that cross much of the PFAS life cycle. This includes the use of electron activated dissociation (EAD) from the ZenoTOF 7600 system as an orthogonal fragmentation mechanism for structural elucidation.

V-3 Tuesday, July 25, 2023 7:15-8:15 am

THERMO FISHER SCIENTIFIC

Location: Grand Ballroom A-D, 2<sup>nd</sup> floor

## NEW ANALYTICAL TOOLS FOR PESTICIDE RESIDUES IN FOOD CONTROL

Prof. Amadeo Rodriguez Fernandez-Alba, **EURL-FV**, EU Reference Laboratory for pesticide residues in Fruits and Vegetables, **University of Almería**, Spain

Richard Fussell, Market Development Manager, **Thermo Fisher Scientific**, Hemel Hempstead, UK

Amadeo will discuss the practical implementation of recent instrument advancements to address the golden triangle of pesticide residue analysis: (i) Sensitivity, (ii) Scope and (iii) Speed. For example, the improvement in sensitivity provided by high-end triple quads to mitigate matrix effects and new high-resolution MS systems which enable simultaneous and sensitive acquisition in both targeted and non-targeted analysis in a very consistent way. The sensitivity achieved is still less than that of triple quad MS, but they still achieve default values of 10 ppb. Dual-column chromatography with two columns connected to one MS not only improves utilization of the MS time but can also reduce the chromatographic analysis time to increase sample throughput without compromising selectivity. Alternatively, it can facilitate optimization of eluent compositions for both positive and negative detection modes, simultaneously, to improve LOQs for an increased number of pesticides without increasing the analysis time.

Richard will close with a brief update on developments in the analysis of polar cationic pesticides, options to either reduce or to eliminate the usage of helium as a GC carrier gas, and a new single software with some unique features for efficient data processing of pesticides data acquired by LC-MS, GC-MS and IC-MS.

V-4 Tuesday, July 25, 2023

12:15-1:15 pm

AGILENT TECHNOLOGIES

Location: Grand Ballroom A-D, 2<sup>nd</sup> floor

## Hydrogen for Pesticide Residue Analysis: How to Convert GC/MS/MS Analysis from Helium to Hydrogen and Meet the MRLs

*Lorna De Leoz, PhD, Global Food Segment Manager, Agilent Technologies*

This presentation will address the key strategies for pesticide analysis using GC/MS/MS with hydrogen as the carrier gas that allow for maintaining sensitivity to meet MRLs. The optimized setup with hydrogen showed improved chromatographic resolution and allowed for precisely matching the retention time with helium. The HydroInert and HES sources were shown to provide best sensitivity and preserve spectral fidelity even for the compounds highly prone to reacting with hydrogen in the source by minimizing or preventing such undesirable reactions. As a result, the same MRM transitions, with the same collision energies for the targets eluting at the same retention times as with helium could be used with hydrogen carrier gas, streamlining the transition from helium to hydrogen. The presented method allowed for quantitation of over 90% of target pesticides at or below the default MRL of 10 ppb in spinach.

V-5 Wednesday, July 26, 2023 7:15-8:15 am

BRUKER

Location: Grand Ballroom A-D, 2<sup>nd</sup> floor

## Higher Throughput, Higher Accuracy, and Higher Sensitivity – New Mass Spectrometric Solutions for Food Analysis

*William Fatigante, Applications Scientist, Bruker Applied Mass Spectrometry*

Bruker Applied Mass Spectrometry continues to develop new solutions to overcome ever-increasing challenges of food safety and quality analysis. Through persistent innovation and diligent refinement of its technology, Bruker has achieved some remarkable improvements in the most critical aspects of analytical workflows: speed, accuracy, and sensitivity. From highly efficient VIP-HESI ion source to extremely fast DART JumpShot ionization; from very robust EVOQ triple quadrupole mass spectrometers to state-of-the-art timsTOF systems; from highly automated software for routine analysis and intelligent software to complete out-of-the-box Target Screener 4D solution – Bruker technology addresses challenges of the day and futureproofs laboratories for the challenges of tomorrow.

Join us for breakfast and this short overview presentation to learn about these and other Bruker innovations for food safety and quality analysis.

**V-6 Wednesday, July 26, 2023, 12 noon-1:00 pm**

**RESTEK**

**Location: Grand Ballroom A-D, 2<sup>nd</sup> floor**

## **Analysis of ultrashort-chain and short-chain PFAS in potable and non-potable waters**

*Shun-Hsin Liang, Senior Scientist II, Restek Corporation*

While the current standard tests are focusing on the PFAS with carbon chains of C4 and up using reversed-phase liquid chromatography (RPLC) methodologies, more studies have shown the prevalence and high levels of ultrashort-chain (USC) PFAS (C1-C3) in environmental aquatic systems. Therefore, a simple and reliable LC method is necessary to fulfill the need for standard analytical workflows of USC PFAS. This presentation will discuss a proposed ASTM method development (WK80687) for C1 to C4 carboxylic acid and sulfonic acid PFAS analysis in tap waters, bottle waters, and wastewaters.

## **Large Volume Injection of Pesticides in Matrix Using Low Pressure Gas Chromatography**

*Jana Hepner, Senior Scientist, Restek Corporation*

Concurrent Solvent Recondensation Large Sample Volume splitless injection (CRS-LV, or LVI) is a sample technique that overcomes the limitation of the maximum sample volume to 1 – 2  $\mu\text{L}$  valid for classical splitless injection. The LPGC configuration with the restrictor/guard column lends itself to the requirements of the CRS-LV and has a potential to improve the sensitivity of the detection. Large volume injection of matrix extract (acetonitrile and acetonitrile – toluene) samples were evaluated in range of 1 – 25  $\mu\text{L}$  for peak shapes and the relationship between the peak area and injection volume was established. The calibration parameters were compared for 5  $\mu\text{L}$ , 15  $\mu\text{L}$  and 25  $\mu\text{L}$  injection.