

2018 NACRW VENDOR SEMINARS

Food and beverage provided by each company

(PRE-REGISTRATION IS REQUIRED)

V-1 Sunday Evening, July 22, 2018, 6:15 p.m. to 7:15 p.m. SCIEX

Location: Vista Ballroom

DuoSpray™ Ionization: A Novel Approach to Analyzing the California Mandated List of Pesticides in Cannabis

KC Hyland, Global Technical Marketing Mgr – Food and Environmental

Legalization of *Cannabis* in the United States is defined by individual states with varying legislation for pesticides to be monitored and at what levels. Legislation for pesticides residue testing usually contains action limits which residues are not allowed to exceed. The California List consists of two categories and expands on Oregon's pre-existing suite of pesticides by adding six additional compounds and generally lowering pesticide action limits relative to Oregon's limits. The panel requires electrospray ionization (ESI) and atmospheric pressure chemical ionization (APCI) to be analyzed in its entirety by LC-MS/MS. The SCIEX DuoSpray™ Ion Source consists of two probe housing components, for ESI and APCI, and can be operated on the front of the SCIEX QTRAP® 6500+ system, providing flow to either probe for controlling the ionization over the chromatographic gradient. Analysis of the CA List in a single injection using positive/negative polarity switching and both ionization techniques is enabled in this manner. Pesticides historically analyzed by gas chromatography can now be captured in a single LC-MS/MS injection as part of a more comprehensive residues panel. Data for all 66 pesticides on the California list in Cannabis flower extract show that Category II action limits were achieved for inhalable products when coupled to a QTRAP® 6500+ system.

V-2 Monday, July 23, 2018, 7:15 to 8:15 am

BRUKER

Location: Vista Ballroom

Full quantitative and qualitative validation of a LC-Q-TOF multiresidue method for 272 pesticides in food samples

André de Kok and Jos Scholten

NVWA - Netherlands Food and Consumer Product Safety Authority, NRL for Pesticide Residues in Food and Feed, Akkermaalsbos 4, 6708WB Wageningen, The Netherlands; a.dekok@nvwa.nl

High-Resolution Accurate Mass (HRAM) Mass Spectrometry, based on e.g. Time-of-Flight (TOF) technology, has considerably improved the possibilities of multiresidue methods, particularly in terms of unlimited-scope of analytes and highest possible level of identification confidence. In this presentation, the full validation of a LC-Q-TOF multiresidue method for 272 pesticides in food products using the NL-method (lettuce and orange) and QuEChERS-method (chicken meat)

for extraction (and cleanup), respectively, will be presented. The fulfilment of the EU AQC SANTE Document validation requirements will be shown. This will also been done for a comparison study for the detection and identification of 155 representative pesticides in 20 different matrices.

Finally, a critical comparison will be shown of our UHPLC-Q-TOF and high-end UHPLC-MS/MS TQ instruments, as to sensitivity, selectivity and requirements for data processing software, and the influence on ease of use for routine application of HRMS-methods will be highlighted.

V-3 Monday, July 23, 2018, 12:15 to 1:15 pm

LECO Corporation

Location: Vista Ballroom

Comprehensive, Non-Target Characterization of Environmental Exposome Samples Using GCxGC & High Resolution Time-of-Flight Mass Spectrometry

Lorne M. Fell, Joseph E. Binkley, Todd S. Richards, LECO –Separation Sciences Applications Centre

Historically targeted analysis has been the primary route to evaluate complex environmental samples. This constrained testing, while effective, has often missed emerging or unexpected compounds within samples. Recent improvements in detection and data processing capabilities of various systems have allowed scientists to more fully evaluate these same samples using non-targeted (NT) techniques. As a result, the EPA is currently conducting a multiple lab, multiple platform evaluation for non-targeted analysis methods in samples designed to mimic the environmental exposome. The project contains two initial phases, first a blinded study is conducted and reported. In phase two the individual standard component lists are provided and the evaluation revised as necessary. Each blind standard is reported to contain between 100-400 spiked analytes with potential for more due to contaminants, intra-sample degradation, or reaction product formation. This presentation describes the systematic logic used for identification of the unknowns, its results, and the lessons learned from the process as it applied to the first round of ten, blinded ENTACT samples for a single platform. The platform used was a comprehensive GCxGC gas chromatograph coupled with a high resolution accurate mass (HRAM) time-of-flight mass spectrometer (TOF-MS) in both electron ionization (EI) and chemical ionization (CI) modes. Deconvolved spectra were matched to existing commercial MS libraries and screened based on the peak's retention index value, molecular ion mass accuracy, and fragment ion formula fidelity. Questions addressed will be : (i) what percentage of each sample was correctly identified, (ii) what instrumentation characteristics contributed most significantly to the identification, and (iii) what impurities, reaction products and degradation products were identified.

V-4 Tuesday, July 24, 2018 7:00 to 8:15 am

THERMO FISHER SCIENTIFIC

Location: Vista Ballroom

Targeted and Non-Targeted MS Methods for Algal Toxins and their Potential Health Effects

At NACRW 2018, Thermo Fisher Scientific is pleased to have two highly respected researchers present their work on toxins produced by cyanobacteria (blue-green algae) blooms and potential health outcomes related to exposure to those toxins.

Dr. Judy Westrick from Wayne State University will provide an overview of algal toxins along with the analytical methods that her laboratory employs for both targeted and non-targeted analysis including LC-MS-MS, LC-IT-HRMS and ELISA.

Dr. David Muddiman from North Carolina State University will discuss research his lab has undertaken that looks at exposure to cyanotoxins in the food web and the possible relationship that exposure has to sporadic amyotrophic lateral sclerosis (ALS).

V-5 Tuesday, July 24, 2018, 12:15 to 1:15 pm

AGILENT TECHNOLOGIES

Location: Vista Ballroom

Application of Enhanced Matrix Removal-Lipid Cartridges for Sample Preparation in Food Analysis

*Limian Zhao, Senior SPP Application Scientist.
Agilent Technologies, Wilmington, DE USA 19808*

Captiva Enhanced Matrix Removal-Lipid (EMR-Lipid) implements a pass-through solid phase extraction (SPE) format for highly selective lipid removal without impacting analyte recovery. Lipid hydrocarbon chains are trapped in the sorbent while analytes pass-through for analysis using a combined mechanism of size exclusion and hydrophobic interaction. The pass-through cleanup is faster and easier than traditional fat cleanup methods and provides high lipid removal efficiency. The cleaner samples improve method reliability and data quality, reduce negative matrix impact on the instrument, and improves the sample analysis productivity.

Trim time not columns – Multiresidue Pesticide analysis with the Intuvo GC/TQ

*Melissa Churley, GCMS Applications Scientist
Agilent Technologies, Santa Clara, CA USA 95051*

The Intuvo 9000GC system provides an entirely new approach to optimize productivity in the GCMS laboratory with innovations such as a compact, no-trim column and easy-to-install, disposable Guard Chip. A new and robust method, coupling the Intuvo 9000GC with a 7000D GC TQ MS system, will be described as we introduce the new Agilent Pesticide and Environmental Pollutants MRM Database and Workflow Kit for the Intuvo GC/TQ. The kit includes a customized retention-time-locked MRM database designed specifically for the Intuvo GC, which includes matrix-matched transitions and retention time information for the multiresidue screening of pesticides in food and easy reference to other consumables needed to stay productive.

Part 1:

What's New and Exciting in 2018 from Waters!

Simon Hird, Principle Scientist, Waters Corporation, Wilmslow, UK

Sample preparation, separation, MS detection, and informatics; it's all important! This presentation will provide an insight into what is new in each of these critical technology areas from Waters in 2018.

Part 2:

Ion Mobility-HRMS Based Screening of Suspected Compounds in Complex Matrices without the Use of Physical Reference Substances

Anton Kaufmann, Official Food Control Authority Zürich, Switzerland

Modern multiresidue methods analyse several hundreds of compounds within a single chromatographic run (e.g. pesticides in fruits). Such methods rely on the use of physical reference compounds in order to confirm suspected peaks. It is very challenging to produce and maintain reference compound solutions containing hundreds of analytes. Hence, there is a strong motivation to move away from relying on physical reference substances.

Data independent acquisition (DIA) can be used to produce product ion information for each observed chromatographic peak in a complex sample. Such product ion data can be used to tentatively confirm suspected analytes by in-silico fragmentation data.

The DIA approach investigated in this presentation was based on ion mobility Q-TOF technology (Vion). This instrument monitors a comprehensive 4-dimensional space consisting of retention time, drift time, m/z and ion abundance. A "chopping" in-silico fragmentation algorithm (MassFragment) is fed with the chemical structures of the targeted compounds (mol file). Each chromatographic peak is tested for the presence of the accurate mass of the precursor and any of the accurate masses of the postulated product ions.

This approach produced encouraging results even when analysing residues in complex matrices (e.g. veterinary drugs in bovine liver extracts).

V-7 Wednesday, July 25, 2018, 12:00 to 1:00 pm

O2SI SMART SOLUTIONS

Location: Vista Ballroom

The Challenge of Designing a Master Calibration Solution for Pesticide Solution Product Verification

Huichen Stavros, Ph.D. and Daniel Biggerstaff, Ph.D.

As a custom reference material manufacturer, we produce approximately 400 solutions weekly with about 25% of those solutions being made for the first time. This places a high demand on generating excellent data quality and high throughput in the quality control laboratory. To facilitate both of these aspects, we have developed GC/MS and LC/HRAMS pesticide calibration method containing approximately 400 and 800 analytes, respectively. Stability data, solvent, pH, and chemistries will be discussed.