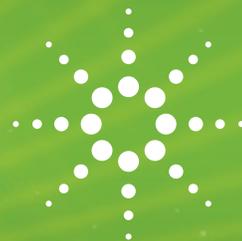


# ENVIRONMENTAL

EMERGING CONTAMINANTS IN WATER AND AIR

e-Seminar series for analysts by analysts

The Measure of Confidence



## Agilent Technologies 2013 Environmental e-Seminar Series

Agilent offers a comprehensive portfolio of innovative solutions – including chromatography, mass spectrometry, atomic and molecular spectroscopy, service, and consumables - all designed to improve the capability and productivity of your environmental lab.

This e-Seminar series features presentations by three thought leaders in the field of environmental analysis. Topics include the analysis of emerging water contaminants using elemental, chromatography, and mass spectrometry techniques. A full abstract for each session is available through the link below. Each session will be run live with a Q&A portion following the presentation.

### Schedule

**NEW!** - March 20, 2013 at 2PM EST

**PCB Arochlor analysis and identification using a GC Triple Quadrupole and MassHunter Software**

Dale Walker

**NEW!** - April 11, 2013 at 2PM EST

**GC Q-TOF analysis of fluorinated alkyl compounds in bio-solid matrix**

Anthony Macherone

**NEW!** - April 25, 2013 at 2PM EST

**Getting the best performance from your GC Triple Quadrupole for the analysis of Pesticides in environmental matrices**

Rafael Acosta

**NEW!** - May 16, 2013 at 1PM EST

**Harmonized GC Triple Quadrupole analysis of steroidal analogues for clinical and environmental monitoring of the exposome**

Anthony Macherone

**NEW!** - June 6, 2013 at 1PM EST

**GC-QQQ use in challenging matrices for detection of compounds in EPA Methods 8270, 8081 and 8082.**

Fred Feyerherm

[Recordings of previous seminars available on demand](#)

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Can't make one of the live seminars? No problem! All sessions will be recorded and available on-demand by following the link above.



Agilent Technologies

## Agilent Technologies 2013 Environmental e-Seminar Series

### Abstracts

#### **PCB Arochlor analysis and identification using a GC Triple Quadrupole and MassHunter Software**

Dale Walker

PCB's are Persistent Organic Pollutants (POPs) which had been widely used until their ban in 1979. Now they can be found in many environmental and biological matrices. Traditional analysis in the past has been done using an ECD. This session will cover the benefit of adding the specificity of a GCQQQ for low level quantitation and the features of MassHunter Software to assist in the Arochlor identification.

#### **GC Q-TOF analysis of fluorinated alkyl compounds in bio-solid matrix**

Anthony Macherone

Fluorotelomer alcohols (FTOH) are used as building blocks for synthetic polymers and oxidize in the environment to fluorinated carboxylic acids, some of which have been found to be toxic. Sensitive and specific analytical methodology is required to study the fate and transport of FTOH in the environment. Herein is presented a GC Q-TOF method for the analysis of FTOH compounds in residual bio-solid from waste water treatment plants.

#### **Getting the best performance from your GC Triple Quadrupole for the analysis of Pesticides in environmental matrices**

Rafael Acosta

Low level pesticide quantitation in environmental matrices can be enhanced using the power of GCQQQ. Pushing levels to their lowest requires special attention to the flow path and use of analyte protectants or matrix matching. We will examine flow path considerations and ways to use analyte protectants. Use of auto samplers and WorkBench to increase through put will be discussed.

#### **Harmonized GC Triple Quadrupole analysis of steroidal analogues for clinical and environmental monitoring of the exposome**

Anthony Macherone

Exposomics is the application of "omics" tools to measure the summation of exogenous and endogenous exposure events over the course one's a lifetime and the correlation of exposure to disease. To this end, targeted panels and non-targeted screening techniques are needed to find, identify and quantitate biological and manufactured chemicals in the environment and in the biological system in an effort to define the dose-response relationship of exposure. Biological systems synthesize steroids for the modulation of multiple biological needs. Exposure to exogenous steroids can disrupt these pathways. Therefore, steroids can be monitored as both a biomarker for disease and exposure. Herein is presented a harmonized GC/MS/MS method for monitoring estradiol in both plasma and environmental water sources.

#### **GC-QQQ use in challenging matrices for detection of compounds in EPA Methods 8270, 8081 and 8082.**

Fred Feyerherm

Challenging environmental matrices such as soil extracts can present problems for trace level detection of target analytes. Traditional analysis in the past has been done using a single quadrupole MS or ECD, but this is prone to matrix interferences. This session will cover the benefit of adding the specificity of a GC-QQQ for ultra low level quantitation of a number of compound types including PAH's, OC pesticides, PCB's, and many others on the 8270 compound list in very difficult matrices.



### Abstracts

#### **Applications of Emerging Spectrochemical Techniques in Environmental Monitoring**

Steve Wilbur, Senior Applications Chemist, ICP-MS Systems

Occasionally a breakthrough technology revolutionizes environmental monitoring. GC/MS was one such technology, ICP, followed later by ICP-MS were others. These technologies all enabled lower detection limits, improved data confidence and increased productivity and resulted in eventual adoption by EPA and other agencies for regulatory compliance monitoring. Last year, two new breakthrough technologies for elemental analysis were introduced by Agilent Technologies. The 4100 microwave plasma atomic emission spectrometer and 8800 triple quadrupole ICP-MS are poised to revolutionize aspects of environmental monitoring. Fundamentals of these technologies will be described along with present and future opportunities using them to further improve the quality and efficiency of environmental monitoring.

#### **Analysis of Environmental Samples with Ultra High Definition LC/QTOF-MS and Accurate Mass: How Much Resolving Po-20130117 1805-1**

Dr. E. Michael Thurman, Emeritus Scientist, US Geological Survey, University of Colorado

European Union regulations for the high resolution analysis of banned veterinary drugs in food and food products requires the use of resolving power equal to or exceeding 10,000 using the 10% valley definition, which is equal to 20,000 resolving power using full width at half maximum (FWHM). Identification points are assigned for each accurate mass with this method of 2 or 2.5 points by MS/MS for a total of at least 4 points for correct identification. The concept of identification points by this system has been advocated for environmental water samples in several publications using LC/QTOF-MS. However, in all published examples of TOF the minimum requirement of 10,000 resolving power at 10% valley (20,000 FWHM) has not been shown by time-of-flight mass spectrometry. The reason is that, until recently, TOF mass spectrometers have not been able to resolve small fragment ions of pharmaceuticals (less than  $m/z$  150) at 20,000 (FWHM). This abstract and talk will show that it is possible to reach and exceed the resolving power requirement of 10,000 at 10% valley (20,000 FWHM) for antibiotics, anabolic steroids, and other pharmaceuticals in aqueous samples using LC/Q-TOF/MS. Furthermore, it is possible to distinguish isobaric product ions of the anabolic steroid, stanozolol, that differ by either  $\text{CH}_2\text{CH}_2$  or  $\text{N}_2$ , which is a mass difference of 0.0252 mass units. This is a fragmentation pattern with resolution that was thought only to be possible with FT/MS or FT/MS Orbitrap instruments. In fact, we were able to exceed published results of both of these instruments with a broader range of  $m/z$  ions from masses as low as  $m/z$  69 to the protonated molecule at  $m/z$  279 giving resolving power exceeding the 20,000 (FWHM) requirement and answering the question of how much resolving power is enough for small molecule work ( $m/z$  less than 300). These analyses are carried out with accurate masses at the less than 1 ppm mass accuracy using both MS and MS/MS techniques.

#### **Trace Contaminant Analysis of Water with On-line SPE LC/MS/MS-20121213 1802-1**

Ralph Hindle, President, Vogon Laboratory Services Ltd; Sheher Bano Mohsin, Senior Application Scientist, Agilent Technologies

Automated on-line solid phase extraction (SPE) coupled with LC/Triple Quadrupole MS/MS enables low level detection of target analytes in water samples. Examples shown include quantitation of trace pharmaceutical and personal care products (PPCPs), pesticides, and emerging contaminants. The automation allows more samples to be analyzed per day while reducing the time and dollars associated with traditional sample prep techniques. Smaller sample volumes also results in substantial cost savings generally associated with water sample collection, transport and storage.

#### **Emerging Water Contaminants: Implications for Water Sustainability-20121108 1803-1**

Dr. Shane Snyder, Professor and Co-Director, Chemical and Environmental Engineering, University of Arizona

The availability of safe freshwater is diminishing at an alarming rate globally. Increasing human population is stressing water supplies and contributing to water pollution. Population density through urbanization also creates unique challenges in both fresh water resources and in waste disposal. These factors coupled with climate changes, including epic droughts and tragic floods, in certain parts of the world have led to the utilization of non-conventional water resources. These resources include desalinated sea water and recycled water to meet potable water needs. Thus, the water quality in many parts of the world is changing. The burgeoning human population taxes not only water resources but also



food supplies, leading to rising demands for irrigation water and consequently to greater potential for water contamination by pesticides, fertilizers, and naturally occurring constituents. Recently, a great deal of attention has been directed towards the discovery that organic contaminants of distinctly human origin can occur in the water cycle, including drinking water. Of particular concern are endocrine disruptors and pharmaceuticals, which have known biological impacts to the environment and human health depending on timing and dose of exposure. In order to characterize the risk of these substances in water, robust and reliable analytical techniques are required in order to determine the exposure. Many existing methods are labor intensive, require large sample volumes (i.e., >1L), and utilize time consuming extraction/concentration/clean-up procedures. Modern analytical instruments can now detect these substances using much faster techniques such as direct water injection and on-line solid-phase extraction. However, measurement provides only the occurrence metric and not the health metric needed to characterize risk. New generations of cellular (in vitro) bioassays have been developed which can screen essentially all receptors in the human genome for activity resulting from mixtures of contaminants in water. This presentation will discuss the current research activities regarding emerging contaminants in water with a focus on analytical and bioanalytical methods to characterize the complex mixtures of these contaminants in the aqueous environment.

### **Minimize Startup Time for Complex Semi-volatiles Analysis with Factory-tested GC/MSD Analyzers -20100928 1803-1**

Mike Szelewski, Application Scientist for Environmental Analysis, Agilent Technologies

Agilent's Semivolatiles DRS Analyzer is designed for the analysis of semivolatile compounds by GC/MSD, with Deconvolution Reporting Software for data reduction. The Semivolatiles DRS database includes the 338 single component compounds and is designed for generic semivolatiles analysis not specific to USEPA methods. An analyzer is pre-configured and tested at Agilent's manufacturing site. Installation time is minimized and productive samples can be run sooner. The hardware and software components are configured for maximum sample throughput including backflush for minimal maintenance. The Agilent Semivolatiles Analyzer is an ideal solution for a new laboratory looking for quick startup.

*On-demand e-Seminar abstracts are available on the [registration page](#)*

