

# PRELIMINARY AGENDA

## Orange County, California | May 10, 2012

Time	Environmental Track	Pharmaceutical Track	Food Track	Petrochemical Track		
8:30 AM	Registration / INnovation Hub					
9:00 AM	Welcome & Introductions: INnovation Hub					
9:30 AM	Optimizing Laboratory Profits with EPA Methods Using Innovative Injection Technology and a New, Most Sensitive GC/MS	Data In, Data Out – Visualization of Data Organized Through an ELN	An Improved Arsenic Speciation Method for Urine and Apple Juice	Guest Presenter: Dr. Nathan Saetviet Elemental Scientific Improved Detection Limits and Reduced Si Speciation with Micro-Flow Analysis of Undiluted Petrochemicals by ICP-OES and microFAST OS		
10:00 AM	Guest Presenter: Joshua Wilhide UMBC Comparative Study: LC-APCI-MS and offline Ambient Ionization with DSA of Explosives	What is the impact of USP 232? Being Prepared to Meet the New Trace Metals Regulation	Guest Presenter: More information coming soon	Utilizing the Gulf Oil Spill to Understand the Degradation Properties of Tar Balls by TGA- FTIR		
10:30 AM	Break / INnovation Hub					
11:00 AM	Answers in Seconds: Analysis of Pesticides in Drinking Water by DSA/TOF	Guest Presenter: Dr. Andre' J. Sommer Miami University ATR Imaging for Problem Solving in Pathology and Pharmaceutical Formulation	Determining Flavors and "Defects" in Beer by Headspace Trap/GC/MS	Accurate, FastD 3606: Optimize Resolution Between Ethanol and Benzene with Ability to Analyze 15 Samples per Hour		
11:30 AM	Guest Presenter: Eduardo Morales Weck Laboratories Evaluation of a Variety of Extraction and Analytical Techniques for the Determination of Pyrethroid Pesticides in the Tissue of Aquatic Organisms	Stress Free Compliance: Simplifying and Speeding up Your Instrument Qualification Process	HPLC Sample Preparation Solutions for INcreased Productivity and Performance	Get out of the Lab! Ensuring Product Quality with Portable Testing		
12:00-1:00 PM	Lunch / INnovation Hub					
1:00 PM	Trace Metals in Drinking Water: Skills and Techniques for Better Analysis	Impurities in your samples? Quick and Easy Identification of Unknowns	Verifying Ingredient Identity and Purity by FT-IR Spectroscopy and SIMCA	Guest Presenter: Dr. Nathan Saetviet, Elemental Scientific Automated Mixing and Sampling of Wear Oil for the Rapid Determination of Trace Metals by ICP-OES		

1:30 PM	Going Paperless: Learn About the Challenges with Paper, the Components of a Paperless Lab and How to Convert to a Paperless Operation	More information coming soon	Is our food really safe? Analysis of Banned Pesticides and Other Dangerous Compounds in our Food and Beverages using TOF with DSA	What's New and Innovative at ASTM: Optimizing Methods
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Note: Presentation titles subject to change.

# **INSPIRING INNOVATION WORKSHOP AGENDA**

Orange County, California | May 10, 2012

Time	Environmental Track	Pharmaceutical Track	Food Track	Petrochemical Track		
2:00 PM	BREAK / INnovation Hub					
2:30 PM	New Atomic Spectroscopy Technologies That Lower Laboratory Costs While Increasing Productivity	Get out of the Lab! Ensuring Product Quality with Portable IR Testing	Guest Presenter: Marian Boardley Marian Boardley Consulting Use of Appropriate Reference Materials for Identification of Dietary Ingredients by IR Spectroscopy	Advances in FT technology for ICP-OES and its Application to High Salt Matrices		
3:00 PM	Nanoparticles in the Environment: Opportunities for Testing by ICP-MS?	Method Optimization and Validation Requirements for Chromatography Methods	More information coming soon	More information coming soon		
1:00 – 4:00 PM	INnovation Hub					

# **Environmental Track**

### Comparative Study: LC-APCI-MS and offline Ambient Ionization with DSA of Explosives

Author & Presenter: Joshua Wilhide, Mass Spectrometry Facility Manager, University of Maryland, Baltimore County

During this presentation, the presenter will discuss running explosive samples on the AxION platform with HPLC and DSA capabilities.

# Evaluation of a Variety of Extraction and Analytical Techniques for the Determination of Pyrethroid Pesticides in the Tissue of Aquatic Organisms

Author & Presenter: Eduardo Morales, Senior Chemist, Weck Laboratories

Due to the intensive agricultural demand and changes in farming practices, environmental pesticide pollution has become a serious problem, particularly in the aquatic ecosystem. The objective of this study is to develop a rugged and reliable extraction and analytical method for the determination of a number of synthetic pyrethroid analogs in fin and non-fin fish tissue by exploring different techniques. Sample preparations consist of a number of different extraction approaches that include Accelerated Solvent Extraction (ASE), ultrasonic extraction (sonication) and QuEChERS. The analytical methodologies evaluated are single quadrupole GC/MS and tandem GC/MS/MS (triple quadrupole mass spectrometry) in both electron impact and chemical ionization modes which when integrated with the appropriate preparation technique produce detection limits in the low parts-per-billion level.

# Going Paperless: Learn About the Challenges with Paper, the Components of a Paperless Lab and How to Convert to a Paperless Operation

Presenter: Phillip Skinner, Director Field Marketing, PerkinElmer Presenter: Rudy Potezone, Executive Director, Global Informatics, PerkinElmer

This session will focus on how to overcome paper-based obstacles and delays in the laboratory by way of an ELN. Explore how environmental labs can improve efficiency while simultaneously reducing errors with the right software. In addition, we'll discover why an ELN should not be considered a stand-a-lone system, and why integrating your lab is of high value.

## **Environmental Track**

### Nanoparticles in the Environment: Opportunities for Testing by ICP-MS?

Author & Presenter: Chady Stephan, Product Specialist (Atomic Spectroscopy), PerkinElmer

Engineered Nanomaterials (ENMs) are synthesized by a manufacturing process that produces and controls ENMs to have at least one dimension in the range of 1 to 100nm in size. ENMs often possess different properties than bulk materials of the same composition, making them of great interest to a broad spectrum of industrial and commercial applications. The widespread use and application of ENMs will inevitably lead to their release into the environment, which raises concern about their potential adverse effects on the ecosystems and, subsequently, human health.

This work describes the versatility of ICP-MS in analyzing Engineered Nanomaterials in the environment. In Standard Mode, an ICP-MS provides accurate composition and concentration measurements. In Single Particle Mode (SP-ICP-MS), it allows the differentiation between ionic and particulate signals, measures particle sizes (if shape is known), and explores agglomeration and size distribution. Coupled with a size separation technique, some information about the surface charge and functionality could be investigated.

### Answers in Seconds: Analysis of Pesticides in Drinking Water

Author: Hayley Crowe, Product Specialist (Mass Spectrometry Detection), PerkinElmer Presenter: Charlie Schmidt, LC/MS Lead, PerkinElmer

Direct Sample Analysis (DSA) time of flight (TOF) system enables an alternative workflow for analyzing water for pesticides, personal care products and other environmental compounds. This new technology provides results in seconds with no chromatography, sample preparation, or method development. You will learn about DSA, TOF, and how the integration of both technologies provides a more productive and easy workflow in any laboratory.

# Optimizing Laboratory Profits with EPA Methods Using Innovative Injection Technology and a New, Most Sensitive GC/MS

Author: Lee Marotta, Sr. Field Application Scientist (Chromatography), PerkinElmer Presenter: Tom Kwoka, Product Specialist (Chromatography), PerkinElmer

This presentation demonstrates how enhancing GC/MS sensitivity can reduce laboratory costs by enabling the collection of smaller sample volumes and still be able to meet and/or exceed EPA criteria. If a significantly smaller sample size is being used, less extraction solvent will be used and less storage space is needed for the same number of samples. In most instances, the concentration step can be avoided, providing additional cost savings for the laboratory.

### Trace Metals in Drinking Water: Skills and Techniques for Better Analysis

Author: Ewa Pruszkowski, Sr. Applications Scientist (ICP-MS), PerkinElmer Presenter: Steve Mangum, Product Specialist (Atomic Spectroscopy), PerkinElmer

Drinking water safety is one of the most important issues in the today's world. The NexION 300 ICP-MS system is well-equipped to handle the demands of U.S. EPA Method 200.8 for the analysis of drinking water samples. It has the flexibility to use the standard or collision/reaction modes to remove spectral interferences, while the method IDLs and MDLs can be met with ease. The analytical accuracy analyzing certified reference standards is excellent and long term stability is superb.

#### New Atomic Spectroscopy Technologies that Lower Laboratory Costs while Increasing Productivity

Author: Paul Krampitz, Sr. Product Specialist (Atomic Spectroscopy), PerkinElmer Abstract: Coming Soon

## **Pharmaceutical Track**

#### ATR Imaging for Problem Solving in Pathology and Pharmaceutical Formulations

Author & Guest Presenter: Dr. Andre' J. Sommer, Professor Director, Molecular Microspectroscopy Laboratory and Analytical Division Coordinator, Miami University

The presentation will focus on the advantages of attenuated total internal reflection (ATR) infrared imaging over transmission and trans-flection imaging methods. Specific examples will include disease detection and metabolite identification in kidney biopsies and the authentication of pharmaceutical formulations.

#### What is the impact of USP 232? Being Prepared to Meet the New Trace Metals Regulation

Author: Lee Davidowski, Sr. Product Specialist (Atomic Spectroscopy), PerkinElmer Presenter: Steve Mangum, Product Specialist (Atomic Spectroscopy), PerkinElmer

This talk will cover the new proposed heavy metals methods, and discuss the requirements for laboratories to meet these regulations. Emphasis will be given to plasma based technology as it is most closely aligned with proposed metals limits and detection capabilities.

#### Data In, Data Out - Visualization of Data Organized Through an ELN

Presenter: Phillip Skinner, Director Field Marketing, PerkinElmer Presenter: Rudy Potezone, Executive Director, Global Informatics, PerkinElmer

The increasing footprint of Electronic Lab Notebooks in biopharmaceutical organizations has led to an evolving role for such systems. ELNs initially provided mostly document management (Word, Excel) capabilities along with specific stoichiometric tools for synthetic chemistry. We will describe the addition of a structured data model into an ELN which allows for the facile capture and management of *in-vitro* and *in-vivo* data. We will describe how that data coming from plate readers is combined with relevant chemical information and exposed for visualization and exploration of such structured relationships.

# **Pharmaceutical Track**

#### Stress Free Compliance: Simplifying and Speeding up your Instrument Qualification Process

Author: Jim Willis, Director, Americas Validation and Compliance Services, PerkinElmer Presenter: Tony Pezzolo, Validation Specialist, PerkinElmer

A Harmonized approach to instrument qualification has numerous advantages such as: productivity, efficiency, cost savings and compliance, to mention a few. The Universal Qualification automates and simplifies the qualification process, thereby allowing more time for you to focus on what is important - Science. The Universal Qualification's ability to generate an electronic file also has the added benefit of being able to support the current industry trend toward the "Paperless Laboratory."

### Impurities in your samples? Quick and Easy Identification of Unknowns

Author: Hayley Crowe, Product Specialist (Mass Spectrometry Detection), PerkinElmer Presenter: Charlie Schmidt, LC/MS Lead, PerkinElmer

Have you ever had an unknown peak or impurity in your sample and needed to figure out what it is? In this session we will provide an easy workflow using LC-TOF in the identification of unknowns. You will learn about time of flight mass spectrometry and how it is commonly used to provide elemental composition for unknowns.

### Method Optimization and Validation Requirements for Chromatography Methods

Author & Presenter: Tony Pezzolo, Validation Specialist, PerkinElmer

A typical chromatography method will likely require changes, adjustments, and optimizations throughout the duration of its lifecycle. Unbeknownst to many, the existing guidance does allow for some method optimizations, without necessitating full method revalidation. The following talk serves as a primer for method validation, and will explore which parameters can be adjusted, and to what extent, without requiring the need for method re-validation.

### Get out of the Lab! Ensuring Product Quality with Portable IR Testing

Author: Dean Brown, Sr. Product Specialist (Molecular Spectroscopy), PerkinElmer Presenter: Sam White, Sr. Product Specialist (Molecular Spectroscopy) PerkinElmer

A portable instrument that a pharmaceutical or nutraceuticals facility can take on to the loading dock to verify incoming raw material would be a valuable asset. For ease of implementation, AssureID mimics existing QA workflows, guiding users through method development, validation and trending and analysis of results. Expertise is built into the software to provide fast data modeling, troubleshooting and method validation without prior knowledge of chemometrics. AssureID also meets the stringent requirements of 21 CFR part 11 compliance.

## **Food Track**

### Use of Appropriate Reference Materials for Identification of Dietary Ingredients by IR Spectroscopy

Author & Guest Presenter: Marian Boardley, President, Marian Boardley Consulting

This presentation focuses on cGMP-compliant (21 CFR 111) use of standard and in-house reference materials, specifically when using those materials as a reference standard for identification of dietary ingredients using IR spectroscopy. The presentation includes a case study using PerkinElmer instruments (mid-IR) to match ground botanical raw materials with available reference standards.

# Is our food really safe? Analysis of Banned Pesticides and Other Dangerous Compounds in our Food and Beverages

Author: Hayley Crowe, Product Specialist (Mass Spectrometry Detection), PerkinElmer Presenter: Charlie Schmidt, LC/MS Lead, PerkinElmer

In this session we will show you a fast and easy way to quickly screen for the presence of pesticides and other dangerous compounds in our food and beverages. Using the new direct sample analysis (DSA) time of flight (TOF) system we can directly analyze samples without chromatography or method development in seconds. By streamlining your workflow using the DSA-TOF you will get results faster, enabling increased productivity and decreased overhead costs.

### Determining Flavors and "Defects" in Beer by Headspace Trap/GC/MS

Author: Lee Marotta, Sr. Field Application Scientist (Chromatography), PerkinElmer Presenter: Tom Kwoka, Product Specialist (Chromatography), PerkinElmer

The brewing process is very interesting, exciting and enjoyable science. In this presentation, we will discuss several solutions for the brewery using headspace trap, GC/MS. The goal is to utilize one instrument to characterize flavor components, measure defects, investigate raw materials, determine brewing completion, accomplish consistency and investigate competitive products.

### Verifying Ingredient Identity and Purity by FT-IR Spectroscopy and SIMCA

Author: Ben Perston, Applications Scientist (Molecular Spectroscopy) PerkinElmer Presenter: Sam White, Sr. Product Specialist (Molecular Spectroscopy) PerkinElmer

Glycerin – Purity and safety of an important ingredient. You can use FT-IR to verify that incoming glycerin is really glycerin and not contaminated with other glycols. AssureID software offers an untargeted screening approach that provides good sensitivity for contaminants even in the presence of natural variability in the raw material.

#### Sample Preparation Solutions for INcreased Productivity and Performance

Author: Mike DiVito, Director, Sample Preparation & Separations, PerkinElmer Presenter: Craig Young, Product Specialist (Liquid Chromatography), PerkinElmer

Sample preparation is arguably the most critical step within the analytical process, impacting the quality of the analysis and often representing up to 60 % of a laboratory technicians timetable. A variety of proven techniques, such as filtration, dialysis, liquid/liquid extraction and Solid Phase Extraction (SPE), are routinely adopted in today's analytical laboratories to resolve the vast array of sample preparation demands. This session will focus on the use of Solid Phase Extraction (SPE) for effective, efficient sample concentration and purification.

## **Food Track**

#### An Improved Arsenic Speciation Method for Urine and Apple Juice

Author: Chuck Schneider, Product Planning Leader (Atomic Spectroscopy), PerkinElmer

Determining the various inorganic and organic arsenic species in urine and juice products has proven to be challenging. Although a variety of chromatographic methods are available, all suffer from any number of limitations, including long analyses times, non-baseline resolved peaks, and expensive LC columns. To address these issues, we have looked at a different approach to the separation chemistry. The initial results are encouraging and indicate that five common arsenic species (AsB, MMA, DMA, AsIII, and As5) can be separated with baseline resolution is less than five minutes in both urine and apple juice matrices. The preliminary work will be presented, although more work is required to validate and characterize the method.

# **Petrochemical Track**

# Improved Detection Limits and Reduced Si Speciation with Micro-Flow Analysis of Undiluted Petrochemicals by ICP-OES and microFAST OS

Guest Presenter: Dr. Nathan Saetviet, Elemental Scientific

The analysis of volatile solvents by ICPOES is challenging because the volatility and vapor pressure of the samples cause plasma instability and quickly deteriorate peristaltic pump tubing. As a result, samples are often diluted in a less volatile solvent and introduced with a chilled spray chamber. However, dilution often puts the desired detection limits out of reach and is time consuming prone to contamination. Furthermore, elements such as Si may have different instrumental response depending upon the organic form of the analyte due to varying transport efficiencies in the spray chamber. By using a micro-flow sample introduction system that has nearly 100% transport efficiency, sample preparation steps are eliminated, detection limits are improved, and elemental speciation effects are reduced or eliminated.

#### Using the Gulf Oil Spill to Understand the Degradation Properties of Tar Balls

Author: Justin Lang, Product Specialist (Molecular Spectroscopy & Thermal Analysis), PerkinElmer and Elizabeth Gardner, University of Alabama, Birmingham

Presenter: Sam White, Sr. Product Specialist (Molecular Spectroscopy), PerkinElmer

Thermogravimetric Analysis coupled to a Fourier Transform Infrared Spectroscopy (TGA-FTIR) was utilized in the study of petroleum pollution in the form of surface residues (tar balls). These surface residues are attributed to the recent BP oil spill. Due to the magnitude of the event, petroleum contamination was reported throughout the gulf coast region. Samples were obtained from Louisiana (Grand Isle), Alabama (Fort Morgan), and Mississippi (Biloxi). The TGA analysis makes it possible to analyze the volatility and percent of petroleum products in the tar balls. Through FTIR, identification of key functional groups associated with the evolved gases is possible.

#### What's New and Innovative at ASTM: Optimizing Methods

Author: Lee Marotta, Sr. Field Application Scientist (Chromatography), PerkinElmer Presenter: Tom Kwoka, Product Specialist (Chromatography), PerkinElmer

There is new and exciting information from ASTM. Several methods are being updated for speed, ease of use and accuracy. The language of these updated methods is simplified and new instrumentation is being used for better, quicker results.

# **Petrochemical Track**

#### Enhanced, Accurate, Fast ... D 3606: Optimized Resolution between Ethanol and Benzene

Author & Presenter: Leeman Bennington, Product Specialist (GC, GC/MS), PerkinElmer

Run 15 samples per hour! The round robin has begun for bringing D-3606 into capillary technology. The separation between Ethanol and Benzene is amazing resulting in more accurate results for benzene. Because of the stability and short instrument runtime, laboratories will enjoy significantly, increased instrument uptime and increased sample throughput.

### Get out of the Lab! Ensuring Product Quality Anywhere, Anytime with Portable Testing

Author: Dean Brown, Sr. Product Specialist (Molecular Spectroscopy), PerkinElmer Presenter: Sam White, Sr. Product Specialist (Molecular Spectroscopy), PerkinElmer

A compact instrument is preferable if and only if performance is not compromised. New innovative software gives one the ability of creating turnkey methods for almost every analysis. Turnkey analysis of IR Lubricating oil analysis, FAME analysis, and Determination of Oil and Grease in Water will be discussed.

### Advances in FT Technology for ICP-OES and its Application to High Salt Matrices

Author: Denise Porter, Product Specialist (Atomic Spectroscopy), PerkinElmer Presenter: Chady Stephan, Product Specialist (Atomic Spectroscopy), PerkinElmer

Conventional plasmas use a helical RF coil for the generation of the RF field. When analyzing high salt solutions with this design, it is common to increase the plasma gas flow to maintain the robustness of the plasma. With the new Flat-Plate technology introduced by PerkinElmer, the plasma characteristics can be maintained at gas flows up to 50% less.