# AGILENT MS TRAINING WORKSHOPS 2014

## 1ST – 2ND OCTOBER 2014

## Hilton Albert Dock, Liverpool, England

As a user of **Agilent organic Mass Spectrometry instrumentation**, you have one of the very best systems for your work. But are you getting the maximum possible performance and productivity from your system, and benefiting from its full capabilities?

As part of Agilent's on-going focus on customer satisfaction we would like to invite you to attend our **MS Workshops 2014** specifically designed for anyone using our organics MS systems. Take this opportunity to get the latest technical and applications related information.

The modular structure to the **2 day program** lets you select topics that are relevant to your daily work, as well as providing the opportunity to interact with our team of specialists to address your questions.

The 2014 venue is conveniently located in the heart of Liverpool with spectacular views over the famous **Albert Dock** and less than a mile from **Liverpool Lime Street Station. John Lennon Airport** is only a 20 minute cab ride away and for international delegates, **Manchester Airport** is accessible with a direct rail link.

The training package includes your accommodation and meals, and if you register and pay before the 31st July costs only £225 plus VAT - a very effective use of your training budget.

We encourage you to **register early** to secure your place as we expect a high attendance at the meeting. Once registered, we'll contact you to request your workshops of choice.

**www.agilent.com/chem/ms_meeting**

**Delegate package** - includes attendance at the Workshops from midday Wednesday 1st to midday Thursday 2nd October, exhibition, refreshments, meals and accommodation for the night of 1st October.

EARLY BIRD WORKSHOP package - £225* + VAT

STANDARD WORKSHOP package - £295 + VAT

* Early Bird package available until 31st July 2014

**More info and Register: www.agilent.com/chem/ms_meeting**

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## Synopses of Workshops

## Wednesday 1st October, Afternoon Session (13:30 - 17:15)

### A. Secrets for successful GC-QQQ pesticide method development

*Dr Kate Mastovska, Covance Laboratories, Madison, WI, USA & Harrogate, UK*

This workshop will discuss tools that can help you develop rugged GC-MS/MS methods or improve performance of your current methods for pesticide residue analysis and other applications. This includes optimization of MS/MS conditions to provide sensitive and selective determination of analytes at low levels in complex matrices. Special attention will be paid to the optimization and use of column back flushing as a time- and cost-effective approach to improve ruggedness of your GC-MS/MS system whilst increasing your sample throughput. The use of analyte protectants leading to more consistent results and other beneficial outcomes, will also be discussed. No GC-MS/MS analysis would be successful without properly optimized GC injection conditions. Our discussion will focus on programmable-temperature vaporization (PTV) technique for direct injection of QuEChERS extracts but other injection approaches applicable to trace-level analysis will be also reviewed.

### B. New developments in highest sensitivity GC and GC-QQQ technology

*Chris Sandy, GC/MS Product Specialist, Agilent Technologies UK*

In recent years, many analytical laboratories have migrated their multi-residue methods from GC/MS employing Selective Ion Monitoring (SIM) to GC/MS/MS systems employing Multi Reaction Monitoring (MRM). The superior selectivity and sensitivity provided by GC/MS/MS has facilitated the implementation of robust and routine multi-residue methods that meet regulatory requirements.

Trace quantitation of analytes in complex sample matrices places demands on all the components of the analytical instrument – GC, MS and Software. This workshop will discuss the very latest developments in GC and MS hardware – including the 7000C and 7010 GC/MS/MS systems – and software that ensure the highest levels of analytical performance and productivity are not only achieved, but also maintained in routine use.

### C. Taking GC and GC/MS to another dimension

*Bryan White, JSB Limited*

What's hidden below the baseline and "interferences" in your sample? When you have isobaric components interfering with your targets or you need to separate aliphatics and aromatics what are your options? With Customisation, GCxGC and Capillary Flow Technology the options are almost limitless. This workshop will explore the possibilities of ensuring error free TPH analysis with no separation in the sample prep, investigating flavours in food and beverage samples with limited prep and give real examples of how you can investigate your sample with creative gas chromatography.

### D. UHPLC Unmasked- UHPLC efficiency at conventional pressures using Poroshell columns

*Kevin Bayly, LC Product Specialist, Agilent Technologies*

This workshop will demonstrate the practical issues of using UHPLC systems with Sub 2 Micron columns and the fact that there is clearly an attractive alternative in the use of superficially porous columns. We will demonstrate how you can take a 'Conventional' HPLC method and convert it into a RRLC method using a Conventional HPLC system with a Superficially Porous phase. We will show how you can achieve a >70% solvent saving with a 4 x Increase in Analysis time all without the need for <2 Micron columns and Ultra High Pressures.

### E. Recommended maintenance for High End LC-MS – daily, weekly, monthly and not at all!

*Rob Woolf, Field Systems Specialist, LC/MS & GC/MS, Agilent Technologies UK*

The engineer's toolbox – tools and techniques for diagnosing instrument faults. A discussion on the techniques an engineer will use to isolate and diagnose instrument faults on high-end LC-MS systems including half-splitting and using diagnostic software and the benefits of pre-emptive maintenance.

### F. Optimization Approaches in Sample Preparation for Environmental and Food Applications

*Dr Joan Stevens, Sample Preparation Applications Scientist, Agilent Technologies*

Determination of trace residues and contaminants in complex matrices, such as environmental and food often requires sample extraction and preparation prior to analysis. Optimizing your sample preparation is advantageous since it offers cleaner extracts and lower levels of detection. Optimization can appear to be very time consuming, but it doesn't have to be if a systematic approach is taken. This approach can also be used to troubleshoot a problematic method. We will discuss how to apply the systematic approach to an existing and new sample preparation method.

### G. High-throughput MassHunter Quant workflows

*Marc Tischler, Software Specialist, Agilent Technologies*

A high-throughput quantitative workflow is the key to realizing lab productivity. This workshop explains how to speed up the analytical process by means of reviewing by exception. Streamline time-consuming steps such as manual integration by filtering batch results with outlier visualization in Batch-at-a-Glance, Compounds-at-a-Glance, and QRS cross-batch trend charting. Finally, the workshop shows how to seamlessly investigate non-target interferences with Unknowns Analysis.

### H. Laboratory compliance across industries – Preparing for audits and managing UKAS accreditation

*Paul Smith, EMEAI Lab. Compliance Productivity Specialist, Agilent Technologies*

Whilst the UK environmental and food sectors have focussed on validating methods for regulated residues and contaminants to achieve UKAS accreditation; the FDA have historically focused on instrument validation on which to build proprietary methods. Bringing 'method validation' and 'instrument validation' together this compliance workshop explores the risks and costs in maintaining UKAS accreditation: Experimental design with UKAS, MCERTS, or DWTS in mind; Audit preparation and management; Emerging audit trends such as data integrity, record keeping, and validating unknown contaminants.

### I. Find the needle, characterize the haystack- smart software for statistical analysis of MS data

*Gordon Ross, LC/MS Specialist, Agilent Technologies UK*

This workshop will focus on the use of differential and multivariate statistical analysis of high resolution accurate mass data to elucidate differential sample composition, trends, food authenticity and sample class prediction. Mass Profiler B.07 software allows impurity identification and discovery of emerging contaminants in environmental and food analysis. Multivariate analysis using Mass Profiler Professional allows differential analysis between multiple sample groups and conditions. This provides a means of highlighting and identifying differential compounds, compounds which behave in similar ways (clustering) and allows Sample Class Prediction - a powerful tool for determining sample authenticity.

## Thursday 2nd October, Morning Session (9:00 – 13:00)

### A. High efficiency screening for trace organics in water samples using a turnkey GC-MS analyzer

*Chris Sandy, GC/MS Product Specialist, Agilent Technologies UK*

In December 2000, the European Commission introduced a new piece of legislation, the Water Framework Directive (WFD 2000/60/EC). Working in collaboration with a major European Environmental Laboratory, Agilent has developed a comprehensive GC/MS analyzer package for the target based, multi-residue screening of environmental water samples using the Agilent 7890B / 5977 bench top GC/MS system. This multi-residue screening analyzer uses a retention time locked, full scan data acquisition method and data processing utilizing the new Target Deconvolution (TD) feature of MassHunter Quantitative software. Data processing includes the use of a unique reference library of electron impact mass spectra that contains more than 1000 compounds, including volatile organic compounds (VOCs) and semi-volatile organic compounds (SVOCs). The GC/MS analyzer facilitates the rapid identification and reporting of GC-amenable organic pollutants in extracted environmental water samples at the sub µg /L concentration range.

### B. Recommended maintenance for High End GC-MS – daily, weekly, monthly and not at all!

*Rob Woolf, Field Systems Specialist, LC/MS & GC/MS, Agilent Technologies UK*

The engineer's toolbox – tools and techniques for diagnosing instrument faults. A discussion on the techniques an engineer will use to isolate and diagnose instrument faults on high-end GC-MS systems including half-splitting and using diagnostic software and the benefits of pre-emptive maintenance.

### C. 21st Century LC - Discovering the hidden dimension in liquid chromatography, a peep at 2D LC

*Kevin Bayly, LC Product Specialist, Agilent Technologies*

Until now, the ultimate in Resolution and Peak Capacity has looked to be achieved using UHPLC. In this Workshop we'll demonstrate how today's advances in HPLC instrumentations now makes 2DLC a more powerful tool to uncover hidden peaks that otherwise could go unresolved. We demonstrate how a 2DLC system is configured and the practical aspects of using a 2DLC system.

## D. Universal Guide to LC/QTOF-MS Methodology-Essential Considerations when planning a screening project using the QTOF

*Dr. Imma Ferrer and Dr. Mike Thurman, University of Colorado, Boulder, USA*

This workshop will address the following topics: (1) Unknown identification of small molecules (less than 1000 molecular weight) by LC/QTOF-MS dealing with pesticides, pharmaceuticals, and surfactants. (2) Sample preparation for LC/MS analysis, and (3) Essential considerations when planning a screening project in a logical series including both targeted and non-targeted screening using accurate mass. These essential considerations consist of building accurate mass databases for targeted analysis and setting windows for accuracy and formula generation. Next will be the discussion of non-targeted unknown analysis and formula generation followed by large database screening, such as ChemSpider. The use of isotopes will be explained in order to shorten the list of possible unknown candidates for identification. MS-MS analysis and fragmentation will be reviewed in order to identify unknowns from non-target analysis by LC/QTOF-MS. Finally, the use of standards and the synthesis of standards will be shown for degradates and metabolite studies. Copies of Application Notes and Research Papers will be available and a book will be on display of unknown analysis by Agilent based LC/QTOF-MS systems.

## E. Highest sensitivity LC-QQQ - experiences with the latest system

*Thomas Glauner, LC/MS Applications Scientist, Agilent Technologies*

At the American Society of Mass Spectrometry conference in June, Agilent presented the latest model of the 6400 LC/MS product line, the 6495 triple quad. Several changes to the ion optics, the collision cell, and the detector further improved the ion transmission, resulting in more sensitivity, better precision and improved robustness.

In this workshop we will explain the technical innovations and their implications for routine lab use. We will discuss instrument tuning, the concept of the instrument detection limit (IDL), the transfer of methods from other triple quad models and summarize the experiences we made in our labs since the market introduction. Finally we will showcase exciting applications from the field of food safety and environmental enabled by the new level of performance the 6495 LC/MS instrument offers.

## F. HPLC GPC cleanup of high matrix samples prior to instrumental analysis

*Cate Jones, Natural Resource Wales*

Analytical method robustness is a key requirement in a high throughput laboratory. Dirty samples can jeopardize reliability if care isn't taken during extraction and clean up. This workshop will cover the use of standard HPLC hardware including fraction collection for the removal of high molecular weight interference from high matrix environmental samples prior to instrument analysis for trace organics. We will show how this technique can be applied to soils, sediment, marine biota, waste waters and effluents and also fatty foods.

### G. Automated Sample Preparation for Polar and Non-Polar Species in Water at Low Levels

*Ray Perkins, Managing Director, Anatune Ltd*

Stir Bar Sorptive Extraction (SBSE) is a convenient way of extracting low-polarity analytes from water; It offers simplicity, high concentration factors and splitless transfer of analytes to the column. As the use of GC-tandem mass spectrometry becomes more widespread, the great selectivity this offers compliments SBSE perfectly. This workshop will begin with a brief introduction and demonstration of SBSE and move on to cover current applications such as :taste and odour compounds in drinking water, extraction of ultra-low levels of cypermethrin and poly aromatic hydrocarbons.

The workshop will also discuss how GC-QqQ, SBEE and automated, micro-scale, solid phase extraction can, together, be used to automate the extraction and analysis of both polar and non-polar analytes in water samples from a variety of sources

### H. Streamline Mass Hunter reporting to LIMS, MS office and database applications operating on the network

*Marc Tischler, Software Specialist, Agilent Technologies*

Analysing large numbers of samples also brings challenges in data management. This workshop will focus on the standard tools that exist for efficiently integrating MassHunter into the laboratory network and LIMS system. It will cover the facilities for making reporting easy in a variety of formats depending on where the data is destined and also looks at new convenience functionality for local work group data storage.

### I. Accurate Mass screening with the new GC-QTOF and screening databases

*Joerg Riener, GC/MS Specialist, Agilent Technologies*

Conventional screening with single quadrupole or tandem quadrupole instruments require extensive method setup and optimization to screen for hundreds of compounds. The combination of Q-TOF technology and an exact mass library eliminates this complexity and provide greater flexibility in screening workflows and high-resolution accurate mass measurements provide higher confidence in screening results. A pesticide PCDL has been developed for the Agilent 7890B GC and 7200 Series GC-QTOF mass spectrometer for food safety and environmental screening employing retention time locking. This workshop will explain the concept, functionally and show the entire workflow. MassHunter PCDL software will be shown which allows content to be easily viewed and edited, making it easier for users to create custom databases for smaller and more specific suites of analytes. Finally the workshop we will showcase this workflow for food safety applications, screening for 700 pesticides in food samples measured on the 7200 GC-QTOF.

**Once you have formally registered, we will ask you to select your workshops of choice. 4 workshops may be chosen from each day, making a total of 8 workshops.**




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