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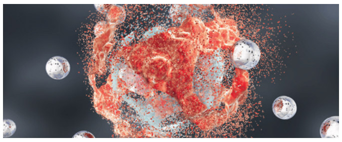

Celebrating the Year of the Periodic Table of Elements

Ed McCurdy, ICP-MS Product Marketing, Agilent Technologies, UK

In this issue of Agilent's ICP-MS Journal, we celebrate the UN/UNESCO International Year of the Periodic Table, which marks 150 years since the periodic system of the elements was proposed by Dmitri Mendeleev. On March 6, 1869 Mendeleev presented the first periodic table containing all 63 known elements, sorted according to their properties. There are now 118 known elements, but only 90 occur naturally. ICP-MS is routinely used to measure most of them.

As scientists continue to research the role and nature of elements, we consider some current uses for ICP-MS including single cell analysis, and report on developments to improve its ease-of-use.

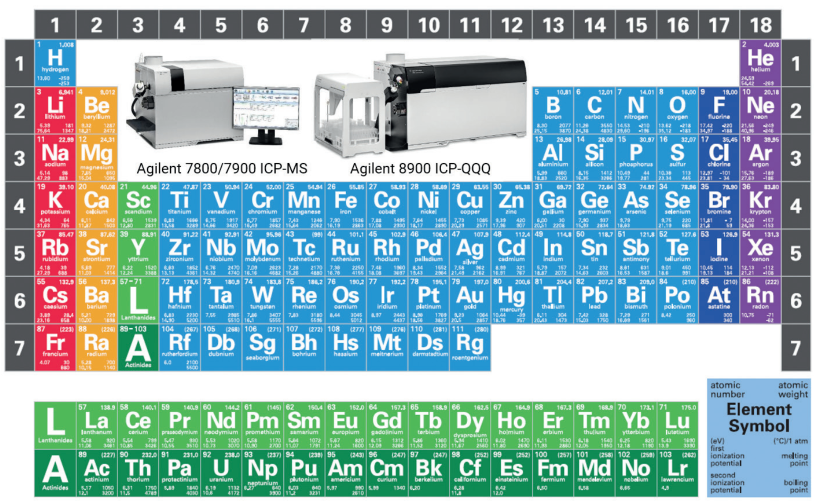

Figure 1. Agilent ICP-MS mass card.

ICP-MS Software Tools and Options to Support Ease-of-Use and Low Cost-of-Ownership

Ed McCurdy, Glenn Woods, and Abe Gutierrez, Agilent Technologies

Introduction

In a previous article in Journal Issue 75, we explained how hardware configuration and operating conditions affect usability and productivity. In this follow-up article, we show how software features and workflows also impact ICP-MS ease-of-use and cost-of-ownership. We also discuss how the recently introduced ICP Go interface simplifies ICP-MS operation, speeding up initial training and streamlining routine operational workflows.

Agilent ICP-MS systems are engineered to give users the highest level of performance. But performance alone is not enough to meet the requirements of routine and commercial laboratories, where ease-of-use and productivity are as important as sensitivity and detection limits. To address this need, ICP-MS MassHunter includes a range of usability and automation features to ensure consistently high levels of performance from day to day and between different operators.

Preset Method and Method Wizard

Preset Methods have been an integral part of Agilent's ICP-MS MassHunter software for many years. They were initially conceived as a way to predefine acquisition settings, QC checks, and report templates for US EPA regulated ICP-MS methods. The method library has been extended over time to provide methods for a range of applications on both single quad and triple quad ICP-MS.

ICP-MS MassHunter's Preset Methods eliminate the unproductive "downtime" for initial method setup and optimization. This is an important time – and cost – saving for laboratories in the commercial sector. For applications not covered by a built-in Preset Method, user-defined settings can be saved as a new batch template. This saves method setup time and ensures consistency, as the acquisition parameters and auto-optimization settings are loaded from the template.

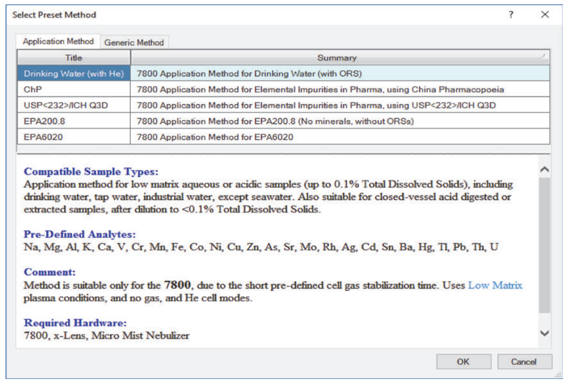

Figure 1. Example of application-specific Preset Method template for the Agilent 7800 ICP-MS. Template predefines analyte/ISTD list, cell modes, integration times, appropriate plasma conditions, and more.

Method automation

Developing a method for a new or unusual sample type for which no Preset Method exists can still be a time-consuming task, especially for labs that are new to ICP-MS. The automated function of ICP-MS MassHunter's Method Wizard can create an optimized method from the analysis of a representative sample or from user responses to a few sample-related questions. The new method can be saved as a template for future use.

Startup and Auto-Optimization

Parameters such as torch alignment, gas flow settings, ion lens tuning, mass calibration, and electron multiplier (EM) detector voltages have a major impact on system performance. But manual optimization of these settings can lead to unwelcome and potentially costly variation in system performance. The solution is to use ICP-MS MassHunter's built-in Startup and auto-optimization routines to ensure that system performance is consistent regardless of operator experience.

Startup can be scheduled to optimize hardware settings (torch position, EM voltages, resolution, and mass calibration), plasma conditions, and ion lens voltages automatically following plasma ignition. Startup ensures that the ICP-MS is permanently calibrated and optimized, eliminating the errors and variability that can occur with manual tuning, and ensuring the instrument is always operating at peak performance. Agilent's plasma correction function (part of the High Matrix Introduction – HMI/UHMI – capability) can also be calibrated during Startup. This ensures that optimum plasma conditions (matrix tolerance, sensitivity, oxide level) are always available for any target sample type.

As part of Startup, a detailed system Performance Report can be generated. This includes a time-stamped entry in a table showing the history of each parameter's value, along with a snapshot of all tune values and meter readings. This history view is extremely valuable in identifying lab environment issues (such as a change in ambient temperature) or to track gradual changes that indicate the need for routine maintenance.

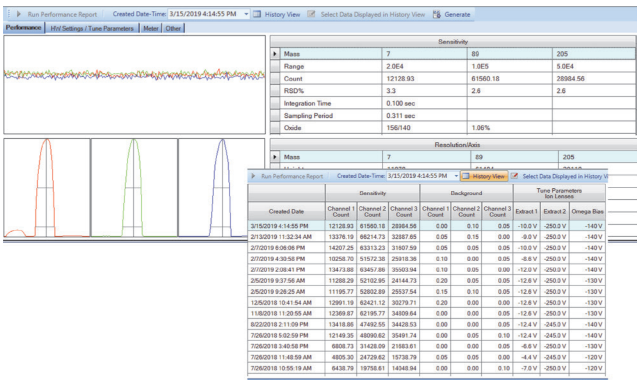

Figure 2. ICP-MS MassHunter Performance Report and history view.

A batch-specific autotune can also be run before each analytical batch, ensuring full traceability of the system performance at the time the samples were analyzed.

ICP Go User Interface

ICP Go was launched with the Agilent 7800 ICP-MS Water Analyzers (*1*), but is also compatible with other Agilent 7700, 7800, and 7900 ICP-MS systems. ICP Go is a new concept in ICP-MS software, providing a radically simplified interface between the operator and the underlying ICP-MS MassHunter software. ICP Go controls the entire analytical run, from igniting the plasma through setting up the run from a predefined or user-defined template, to data analysis and reporting.

Urgent samples can be inserted into the Queue for immediate analysis, so in-run flexibility is not compromised.

ICP Go is browser-based, replacing the ICP-MS Mobile App, which is no longer available. Connection to the ICP-MS can be from any compatible network-connected device. This is beneficial in busy laboratories, where a user might want to monitor instrument status and run progress on several ICP-MS systems remotely.

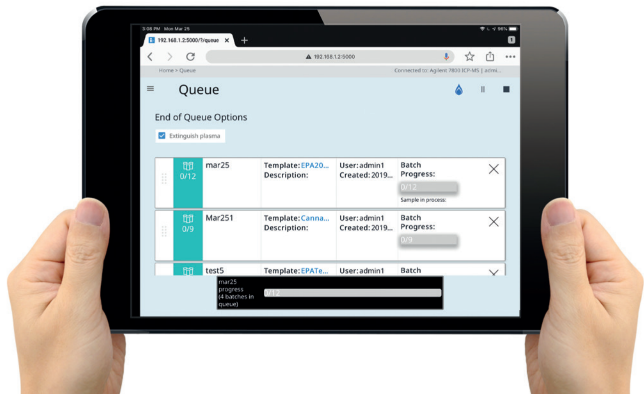

Figure 3. ICP Go user interface provides simple, touch-compatible control of Agilent ICP-MS from PC, laptop, tablet, or smartphone.

ICP Go is so simple and intuitive that novice users can be productive in just 15 minutes. The clear screen layout and simple workflow also make it easy for operators to be cross-trained, supporting staffing flexibility in the lab.

ICP Go is installed alongside the ICP-MS MassHunter software, so full functionality is still available if necessary for new method development or non-routine analyses.

Conclusions

ICP-MS MassHunter's Preset Methods, Method Wizard, and comprehensive auto-optimization routines – plus the ICP Go user interface – set a new standard for simple ICP-MS setup and routine operation.

Laboratories benefit from shorter training times and more consistent performance, improving productivity. Cross-training of staff is also easier, maximizing operational flexibility and staff utilization.

Reference

Agilent ICP-MS Journal 75, 5994-0572EN

Measuring the Elemental Content of Single Cells using the Agilent 7900 ICP-MS

Tetsuo Kubota, Agilent Technologies, Japan

Measuring Elements Present in Intact Single Cells

Expanding the understanding of the role metals play in cell biology is an emerging field of study. Many elements are essential for cell health, and an imbalance, deficiency, or excess may disrupt natural cell processes. Traditional bulk analysis methods for measuring metals in cells rely on sample solubilization, extraction, or digestion, followed by analysis by atomic spectroscopy. The sample preparation step destroys the individual cell structure, so the reported metal concentration results are derived from the mean values measured from thousands of cells.

In single cell-ICP-MS (scICP-MS), intact cells contained in the sample liquid are nebulized so each cell is suspended in an aerosol droplet. Individual cells are introduced into the plasma using an approach similar to the well-established method used for single nanoparticle analysis by ICP-MS (spICP-MS). As each cell-containing aerosol droplet passes through the plasma, the ions produced from the metal content of the cell are detected as a discrete signal pulse using time resolved analysis (TRA). The intensity of the signal is proportional to the mass of the analyte ions present in the cell. If the cell transport efficiency is known, the number of cells that contain the analyte (or analytes) of interest can be determined, together with the analyte concentrations per cell (*1*).

Experimental

Instrumentation

An Agilent 7900 ICP-MS fitted with the optional Integrated Sample Introduction System (ISIS 3) was used. The 7900 ICP-MS provides optimum conditions for acquisition of the short-duration signals that are characteristic of single cell and single particle applications. It combines very high sensitivity with short (0.1 ms) dwell times, enabling fast TRA mode. Fast TRA allows single element acquisition at a sampling rate of 10,000 measurements per second with no settling time between measurements. Very high sensitivity is essential to allow detection of attogram (ag, 1.0×10^{-18} g) levels of analytes in single cells.

The 7900 ICP-MS was fitted with a quartz torch with small (1.0 mm) internal diameter injector and standard nickel cones. An AIF-3 triple tube nebulizer and spray chamber (both from S.T. Japan) were specially designed for the introduction of intact cells to the ICP-MS. A syringe pump (AS ONE Corporation, Japan) was fitted to the ISIS 3 to control the low sample flow rate to the ICP-MS.

Sample, standards and reference material (RM)

A yeast cell sample was prepared in an aqueous solution. A silver nanoparticle RM (Merck Sigma Aldrich) with a nominal particle size of 100 nm was used to measure the nebulization efficiency. The RM was diluted to a particle concentration of 1.0 ppb with 0.25% ethanol. Ionic standards for Ag, Zn, Fe (Kanto Chemicals, Japan), P, and S (SPEX CertiPrep) were prepared at concentrations of 5 ppb for Ag, 10 ppb for Zn and Fe, and 100 ppb for P and S, in 1% HNO_3. The standards were used to measure the elemental response factor, which is used to convert the measured analyte counts per cell to analyte mass in attograms per cell.

Multi-element acquisition for single cell analysis

Method setup, acquisition, and data processing were performed using the Rapid Multi-Element Nanoparticle Analysis mode of the Single Nanoparticle Application Module of Agilent ICP-MS MassHunter software. Originally developed for single nanoparticle analysis, the software is equally suited to analysis of the elemental content of single cells.

ICP-MS MassHunter includes a Method Wizard, which guides the user through the entire setup process and automatically provides or calculates the required method parameters. Using the software module, multi-element data is collected and combined into a table in ICP-MS MassHunter's Data Analysis pane, shown in Figure 1.

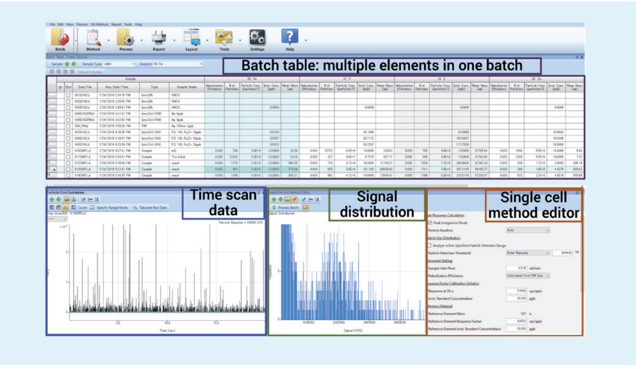

Figure 1. ICP-MS MassHunter data analysis overview. Final single-cell analysis results are reported in tabular and graphical formats.

The overview screen provides comprehensive information about each of the analytes measured in the cells. For example, the number of cells containing each analyte, the nebulization efficiency, signal distribution, mean mass of analytes in each cell, and ionic concentrations external to the cell. Being able to measure multiple elements in a single acquisition saves time and reduces the sample volume required for each analysis (*2*). The total acquisition time was 240 s from a sample volume of approximately 100 µL. If each analyte had been determined individually, the acquisition time would have been 640 s, requiring a sample volume of 400 µL.

Results and Discussion

Cell nebulization and transport efficiency

To establish the cell transport efficiency, the number of cells calculated by ICP-MS was divided by the number of cells counted by microscope. Using this method, the cell transport efficiency was found to be 25%. Ensuring a high number of cells are nebulized and analyzed improves the accuracy of the data.

Signal distribution

Single cells were analyzed using scICP-MS in multi-element mode. The signal distributions for $^{31}P^+$, $^{34}S^+$, $^{56}Fe^+$, and $^{66}Zn^+$ are shown in Figure 2. By rinsing the cells well during the centrifugation and buffer exchange steps of the sample preparation procedure, signals for each element in single cells can be clearly distinguished from the background.

Mean mass

The mean mass data for P, S, Fe, and Zn shown in Table 1 was automatically calculated by the ICP-MS MassHunter software. In addition to P and S, which are major components of nucleic acid compounds and proteins, Fe and Zn were measured at sub-femtogram (fg, 1.0×10^{-15} g) levels per cell.

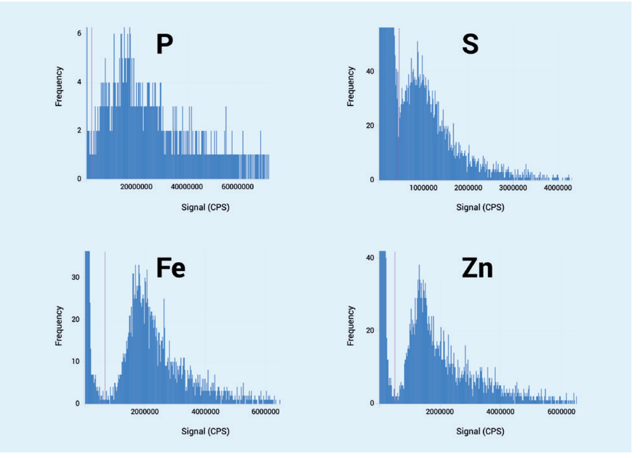

Figure 2. Signal distribution of four analytes in single cells.

Table 1. Mean mass (attograms) and precision of each analyte in single cells (n=3).

Analyte	Mean mass (ag)	RSD (%)
P	70,800	2.4
S	54,900	16.1
Fe	485	0.7
Zn	873	2.6

Conclusions

The Agilent multi-element scICP-MS method enables the role of multiple metals in cell biology to be measured and explored in detail. The technique provides valuable information on the intrinsic metal content and metal associations in individual cells. scICP-MS can also be used to research the uptake, accumulation, and release of metals and metal-containing nanoparticles from cells.

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1. S. Meyer, A. Lopez-Serrano, H. Mitze, et al., Single-cell analysis by ICP-MS/MS as a fast tool for cellular bioavailability studies of arsenite. *Metallomics*, 2018, 10, 73
2. Michiko Yamanaka and Takayuki Itagaki, Measuring Multiple Elements in Nanoparticles using spICP-MS, Agilent Technologies publication, 2018, 5994-0310EN

Researcher Wins IUPAC-Solvay International Award for PhD Thesis on ICP-MS/MS Method Development

Sayuri Otaki, ICP-MS Marketing Manager, Agilent Technologies, Japan

Dr. Eduardo Bolea-Fernandez (pictured), a postdoctoral researcher in the Atomic and Mass Spectrometry (A&MS) research unit at Ghent University, Belgium, won a IUPAC-Solvay International Award for Young Chemists in 2018.

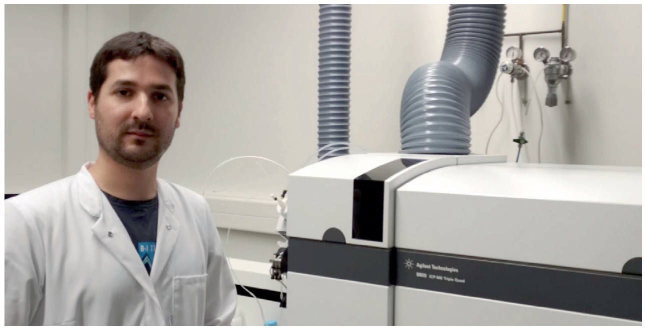
Only five prizes are awarded each year, based on the best PhD theses in the chemical sciences, as described in a 1000-word essay. For the 2018 award, there were 45 applications from individuals receiving their PhD degrees from institutions in 15 countries.

Eduardo's PhD on "Method development for ultratrace elemental and isotopic analysis using tandem ICP-mass spectrometry (ICP-MS/MS)" was supervised by Prof. Dr. Frank Vanhaecke, Prof. Dr. Martín Resano, and Dr. Lieve Balcaen. While the PhD was carried out at Ghent University, Belgium, Eduardo also worked closely with colleagues based at the University of Zaragoza, Spain.

As well as completing his PhD thesis, Eduardo has (co-) authored 17 articles in peer-reviewed international journals. Details of his papers based on ICP-MS/MS are provided in the bibliography. His current postdoctoral research activities involve an extension of the capabilities of ICP-MS/MS to determine ultratrace level elements in dissolved and nanoparticulate form and the analysis of individual cells. Working within the A&MS group at Ghent University he combines these topics with high-precision isotopic analysis of mercury using multi-collector ICP-MS in an environmental context.

Eduardo will receive a cash prize of USD 1000 and travel expenses to the 47th IUPAC World Chemistry Congress, 7 to12 July 2019, in Paris, France. He will also present a poster describing his award-winning work and submit a short critical review on aspects of his research topic, to be published in Pure and Applied Chemistry.

More information on the IUPAC-Solvay prize



- Characterization of SiO_2 nanoparticles by single particle-inductively coupled plasma-tandem mass spectrometry, *J. Anal. At. Spectrom.*, 2017, 32, 2140-2152
- Overcoming spectral overlap via inductively coupled plasma-tandem mass spectrometry. A tutorial review, *J. Anal. At. Spectrom.*, 2017, 32, 1660-1679
- Determination of ultra-trace amounts of prosthesis-related metals in whole blood using volumetric absorptive micro-sampling and tandem ICP-Mass Spectrometry, *Anal. Chim. Acta.*, 2016, 941, 1-9
- Laser ablation-tandem ICP-mass spectrometry for direct Sr isotopic analysis of solid samples with high Rb/Sr ratio, *J. Anal. At. Spectrom.*, 2016, 31, 464-472
- Tandem ICP-mass spectrometry for Sr isotopic analysis without prior Rb/Sr separation, *J. Anal. At. Spectrom.*, 2016, 31, 303-310
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- Interference-free determination of ultra-trace concentrations of arsenic and selenium using methyl fluoride as a reaction gas in ICP-MS/MS, *Anal Bioanal Chem*, 2015, 407: 919
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- Accurate determination of ultra-trace levels of Ti in blood serum using ICP-MS/MS, *Anal Chim Acta*, 2014, 809, 1-8

Reflections on the European Winter Plasma Conference 2019

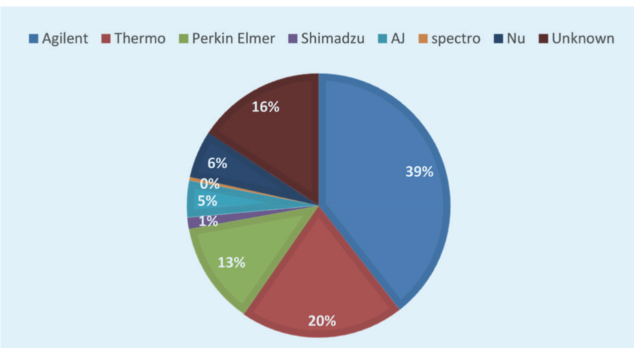
Sayuri Otaki, ICP-MS Marketing Manager, Agilent Technologies, Japan

Nanoparticle Analysis Among Highlights in 2019

The 18th European Winter Conference on Plasma Spectrochemistry (EWCPS) was held in Pau, France in February 2019. Around 550 people traveled from all over the world to discuss the major topics of interest in plasma spectrochemistry. Nanoparticles remained a hot topic at this conference and there were presentations and lively discussions on measurement devices, analytical methods, single cell analysis, and laser ablation imaging. Looking forward to future conferences, fields of interest are expected to include lithium ion batteries and emerging pollutants from high-technology industries.

ICP-MS Poster Review

Almost 290 posters were presented at the six-day conference. Of the 223 posters that used ICP-MS, almost 40% used Agilent instrumentation, with ICP-QQQ instruments (8800 or 8900) used in around a third of these.



Agilent Events and Award Ceremonies

Agilent was delighted to welcome delegates to its various events including the lunchtime seminar "Pushing Boundaries in Life Science Research" (pictured). Dr. Björn Meermann from the Federal Institute of Hydrology (BfG) Germany spoke about "Automated Single Algae ICP-MS" and Panayot Petrov from LGC, UK explained "Metrological Applications of ICP-QQQ in Life Sciences".

Agilent has been sponsoring the European Award for Plasma Spectrochemistry since 2002 and the European Rising Star Award for Plasma Spectrochemistry since 2017. This year's "Plasma Award" went to Prof. Jose Ignacio Garcia Alonso, Department of Physical and Analytical Chemistry, University of Oviedo, Spain for his extensive work on plasma spectrochemistry. Ass. Prof. Magdalena Matczuk, Department of Chemistry, Warsaw Technical University, Warsaw, Poland was awarded the Rising Star Award.

Prof. Alonso (left) and Ass. Prof. Matczuk (right) receiving their awards from Ryszard Lobinski, Conference Chair, and Sayuri Otaki, Agilent Technologies.

Both awards aim to support plasma spectrochemical developments and applications in Europe.

Sponsorship of these two prizes underlines Agilent's continued commitment to supporting high-quality research and innovation in plasma spectrochemistry, at all stages of a scientist's career.

The next WPC will take place in Tucson, Arizona, USA in January 2020, and the next EWPCS will take place in Ljubljana, Slovenia, in February 2021.

On-Demand Webinars

Title: **What's the BIG DEAL about Nanoparticles in Water: spICP-MS for Identification and Occurrence in Water Treatment Plants**
Speaker: Dr. Arturo A. Keller, Bren School of Environmental Science & Management, University of California, Santa Barbara, USA
Host: Spectroscopy

Register here

Title: **Determination of the Geographic Origin of Spices Using ICP-OES, ICP-MS, and Mass Profiler Professional**
Speakers: Lindsey Whitecotton and Jenny Nelson, Agilent Technologies
Host: Agilent Technologies

Register here

Title: **ICP Go – Fast, Easy, Go! – Elemental Analysis Made Easy**
Speaker: Bert Woods, Agilent Technologies
Host: Agilent Technologies

Register here

Webinar Executive Summary

Title: **How to streamline implementation of ICP-MS for regulated water analysis**
by Gregory Lecornet and Ed McCurdy, Agilent Technologies
Publisher: Spectroscopy

Download here

Agilent ICP-MS Publications

- **Application compendium:** Fourth Edition of Handbook of ICP-QQQ Applications using the Agilent 8800 and 8900, 5991-2802EN
- **Application note:** Routine Analysis of Fortified Foods using the Agilent 7800 ICP-MS: Simple and robust quantitative analysis of 28 elements in food digests using helium mode, 5994-0842EN
- **Application note:** Simultaneous Iodine and Bromine Speciation Analysis of Infant Formula by HPLC-ICP-MS: Determination of four halogen species in less than 6.5 minutes, 5994-0843EN
- **Application brief:** Single Cell Analysis using Agilent 7900 ICP-MS in scICP-MS Mode, 5994-0845EN
- **Case study:** Looking Far and Near: Agilent helps researcher examine the short- and long-term effects of nanoparticles, 5994-0666EN

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