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The Measure of Confidence



Agilent Technologies

New Revision of G7201A MassHunter Software for the Agilent 7700 Series ICP-MS

Ed McCurdy

ICP-MS Product Marketing,
Agilent Technologies, UK

A new revision of ICP-MS MassHunter software has been released for the 7700 Series, building on the success of the existing platform and adding many new features.

The previous revision of ICP-MS MassHunter (see Journal issue #43) has been shipping with new 7700 Series instruments since late 2010. A new revision of MassHunter for the 7700 has just been released, incorporating many new features resulting from on-going product enhancements and extensive feedback from existing users.

MassHunter Key Features

The major developments in the new revision are:

- Greater flexibility in acquisition modes and data processing
- More real-time status information displayed during autotuning and system optimization
- New user interface and enhanced functionality for chromatographic data analysis
- Support for many new Agilent LC 1200 Infinity modules

Enhanced Acquisition and Data Analysis Modes

The new revision of MassHunter adds more flexible HMI (High Matrix Introduction) for the 7700x, with pre-set plasma conditions supporting variable aerosol dilution.

The availability of user-settable sweeps per replicate (from 1 to 1000) also simplifies setup for advanced applications such as faster discrete sampling with the ISIS integrated sample introduction system (ISIS-DS).

The configuration and use of correction equations has also been enhanced significantly, with simple checkbox controls to switch on/off individual or all corrections. Simple editing of correction equations from

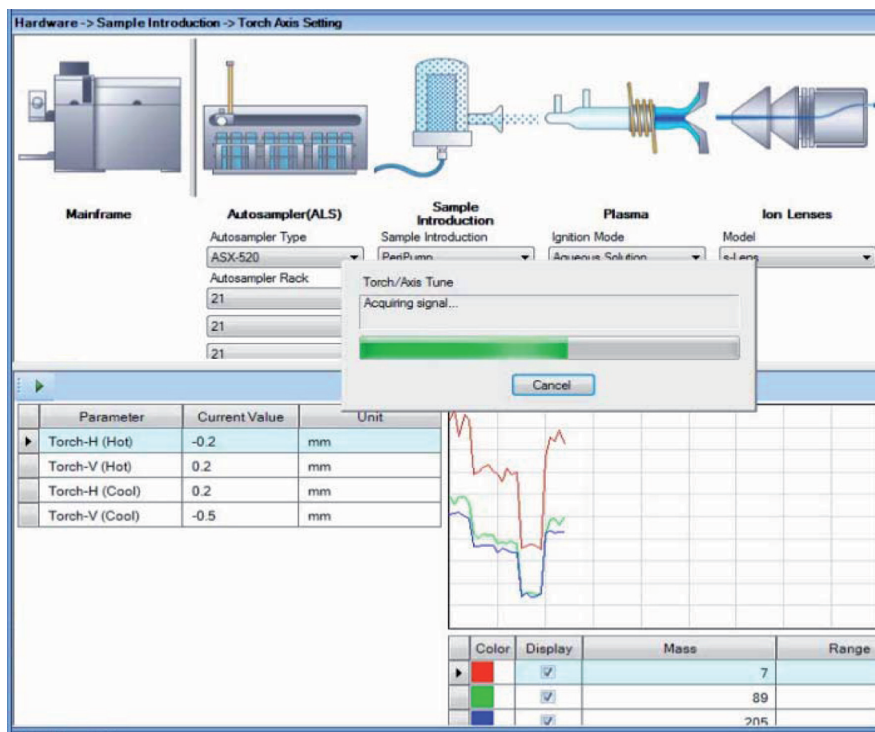


Figure 1. Auto tune Status Display

within the data analysis batch is now also supported.

Tune Status Visualization

7700 users know that the Hardware optimization and autotune algorithms work exceptionally well to deliver consistent high performance. But many users like to see the current signal and the tuning status during optimization, so in the newest revision of MassHunter we have added visualization for many common tune functions, as shown in Figure 1.

Calibration Report

ICP-MS MassHunter now includes a flexible calibration report tool, which allows a user-set page layout for calibration summary reports, and can include full details of curve fit, calculated BEC, DL, calibration standard read back, cps, RSD, etc. (below).

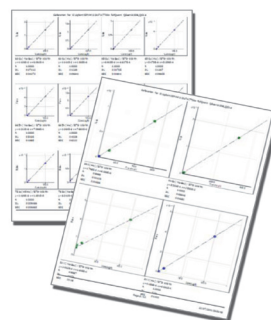


Figure 2. Flexible calibration summary printout options

Compliance

ICP-MS MassHunter G7201A integrates with a new version of Agilent's OpenLAB ECM software for compliance with regulatory requirements in pharmaceutical and other industries. In combination with the optional User Access Control module (G7207A) and OpenLab ECM, ICP-MS MassHunter (Full Version only) can provide a solution that satisfies all the regulatory requirements of 21 CFR Part 11.

Mass Profiler Professional Statistical Processing for MS Data

All MassHunter data (from ICP-MS, GC/MS and LC/MS) is compatible with Agilent's Mass Profiler Professional (MPP) data mining and statistical processing software. The MPP data export function in ICP-MS MassHunter is shown in Figure 3.

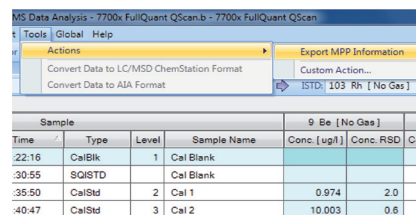


Figure 3. MPP data export

Typically used for multi element data such as MassHunter's QuickScan or semi-quant data, MPP is ideal for

applications such as food provenance and authentication, where samples can be distinguished by their trace element profiles.

Agilent 1200 Infinity LC support

The previous revision of ICP-MS MassHunter provided direct control of some Agilent LC modules, but the new revision adds support for many more LC modules, as shown below.

Agilent 1200 Infinity Modules Supported	Part Number
1200 Isocratic pump	G1310A
1260 Isocratic pump	G1310B
1200 Binary pump	G1312A
1260 Binary pump SL	G1312B
Solvent Selection Valve	G1312B, #031
Quaternary pump	G1311B
1200 standard ALS	G1329A
1260 standard ALS SL	G1329B
High performance ALS SL	G1367E
Thermostat for 1200 ALS	G1330B
Micro Degasser	G1379B
Ti-based iron-free Quaternary Pump	G5611A
Bio-Inert metal-free ALS	G5667A

Unsupported modules can still be controlled using a co-resident LC/GC ChemStation or the LC Instant Pilot.

Direct control of the LC (or GC) simplifies speciation applications with the 7700. The LC modules are configured directly from the 7700 Hardware pane (Figure 4). Method

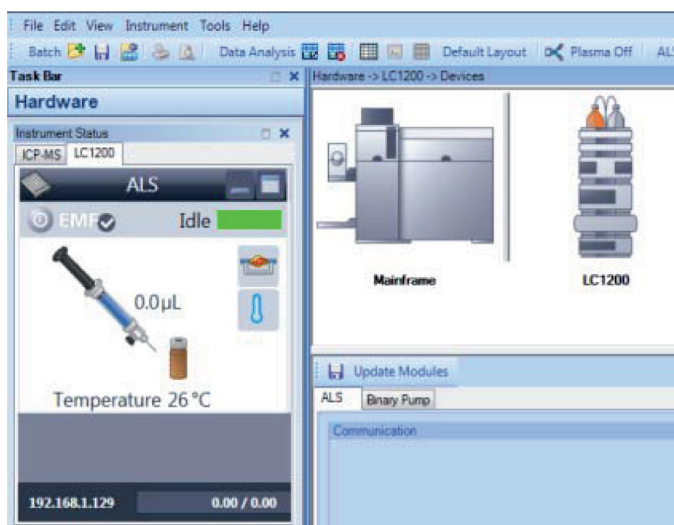


Figure 4. LC Hardware setup

settings, run control and autosampler vial position selection are all done within the ICP-MS MassHunter software, providing seamless operation of the coupled system.

Chromatographic data analysis

The new revision of ICP-MS MassHunter also adds significantly enhanced functionality in chromatographic data analysis (DA). A new Integration Parameters pane has been added to the DA Method Editor. The new pane combines the chromatogram display, the integration parameters and the peak/compound table, so all method settings can be viewed together (Figure 5).

Peaks from any chromatogram may be added to the peak list for the batch, and integration parameters can be modified for individual compounds, selected EIC masses or

applied to all peaks. The peak list can be filtered to show TIC, EIC or "All".

New peak select and integration tools are also provided, including adding chromatogram regions for peak-sum and area-sum integration. Individual named compounds within these regions can also be processed as standalone compounds.

Availability

The new revision of ICP-MS MassHunter will be shipped as standard with all new 7700 Series ICP-MS instruments from November 2011, and will be available as an upgrade for all existing 7700 Series users shortly afterwards. All existing G7201A users will be offered a free update, while 7700 Series users with earlier software revisions (G7200B) can purchase an upgrade to the new revision.

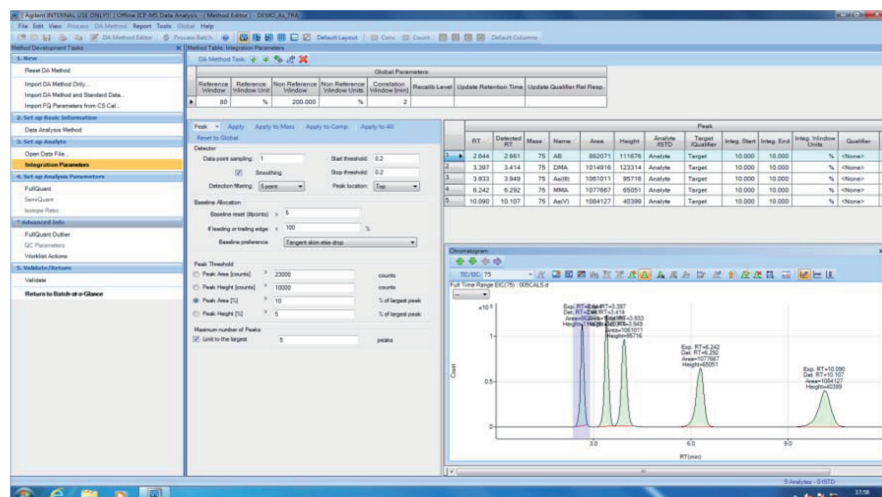


Figure 5. Chromatographic Data Analysis Method Editor screen

Enhanced Analysis of Organic Solvents using the Agilent 7700 Series ICP-MS

Ed McCurdy, Tetsuya Kanda, Kazuo Yamanaka, Yu-Hong Chen and Junichi Takahashi

Agilent Technologies

The Agilent 7700 Series ICP-MS has gained an excellent reputation for its tolerance to organic solvent samples. Now, updates to the hardware and firmware, and a new revision of ICP-MS MassHunter software, further enhance the performance of the 7700 for routine analysis of volatile organic solvents.

Organic Solvents and ICP-MS

Analysis of trace elements in organic solvents has traditionally been regarded as an application more suited to Inductively Coupled Plasma-Optical Emission Spectroscopy (ICP-OES) rather than ICP-Mass Spectrometry, and petrochemical industry methods defined by organization such as ASTM still typically recommend ICP-OES.

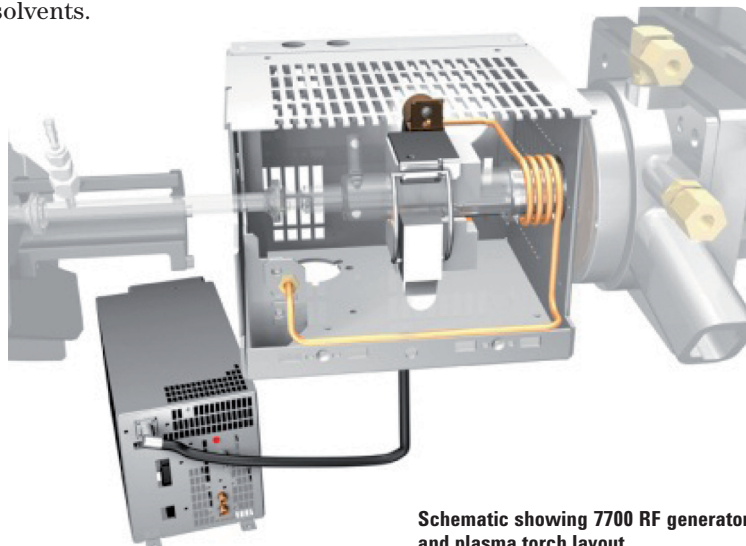
However, in many emerging applications such as semiconductor, pharmaceutical, process control and speciation (e.g. LC-ICP-MS with organic mobile phases), ICP-OES does not provide low enough detection limits for some of the elements of interest. Consequently there is increasing interest in a robust routine ICP-MS method for low level (ppb and sub-ppb) analysis of trace metals in organic solvents.

Overcoming the Challenges

The measurement of organic solvents that are not miscible with water is challenging for ICP-MS:

- Some of the standard (aqueous) sample introduction components use materials that are not tolerant of some solvents, and so must be replaced with solvent-resistant alternatives. Solvent resistant components are included in the organic solvent introduction kit for the 7700, and Pt interface cones are also available.
- Organic solvents typically have a much higher vapor pressure than aqueous solvents, which makes it difficult to light and sustain the plasma, especially at high solution flow rates (e.g. 1 mL/min). The 7700 includes a unique frequency-matching RF generator that provides excellent tolerance to solvents. A Peltier-cooled spray chamber is also standard, and chilling the chamber to -5°C helps to reduce the vapor pressure so solvents can be introduced.
- The presence of a very high level of carbon (from the solvent) and the absence of oxygen (from the lack of water) means that soot can deposit on the interface cones, leading to orifice clogging and rapid loss of sensitivity. The optional 5th gas line of the 7700 delivers a precisely controlled flow of oxygen (at 20% in argon) to the plasma, ensuring that the carbon matrix is decomposed and soot deposition doesn't occur. Pt cones must be used when O_2 is added to the plasma.

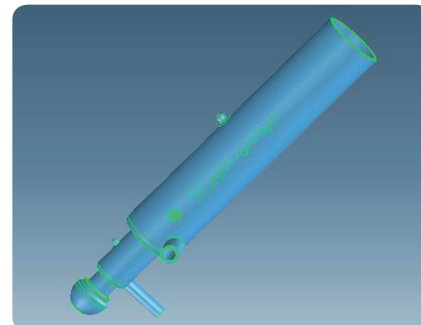
In addition, Agilent R&D and Applications Specialists have



Schematic showing 7700 RF generator and plasma torch layout

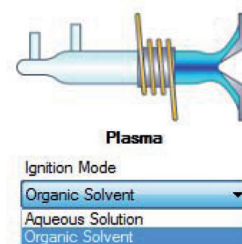
recently developed new hardware, firmware, software and analytical methodology to permit the routine analysis of highly volatile organic solvents using the Agilent 7700 Series ICP-MS.

7700 Series Plasma Torch



Previously, the 7700 has used a very narrow (1 mm internal diameter (ID)) torch for the most volatile solvents, in place of the standard 2.5 mm torch used for aqueous samples. However, the 1 mm ID torch leads to lower sensitivity and therefore poorer DLs. A new 1.5 mm ID organics torch (pictured) has now been developed for the 7700, providing higher sensitivity than the 1 mm torch while maintaining plasma tolerance to volatile solvents.

Firmware and Software



The process of igniting the plasma may seem straightforward, but organic solvents present a particular challenge. The build-up of solvent vapor in the spray chamber can affect the plasma ignition process, while the requirement to add the O_2/Ar option gas adds another ignition variable.

A new revision of MassHunter software and modified firmware in the 7700 now provides optimized flow rates and timings for the carrier, make-up and option gas parameters during the ignition sequence. This greatly increases the tolerance of the plasma to solvents and allows the plasma to be ignited reliably even with very volatile organic solvents.

Analysis of Naphtha Samples

Very volatile solvents such as petroleum ether (benzene), naphtha and acetone provide a major analytical challenge for ICP-MS, but the new developments on the 7700 now allow solvents such as these to be analyzed routinely. Typically these samples are diluted in a less-volatile solvent, to ensure that aspiration rates are not affected by variable sample viscosity. However, if samples are of a similar solvent type, it is possible to use a standard addition or matrix matched calibration and run these highly volatile solvents directly without any dilution on the 7700.

Calibrations for organic solvent analysis are typically prepared by weight from organometallic standards such as the Conostan (SCP Science, Quebec, Canada) S-21 blend of 21 elements. Many elements of interest in petrochemical applications are included in this blend, and other elements such as Hg and As are available as single element standards. The calibrations shown (Figure 1) include the elements V, Ni, As and Hg, all demonstrating low ng/kg (ppt) detection limits.

In addition to the difficulties associated with high solvent vapor pressure, the presence of high levels of carbon in the organic sample matrix leads to new polyatomic interferences that can affect some analytes, notably $^{12}\text{C}_2$ on ^{24}Mg , $^{12}\text{C}^{16}\text{O}$ on ^{28}Si and $^{40}\text{Ar}^{12}\text{C}$ on ^{52}Cr . These interferences can be reduced or removed effectively using the

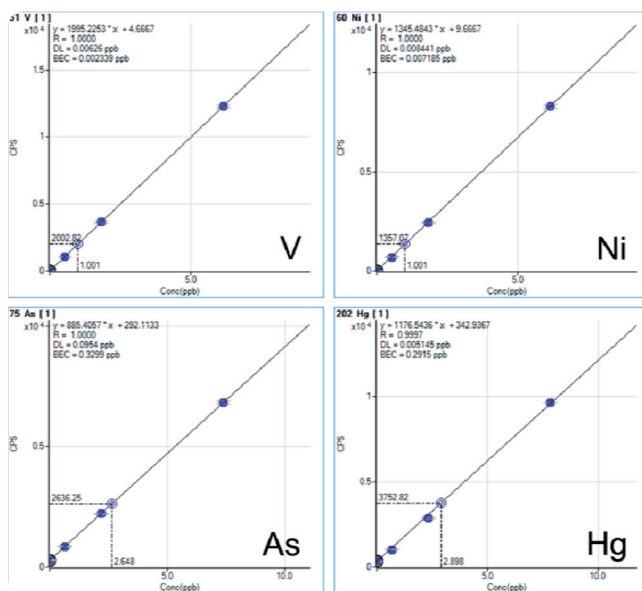


Figure 1. Calibration for V, Ni, As and Hg in naphtha, showing low ng/kg (ppt) detection limits

standard He mode of the 7700 or, for the lowest detection limits using the optional H_2 cell gas line.

The new 7700 Series torch, firmware and software revision even allow routine analysis of volatile solvents using cool plasma (7700s only), which provides a further option for reducing interferences in the highest purity semiconductor solvents.

The stability plot (Figure 2) shows the long-term signal stability (more than 1 hour) for a 1 ng/g multielement spike (S-21 plus other elements) in a naphtha sample. All elements were measured in the standard He mode, and excellent stability was achieved

for all elements, including those that can suffer from polyatomic overlaps in organic solvents (Mg and Cr).

Conclusions

The already impressive performance of the 7700 for organic solvent samples has been further enhanced through developments in torch design, updated firmware and a new revision of ICP-MS MassHunter software with modified plasma ignition parameters.

The new developments provide the 7700 with unmatched tolerance to organic solvents, allowing routine analysis of undiluted highly volatile organic solvent samples.

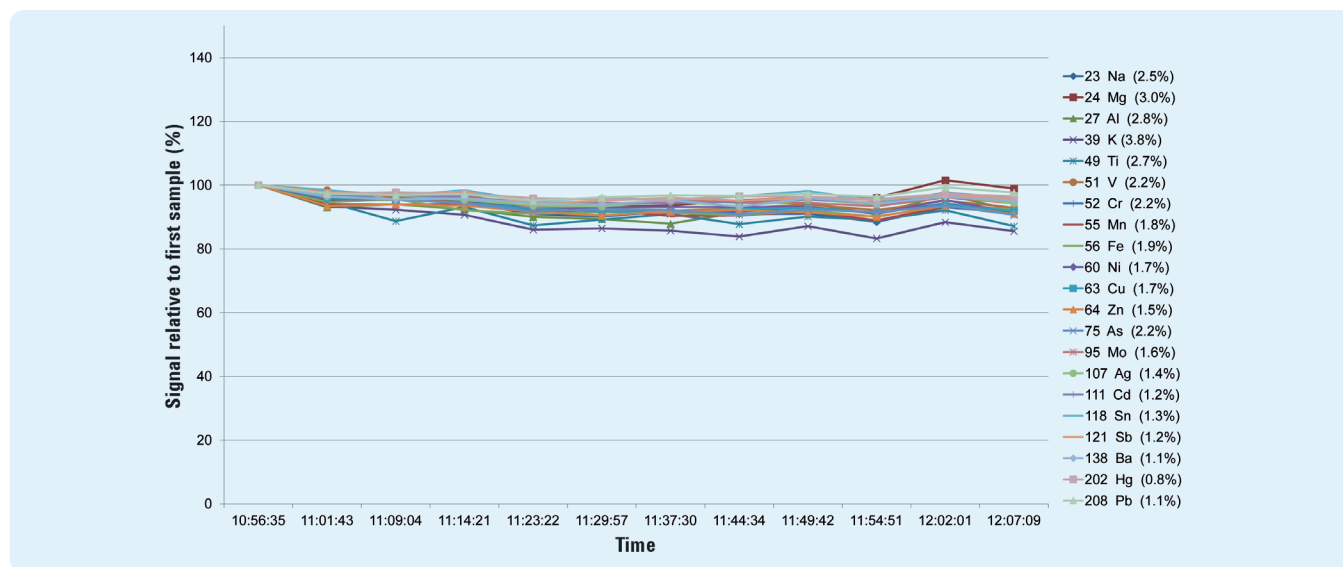


Figure 2. Long-term stability (70 mins) and %RSD of Conostan S-21 spike recovery in naphtha sample. All elements were spiked at 1 ng/g (ppb) and measured in He mode.

Agilent 4100 MP-AES Expands Agilent's Atomic Spectroscopy Portfolio

Craig Taylor and Eric Vanclay

Agilent Technologies, Australia

Microwave Plasma-Atomic Emission Spectroscopy (MP-AES) is a completely new instrumental technique for the direct, fast, sequential determination of multiple elements in aqueous and organic samples. It has been designed to improve the analytical performance and productivity when compared with flame atomic absorption spectroscopy (AAS), while decreasing operating costs by eliminating the need for flammable and expensive gases. The nitrogen based microwave plasma operates from a compressed air supply and nitrogen generator, resulting in a significant reduction in operating costs and allowing installation in mobile labs or remote locations where gas supplies may not be available, or on sites where flammable gases are not permitted due to safety concerns.

The state-of-the-art Agilent 4100 MP-AES (Figure 1) is an atomic emission instrument, so it also eliminates the need for costly consumables such as the hollow cathode lamps used in the traditional AAS techniques. MP-AES offers greater sensitivity, superior linear dynamic range, lower detection limits and faster analysis compared to conventional flame AAS, and provides a cost-effective alternative when the number of elements per



Figure 1. Agilent 4100 MP-AES

sample does not justify switching to an ICP-based technique (Figure 2).

Typical applications for MP-AES include mineral ore assays, petrochemical and chemical testing, food and beverage analysis, and feed and fertilizer monitoring.

Which Technique is Right for You?

Agilent is committed to continuous investment in atomic spectroscopy and now provides the most comprehensive and innovative range of instruments for inorganic analysis of liquid samples including: Flame AAS; Fast Sequential Flame AAS; Graphite Furnace AAS (GFAAS); Vapor Generation AAS; MP-AES; simultaneous ICP-OES and ICP-MS.

Selecting the best technique for any given application will depend on a number of factors such as the required detection limits, number of elements per sample, sample

throughput, analytes measured, linear dynamic range, regulatory compliance, and available budget but often the two main considerations are:

1. How many samples do you need to measure each day, and how many elements in each sample?

- Many samples or many elements per sample (multi-element analysis). Typically labs will use ICP-OES or ICP-MS – and now MP-AES.
- Few samples or few elements per sample (single-element analysis). Typically labs will use Flame AAS or GFAAS.

2. What detection limits do you need?

- Low detection limits (low/sub-ppb or ppt = ultra- trace level analysis). Typically labs will use GFAAS (few elements) or ICP-MS (many elements).
- High detection limits (above 1 ppb = trace, minor/major level analysis). Typically labs will use Flame AAS (few elements per sample), MP-AES (medium number of elements per sample) or ICP-OES (many elements per sample).

With the combination of traditional AAS and ICP-OES instruments, plus the remarkable 7700 Series ICP-MS and the revolutionary 4100 MP-AES that literally runs on air, Agilent now delivers robust and reliable solutions to practically any application need across a broader range of industries and geographies.

More Information

Learn more at:

www.agilent.com/chem/RunsOnAir

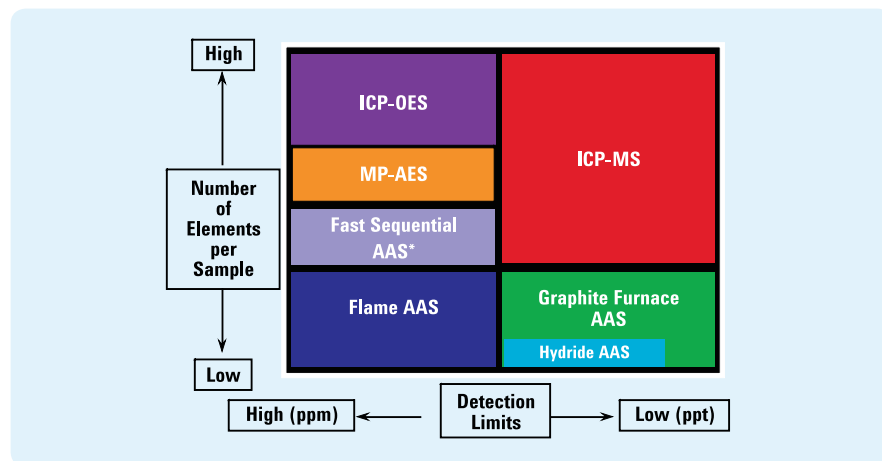


Figure 2. Number of analytes vs detection limit capability

*Note: Agilent's exclusive Fast Sequential AAS doubles sample throughput compared to conventional FAAS.

Proud Moment As 5000th Agilent ICP-MS Goes to Work in Canada

Mina Tanoshima

ICP-MS Product Marketing,
Agilent Technologies, Japan

The total number of ICP-MS systems manufactured by Agilent since the first 4500 Series instrument was sold in 1994 has now passed the major milestone of 5000 units. The 5000th unit – a 7700x – is up and running in the Environmental & Minerals Services lab of SGS Canada Inc. based in Ontario. Analyst Rob Irwin is pictured with the instrument.



SGS Canada's ICP-MS analyst Rob Irwin with the Agilent 7700x ICP-MS

SGS is a leading inspection, verification, testing and certification company that operates a network of over 1,250 offices and laboratories around the world. The Minerals Services lab provides a broad spectrum of services for the analysis of coal and coke, precious and base metals, steel and steelmaking raw materials, bio-fuels, fertilizers, cement, industrial minerals and diamonds.

SGS purchased the 7700x to strengthen their ICP-MS capacity. Initially, they plan to use the HMI capability of the 7700x to develop new methods for the determination of rare earth elements following different sample preparation procedures.

Further Information

Visit the SGS group web site at:
www.sgs.com

Agilent Malaysia Hosts Inaugural ICP-MS User Group Meeting

Steven Pang

Elemental Spectroscopy Applications Engineer,
Agilent Technologies, Malaysia



Participants enjoying the first Agilent ICP-MS User Group Meeting in Kuala Lumpur

Agilent Technologies Malaysia hosted its inaugural ICP-MS User Group Meeting at the Le Meridien Hotel, Kuala Lumpur, on August 24, 2011. Approximately 30 Agilent ICP-MS users attended this event which was opened by Agilent Malaysia Country Manager, Mr. Soh Lam Seng.

A user presentation was given by Dr. Koh Yew Ming from ALS Technichem Malaysia (ALSTM) who neatly summarized their experience with their Agilent 7500ce for ultratrace environmental analysis over the last 5 years. Perhaps his most notable remark was with over 250,000 samples processed since 2006, and very little downtime, ALSTM has no reason not to select the Agilent 7700x for their second ICP-MS system!

The guest speaker was Mr. Katsuo Mizobuchi from Agilent Technologies Japan who shared information on the determination of food provenance using Agilent's Mass Profiler Professional (MPP) software. Katsuo also provided some useful tuning tips and tricks for Agilent ICP-MS systems. Other Agilent speakers included Ms. Chow Mee Ling (Spectroscopy Product Specialist), Mr. Liew Ting Wai (Customer Engineer), and Mr. Steven Pang (Elemental Spectroscopy Applications Engineer).

Agilent ICP-MS Publications

To view and download the latest ICP-MS literature, go to www.agilent.com/chem/icpms and look under “Literature Library” and search using the title or publication number.

- **Application Note:** On-line isotope dilution analysis with the 7700 Series ICP-MS: Analysis of trace elements in high matrix samples, 5990-9171EN
- **Application Note:** Low-level speciated analysis of Cr(III) and Cr(VI) using LC(IC)-ICP-MS, 5990-9366EN
- **Application Note:** Proposed new USP general chapters <232> and <233> for elemental impurities: The application of ICP-MS for pharmaceutical analysis, 5990-9382EN
- **Application Note:** Validating the Agilent 7700x ICP-MS for the determination of elemental impurities in pharmaceutical ingredients according to draft USP general chapters <232>/<233>, 5990-9365EN
- **Technical Overview:** ICP-MS MassHunter WorkStation software (G7201A) for the Agilent 7700 Series ICP-MS, 5990-9372EN
- **Advertorial:** Regulatory Compliance for ICP-MS: Generating, Storing and Protecting Electronic Records in Regulated Laboratories, 5990-9073EN

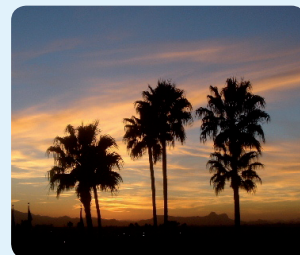
Coming soon

- **Application Note:** Simplified Drinking Water Analysis using the Agilent 7700e ICP-MS with Preset Methods
- **Application Note:** Trace elemental analysis of distilled alcoholic beverages using 7700x ICP-MS with octopole collision/reaction cell

Join Agilent Technologies at the 2012 Winter Plasma Conference

Tucson, Arizona. January 9 - 14, 2012.

Once again, Agilent has planned an exciting line up of activities that you will not want to miss:



Monday Night - stop by and visit the Agilent Booth and be among the first to see our ground-breaking new technology for interference removal in ICP-MS.

Lunch and Learn - come by our booth for an opportunity to learn about the latest developments from Agilent Technologies:

- **Monday lunch:** MP-AES Technology: A revolution in plasma emission spectroscopy that runs on air!
- **Tuesday lunch:** Agilent's latest technology for interference removal in ICP-MS: Take a closer look at the new technology we unveiled on Monday night.
- **Wednesday lunch:** Agilent's Atomic Spectroscopy Family: Learn more about the growth of the Agilent Atomic Spectroscopy portfolio.

Tuesday Night – spend the evening with Agilent at our world-famous User Meeting.

Please see the Winter Plasma Conference Program guide or visit the Agilent booth to check for specific venues for each event.

Conferences. Meetings. Seminars.

2012 Winter Conference on Plasma Spectrochemistry

January 9-14, 2012, Tucson, Arizona, USA

www.icpinformation.org

Pittcon 2012

March 11-15, 2012, Orlando, Florida, USA

www.pittcon.org

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