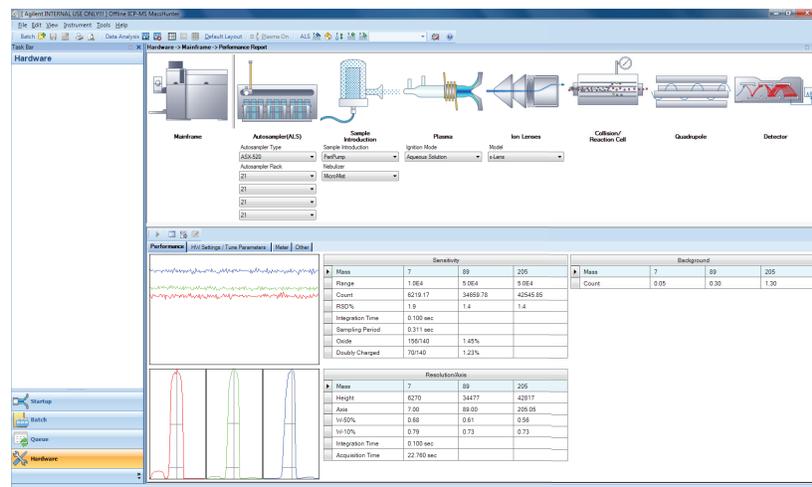


ICP-MS MassHunter WorkStation Software (G7201A) for the Agilent 7700 Series ICP-MS

Technical Overview



Introduction

Agilent's MassHunter is powerful, easy-to-learn software that provides a common platform across Agilent's LC/MS, GC/MS and ICP-MS systems. The common user interface and standard terminology simplifies the transfer of skills across the laboratory.

The latest revision of ICP-MS MassHunter software (G7201A, A.01.02) provides configuration, setup and control of the Agilent 7700 Series ICP-MS hardware and accessories, together with method setup, acquisition, data processing and reporting, all through a modern, integrated and intuitive user interface.

ICP-MS MassHunter Workstation is supplied as standard with all new 7700 Series instruments, and the new revision is available as an upgrade for all 7700 instruments already in use.

Overview

Agilent's ICP-MS MassHunter uses a familiar screen layout with a taskbar on the left and the application pane and associated toolbar icons and menu commands on the right. The software has been developed to provide simple operation in common, routine applications, while maintaining the flexibility required for advanced functionality in research use.

Many routine applications are well-defined and consistent, so acquisition parameters can be pre-defined and used repeatedly. ICP-MS MassHunter provides a range of built-in pre-set methods and autotuning functions that simplify method setup and ensure consistent operation even with multiple operators.

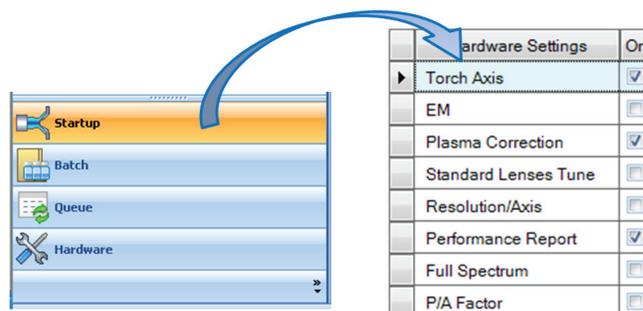
At the same time, many 7700 Series ICP-MS instruments are used for advanced applications, where flexibility is necessary and specialized functionality may be needed to suit individual requirements.

ICP-MS MassHunter is supplied as a "Core" version (included with the 7700e instrument), which provides a simplified user interface and streamlined operation for common, routine and well-defined applications. An upgrade to the "Full" version is available. The "Full" version supplied with the 7700x and 7700s models delivers high levels of flexibility and advanced functionality, and can be upgraded with optional software modules.

Startup and hardware optimization

Both "Core" and "Full" versions of ICP-MS MassHunter provide full control of the 7700 Series ICP-MS, including automated Startup and optimization, and automated, unattended system shutdown at the end of a sequence.

Startup provides a simple, user-configured schedule of system optimization and performance checks to be run following plasma ignition. A pre-defined warmup period and standard operating conditions deliver a consistent record of system performance.



Startup is particularly useful in busy commercial laboratories, as it ensures that performance is optimized consistently from day to day, and is independent of operator experience.

Startup tasks such as Torch Axis (horizontal and vertical alignment with the interface) and Plasma Correction can be followed by generation of a Performance Report, which gives a continuing record of system performance.

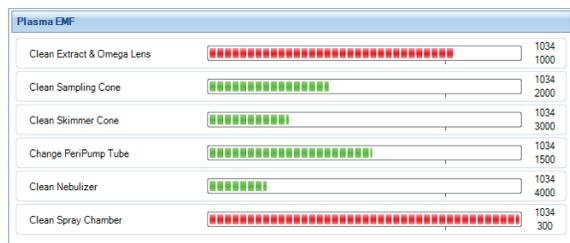
The Performance Report provides a graphical display of key system performance parameters (sensitivity, oxides, background, mass calibration and resolution). The report also includes a History view, which allows users to monitor the daily performance over time. In addition to this daily performance check, the Performance Report saves all the current tune and meter values, giving a complete record of system settings.

The Hardware pane contains a graphic of the main instrument components, providing the user interface for all hardware-related functions including:

- System configuration and communication
- Hardware optimization
- Maintenance tasks such as leak checks
- Early Maintenance Feedback (EMF)
- Diagnostics
- Performance Reports

The instrument graphic updates automatically when different system introduction hardware (alternative autosampler or LC or GC modules) is selected.

Pre-defined Early Maintenance Feedback (EMF) checks are included, providing a flexible monitor of system running time. All major maintenance items are monitored as standard, and additional user-settable maintenance flags can be defined.



A built-in maintenance log allows users to record routine maintenance actions for lab management and audit purposes; full system error logging is included, with a plain text log of all errors. Remote diagnostic capability is available, and simple archive and restore functions provide easy access to system data for support investigation.

Using a single user interface for all system setup, maintenance and diagnostic functions ensures that users have all the information on system operation easily available at all times.

Batch

The Batch pane (below) brings together all the information required for a sample analysis session or experiment, including peripump program, tune modes, acquisition masses, integration times, sample list, and data analysis (calibration) parameters. All these parameters are saved in the Batch and can be recalled for use in subsequent sample analyses.

The Batch concept is a major innovation of the ICP-MS MassHunter platform, as it simplifies file management and ensures that consistent conditions can be used for regular or routine sample analysis. A periodic table interface (below) allows users to easily select analytes and internal standard masses. A user-editable database pre-defines the preferred isotope for each analyte, and the prohibited masses for each tune mode, simplifying method setup.

Complete flexibility is provided for the user to select any analyte or isotope to be acquired in any tune step or gas mode. Each analyte can be acquired in multiple tune steps for method development, and tune steps may be run in any order, with a user-settable stabilization time between each step.

Mass	Element Name	Monitor	Integ Time (Sec)	Integ Time (Mass (Sec))
7	Li	<input checked="" type="checkbox"/>	0.30	N/A
9	Be	<input checked="" type="checkbox"/>	0.30	N/A
27	Al	<input checked="" type="checkbox"/>	0.30	N/A
51	V	<input checked="" type="checkbox"/>	0.30	N/A
52	Cr	<input type="checkbox"/>	N/A	N/A
53	Cr	<input type="checkbox"/>	N/A	N/A
54	Fe	<input type="checkbox"/>	N/A	N/A
55	Mn	<input type="checkbox"/>	N/A	N/A
56	Fe	<input type="checkbox"/>	N/A	N/A
59	Co	<input type="checkbox"/>	N/A	N/A
60	Ni	<input type="checkbox"/>	N/A	N/A
63	Cu	<input type="checkbox"/>	N/A	N/A
66	Zn	<input type="checkbox"/>	N/A	N/A
75	As	<input type="checkbox"/>	N/A	N/A
77	Se	<input type="checkbox"/>	N/A	N/A
78	Se	<input type="checkbox"/>	N/A	N/A
111	Cd	<input type="checkbox"/>	0.30	N/A
205	Tl	<input checked="" type="checkbox"/>	0.30	N/A
208	Pb	<input type="checkbox"/>	0.30	N/A
238	U	<input type="checkbox"/>	0.30	N/A

Data acquisition parameters

Both versions of ICP-MS MassHunter provide a range of data acquisition modes:

- Single mass monitoring
- Peak jumping
- Scanning
- Segmented scanning

The number of sweeps per replicate (variable from 1 to 1000), number of replicates per sample, peak pattern and integration times are all user-settable, allowing full flexibility for spectrum (peak profile view) analysis. Acquisition times can be optimized for quantitative, fast discrete sampling, semi-quant, and ratio (“Full” version only) acquisitions.

A Quick Scan acquisition (MassHunter “Full” version only) can be selected to run for any tune step, giving a rapid screen for each sample, in addition to the main quantitative or isotope analysis measurement.

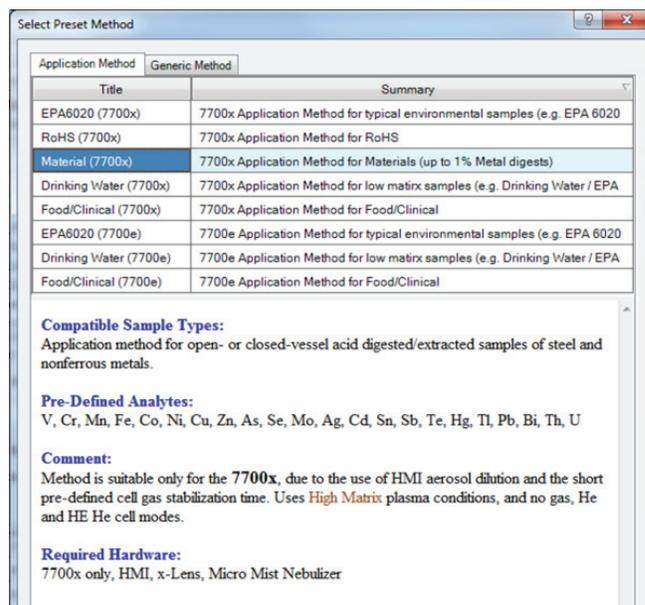
MassHunter “Full” version also provides flexible Time Resolved Analysis (TRA), with user-set acquisition and tune conditions for each time program step.

Pre-Set Methods

A new Batch can be created from a blank template, an existing Batch, or one of several instrument-specific Pre-Set Methods that ship with the software.

Pre-Set Methods pre-define all critical parameters for many typical applications, with appropriate methods provided for each 7700 Series model. In addition to the analyte list, integration times and cell gas modes, the Pre-set Methods define the default values and tuning ranges for the autotune parameters, ensuring that the system is perfectly optimized every time for the chosen application’s target sample type.

A unique feature of Pre-Set Methods on the 7700 is the use of Pre-Set Plasma conditions, which allow plasma settings for different sample types to be pre-selected and used repeatedly, based on a “plasma map”, which is automatically calibrated for each instrument. This ensures consistent operation for a particular instrument,



and is also essential to allow the autotuned plasma conditions to be replicated accurately across all 7700 instruments.

Tuning

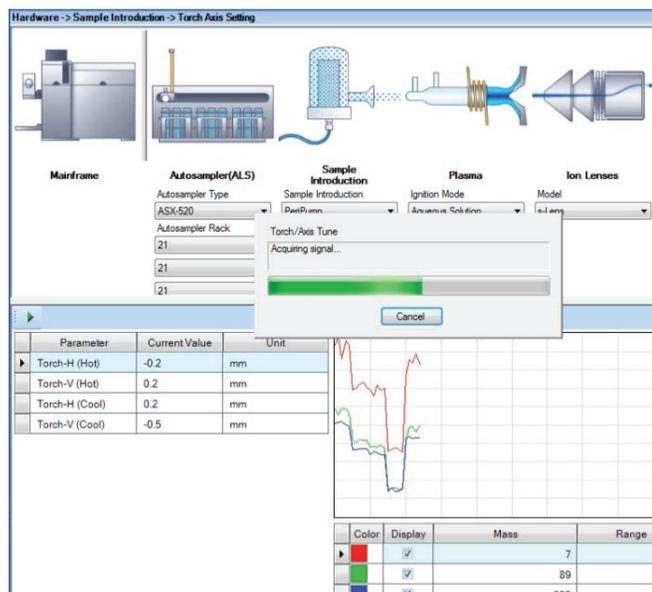
The typical mode of operation for routine applications uses sophisticated autotune functions to optimize the 7700 system reliably for the selected application.

Expert Autotuning simplifies system optimization to ensure consistent and reproducible performance from day to day, even with multiple operators.

In non-standard or less routine applications where specific tuning requirements are not provided within the Pre-Set Methods and autotune framework, manual tuning may be preferred. ICP-MS MassHunter (“Full” version) provides a flexible tuning setup pane that allows full manual control of all parameters or subsets of parameters. This includes the settings normally adjusted automatically using Hardware optimization, such as quadrupole and electron multiplier (EM) voltages. Users can choose which parameters are displayed and which should be applied to all tune steps (Batch-wide Parameters).

A batch-specific Tune Report can be viewed or generated at any time, or run automatically as part of a Batch acquisition.

During system optimization, the system status and current signal display indicate autotune progress.



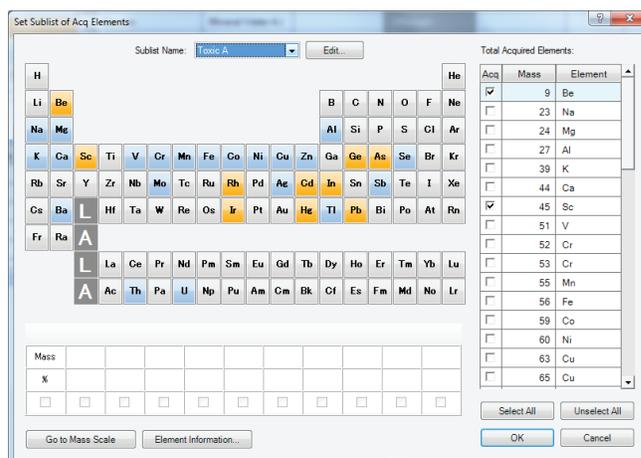
Sample list

The Batch also contains the sample list or sequence, allowing the sample list template to be saved and reused easily for subsequent sample batches, for example by importing a new sample list from a LIMS.

Sample list controls include flexible dilution factor calculation (for example, based on imported wt/vol values), variable numbers of replicates per sample, autosampler vial selection for integrated accessories (such as Agilent LC and GC systems) and common edit functions including cut/paste, copy, insert, fill down, and skip samples. Autosampler vial positions may be entered manually, pasted or imported from a CSV file, or selected from an intuitive autosampler vial map that updates automatically according to the current instrument configuration.

Sublists can be defined, to customize the acquisition for individual samples or groups of samples. Sublists allow the acquired analytes to be modified while retaining the global calibration for the batch. This means that several different sample types or acquisition methods can be measured in a single batch, against a single global calibration.

In the screenshot below, the selected sublist (Toxic A) contains only the analytes highlighted in orange, while the full element suite (all elements selected in the batch) also includes those elements in blue.



Full access to the sample list is retained while the sequence is running, allowing the current sequence to be paused for editing, for example to add a rush sample or change the order of samples awaiting analysis.

The user can choose at which point the current batch is paused. For example, the sequence can be set to pause after the calibration block so the calibration can be checked before continuing the sequence.

Data analysis (calibration) setup

As well as the settings required for sample acquisition, the Batch contains the calibration information, allowing real-time calculation of results as each sample is acquired.

The calibration table can be imported from an existing batch, so the same calibration standard levels can easily be re-used for different sample batches. Advanced functions are provided, such as user-selectable minimum reporting levels, built-in or user-entered reporting units, and flexible internal standard and calibration curve fit selection.

Setup of the calibration is simplified with shortcut tools such as copy/paste, fill-down, fill across and "Multiply Conc". This function allows the calibration table to be filled in automatically, based on a single standard level.

Queue

The Queue pane is divided into three sections (below). The top section contains the interactive Queue or schedule, which lists all the Hardware tasks (such as the performance checks run during Startup) and Batches awaiting analysis. The scheduled tasks and Batches waiting in the Queue list can be moved, edited or deleted, allowing full flexibility to control the analysis.

The lower section is divided into the interactive Sample List for the current Batch, and the real-time display showing the signal during acquisition of the current sample.

The real-time display view also includes a Monitor function, which displays the signals for several user-selected masses in the period between acquisitions. As well as a visual rinse monitor, this provides an indication that the next sample has reached a steady signal before acquisition.

In TRA acquisitions ("Full" version only) the real-time display includes a Snapshot function to transfer the current sample acquisition data to the Data Analysis pane for processing while the acquisition completes.

The screenshot displays three main windows from a chromatography software interface:

- Queue Window:** Shows a list of tasks with columns for Task Name, Status, Calibration Inport, Start Time, End Time, Start Line, End Line, and Current Line.

Task Name	Status	Calibration Inport	Start Time	End Time	Start Line	End Line	Current Line
HW Settings: Torch Axis	Succeeded		5/13/2010 9:29 AM	5/13/2010 9:30 AM			
HW Settings: Plasma Correction	Succeeded		5/13/2010 9:34 AM	5/13/2010 9:36 AM			
Performance Report	Succeeded		5/13/2010 9:39 AM	5/13/2010 9:43 AM			
Water	In Process		5/13/2010 5:30 PM		Calibrati	Unkno	Calibration
- Sample List Window:** Shows the current batch's acquisition order and calibration standards.

Sequence Flow	Sample Type	Sample Name	Comment
1	CalBlk	Calib Blank	1
2	CalStd	Calib 10ppb	1
3	CalStd	Calib 5ppb	1
4	CalStd	Calib 10ppb	1
5	Sample	Rinse	1
6	Sample	Extra rinse	1
- Real Time Display - Water b Window:** Shows a chromatogram plot of signal intensity versus Time [min]. Below the plot is a table of monitored masses.

Color	Display	Mass	Range	Count	Avg Count	RSD [%]
Red	<input checked="" type="checkbox"/>	TIC	5.0E6	3446473	932665	80.6
Orange	<input checked="" type="checkbox"/>	7	1.0E6	531954	282239	88.0
Green	<input checked="" type="checkbox"/>	27	1.0E6	599934	333605	80.6
Blue	<input checked="" type="checkbox"/>	205	1.0E6	538416	316819	79.2

Data analysis

Data Batch view

After each sample acquisition is completed, the results are automatically displayed in a Data Batch view, which has a flexible, user-selectable table format illustrated below.

The Data Batch table is updated in real-time during sequence analysis, and the display includes the sample header information, sample data (counts, concentration, SD, %RSD), internal standard counts and recovery, LabQC recovery, calibration plots (either summary or detail) and outlier flags. Outliers can be user-configured and the data can easily be filtered based on outlier flag status.

The batch table is interactive, allowing users to move up and down the table to display the current sample spectrum/chromatogram, the internal standard recovery for the current sample, and the calibration curve for the current analyte.

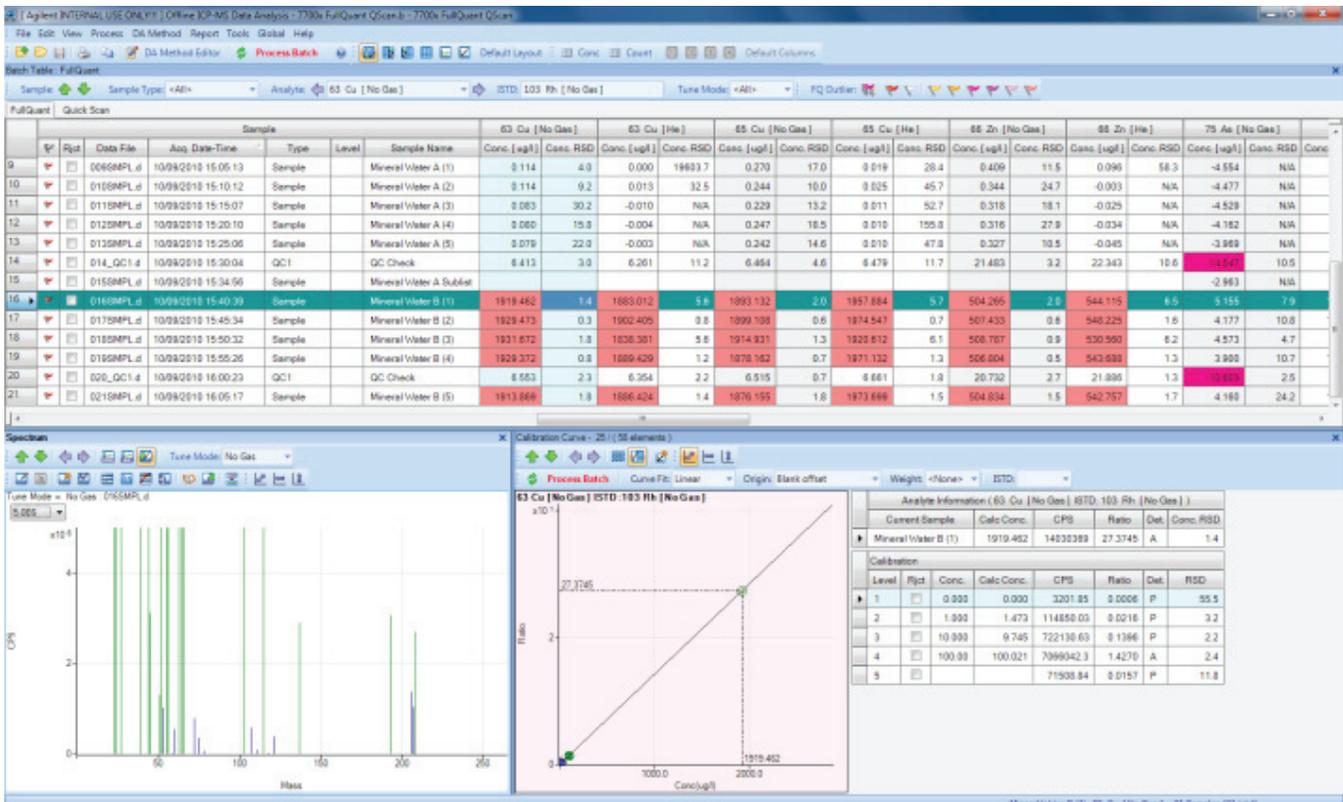
Calibration

Data acquired using MassHunter is available for processing using any data analysis mode. For example, data acquired for quantitative analysis may also be processed using isotope ratio analysis*, or semi-quantitative calibration, to give approximate concentrations for uncalibrated elements. The calibration method may be changed and the data reprocessed at any time during or post-acquisition.

Calibration modes include external calibration, method of standard additions, semi-quantitative calibration, isotope ratio*, and Isotope Dilution (IDMS)*.

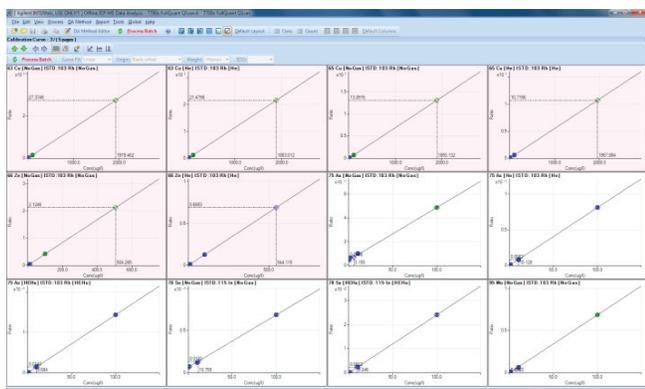
Calibration curve fit options include linear, linear through zero, linear through the blank, weighted least squares, log and second order.

* "Full" version only.



Users have full flexibility to change the curve fit, exclude individual points, change internal standards or switch internal standard correction on or off. The curve is updated immediately and any changes are easily applied to all samples in the batch.

Recalibrations during the sequence are applied automatically to the samples run after the recalibration, including converting standard addition to external calibration, isotope ratio mass bias correction, and semi-quantitative calibration.



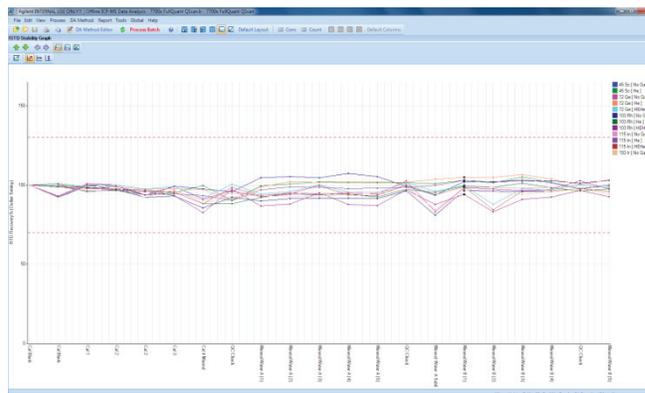
Calibration curves can be shown as a summary (12 plots, shown above), or as individual plots. Elements with an outlier flag for the current sample are also highlighted (red shading) in the calibration plots.

Full curve statistics are available, including counts for each point, calibration recovery (read-back), background equivalent concentration (BEC) and detection limit (DL).

The concentration of the currently selected sample is shown on the calibration plot and the displayed concentration updates for the current sample as the user scrolls through the Data Batch table.

Internal standard recoveries

The lower left section of the data analysis pane contains the graphical display, which is typically either the current sample spectrum/chromatogram or the internal standard (ISTD) recovery plot. The internal standard recovery plot is also linked to the batch table, so the ISTDs for the currently selected sample are highlighted on the plot (shown in the next figure).

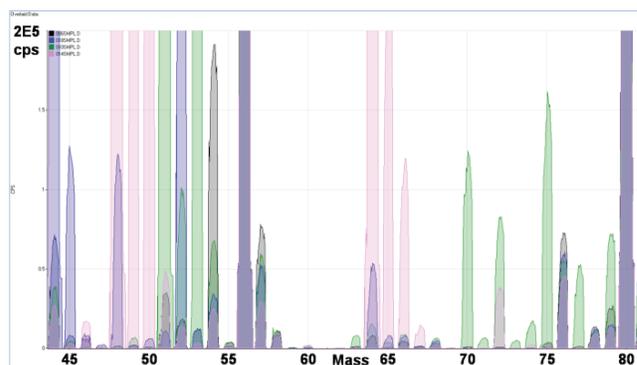


Spectrum analysis

Simple spectra are one of the most beneficial characteristics of ICP-MS, especially when combined with interference removal using helium (He) mode.

The spectrum analysis tools in ICP-MS MassHunter provide an ideal interface to view and interpret these simple spectra. Advanced tools include:

- Full control of scale, log/linear, zoom and scroll functions for the displayed spectrum.
- Unlimited isotopic templates displayed on the spectrum, with automatic recalculation of the templates for the current sample, as the user scrolls up and down the Data Batch table.
- Data comparison, using overlays of the spectra for different tune steps/modes from the same sample, or of different samples. In the example below, the background peaks in several different sample matrices are shown in different colors on the overlaid spectrum (all in no gas mode).



A major enhancement in the latest revision of ICP-MS MassHunter is the integrated chromatographic data analysis method setup pane (below).

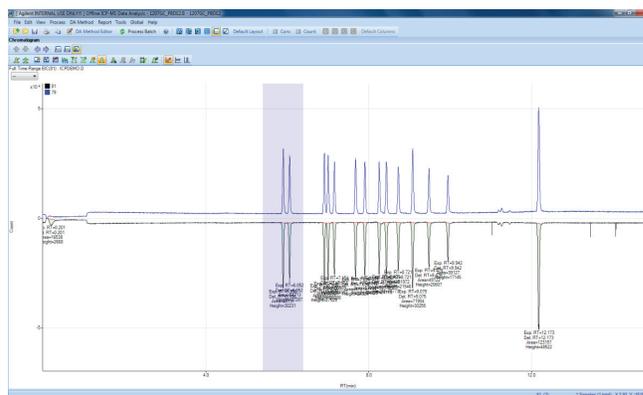
The method setup pane now includes a batch-wide peak/compound list, an interactive table which links seamlessly to the sample chromatograms in the batch. Integration can be based on the total ion chromatogram (TIC) or individual extracted ion chromatograms (EICs), and integration parameters can be applied globally, per mass, or per compound.

The new integration parameter pane provides full chromatographic method functionality, including advanced peak detection, baseline allocation and threshold controls to ensure that peaks are detected reliably, even for the variable peak shapes that are common in many chromatographic applications.

Integration window start and end points can be adjusted to ensure that compounds remain correctly identified if retention times shift during the analysis.

An "Auto-Review" function is included in the Integration Parameter setup pane, to scroll through the samples allowing the user to check that all peaks were detected correctly. A similar function is provided in the Batch data table.

Chromatogram display options provided in ICP-MS MassHunter include blank subtraction, signal-to-noise calculation, chromatogram overlay and invert (illustrated below).



The screenshot shows the software interface with the 'Method Table: Integration Parameters' pane open. The pane is divided into several sections: Global Parameters, Peak detection settings, Baseline Allocation, and Peak Thresholds. A table below the pane lists the detected peaks with their retention times, masses, names, areas, heights, and integration parameters.

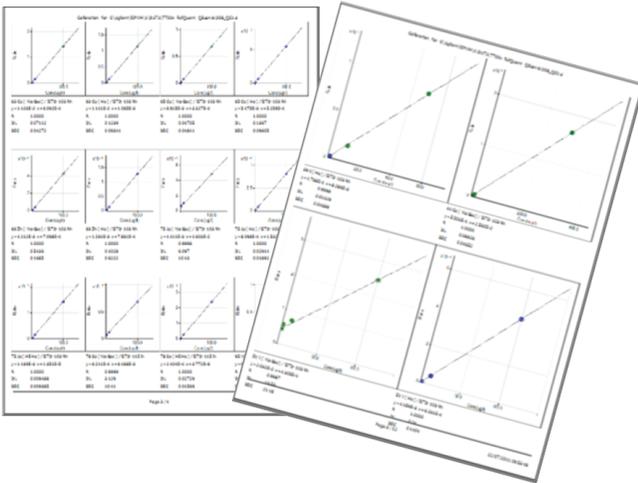
RT	Detected RT	Mass	Name	Area	Height	Analyte /STD	Target /Qualifier	Integ. Start	Integ. End	Integ. Window Units	Qualif	
1	1.798	4.518	1.798-4.518	75	771933	96171	Analyte	Target	1.798	4.518	%	<None>
2	2.644	2.644	75	AB	345515	45378	Analyte	Target	10.000	10.000	%	<None>
3	3.397	3.397	75	DMA	414105	50327	Analyte	Target	10.000	10.000	%	<None>
4	3.933	3.933	75	As(III)	431256	39083	Analyte	Target	10.000	10.000	%	<None>
5	6.242	6.258	75	MMA	440612	26719	Analyte	Target	10.000	10.000	%	<None>
6	10.090	10.107	75	As(V)	441477	16458	Analyte	Target	10.000	10.000	%	<None>

The 'Chromatogram' window shows a Total Ion Chromatogram (TIC) with several peaks. The peak at 6.242 minutes is highlighted, and its integration parameters are displayed: RT(Expected)=6.242, RT(Detected)=6.288, Area=440612, Height=26719. Other peaks are also labeled with their respective parameters.

Reporting

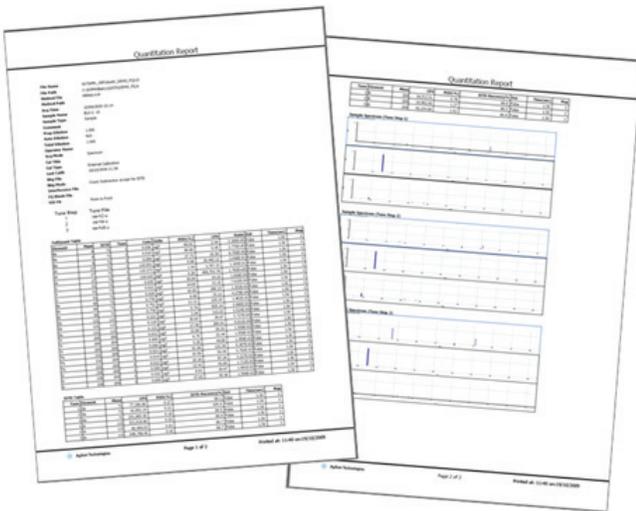
Calibration report

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



Flexible results report format

MassHunter also includes a flexible, user-configurable report layout for sample results. Built-in reports include quant, semi-quant and isotope ratio reports for individual samples, and a flexible quick batch report for full or selected batch table data.

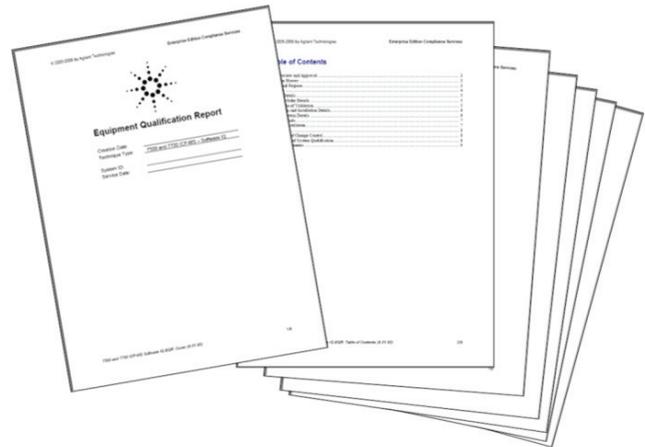


In addition to printed reports, the sample data and batch table are compatible with electronic reporting, with direct export to Microsoft® Excel (supplied), and file formats such as .csv and .txt providing simple connection to LIMS and other electronic report packages.

Compliance

Software qualification

Validation tools for installation qualification (IQ) and operation qualification (OQ) are available for both versions of ICP-MS MassHunter, providing full documentation for audit purposes.



21 CFR Part 11

In combination with the optional User Access Control module (G7207A) and Agilent's OpenLab ECM software, ICP-MS MassHunter ("Full" version) can provide a solution that satisfies all the regulatory requirements of 21 CFR Part 11.



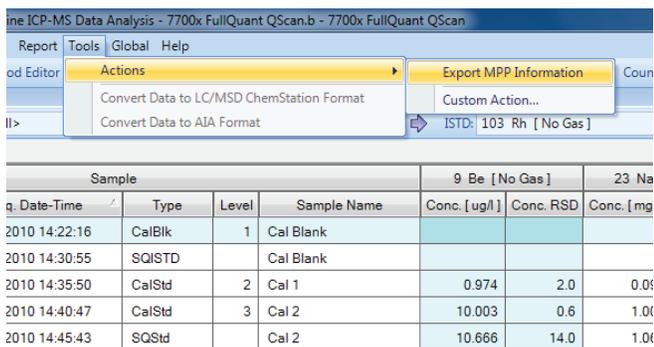
OpenLAB

CAPTURE • ANALYZE • SHARE

Mass Profiler Professional

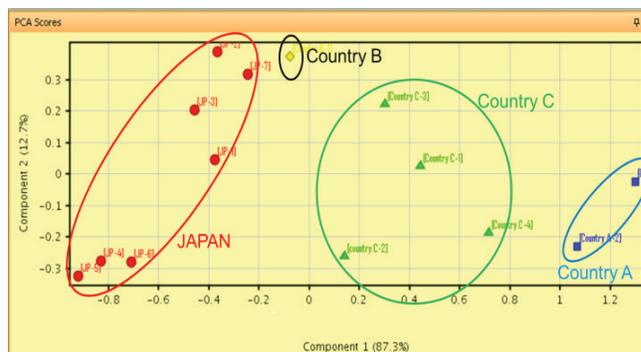
Statistical processing for MS data

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. MPP includes support for ICP-MS MassHunter's quantitative and QuickScan data formats, simplifying data transfer.



Sample							9 Be [No Gas]	23 Na
q. Date-Time	Type	Level	Sample Name	Conc. [ug/l]	Conc. RSD	Conc. [mg		
2010 14:22:16	CalBlk	1	Cal Blank					
2010 14:30:55	SQISTD		Cal Blank					
2010 14:35:50	CalStd	2	Cal 1	0.974	2.0	0.00		
2010 14:40:47	CalStd	3	Cal 2	10.003	0.6	1.00		
2010 14:45:43	SQStd		Cal 2	10.666	14.0	1.00		

The MPP data export function is shown in the previous figure, and below is an example of a PCA (principle component analysis) plot showing the geographical origin of rice samples distinguished by their trace element profiles.



Conclusions

The new revision of ICP-MS MassHunter software (G7201A, A.01.02) provides many ease-of-use, functionality and productivity benefits for Agilent 7700 Series users. It is supplied as standard with all new 7700 Series instruments, and is also available as an upgrade for all 7700 instruments already in use.

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