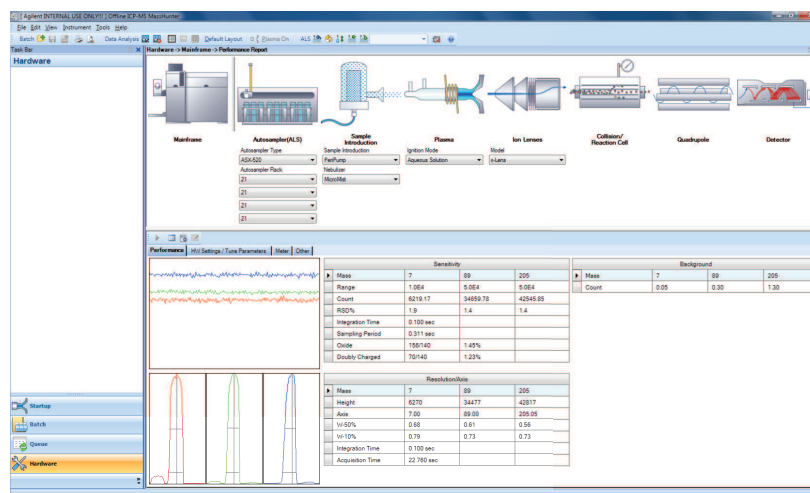# ICP-MS MassHunter WorkStation Software (G7201A) for the Agilent 7700 Series ICP-MS

## 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.

**Agilent Technologies**

## 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.
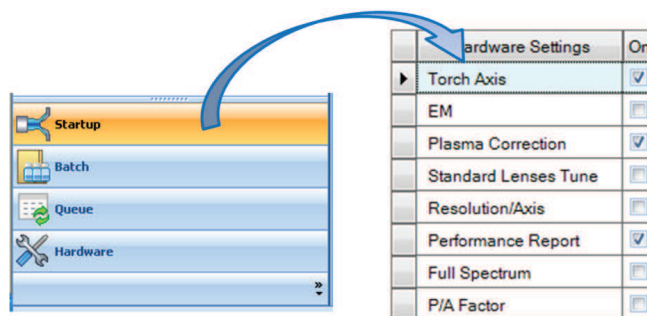


Startup is particularly useful in busy commercial laboratories, as it ensures that performance is optimized consistently from day to day, and is independent of operator experience.

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.
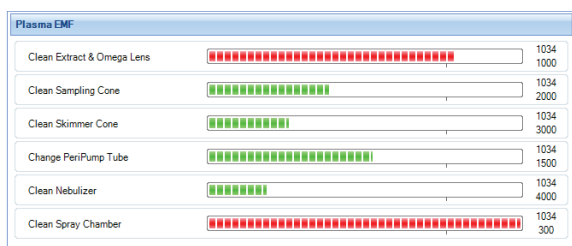


A built-in maintenance log allows users to record routine maintenance actions for lab management and audit purposes; full system error logging is included, with a plain text log of all errors. Remote diagnostic capability is available, and simple archive and restore functions provide easy access to system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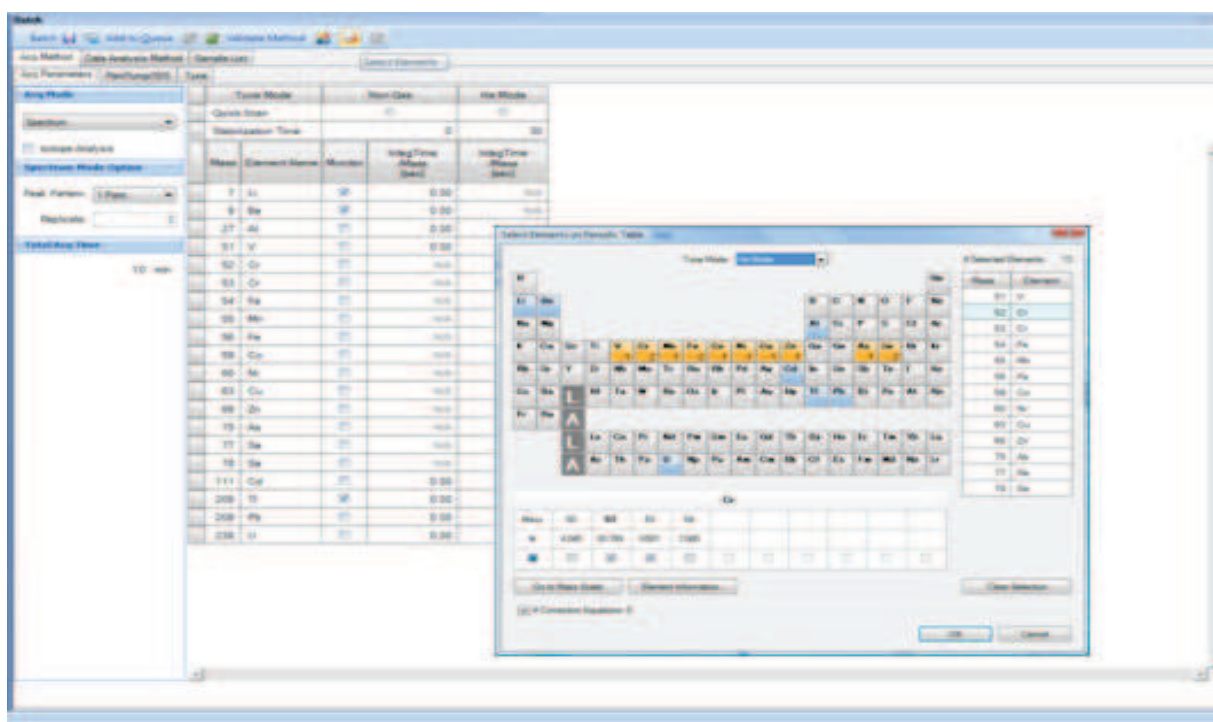
**Data acquisition parameters**

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,
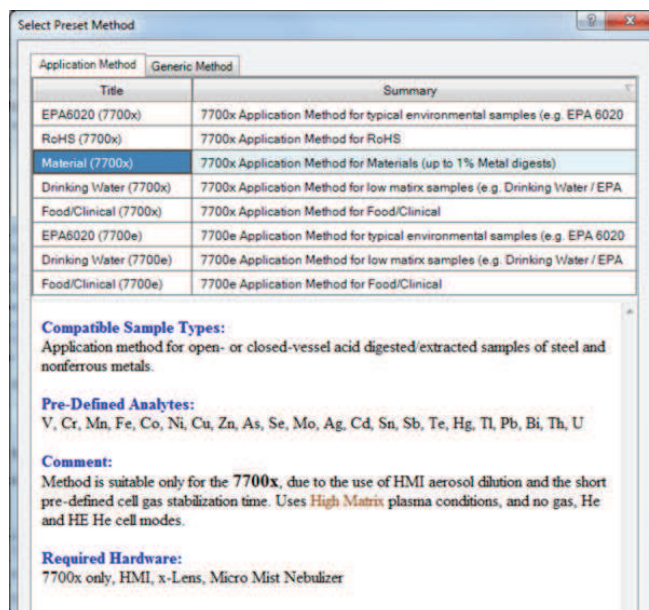


and is also essential to allow the autotuned plasma conditions to be replicated accurately across all 7700 instruments.

**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.

4

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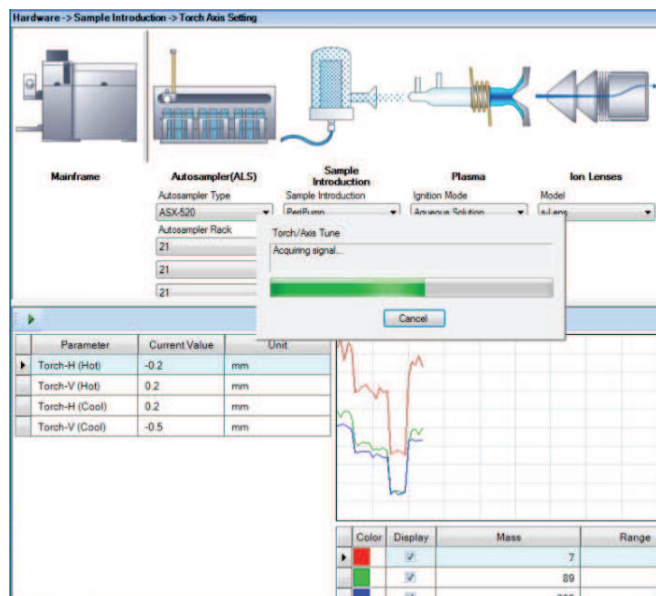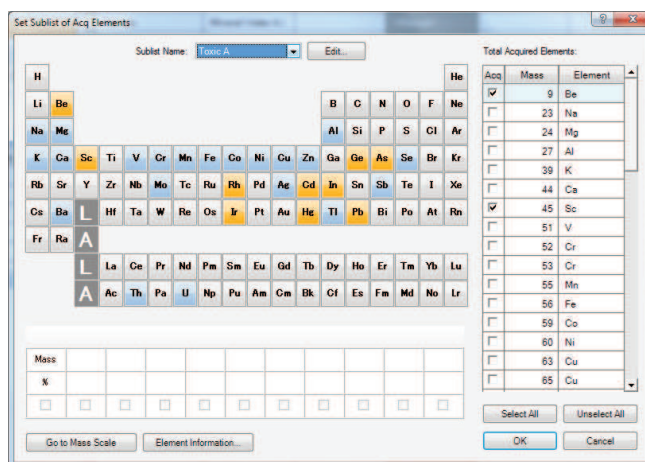


### Sample list
The Batch also contains the sample list or sequence, allowing the sample list template to be saved and reused easily for subsequent sample batches, for example by importing a new sample list from a LIMS.

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.
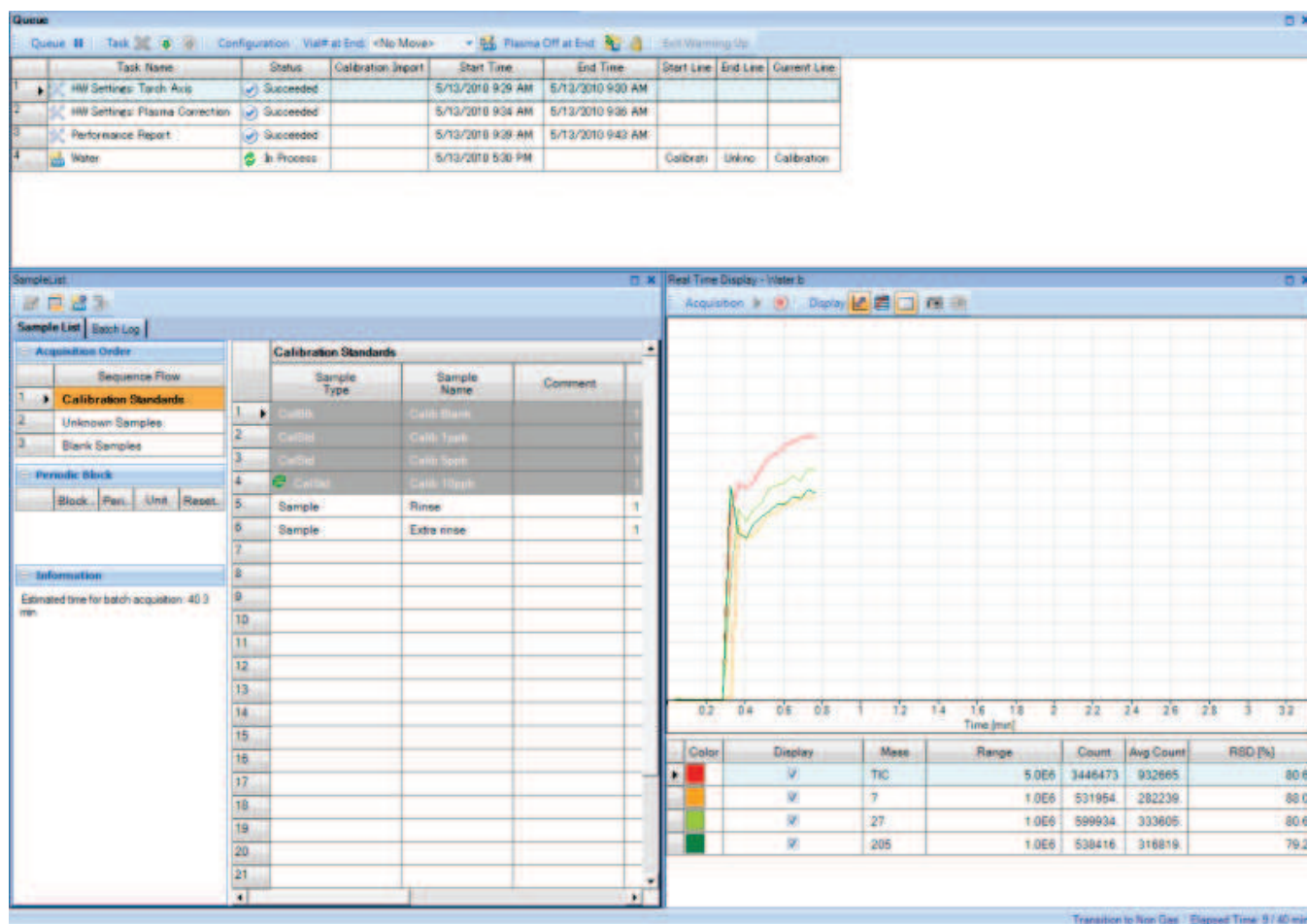
## Data analysis

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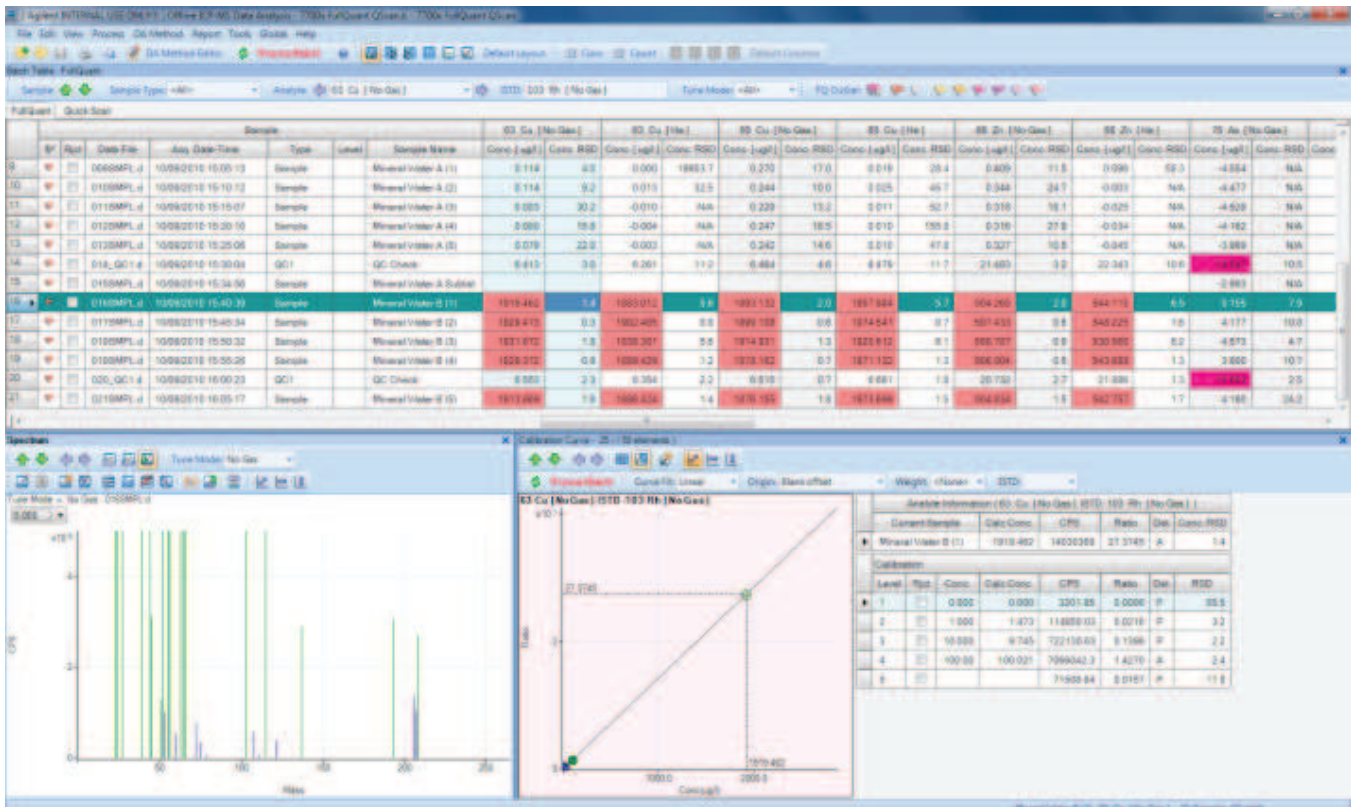
Users have full flexibility to change the curve fit, exclude individual points, change internal standards or switch internal standard correction on or off. The curve is updated immediately and any changes are easily applied to all samples in the batch.

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.
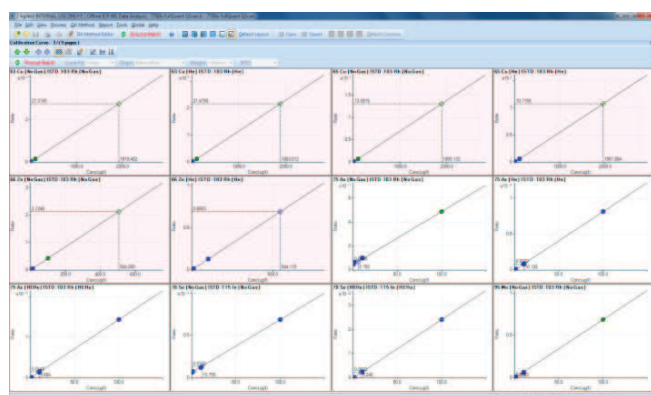


Calibration curves can be shown as a summary (12 plots, shown above), or as individual plots. Elements with an outlier flag for the current sample are also highlighted (red shading) in the calibration plots.

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).
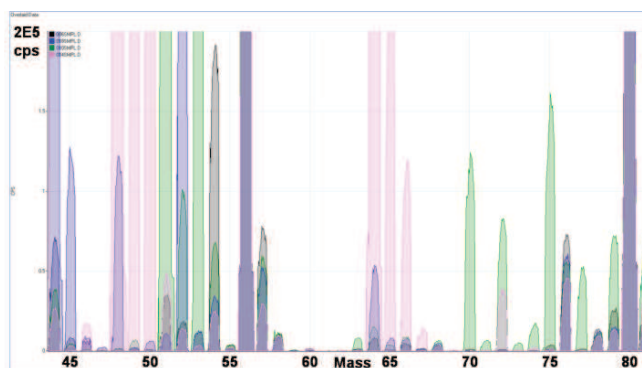
## QuickScan acquisition ("Full" version only)

Rapid screening acquisitions are a particularly valuable tool for 7700 users, as the spectrum in the normal He mode is essentially free from polyatomic interferences.
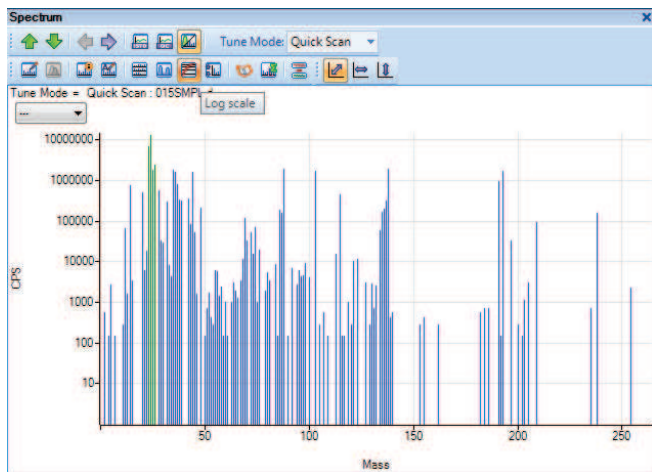


A QuickScan acquisition can be added to any tune step of a spectrum acquisition, to give semi-quantitative concentrations for all elements.

# Chromatographic Analysis with ICP-MS

The optional Chromatographic Analysis module (available for the "Full" version only) supports a range of hyphenated 'speciation' analysis with ICP-MS. In addition to data processing for ICP-MS chromatographic data, direct hardware setup and run control for many common Agilent LC and GC modules is provided from within the ICP-MS MassHunter software (below).
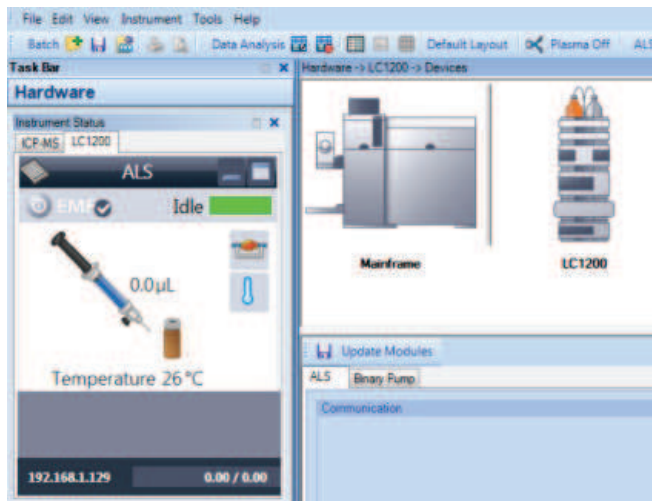


Advanced chromatographic functions include:

- Direct setup and run control for common Agilent 7890 GC and 1200 Infinity LC modules (see Specifications for full list of supported modules)

- Point-to-point ISTD correction

- Retention time recalibration

- Snapshot data analysis of current sample

- Integrated method integration parameter setup

- Batch-wide peak/compound list

- Peak-sum and area-sum integration

- Integration per compound using user-selectable integration parameters

- Compound-independent calibration (CIC)

- Signal-to-Noise calculation

## Data analysis for chromatography

Chromatographic data analysis in ICP-MS MassHunter uses the same interactive data table format as spectrum data (below). The current chromatogram is displayed and updated as the user scrolls through the sample list, and outlier functions and calibration options are provided as for spectrum mode.
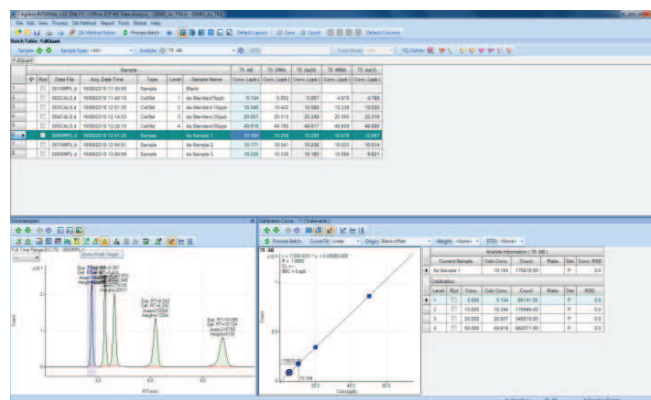
A major enhancement in the latest revision of ICP-MS MassHunter is the integrated chromatographic data analysis method setup pane (below).

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).
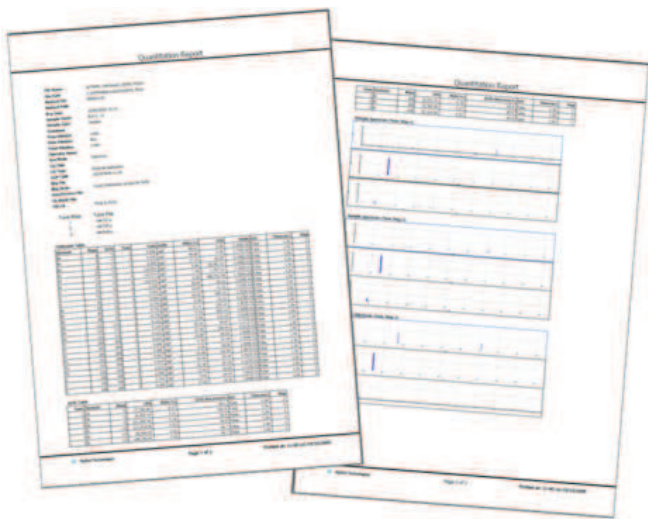
# Reporting

### 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.
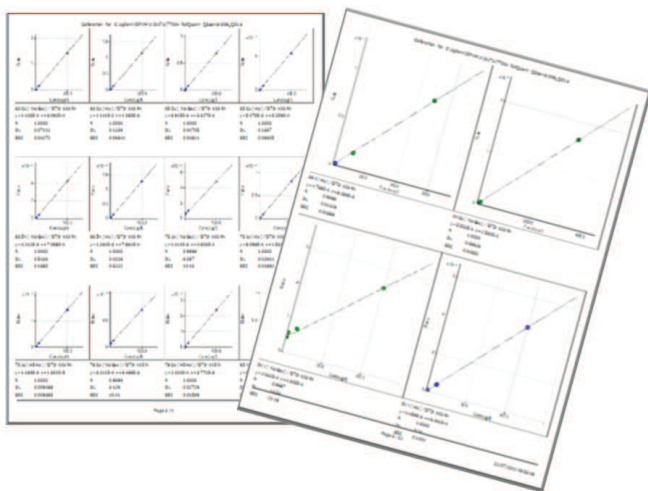


### Flexible results report format
MassHunter also includes a flexible, user-configurable report layout for sample results. Built-in reports include quant, semi-quant and isotope ratio reports for individual samples, and a flexible quick batch report for full or selected batch table data.



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.
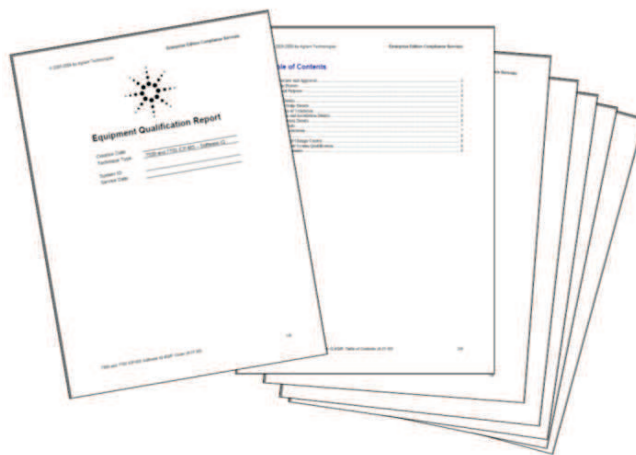


### 21 CFR Part 11
In combination with the optional User Access Control module (G7207A) and Agilent's OpenLab ECM software, ICP-MS MassHunter ("Full" version) can provide a solution that satisfies all the regulatory requirements of 21 CFR Part 11.
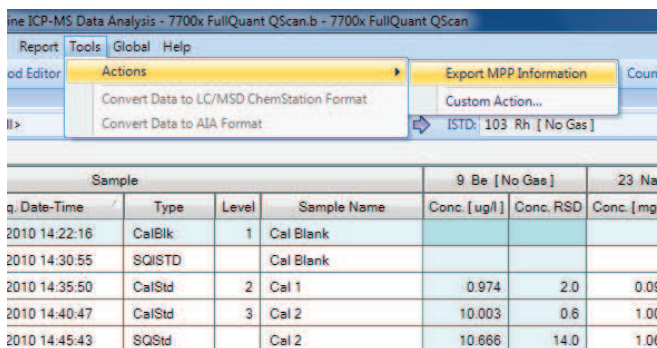
## Mass Profiler Professional

### 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.



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.
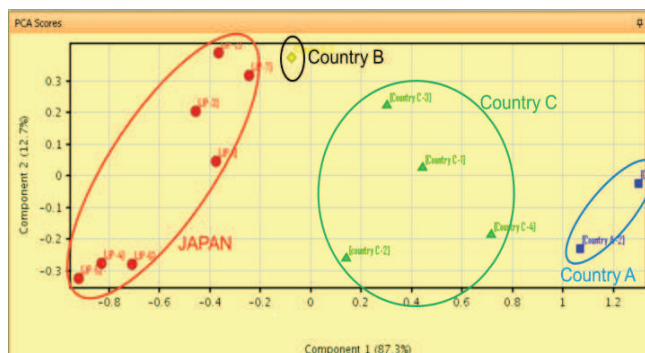


## Conclusions

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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