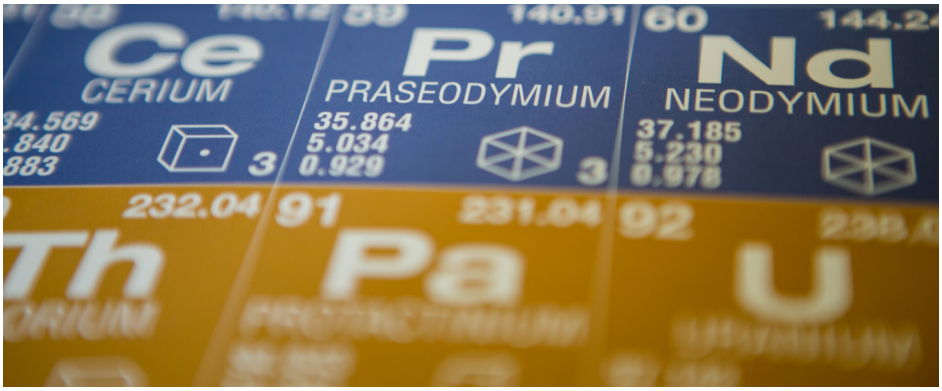
Technical Overview

Agilent ICP-MS IntelliQuant Analysis

An overview of QuickScan, IntelliQuant, and Star Rating



Introduction

Introduced in Agilent ICP-MS MassHunter version 4.6, IntelliQuant for ICP-MS provides an automated semiquantitative analysis for every sample. Calibration and background correction are automatically made with no user intervention, and data is presented in an easily understood periodic table heat map format and a comprehensive data table.

IntelliQuant is possible because a QuickScan can be performed when measuring each sample. The optional two second QuickScan acquires a complete mass spectrum of the entire measurable mass range, facilitating semiquantitative and Total Matrix Solids (TMS) calculations of every sample.

TMS levels are calculated from the IntelliQuant data. Similar to Total Dissolved Solids (TDS), TMS is the sum of the key matrix elements in each sample.

Included in the TMS calculation are the elements typically considered to contribute to matrix effects, such as ionization suppression and matrix deposition on interface cones and lenses. Gas elements, including elements in acids such as HCl and HNO_3, do not cause appreciable matrix effects in ICP-MS, so they are excluded from the calculation.

Interference removal

ICP-MS data would not be useful if matrix-derived interferences were present to bias the results. As default, ICP-MS MassHunter acquires QuickScan data in helium kinetic energy discrimination (KED) mode. KED removes polyatomic interferences without needing selective reaction chemistry and is applicable to virtually all polyatomic interferences—the major contribution of spectral interferences in ICP-MS.

Helium KED depends on the instrument design as a whole to operate effectively. For further information, see publication 5994-1171EN.

IntelliQuant data analysis

By default, the QuickScan function is enabled in helium KED mode. Although QuickScan can be disabled, it only adds two seconds to the total analysis time and provides a wealth of extra data. The analyst needs no expertise or interaction, as IntelliQuant selects the most appropriate standard to calibrate the semiquantitative response.

The semiquantitative concentrations for every measurable element are calculated in each sample and displayed in a data table, as well as an easily understood periodic table heat map.

The heat map is automatically updated with the TMS and concentration data when a sample is selected. Users can click on specific elements to view greater detail for that element.

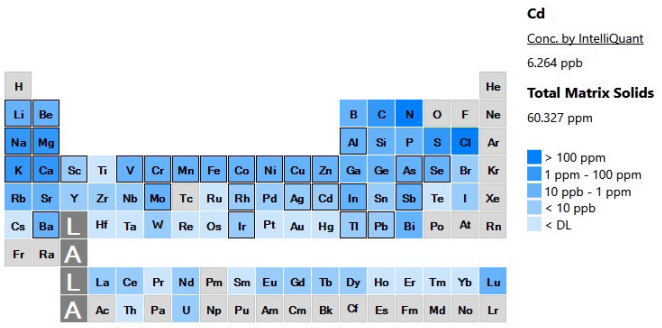


Figure 1. IntelliQuant heat map example displaying the semiquantitative data for all measurable elements within a sample.

Recording the semiquantitative data for every sample means that the analyst has access to a far richer data set than quantitative measurement alone. The data can be used to investigate unusual samples or unexpected results without having to change or disturb the lab workflow.

For example, if a suspect sample requires a full elemental screening, it can be added to the standard, routine method with IntelliQuant enabled, and no changes needed.

IntelliQuant Star Rating

A new feature introduced into ICP-MS MassHunter 5.3 is the innovative Star Rating system. A single button press is all that is needed to display the star rating summary view.

When enabled, ICP-MS MassHunter will evaluate every quantitative element and isotope measured in helium mode. It then assesses the data quality of each isotope and displays the level of confidence in the data using an easily understood star rating system. Five stars indicate high confidence in the result for that isotope.

Confidence in your results

In calculating the star rating, IntelliQuant uses multivariate data including:

- Spectral interferences
- Measurement precision
- Detection limits and backgrounds
- Calibration quality

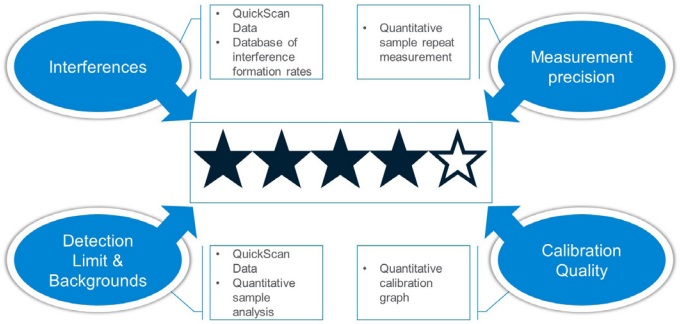


Figure 2. IntelliQuant star rating uses multivariate analysis to calculate a confidence level for the quantitative sample data

Interference database

Spectral interferences are calculated using the full scan data acquired by the QuickScan function. The spectrum is filtered through a comprehensive database of real interferences. The database holds details of the interference formation rates in the different preset plasma conditions (low-matrix, general purpose, or UHMI) for no gas and helium collision modes.

IntelliQuant then uses the QuickScan data to estimate any interference contribution from unknown or unexpected elements. It factors the relative intensity of a possible interference against the analyte signal to evaluate whether the contribution is significant.

This feature is useful for atomic interferences such as doubly charged elements (M^{2+}) where helium collision mode is ineffective. For a doubly charged interference to form at appreciable levels, several factors must occur simultaneously.

The original element must have a twofold higher mass, a low second ionization energy, and a relatively high concentration. These factors are less common for most samples but are often overlooked.

A good example is the contribution of doubly charged Rare Earth Elements (REEs) to the apparent signal of the key elements arsenic (As) and selenium (Se). Many samples do not have appreciable concentrations of REEs, and most regulated methods do not require analysis of REEs.

This means that if a sample contains any REEs, they can be easily overlooked as there is no analytical data for them. However, IntelliQuant and QuickScan will automatically assess the full mass spectrum for every sample and highlight any concerns.

Total data assessment

IntelliQuant star rating is more than an interference finder; it assesses all important factors of the analysis, such as measurement precision and calibration quality. It also factors in the limit of quantitation (LOQ) and background equivalent concentration (BEC) for each analyte down to the isotope level.

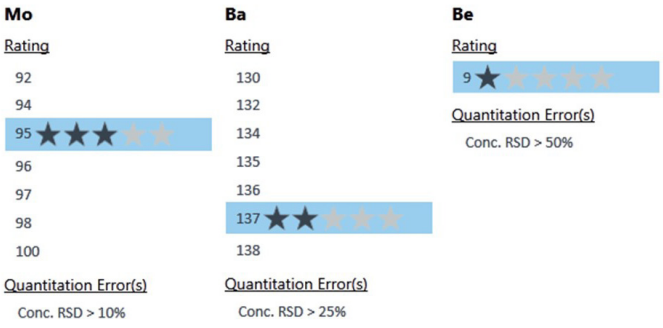


Figure 3. Examples of IntelliQuant star rating of isotopes with various levels of poor measurement precision.

For example, a sample or element with no interferences but poor measurement precision due to the sample running out will be given a lower star rating than a similar sample with good precision. This simple data assessment takes the chore away from the analyst allowing them to focus on other aspects of their work.

Testing IntelliQuant functionality

IntelliQuant was tested using multiple real-world sample batches to verify the robustness and reliability of the algorithms used. An example of interference identification is detailed here.

To assess accuracy, a standard reference material (SRM), NIST 1643f (trace elements in water), was used. The sample was then spiked at increasing concentrations of REEs (0.1, 1.0, and 10.0 ppm), and each solution was measured in duplicate.

Of the certified elements, both As and Se can suffer interferences from doubly charged neodymium (Nd) and samarium (Sm). Table 1 shows the analytical effect and recoveries for As and Se at the various REE spike levels.

Table 1. Effects of Nd^{2+} and Sm^{2+} interferences on the recovery of As and Se for a spiked NIST 1643f SRM. Concentrations are presented as ppb and recoveries as % of the certified value.

	75 As		78 Se	
Certified value	57.42	% Rec	11.70	% Rec
NIST 1643f	58.93	103	11.99	102
NIST 1643f	58.11	101	11.82	101
NIST 1643f + 0.1ppm	61.07	106	55.31	473
NIST 1643f + 0.1ppm	61.86	108	56.15	480
NIST 1643f + 1ppm	93.41	163	447.94	3829
NIST 1643f + 1ppm	93.59	163	447.79	3802
NIST 1643f + 10ppm	518.86	904	6170.19	52737
NIST 1643f + 10ppm	548.79	956	5994.33	51234

The interference effect, particularly for the lower concentration REE samples, may not be obvious to the analyst. However, IntelliQuant successfully identified the interferences using the QuickScan data. Figures 5a-d display how IntelliQuant identified the interferences on As.

The unspiked NIST 1643f displays no problems, and the results for As and Se both gave five stars. Helium collision mode successfully removed any polyatomic interferences, as confirmed by the analytical data in Table 1.

Increasing the REE concentration to 0.1 ppm had little effect on As, although IntelliQuant did detect possible interferences and downgraded the result to four stars. Selenium experienced interferences at every spike level tested, indicated by a single-star rating (Figure 4).

Subsequent spikes increased the interference on As (and Se), and each level of severity degraded the star rating confidence for that measurement.

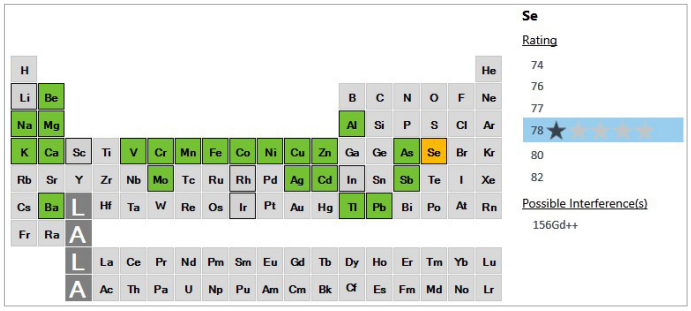


Figure 4. NIST1643f SRM with 0.1 ppm REE spike. Selenium displays a single star rating indicating severe interferences from Nd^{2+} and Sm^{2+}.

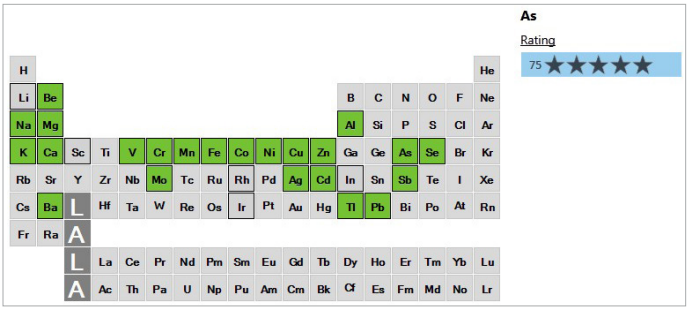


Figure 5a. Unspiked NIST1643f SRM. All elements in the IntelliQuant star rating heat map are green, indicating no problems. Arsenic shows a five-star rating indicating no known problems.

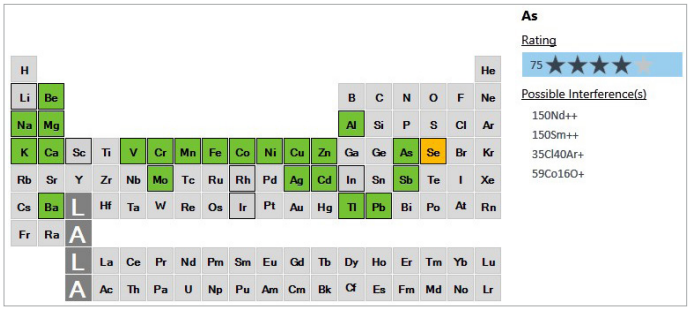


Figure 5b. NIST1643f SRM with 0.1 ppm REE spike. Selenium displays a problem (orange cell), and the star rating for As has degraded, indicating a possible low-level interference from Nd^{2+} and Sm^{2+}.

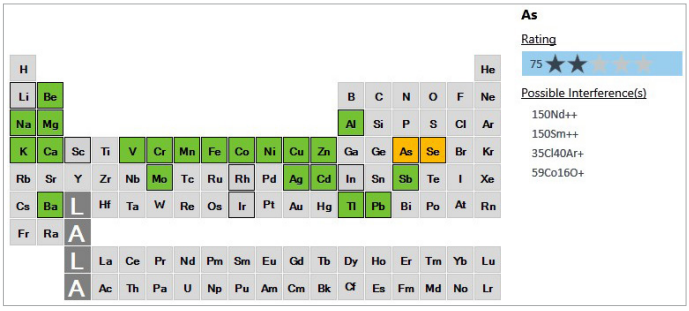


Figure 5c. NIST1643f SRM with 1 ppm REE spike. Confidence in the As result has degraded to two stars and is displayed in orange, indicating a strong interference from Nd^{2+} and Sm^{2+}.

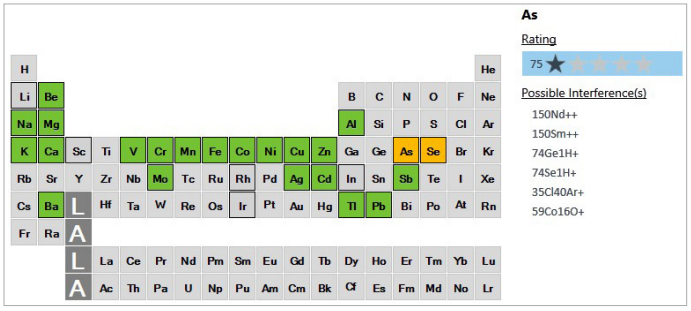


Figure 5d. NIST1643f SRM with 10 ppm REE spike. Confidence in the As result is low, a single star indicates a severe interference from Nd^{2+} and Sm^{2+}.

Table 2 displays the results and recoveries for the unspiked SRM. All recoveries were acceptable and IntelliQuant did not identify any measurement issues for the unspiked sample.

Table 2. Recovery data for the NIST1643f SRM. Certified concentrations (Cert) and measured concentrations (Conc) are displayed as µg L^{-1}.

Element	Cert	Conc	%Rec
9 Be	13.67	13.67	**100**
23 Na	18.83	20.21	**107**
24 Mg	7.454	8.169	**110**
27 Al	133.8	140.4	**105**
39 K	1.932	2.113	**109**
44 Ca	29.43	30.36	**103**
51 V	36.07	35.17	**98**
52 Cr	18.50	18.42	**100**
55 Mn	37.14	37.18	**100**
56 Fe	0.09	0.097	**104**
59 Co	25.30	25.40	**100**
60 Ni	59.8	60.1	**101**

Element	Cert	Conc	%Rec
63 Cu	21.66	21.78	**101**
66 Zn	74.4	76.3	**103**
75 As	57.42	58.93	**103**
78 Se	11.700	11.990	**102**
95 Mo	115.3	125.3	**109**
107 Ag	0.9703	0.977	**101**
111 Cd	5.89	5.88	**100**
121 Sb	55.45	55.35	**100**
137 Ba	518.2	527.1	**102**
205 Tl	6.892	6.812	**99**
208 Pb	18.488	18.569	**100**

IntelliQuant interference simulator

The interference simulator in ICP-MS MassHunter 5.3 and later allows the analyst to test for simulated interferences in various matrices without running a sample—or even turning on the plasma.

Using the interference database created for the star rating, the IntelliQuant simulator calculates potential interferences in the selected cell and plasma modes.

The user can select from example matrices, make any desired edits, and save them as a custom sample matrix.

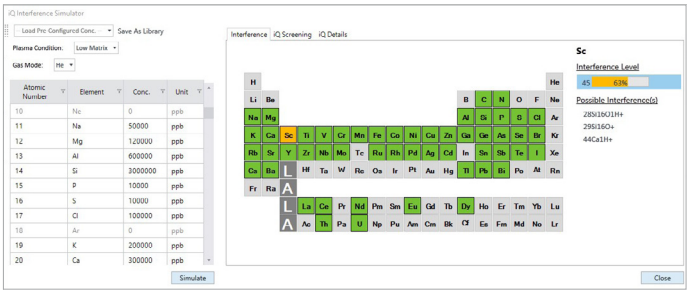


Figure 6. The IntelliQuant interference simulator allows the user to experiment without preparing solutions or even turning on the plasma.

Data compatibility

IntelliQuant and star rating are compatible with any QuickScan data acquired using ICP-MS MassHunter. This compatibility means that all data, regardless of instrument type or age, can be reprocessed using IntelliQuant[1].

The features are compatible with data from the Agilent 7700, 7800, 7850, and 7900 ICP-MS and the Agilent 8800 and 8900 ICP-QQQ.

[1] *Performance will depend upon using preset plasma conditions and helium collision mode.*

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