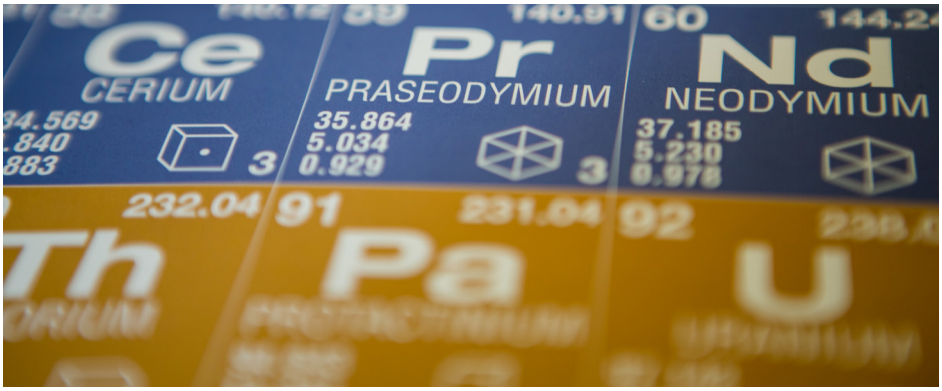
Technical Overview

Agilent ICP-MS IntelliQuant Analysis

An overview of IntelliQuant and Star Rating



Introduction

Agilent IntelliQuant for ICP-MS provides an automated semiquantitative analysis for every sample. Calibration and background correction are performed automatically with no user intervention, and the results are shown both visually and in a comprehensive data table.

IntelliQuant takes the stress out of reviewing unknown sample results by assessing interferences, precision, calibrations, and more. By presenting the data in an easily understood Periodic Table heatmap format and providing an intuitive star rating system, IntelliQuant is a vital tool in any ICP-MS laboratory.

IntelliQuant rapidly screens each sample and acquires a full mass spectrum across the entire measurable mass range. This screening enables semiquantitative analysis and the calculation of Total Matrix Solids (TMS) for each 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.

Data quality

ICP-MS data can become unreliable if matrix-derived interferences exist, leading to biased results. Typically, Agilent OpenLab ICP-MS collects IntelliQuant data using helium (He) kinetic energy discrimination (KED) mode. This mode eliminates polyatomic interferences without needing specific reaction chemistry and is effective against nearly all such interferences, which are the main spectral interferences in ICP-MS.

The effectiveness of He KED relies on the overall design of the instrument. The new Agilent 9500 Triple Quadrupole ICP-MS (ICP-QQQ) includes Advanced Helium Mode (AHM), a high-sensitivity He KED mode that offers enhanced interference removal, greatly increasing data reliability.

For further information, see Agilent publications 5994-1171EN and 5994-8985EN.

IntelliQuant data analysis

By default, the IntelliQuant function is enabled in He KED mode. Although IntelliQuant can be disabled, it adds only two seconds to the analysis time and offers extensive additional data. No expertise or user interaction is required from the analyst, as IntelliQuant automatically chooses the best standard for calibrating the semiquantitative response. The semiquantitative concentrations for all measurable elements are calculated for each sample and displayed in a data table and a clear periodic table heat map (see Figure 1). The heat map updates automatically with the TMS and concentration data once a sample is selected. Users can click on individual elements for more detailed information.

Recording semiquantitative data for every sample means the analyst has access to a far richer data set than quantitative measurements alone. The data can be used to investigate unusual samples or unexpected results without altering or disrupting 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 are needed.

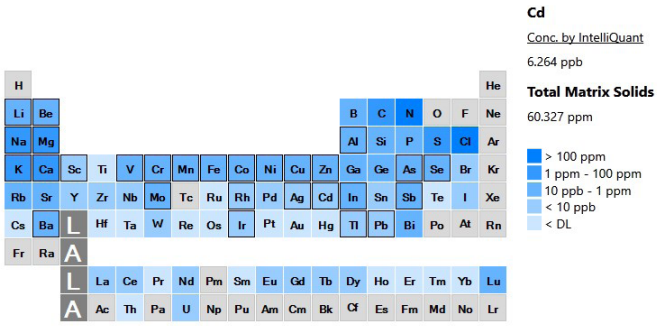


Figure 1. IntelliQuant heat map example showing semiquantitative data for all measurable elements within a sample.

IntelliQuant Star Rating

With IntelliQuant activated, data analysis is enhanced by the innovative star-rating system, offering a clear and intuitive evaluation of analytical results.

A single button press is all that is needed to display the star rating summary view.

When enabled, OpenLab ICP-MS will evaluate every quantitative element and isotope measured in He 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 (Figure 2), including:

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

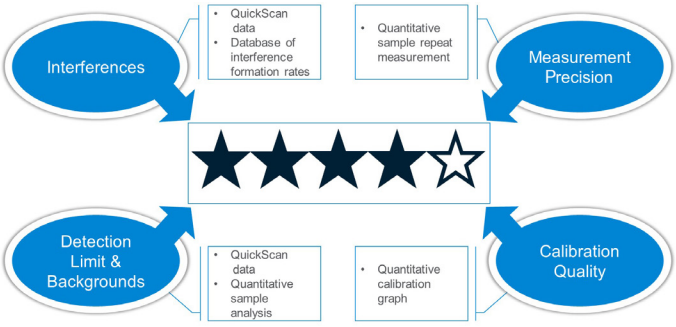


Figure 2. IntelliQuant star rating uses multivariate analysis to calculate a confidence level for the quantitative sample data.

Interference database

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

IntelliQuant then uses the full-scan data to estimate any interference contribution from unknown or unexpected elements. It factors in the relative intensity of potential interferences against the analyte signal to determine whether the contribution is significant.

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

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

An example is the contribution of doubly charged Rare Earth Elements (REEs) which can influence the apparent signals of key elements like arsenic (As) and selenium (Se). Many samples do not have appreciable REE concentrations, and most regulatory methods do not mandate REE testing.

So, if a sample contains REEs, they may be missed since no specific analysis data is usually available. However, IntelliQuant automatically evaluates the entire mass spectrum for each sample and flags any potential issues.

Total data assessment

IntelliQuant star rating goes beyond simply identifying interferences; it evaluates all essential aspects of the analysis, including measurement precision (see Figure 3) and calibration quality. Additionally, it considers the limit of quantitation (LOQ) and background equivalent concentration (BEC) for each analyte, extending to the isotope level.

Figure 3. Examples of IntelliQuant star ratings for isotopes with varying 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 with multiple real-world sample batches to verify the algorithms` robustness and reliability. 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.

Among the certified elements, both As and Se can be interfered with by 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	% Recovery	11.70	% Recovery
NIST 1643f	58.93	103	11.99	102
NIST 1643f	58.11	101	11.82	101
NIST 1643f + 0.1 ppm	61.07	106	55.31	473
NIST 1643f + 0.1 ppm	61.86	108	56.15	480
NIST 1643f + 1 ppm	93.41	163	447.94	3829
NIST 1643f + 1 ppm	93.59	163	447.79	3802
NIST 1643f + 10 ppm	518.86	904	6170.19	52737
NIST 1643f + 10 ppm	548.79	956	5994.33	51234

The interference effect, particularly in lower-concentration REE samples, may not be obvious to the analyst. However, IntelliQuant successfully identified the interferences using the full scan data (Figures 4 and 5).

Figures 5a-d display how IntelliQuant identified the interferences on As. The unspiked NIST 1643f shows no problems, and the results for As and Se both received 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 detected possible interferences and downgraded the result to four stars. Se showed an interference at every spike level tested, as indicated by a single-star rating (Figure 4).

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

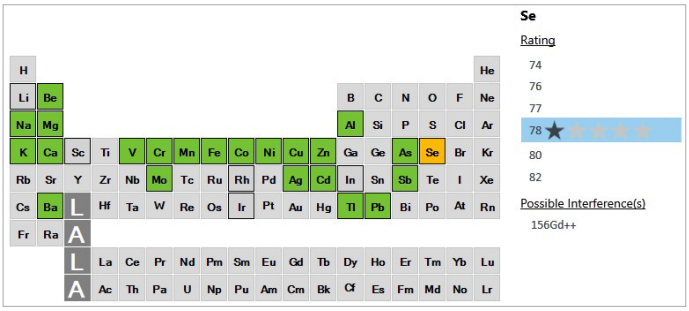


Figure 4. NIST1643f SRM with 0.1 ppm REE spike. Selenium displays a single star rating indicating severe interferences from Nd^{2+} and Sm^{2+}.

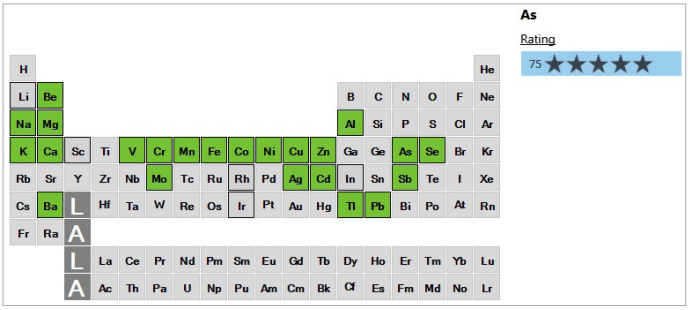


Figure 5a. Unspiked NIST1643f SRM. All elements in the IntelliQuant star rating heat map are green, indicating no problems. Arsenic shows a five-star rating, indicating no known problems.

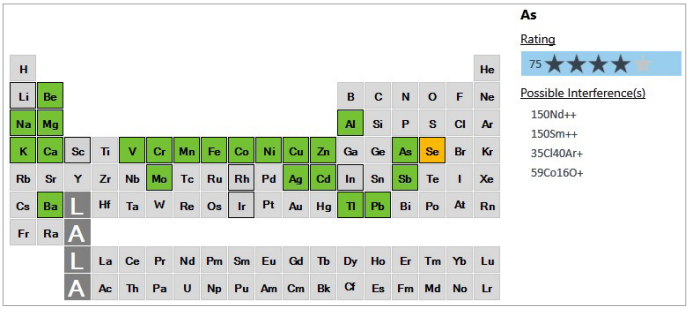


Figure 5b. NIST1643f SRM with 0.1 ppm REE spike. Selenium displays a problem (orange cell), and the star rating for As has degraded, indicating a possible low-level interference from Nd^{2+} and Sm^{2+}.

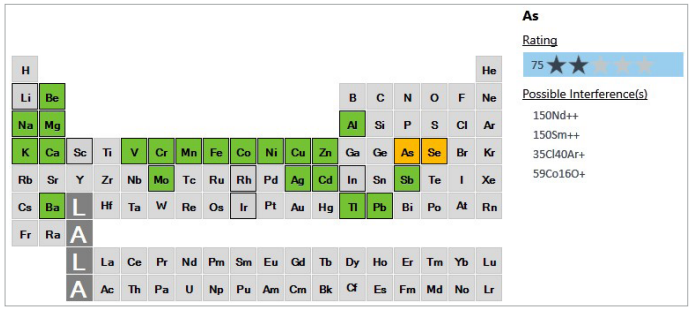


Figure 5c. NIST1643f SRM with 1 ppm REE spike. Confidence in the As result has degraded to two stars and is displayed in orange, indicating a strong interference from Nd^{2+} and Sm^{2+}.

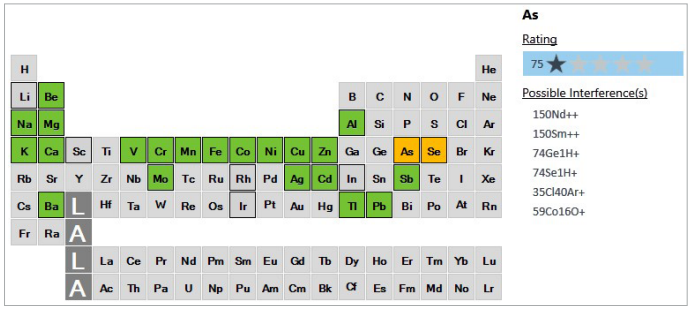


Figure 5d. NIST1643f SRM with 10 ppm REE spike. Confidence in the As result is low; a single star indicates a severe interference from Nd^{2+} and Sm^{2+}.

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.

Element	Cert	Conc	% Recovery
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
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 OpenLab ICP-MS 1.1 or later (or Agilent ICP-MS MassHunter 5.3 and later) enables analysts to test for simulated interferences across different matrices without needing to run a sample or even turn on the plasma. It uses the interference database, created for the star rating, to calculate potential interferences in the chosen cell and plasma modes.

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

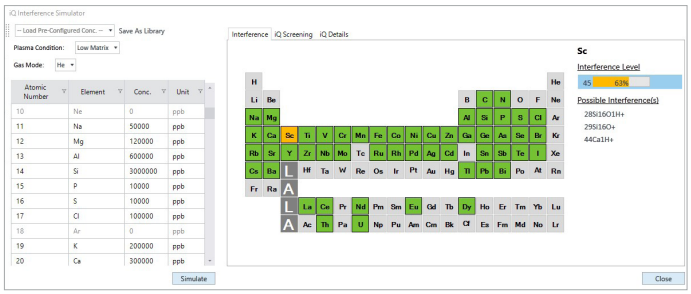


Figure 6. The IntelliQuant interference simulator allows the user to experiment without preparing solutions or even turning on the plasma.

Data compatibility

IntelliQuant functionality in OpenLab ICP-MS is compatible with data acquired on a wide range of Agilent ICP-MS instruments, including the 7800, 7850, and 7900 ICP-MS, as well as the 8900 and 9500 ICP-QQQ systems, provided that the data includes IntelliQuant screening measurements acquired in no gas or He collision mode.

OpenLab ICP-MS software can open and reprocess batch data originally acquired with ICP-MS MassHunter software. When Quick Scan data are present, the IntelliQuant semiquantitative analysis can be applied during data review, enabling additional elemental screening information to be extracted without remeasuring samples.*

** Performance will depend upon using preset plasma conditions and He collision mode.*

www.agilent.com/chem/icp-ms

DE-014936

Published in the USA, June 01, 2026
5994-7441EN

Agilent
Trusted Answers