Technical Overview

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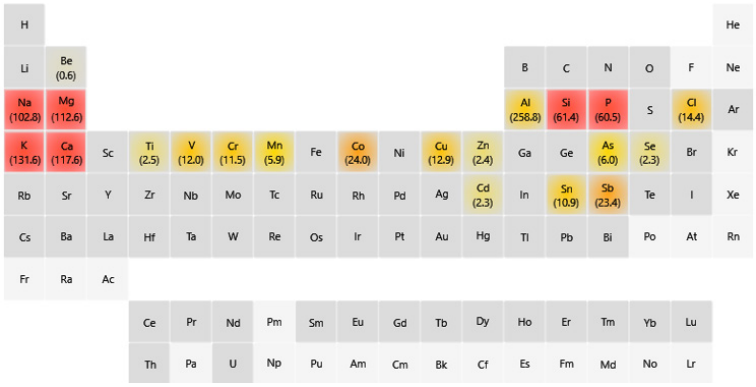
Agilent IntelliQuant Software

For greater sample insight and simplified method development



Introduction

While quantitative elemental analysis remains the main use of ICP-OES instrumentation, semiquantitative analysis provides extra information, allowing the analyst to learn more about their samples. However, collecting and interpreting semiquantitative data on many ICP-OES instruments can be as time-consuming as collecting fully quantitative data. Users of these types of ICP-OES instruments probably don't realize the full potential of semiquantitative data acquisition.

The Agilent 5800 and 5900 ICP-OES instruments include IntelliQuant—a powerful, dedicated semiquantitative analysis tool that allows you to understand the elemental content of your sample better. IntelliQuant can be used to improve traditional quantitative methods or to provide standalone semiquantitative results quickly and with minimal setup.

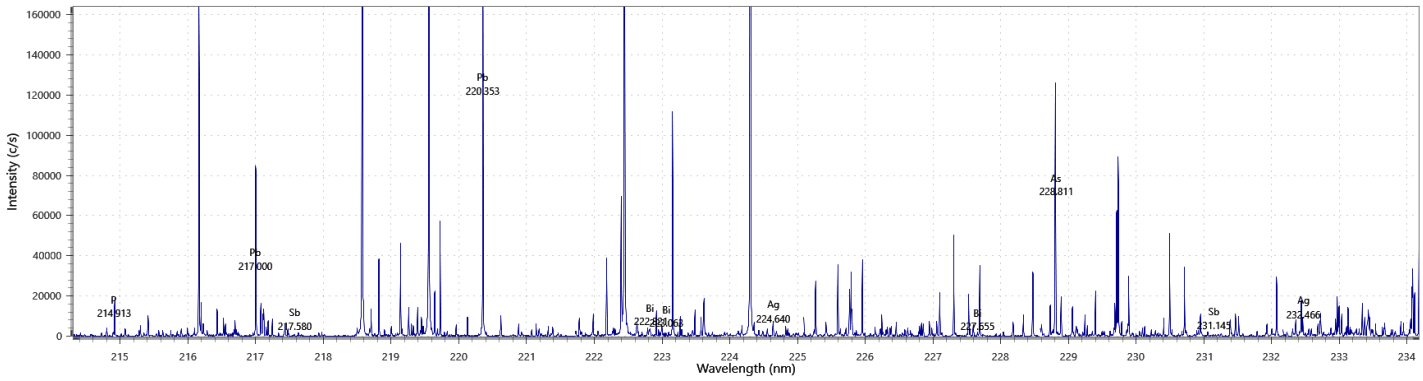


Figure 1. Section of the full-spectrum scan data collected by IntelliQuant. The information provides useful analytical insight into the sample, helping with method development.

What is IntelliQuant?

Part of Agilent ICP Expert software, IntelliQuant is a fast semiquantitative data acquisition routine for ICP-OES (*1*). IntelliQuant collects data across the entire spectral range from 167 to 785 nm for every sample, providing comprehensive data that is not available from all ICP-OES instruments. When performed as part of a quantitative method, an IntelliQuant scan provides quick sample insight.

The section of a full spectrum scan in Figure 1 shows the relative abundance of the elements in a sample obtained using IntelliQuant. This information can be used to develop methods that avoid spectral interference, determine possible dilution factors, assist in determining the calibration range for each element, and which plasma view to use.

Automatic element identification

After a full-spectrum scan has been collected, the advanced IntelliQuant algorithms identify which elements are present in each sample. No user-input is required, as the process is fully automated. The algorithms use a database of atomic and ionic emission lines to separate analyte peaks from noise and interferences.

Choosing the best wavelengths

Once a sample has been measured by IntelliQuant, the Star ranking feature provides a list of the best wavelengths to use for the analysis of every element present in the sample. It also gives a star ranking to each wavelength to help identify interferents, as shown in Figure 2. By determining whether a potential interferent element is present in a sample, IntelliQuant makes wavelength selection for reporting or for adjusting a quantitative method much easier. Also, users can avoid reporting results that have been affected by an interference.

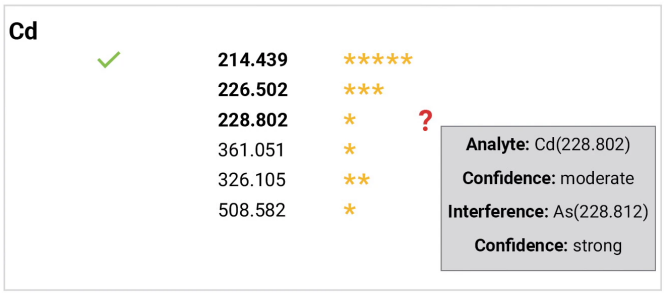


Figure 2. IntelliQuant indicates the best analyte wavelength with a high star ranking and a green tick. It also highlights suspected interferences on analyte wavelengths using a low star ranking. Potential spectral overlaps can be identified by hovering over the red question mark.

Semiquantitative concentration results

IntelliQuant includes premeasured calibrations that can be used to calculate a semiquantitative result for every element that is detected in a sample. Calibrations are provided for all available viewing modes (axial, radial, Vertical Dual View, and Synchronous Vertical Dual View) to ensure that all users have access to a default calibration suitable for their instrument. For improved accuracy, default or any existing calibrations can be updated by remeasuring individual standards, or adding and measuring more calibration standards after the initial collection. This flexibility is essential for users who want to regularly update the calibration for a subset of elements only, rather than for all elements.

An Agilent IntelliQuant Calibration Kit is also available that provides a set of ready made solutions that can be measured directly or used for greater accuracy to prepare matrix-matched standards for complex samples.

Also, users can easily create and measure their own IntelliQuant calibrations. User-defined calibrations can be fully customized and can include any set of elements measured over the user's desired concentration range.

Smart Views

The Smart Views function provides a simple way for users to filter their IntelliQuant data to show only those results that are of interest, preventing important data insights from being overlooked. Concentration-based color thresholds can be defined in Smart Views to visually alert users to results that are abnormally high or low compared with the user-defined values. Users can also choose exactly which elements' results they wish to view and can even define concentration-based rules to select which solutions are shown in the results-grid. For example, if an analyst analyzes 500 solutions using IntelliQuant, they can use Smart Views to instantly filter the results-list to display only those solutions that contain a key element above a specified concentration.

Users can change which Smart Views is applied to their results at any time, or create and save a new Smart Views, even as data is being collected.

Sample insights with IntelliQuant

IntelliQuant provides important sample insight that can be used in different ways, depending on the aims and scope of the analysis.

Sample screening

IntelliQuant can identify and calculate semiquantitative results for up to 70 elements in unknown and uncharacterized samples within seconds, making it an ideal sample screening tool. By displaying the results in a color-coded periodic table, users can see at-a-glance which elements are present in the sample—and at what concentration-level (Figure 3). Using the default settings, elements present at low concentrations are colored yellow, medium concentration are orange, and high concentration are red. However, these concentration thresholds can be custom-defined in Smart Views.

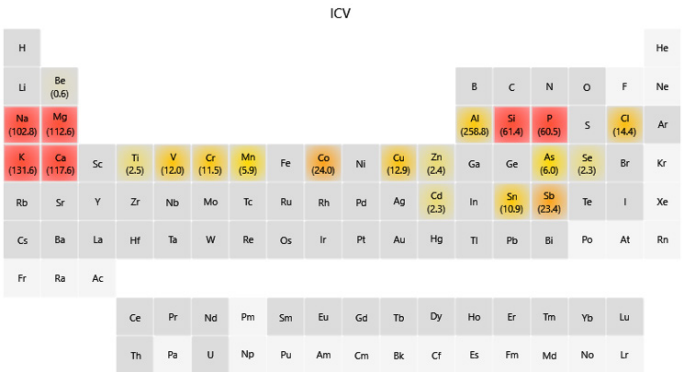


Figure 3. IntelliQuant allows users to visualize the content of their samples and applies color-coding to detected elements based on user-defined concentration thresholds.

Help identify sample preparation issues

IntelliQuant can be used to identify sample preparation issues. For example, failure to add the correct amount of hydrochloric acid during sample digestion can lead to a potentially inadequate sample digestion and the generation of incorrect results. This error can be difficult to detect. However, IntelliQuant can be set up to flag low chlorine results in samples. By quickly checking the IntelliQuant results, analysts can identify whether Cl is present and know that the digestion was done correctly, before the results are reported. The same approach is suitable for most acids used for sample digestion.

While IntelliQuant is an ICP-OES technique, there is no reason to limit its application to ICP-OES-specific samples. IntelliQuant can provide insight into samples that have been prepared for analysis by ICP-MS, AAS, chromatography, or even titration.

Quality control of reagents

Preparation differences between batches of a reagent are a common cause of variation in analytical results. With IntelliQuant, users can easily compare the composition of two or more reagent batches as soon as they are prepared. Any differences will be instantly highlighted, allowing potential issues to be addressed before they affect the quality of the final results. IntelliQuant is a simple way to confirm the quality of reagents used for analyses by ICP-OES or other analytical techniques.

Simplify method development

The IntelliQuant interference avoidance algorithm presents users with detailed information about possible interferences for each detected element, which wavelengths they affect, and which wavelengths are likely to be interference-free.

This information is useful for method development, providing the analyst with immediate insights into the sample components and concentrations. With ICP Expert these insights can easily be used to rapidly start acquiring quantitative data.

Label	Date	Al mg/L	As mg/L	Ca mg/L	Cu mg/L	Fe mg/L	K mg/L	Mg mg/L	Mn mg/L	Na mg/L	P mg/L	Pb mg/L	S mg/L	Sb mg/L	Si mg/L	Ti mg/L	Zn mg/L	Cl Unadj	N %
Soil 1	2019-08-05 12:30:30	176.23 o	23.44	38.35	62.19	604.17	71.31	63.13	30.82	10.52	16.73	79.87	112.95	10.52	10.50	12.29	54.48	2.44	2.36 o
Soil 2	2019-08-05 12:30:51	181.58 o	24.20	36.02	53.64	645.12	72.89	65.04	31.47	10.23	15.19	83.64	112.69	10.23	11.48	12.94	55.89	2.20	2.42 o
Soil 3	2019-08-05 12:31:31	187.33 o	24.21	38.17	53.70	657.96	73.71	66.85	33.25	10.38	14.97	83.96	114.23	10.38	10.70	15.08	54.76	2.21	2.63 o
Soil 4	2019-08-05 12:32:17	199.84 o	23.90	40.33	53.45	708.05	85.68	71.60	32.71	11.05	14.62	83.32	112.50		9.03	16.94	52.60		2.20 o
Soil 5	2019-08-05 12:33:23	186.25 o	23.49	37.04	47.33	657.96	74.23	64.89	31.31	10.49	13.55	81.71	110.29	10.49	10.92	13.98	52.00	2.49	2.51 o

Figure 4. Software screen from an IntelliQuant analysis, highlighting some issues with 'Soil 4'. Note the absence of Sb and Cl in this sample.

Assist with result validation

The interference algorithm can also be used as a powerful tool to assist with the validation of results in established methods. If an analyst is unsure whether a result in their quantitative method has been affected by an interference, IntelliQuant can provide extra information. By identifying likely interferences on the wavelength of the element used in the quantitative method, IntelliQuant can identify which element is causing the interference.

The analyst may then choose to address the interferences in one of several ways. They may avoid it by selecting a different wavelength or correct it using Fast Automated Curve-fitting Technique (FACT) or Inter Element Correction (IEC).

Help identify chemical incompatibilities within a sample

When sample analysis results are lower than expected, there may be several causes of the error, including chemical incompatibilities between elements in the sample. IntelliQuant can be used to identify when chemical incompatibilities between elements are a potential issue. For example, a quantitative analysis result for barium may appear low. It is possible that high sulfate levels in the sample may have caused barium to precipitate before the measurement could be performed. Sulfur may not have been a part of the quantitative method, but it will be identified and semi-quantified by an IntelliQuant analysis. The IntelliQuant results would provide all the information needed to identify the issue, avoiding the inclusion of incorrect data in the final sample analysis report.

Example analysis

In the following example, five replicates of a soil sample were digested using aqua regia and analyzed using an Agilent 5900 SVDV ICP-OES and IntelliQuant. The semiquantitative concentration results for all detected elements in the duplicate samples show good repeatability in all cases, apart from some elements in Soil 4.

The Smart Views routine was used to filter the results. Figure 4 was developed to report results for the most important elements of interest in soil. The results-grid flags a problem with Sb and Cl in Soil 4. The absence of Cl suggests that the sample was wrongly prepared, using only nitric acid rather than aqua regia.

Using IntelliQuant it is possible to obtain this type of sample insight with only one or two clicks of the mouse. IntelliQuant with Smart Views allows the user to quickly and easily identify abnormal results and investigate them before any incorrect data is reported.

Reference

1. Agilent ICP Expert Software: Powerful software with smart tools for ICP-OES, Agilent publication, 5994-1517EN

www.agilent.com/chem/icp-oes

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Printed in the USA, April 18, 2022
5994-1516EN

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