Agilent

Trusted Answers

Agilent IntelliQuant Screening

Smarter and quicker semiquantitative ICP-OES analysis

Introduction

The standard Agilent IntelliQuant semiquantitative analysis tool that is included in the base ICP Expert software gives users extra insight into their samples by collecting and interpreting full-spectrum measurements, with minimal user input (*1*). IntelliQuant Screening, which is part of the Pro pack for ICP Expert, expands IntelliQuant functionality even further (*2*). IntelliQuant Screening allows users to start collecting data within seconds, without having to choose which elements or wavelengths to analyze and rapidly transfer those insights to a quantitative method.

Snapshot mode

IntelliQuant Screening collects full-spectrum data at an even faster rate than the standard version of IntelliQuant using 'Snapshot' mode. This new measurement mode uses the speed and power of the third generation Agilent VistaChip III CCD detector to produce a full-spectrum scan of each sample in less than five seconds of total measurement time.

After the full-spectrum measurement for each sample has completed, IntelliQuant checks the data and automatically determines which wavelength provides the best result for each element. The IntelliQuant algorithm assesses the intensity of the analyte peak, the consistency of the local background of the peak, and the likelihood of spectral interference from other elements found in the sample. IntelliQuant reports high quality, reliable results, without requiring any spectroscopic knowledge from the user. Analysts can be sure that the data is based on interference-free measurements, which are within the valid range of intensities that can be measured in Snapshot mode.

Trend analysis and sample screening

ICP-OES is often used for semiquantitative trend analysis studies in many industries. Trend analysis is used to assess the relative results between batches of samples or changes to solutions over time. IntelliQuant Screening improves the trend analysis capabilities of ICP-OES in several ways.

Users of IntelliQuant Screening can access all the standard IntelliQuant Smart Views functions plus extra graphics for trend analysis. The new visualization options include a pie, bar chart and a scatter chart graphic. The analyst can easily switch between seeing the results as concentrations to viewing them as percentages of the total measured sample content. Figure 1 shows semiquantitative results for selected elements in NIST 2782 industrial sludge standard reference material as percentages. Presenting the results in a visualized way allows users to quickly assess any outliers and investigate the cause. An elevated concentration of an element may be due to a sample preparation error or an atypical sample.

Rapid sample screening

With the Agilent AVS 6/7 valve system, IntelliQuant Screening in Snapshot mode allows users to perform full spectrum measurements at a rate of 15 seconds per sample. This technique provides quick sample insight, which is useful when assessing samples to see if they are suitable for analysis using a different technique, such as ICP-MS. Screening samples can potentially save time by avoiding issues that may otherwise arise due to sample content or concentration.

Smart Views

The Smart Views function of IntelliQuant provides a simple way for users to filter their screening 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.
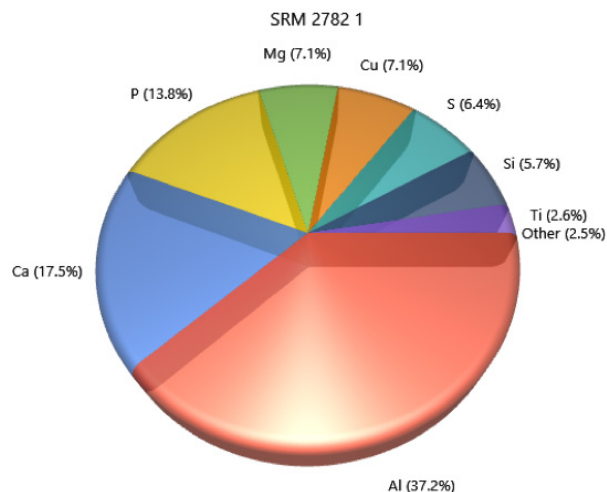

Figure 1. Sample percentage composition chart for user-selected elements generated in real time within the IntelliQuant Screening interface.

Method development

IntelliQuant Screening is useful for technically challenging and time-consuming method development, as it requires no selection of elements and no prior knowledge of the contents of the samples. Method development has traditionally been the domain of more experienced analysts, requiring a great deal of knowledge of ICP-OES. This is no longer the case, as IntelliQuant Screening provides all the tools necessary for less experienced operators to develop quantitative methods.

IntelliQuant Screening uses an easy-to-interpret star ranking system to indicate which analyte wavelengths are likely subject to spectral interferences, background shifts, or poor sensitivity for the samples being measured (displayed in Figures 2 and 3). Analyte wavelengths that are non-interfered or likely to give better sensitivity relative to other wavelengths receive a higher star ranking. Interfered wavelengths or wavelengths with poor sensitivity receive a lower star ranking. Recommended wavelengths for all samples measured in IntelliQuant Screening can be easily transferred into a quantitative ICP Expert method.
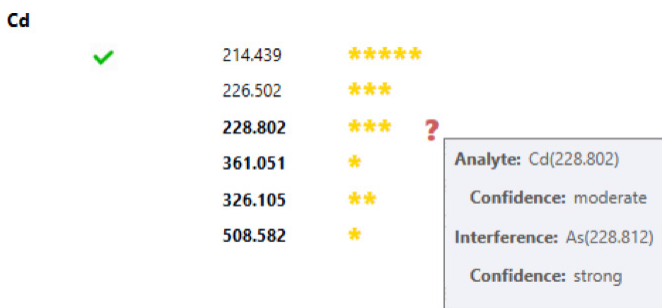
Cd

✓	214.439	★★★★★
	226.502	★★★
	228.802	★★★ ❓
	361.051	★
	326.105	★★
	508.582	★

> Analyte: Cd(228.802)
>
> Confidence: moderate
>
> Interference: As(228.812)
>
> Confidence: strong

Figure 2. IntelliQuant indicates the best analyte wavelength with a high star ranking and the 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.

Rapid sample screening

The IntelliQuant Screening method development workflow can be represented in three easy steps:

1. Run your samples using IntelliQuant Screening

Setting up an IntelliQuant Screening run for your unknown samples is simple and intuitive. No method customization is required—just add your samples and start measuring.

2. Add the recommended wavelengths to the quantitative method

After each sample measurement, the IntelliQuant user-interface displays a list of recommended wavelengths for every element detected in the sample. The IntelliQuant star ranking system is a simple way to determine which wavelengths are likely to give the best result for any element in a sample. IntelliQuant gives a "green tick" to the best wavelength.

Several wavelengths may receive the same star ranking as the IntelliQuant preferred-wavelength (with the green tick). Using ICP Expert, the most common recommended wavelengths can be added to a quantitative method.
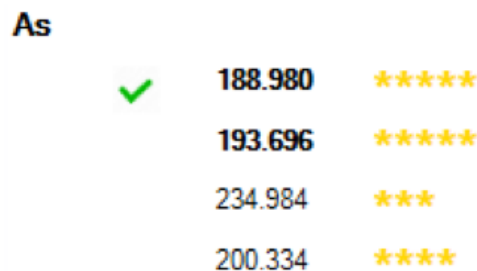
As

✓	188.980	★★★★★
	193.696	★★★★★
	234.984	★★★
	200.334	★★★★

Figure 3. IntelliQuant gives a five-star ranking to the result from two arsenic wavelengths, indicating that both wavelengths are suitable for the quantitative method.

3. Run the quantitative method with IntelliQuant enabled

With the wavelengths recommended by IntelliQuant, from the screening of representative samples, you can now complete construction of the quantitative worksheet. It is advisable to prepare for unexpected sample variation by ensuring that there is more than one wavelength selected for each element (when available) to achieve interference free results for all samples in your new method.

When you analyze unknown samples using the new quantitative method, you can continue to perform IntelliQuant measurements. The IntelliQuant data will allow you to investigate any interferences that arise, which weren't present in the samples used during the method development process. This insight allows you to refine the method by selecting more wavelengths or to correct for the identified interferences using Fast Automated Curve-fitting Technique (FACT) or Inter Element Correction (IEC).

References

1. Agilent IntelliQuant Software: For greater sample insight and simplified method development, Agilent publication, 5994-1516EN

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

Agilent

Trusted Answers