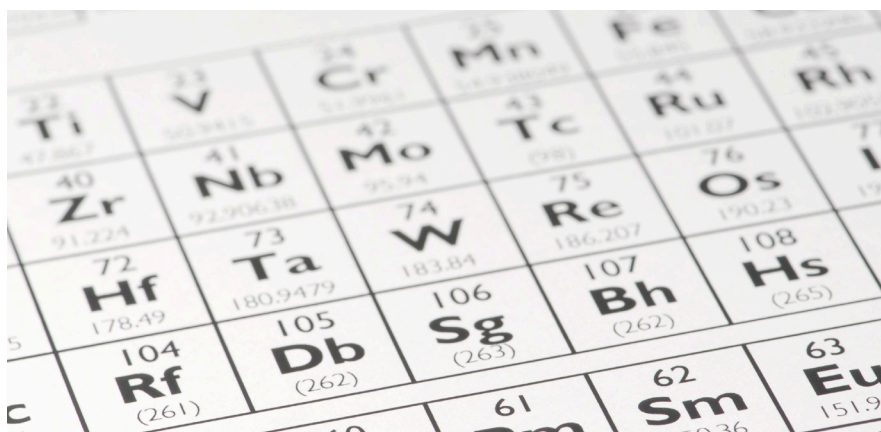# Rapid Sample Assessment and Simplified Method Development with IntelliQuant

Technical Overview

Introduction

In addition to routine quantitative elemental analyses using ICP-OES, analytical laboratories often want to quickly identify other elements in their samples. For example:

- Food testing labs analyzing a routine set of elements want to be aware of the presence of additional elements that may be of concern from a quality control perspective

- Mineral testing labs want to be sure no unexpected precious metal group (PMG) or other valuable metals go unnoticed

- Analysts developing ICP-OES methods need a way to find out all the elements present in their sample to simplify method development

Agilent's IntelliQuant is a software feature that identifies and calculates an approximate concentration (semi-quantifies) for up to 70 elements in a sample, expanding the capabilities of a classic ICP-OES analysis.

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Using IntelliQuant, analysts can quickly check the approximate concentration of many elements in their sample, without changing their routine methods or preparing additional multi-element standards, which can be technically challenging and time consuming.

IntelliQuant is available on all Agilent 5110 ICP-OES and 5100 ICP-OES systems and is fully integrated into ICP Expert software (version 7.3 and later).

How does IntelliQuant work?

Identify up to 70 additional elements in one fast full wavelength scan
In addition to the standard detector read for quantifying selected elements in a sample, IntelliQuant can take a full wavelength scan from 167 to 785 nm. The end result is both the quantitation of the elements defined in the method as well as identification and semi-quantitation of up to 70 additional elements—all with just two readings of Agilent's VistaChip II CCD detector and as little as 15 additional seconds of measurement time per sample.

Default or custom calibration
IntelliQuant includes default calibrations, available for axial, radial and Synchronous Vertical Dual View modes. These factory calibrations allow the estimation of up to 70 elements in a sample without the need to analyze any additional standards.

If you want more accurate results without additional sample preparation, it's possible to update the default IntelliQuant calibrations by using a set of multi-element standards in Agilent's IntelliQuant Calibration Kit. This kit includes multi-element standards which are measured to update the default IntelliQuant calibration for all 70 elements, which is ideal for labs requiring more accurate semi-quantitative analysis without time consuming standard preparation.

For full flexibility a custom IntelliQuant calibration can be measured and stored. This calibration can be fully customized to contain any set of elements over the desired calibration range.

This feature allows you to create a calibration from standards that are matrix-matched to your samples, giving better accuracy.

Any updated or new IntelliQuant calibration is measured in the standard quantitative analytical sequence, meaning no separate analyses or additional worksheets are required.

What does IntelliQuant allow you to do?

Perform rapid screening
IntelliQuant is an ideal rapid sample screening tool. It identifies and semi-quantifies up to 70 unknown elements and takes as little as 15 additional seconds per sample.

The IntelliQuant interface features a periodic table heat map that shows which elements have been found in a sample (Figure 1). Elements present at low concentrations are coloured yellow, medium concentration are orange and high concentration are red.
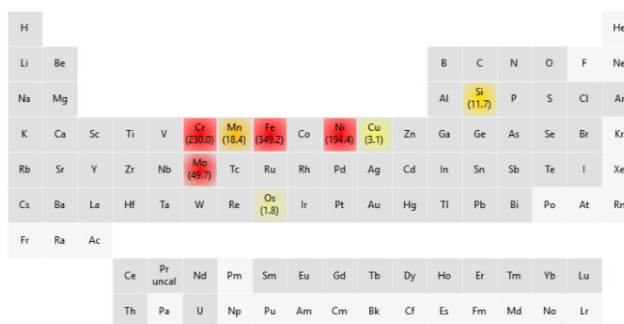

Figure 1. IntelliQuant generates a heatmap to visually present the relative concentrations of elements present in a sample

The heat map is easily customizable. For example, a food testing laboratory may set the high concentration limit as the maximum regulated concentration for a specific element, so non-compliant samples will be displayed with red on the periodic table.

A full wavelength spectrum (Figure 2) is also displayed after the scan, providing more information about the elements present and any potential intereferences. The peak detection threshold (the minimum peak height for an elemental wavelength to be included in the determination), can be set for all or some elements.
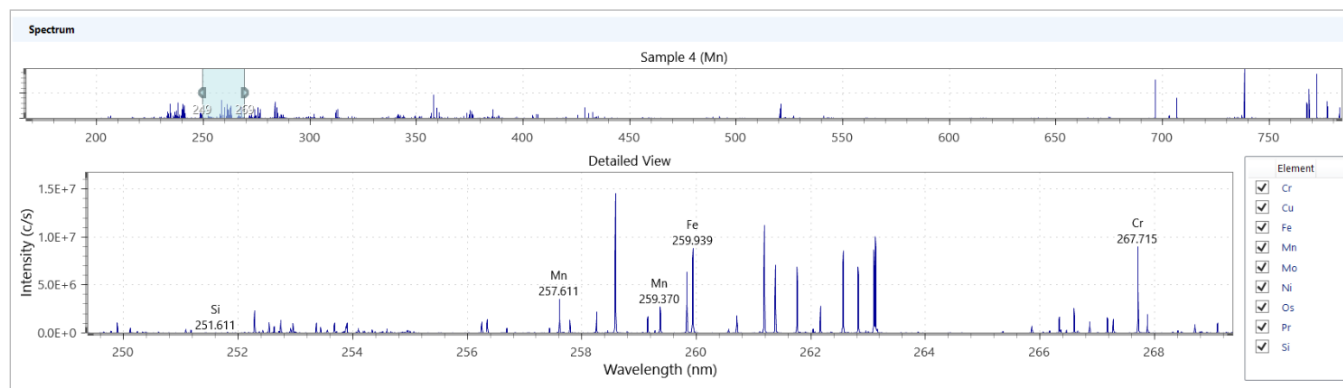
Figure 2. The IntelliQuant interface displays the full wavelength scan of the sample (top) and a detailed spectrum view of any selected wavelength range from the full scan, which includes labeled element peaks (bottom).

Simplify method development

When developing an ICP-OES method it's useful to know if any unknown elements are present, as they may cause spectral interferences with the elements of interest. The full scan obtained by IntelliQuant can guide wavelength selection, avoiding such interferences, thus simplifying the method development process.

IntelliQuant is also useful when the elements in a sample are completely unknown. The full wavelength scan generated can be used to determine which elements are present, allowing the analyst to then decide which should be quantitatively analyzed in a full ICP-OES analysis.

IntelliQuant data can also be used to identify appropriate calibration ranges for each element.

Address unexpected results

As the instrument reads all wavelengths for all elements during an IntelliQuant analysis, any wavelength used for semi-quantitative analysis can be changed after the analytical run is complete. This allows you to retrospectively analyze data at any time after the initial analysis.

For example, if a spectral interference is observed in an IntelliQuant spectrum an alternative wavelength can be selected and the concentration of the element is quickly and automatically reprocessed.

Example analysis

Five pre-digested Certified Reference Materials (CRMs), representing a range of sample types were analyzed using IntelliQuant on an Agilent 5110 SVDV ICP-OES. Results were obtained using an updated IntelliQuant calibration, with the IntelliQuant Calibration Kit multi-element standards being measured on the instrument during a standard analytical run. All measurements were taken in the Synchronous Vertical Dual View (SVDV) mode of the instrument.

Semi-quantitative recoveries for all elements in the food CRMs are shown in Table 1. Results for environmental CRMS are shown in Table 2. IntelliQuant's retrospective wavelength selection capabilities were utilized to avoid spectral interferences and achieve optimum semi-quantitative accuracy.

By changing the wavelengths used to estimate the concentrate of those elements that were being impacted by interference, it was possible to achieve recoveries for almost all measured elements in the five CRMs within ± 20% of the certified value. The accuracy of these results demonstrate IntelliQuant's potential as an extremely useful rapid screening tool.

References

CCD and CID solid-state detectors, Agilent publication 5991-4854EN, (2014).

Table 1. IntelliQuant semi-quantitative recoveries for elements in two food CRMs.

Element & wavelength (nm)	Orchard Leaves (CRM-OL)		Powdered Milk Solution (CRM-MP)	
	CRM Value (µg/mL)	IntelliQuant Value (µg/mL)	CRM Value (µg/mL)	IntelliQuant Value (µg/mL)
Aluminum 237.312	3	3	0.02	–
Arsenic 188.98	0.1	0.07	0.002	–
Barium 614.171	0.5	0.5	–	–
Cadmium 214.439	0.001	–	–	–
Calcium 318.127	200	204	130	136
Chromium 205.56	0.03	0.03	0.0003	–
Cobalt 230.786	0.002	–	0.0004	–
Copper 213.598	0.1	0.09	0.007	–
Iron 273.358	3	3	0.02	–
Lead 217.000	0.5	0.5	0.002	–
Magnesium 277.983	60	57	12	12
Manganese 293.931	1	1	0.003	–
Nickel 231.604	0.01	–	–	–
Phosphorus 177.434	20	20	100	99
Potassium 766.491	150	140	170	153
Selenium 196.026	0.0008	–	0.001	–
Silicon 243.515	5	7	–	––
Sodium 589.592	1	1	50	44
Vanadium 311.837	0.005	–	–	–
Zinc 334.502	25	30	0.5	0.6

Table 2. IntelliQuant semi-quantitative recoveries for elements in three environmental CRMs.

Element & wavelength (nm)	Estuarian Sediment Solution (CRM-ES)		Soil Solution B (CRM-SOIL-B)		Soil Solution A (CRM-SOIL-A)	
	CRM Value (µg/mL)	IntelliQuant Value (µg/mL)	CRM Value (µg/mL)	IntelliQuant Value (µg/mL)	CRM Value (µg/mL)	IntelliQuant Value (µg/mL)
Aluminum 237.312	700	705	700	720	500	534
Antimony 206.834	0.004	–	0.4	0.3	0.03	–
Arsenic 188.98	0.1	–	6	5	0.2	0.1
Barium 614.171	–	–	7	6.48	5	5
Beryllium 313.107	0.02	0.04	–	–	–	–
Cadmium 214.439	0.0004	–	0.2	0.2	0.003	–
Calcium 318.127	80	75	125	118	350	331
Chromium 205.56	0.8	0.8	0.4	0.4	–	–
Cobalt 230.786	0.1	0.1	0.1	0.1	–	–
Copper 213.598	0.2	0.2	3	3	0.3	0.3
Iron 273.358	350	288	350	309	200	189
Lead 217.000	0.3	–	60	58	0.4	0.3
Magnesium 277.983	100	89	80	74	70	62
Manganese 293.931	4	4	100	89	0.1	0.2
Nickel 231.604	0.3	0.3	0.2	0.2	0.3	0.3
Phosphorus 177.434	5	5	10	10	10	9
Potassium 766.491	150	150	210	189	200	192
Selenium 196.026	0.05	–	–	–	0.01	–
Silicon 243.515	3000	2430	3000	2460	3000	2390
Sodium 589.592	200	146	100	86	70	65
Thorium 283.73	0.1	–	0.1	–	0.1	–
Uranium 385.957	–	–	0.25	–	0.01	–
Vanadium 311.837	1	0.9	0.8	0.7	0.1	0.09
Zinc 334.502	1.5	1.6	70	74	1	1

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