

ICP-Optical Emission Spectroscopy

KEY BENEFITS

- Fully customizable interface for efficient and reliable semi-quantitative analysis
- Provides quick screening of new or previously analyzed samples for elemental composition
- Displays the data in heatmap overlays of the periodic table
- A powerful tool for method development and investigations

Knowing the Unknowns with SmartQuant, a Powerful Semi-Quantitative Tool for ICP Analysis

Introduction

When presented with a completely unknown sample, creating a method to accurately analyze its elemental

composition can be daunting. Determining which wavelengths work best for your target analytes or what calibration range is required can be a case of trial and error. In the same regard, even samples that are routinely analyzed can occasionally present challenges in the form of unexpected results from new or unknown interferences. But what if there was a tool that could aid in these situations? What if you could know the unknown in just a few clicks of a mouse? That is where SmartQuant™ can help.

What Is SmartQuant?

SmartQuant is a powerful semi-quantitative analysis software tool that comes standard in Syngistix for ICP software version 5.5 or higher. Utilizing the Universal Data Acquisition (UDA) feature built into every PerkinElmer Avio® 500/550/560 Max fully simultaneous ICP-OES, thousands of analytical wavelengths can be captured with every analysis. SmartQuant takes this data and displays it in a visual way with a customizable user interface. The software applies a user selectable SmartQuant calibration to provide semi-quantitative data in the form of color-coded heatmaps and data tables as well as the ability to view spectral graphs for wavelengths of the measurable elements in potentially any sample.

The Benefits of Knowing the Unknowns

By displaying semi-quantitative concentration data visually, SmartQuant provides users the ability to quickly identify key components within samples and the relative amount present, as well as comparing multiple wavelengths of the same element. Greater than 70 elements can be evaluated in any sample, in both axial and radial views. This is invaluable information whether developing new methods, investigating issues with previously analyzed samples, or troubleshooting. SmartQuant provides two convenient ways to screen samples – SmartScan and SmartQuant Data Review.

SmartScan provides rapid screening of an unknown sample. You simply provide a name for the sample, choose a calibration to

apply, a database to save to, an autosampler position where the sample is placed, and click the “Scan” button. The periodic table is then overlaid with a heatmap representing the concentrations of elements. Semi-quantitative concentration values are also displayed below each element symbol included in the scan (Figure 1).

SmartQuant Data Review applies a semi-quantitative calibration to any previously analyzed UDA samples to view the composition of the samples beyond what was quantified by the original calibration. All the displayed information is interactive (Figure 2). By clicking on a sample table row, a spectrum or an element symbol, all other displays will “snap” to the related data. As well, clicking on spectra can include or exclude that wavelength from the concentration calculation in the heatmap. If desired, the data table can be quickly and easily exported as an excel spreadsheet.

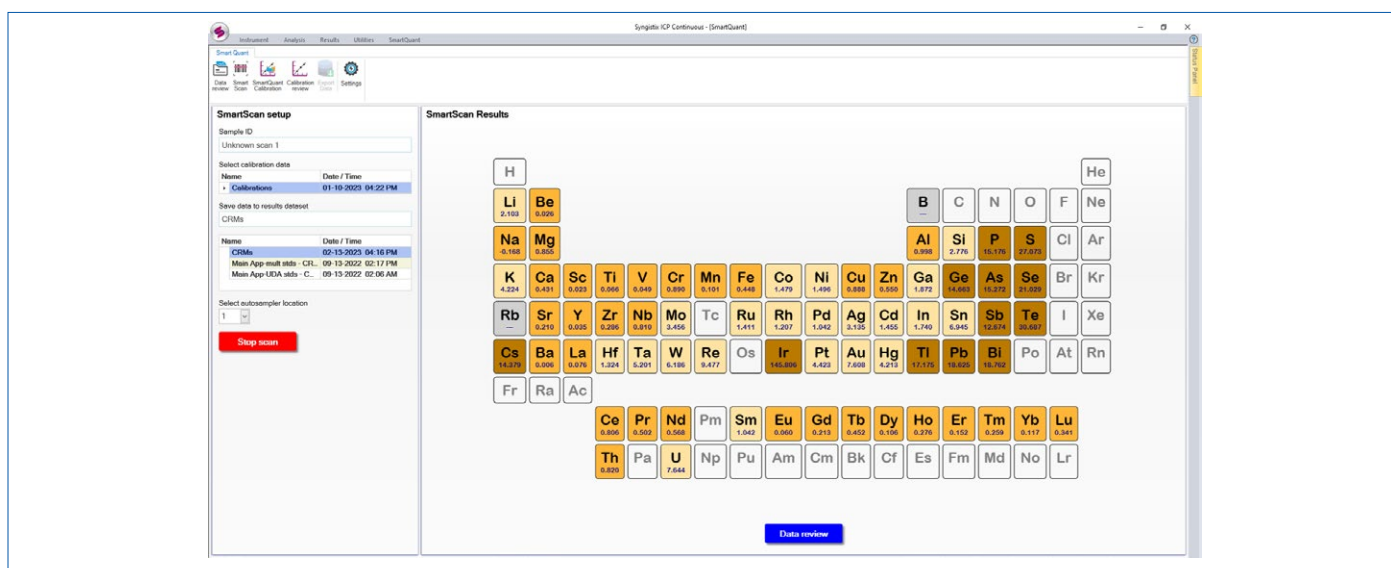


Figure 1: Example of SmartScan results with heatmap.

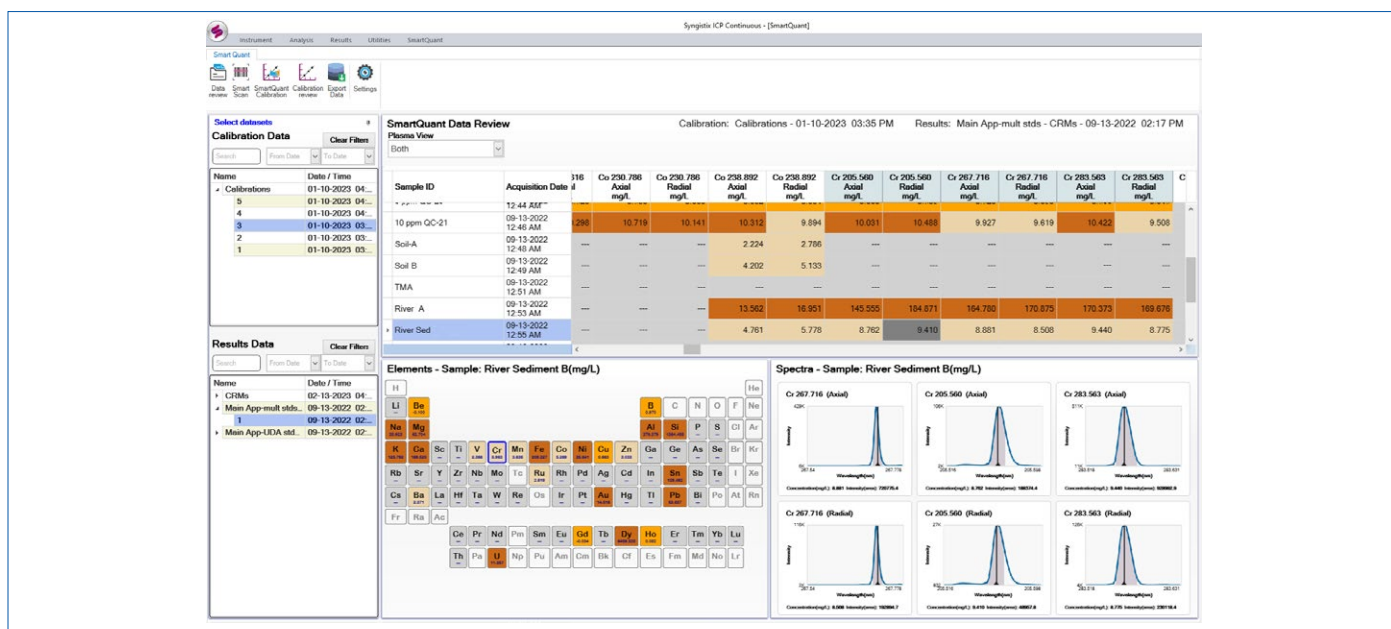


Figure 2: Example of SmartQuant Data Review.

Investigating Erroneous Results

Although the goal of most methods is to be robust and deliver reliable data, there are occasions where unexpected interferences can cause questionable results. SmartQuant Data Review can help in these investigations by visually highlighting discrepancies and allowing users to dive into the spectral data directly. In an

example, Figure 3a shows a QC sample where all wavelengths of cobalt are showing matching results. However, erroneously high concentrations of cobalt are identified in a sample for just one wavelength of cobalt in both axial and radial views (Figure 3b). The spectra show that there is a large shoulder interference on Co 238.882 nm, explaining the false positive results.

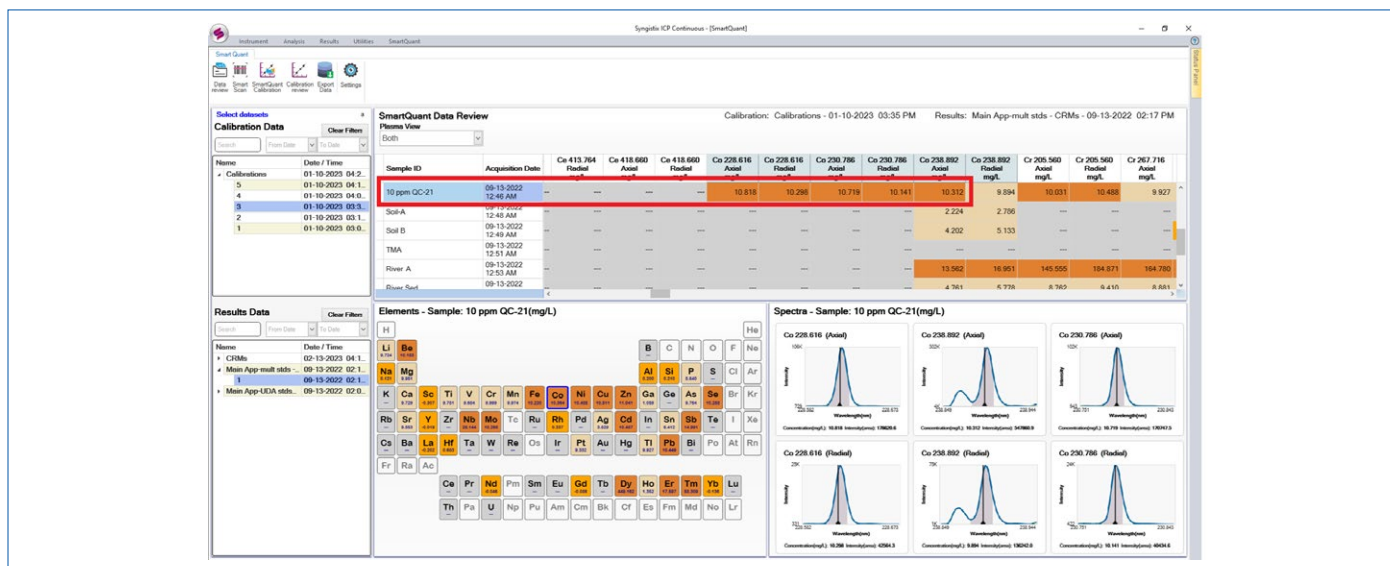


Figure 3a: Example of SmartQuant Data Review, showing the 10 ppm QC standard has matching values for all included cobalt wavelengths.

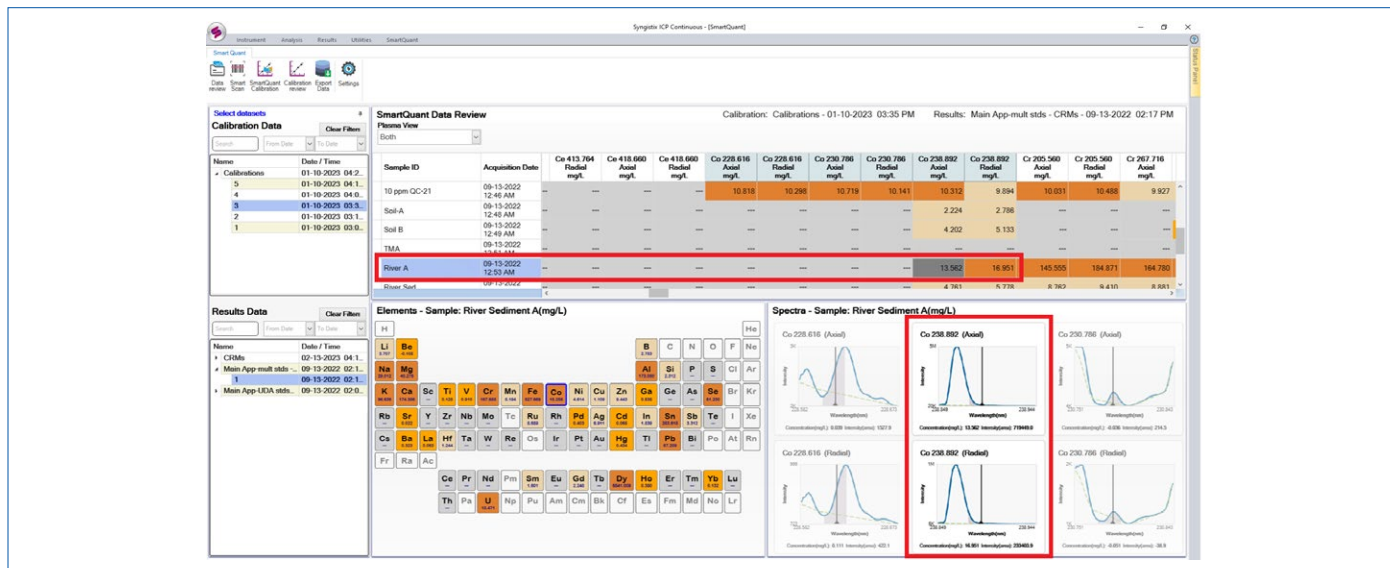


Figure 3b: Example of SmartQuant Data Review, showing a large interfering wavelength near the target wavelength of Co 238.882 nm, causing an erroneously high result for this wavelength of cobalt. All other wavelengths are below the threshold level selected.

Your Data, Your Choice

Tailoring your preferences to ensure an optimal workflow, custom settings allow for managing how your data is handled and how it is displayed (Figure 4). Customize the heatmaps and data ranges to your needs. Set a threshold level to disregard data below a signal-to-background ratio of your choosing. Even customize the colors and decimal places display settings that help you best visualize your data.

Calibrations That Are Fit-For-Purpose

While a universal calibration is convenient, sometimes greater specificity is beneficial. Choose from either using default calibration methods or create a custom calibration method (Figure 5) by importing the method parameters and settings from your current methods. Basing a SmartQuant calibration off an existing quantitative method allows you to use plasma parameters suited to the sample matrix and select the calibration standards to be used. Custom calibrations can include single or multiple points and can be specified on an element-by-element basis, providing increased accuracy. The analyte list can be edited using the interactive periodic table.



Figure 4: SmartQuant, a fully customizable interface.

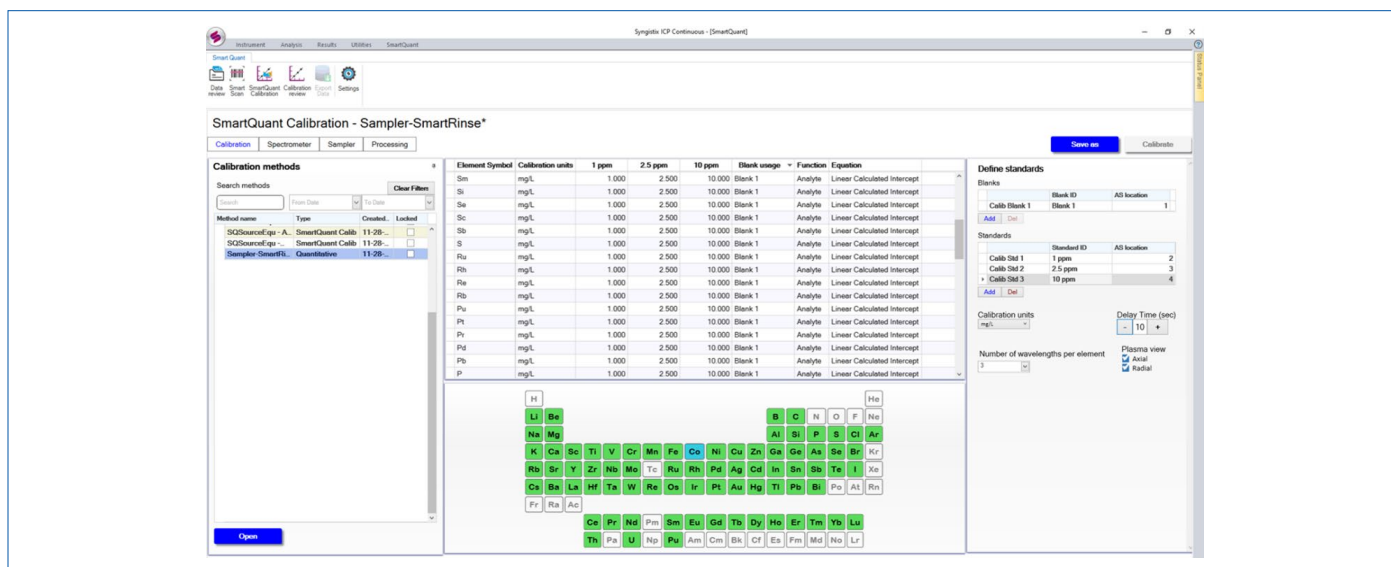


Figure 5: Create custom SmartQuant calibrations by importing settings from existing methods and selecting the elements and calibration standards to be used.

With the option of using custom calibrations, a means to review these calibrations can be useful. Calibration Review (Figure 6) does just that, allowing review of the calibration that has been created to be used and the ability to view down to individual wavelengths. Calibration statistics such as correlation coefficient and residual values are also viewable for any wavelength in the calibration.

Summary

SmartQuant, a powerful semi-quantitative analysis software tool available in Syngistix for ICP version 5.5 or higher, leverages the UDA capability built into every Avio® 500/550/560 Max fully simultaneous ICP-OES to aid in your understanding of the elemental composition within your samples and in interpreting the data. It can help by quickly screening new sample types or

previously analyzed samples for elemental composition and then displaying the data in heatmap overlays of the periodic table, semi-quantitative concentrations displayed in a data table, and spectral images of any wavelength in any sample when drilling-down into the data.

SmartQuant also allows you to customize how you view and screen your samples, providing both pre-defined methods or the option of converting your existing methods to match your plasma conditions and settings to sample types of interest, as well as customizable calibrations to suit your needs. Customization extends to how your heatmaps are displayed, threshold filters to reduce marginal results, and resizable panels with fully interactive data, allowing users to investigate by clicking on what catches their attention.

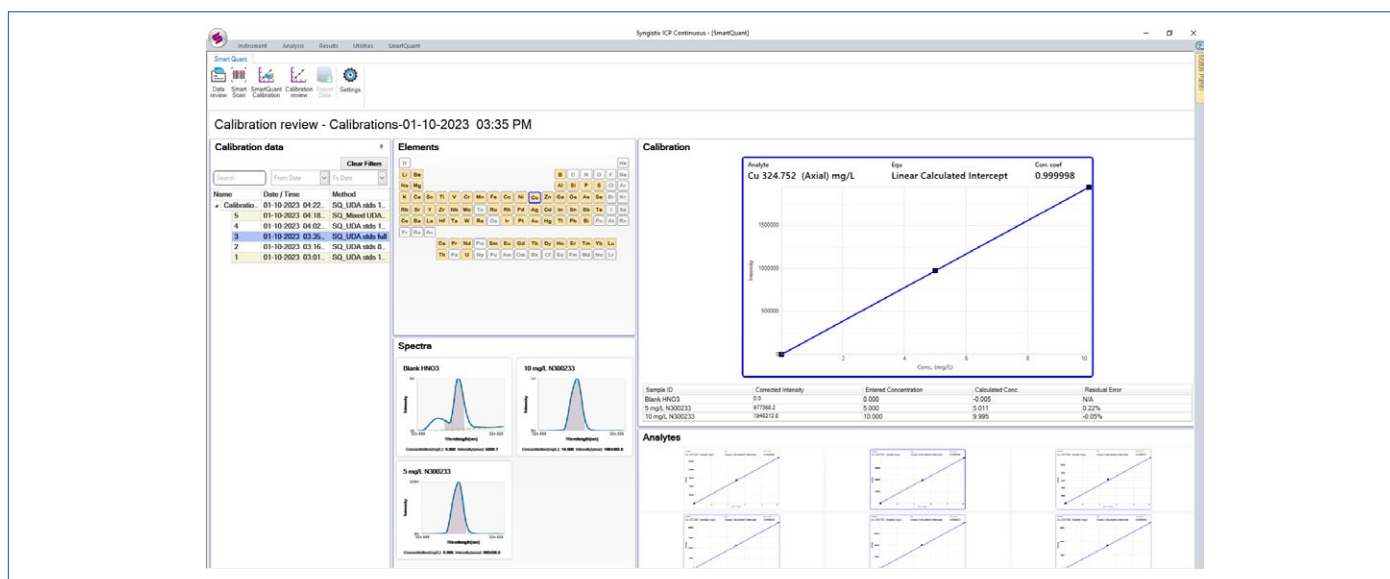


Figure 6: Calibration Review provides access to the calibration curves within any SmartQuant calibration.