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Trace elemental analysis

Thermo Scientific iCAP PRO Series ICP-OES
Discover more with the SemiQuant feature of Thermo Scientific Qtegra ISDS Software

Semi-quantitative analysis can be carried out by inductively coupled plasma-optical emission spectroscopy (ICP-OES) and involves determining the relative concentrations of elements in a sample rather than obtaining precise quantitative measurements. The semi-quantitative approach is often used for rapid screening of samples or for identifying elemental composition trends rather than obtaining exact concentrations.

Interpretation of semi-quantitative analysis may involve identifying major and minor elements present in the sample, detecting elemental trends or patterns, or comparing the elemental composition of different samples.

What is SemiQuant?

The SemiQuant feature within the Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software is a data acquisition tool leveraging Artificial Intelligence and employing deep neural networks to simplify the complex process of intra- and inter-element correction, selecting only non-interfered peaks, automatically. This supports fast screening of samples to gain insights into sample composition. It can be a useful aid in method development and enables the collection and archiving of approximate elemental concentrations of a broader range of analytes in the samples in case they can be of interest at a future date.

Its unique implementation allows users to get a good understanding of the presence of certain elements in their sample and also offers the concentration amount and a level of confidence for the given concentration to allow the best possible interpretation of the results.

All SemiQuant results are obtained without the need to run any calibration solutions.

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How can SemiQuant be used?

SemiQuant analysis can be a valuable tool during method development in several ways:

- **Preliminary screening –** SemiQuant analysis allows for rapid screening of samples to determine their elemental composition. During method development, this can help identify the presence of major and minor elements in samples, providing insights into the scope of the method and potential interferences.

- **Evaluation of sample preparation methods –** Different sample preparation methods may be required depending on the matrix and elements of interest. SemiQuant analysis can be used to assess the effectiveness of various sample preparation techniques, such as digestion methods, extraction procedures, or dilution factors. This allows users to optimize sample preparation protocols for subsequent quantitative analysis.

- **Assessment of method performance –** SemiQuant analysis provides an initial assessment of method performance, including precision, accuracy, and detection limits. By comparing SemiQuant results obtained from different samples, users can evaluate the robustness and reliability of the method before proceeding to quantitative analysis.

- **Identification of interferences –** During method development, it is essential to identify and mitigate potential interferences from matrix components. The SemiQuant feature can help detect elements that can cause interferences on the wavelengths selected for quantitative analysis.

SemiQuant integration within Qtegra ISDS Software

The SemiQuant feature within the Qtegra ISDS Software is simple to use, and results can be obtained with just three simple steps.

Step 1: Select elements of interest or simply all elements that can be analyzed by the SemiQuant feature

Step 2: Select specific or all samples in the sample list for collection of SemiQuant results

Step 3: View results and make informed decisions with the help of visual aids. Multiple views are available, which give a broad overview of elemental composition up to detailed results for each element.
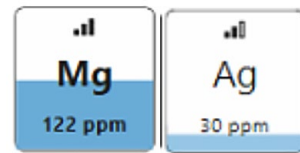
Figure 2. Element View showing SemiQuant result in concentration (ppm) and confidence level

Figure 1. Periodic Table View for the selection of SemiQuant elements

SemiQuant results

Different multielement solutions were measured with the SemiQuant feature.

For the majority of elements, the concentrations determined by the SemiQuant feature were within ±15% of the expected values. The accuracy of the semi-quantitative results may differ in varying matrix samples; however, typically the SemiQuant measurements are within ±30%.
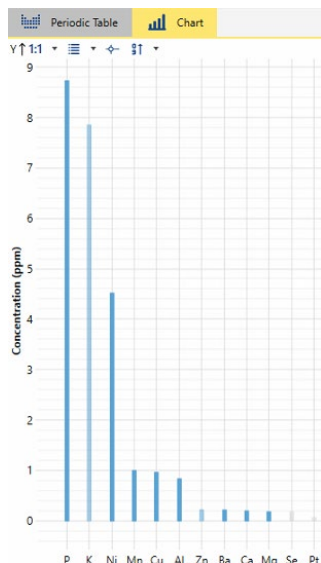

Figure 3. Chart view of SemiQuant results

Table 1. SemiQuant concentration results for multielement solution 1 in mg/L

Element	Expected concentration	SemiQuant measured concentration	Recovery in %
Al	20	18	90
Ba	20	21	105
Co	5	5.3	106
Mn	5	4.6	92
Ni	5	4.7	94
V	5	4.9	98
Zn	5	5	100
Cu	2.5	2	80
Cr	2	2	100
Be	0.5	0.47	94
Cd	0.5	0.57	114

Table 2. SemiQuant concentration results for multielement solution 2 in mg/L

Element	Expected concentration	SemiQuant measured concentration	Recovery in %
Cu	11	11	100
Fe	20	18	90
Pb	10	11	110
As	1	0.95	95
Al	1	0.94	94
P	10	8.5	85
Zn	0.2	0.21	105
Ni	5	4.4	88
Mn	1	0.95	95
Mg	0.2	0.17	85
Ba	0.2	0.21	105
Ca	0.2	0.23	115

Table 3. SemiQuant concentration results for low-level multielement solution in mg/L

Element	Expected concentration	SemiQuant measured concentration	Recovery in %
Al	0.01	0.01	100
Be	0.035	0.039	111
Co	0.008	0.008	100
Ga	0.01	0.011	110
Mg	0.01	0.01	100
Mn	0.006	0.006	100
Ni	0.015	0.014	93
Sc	0.008	0.007	88
Sr	0.005	0.006	120
Zn	0.02	0.02	100

The SemiQuant feature is unleashing the full potential of the iCAP PRO Series CID detector with a groundbreaking AI approach. It harnesses the full emission spectrum to identify any signal interferences and decipher the elemental concentrations, delivering valuable insights and preliminary data. By leveraging the advantages of the SemiQuant feature during method development, users can streamline the optimization process, improve method performance, and enhance the quality of analytical results.

Learn more at **thermofisher.com/icp-oes**