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TECHNICAL NOTE 43399

Linear dynamic range performance of the Thermo Scientific iCAP Qnova series ICP-MS

Keywords
CCT, iCAP RQ ICP-MS, iCAP TQ ICP-MS, KED, Linear dynamic range, Resolution, Skimmer inserts

Introduction

ICP-MS is a technique with high sensitivity and specificity and is typically used in applications where the lowest limits of detection are required. 'Real world' samples contain a very wide range of element concentrations, sometimes greater than 10 orders of magnitude, which makes complete quantitation of all analytes in a single measurement particularly challenging.

This Technical Note details the range of techniques available with the Thermo Scientific™ iCAP™ Qnova series ICP-MS instruments for meeting ng·L^{-1} detection goals for trace elements while optimizing sensitivity for specific matrix analytes during a single data acquisition. The unique combination of hardware and Thermo Scientific Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software control provides the user with a complete analysis of the sample during one sample acquisition.

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The mass spectrometer detector

The detector of both the Thermo Scientific™ iCAP™ RQ ICP-MS and Thermo Scientific™ iCAP™ TQ ICP-MS utilizes a simultaneous combination of Pulse and Analog Counting with accurate Cross Calibration to provide the analyst with a Linear Dynamic Range (LDR) of 10 orders of magnitude.

The very high sensitivity and very low detector background count rate of both systems means that it is capable of ultratrace element analysis at ng·L^{-1} levels and below. The wide LDR means that the most sensitive elements will have a linear calibration up to ~5 ppm and we show that for less sensitive elements or attenuated signals we can calibrate up to 5000 ppm.

Linear dynamic range detector performance

To demonstrate the linearity of the detector ^{175}Lu was chosen as the analyte since very low blanks can be measured for this element. This linearity will apply to any isotopes measured up in the count rate range of 0.1 cps to over 10^9 cps (equivalent to over 10 orders of linear dynamic range) (Figure 1). The built-in linearity may also be combined with a choice of interface technology to meet the analytical goals of the user.

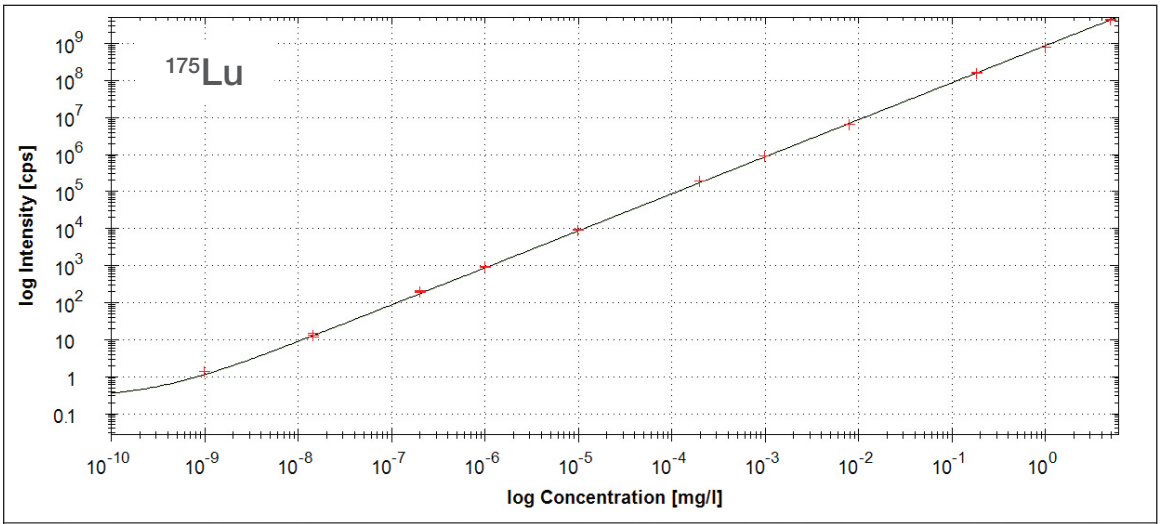
High concentration calibration

The iCAP Qnova series ICP-MS instruments have a range of skimmer inserts (Figure 2) to customize the extraction of ions from the argon plasma. The interchangeable skimmer inserts are a simple and cost effective way to tailor the instrument to the user's application(s).

Robust 4.5 mm	High Matrix 3.5 mm	High Sensitivity 2.8 mm

Figure 2. Skimmer Cone Inserts.

Compared with the standard 3.5 mm skimmer cone insert, the 4.5 mm insert enables measurement of higher concentrations of matrix elements while maintaining the simultaneous measurement of ultratrace elements in the ng·L^{-1} range.



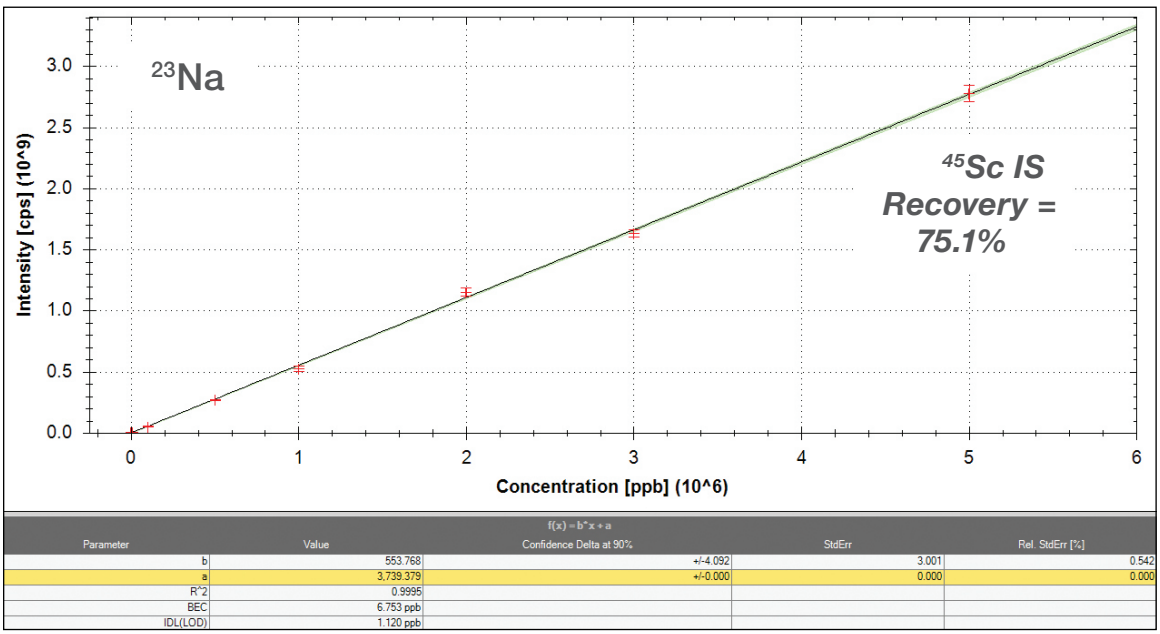
f(x) = b*x + a

Parameter	Value	Confidence Delta at 90%	StdErr	Rel. StdErr [%]
b	848,679,202.040	+/-5,606,796.990	4,112,363.935	0.485
a	0.267	+/-0.000	0.000	0.000
R^2	1.000			
BEC	0.000 mg/l			
IDL(LOD)	0.000 mg/l			

Figure 1. ^{175}Lu calibration curve in log scale from 1pg·L^{-1} to 5 mg·L^{-1}. The background of the blank was <0.3 cps, with over 10 orders of magnitude dynamic calibration range to 5 mg·L^{-1} at 8.57 Gcps with an excellent correlation coefficient of R^2=1.000.

Figure 3 shows calibration of ^{23}Na from 0.0005 to 0.5% using the 4.5 mm skimmer cone insert. Since Na is monoisotopic with a relatively low ionization potential, ICP-MS response is typically very sensitive. This calibration curve demonstrates that it is possible to measure a very wide range of concentrations for sensitive elements, maintaining excellent linearity (as shown by the R^2 of 0.9995) with a low BEC of 6.7 ppb. In addition, the robustness of the interface is demonstrated by the excellent ^{45}Sc Internal Standard recovery of 75.1% at the 5000 ppm ^{23}Na concentration.

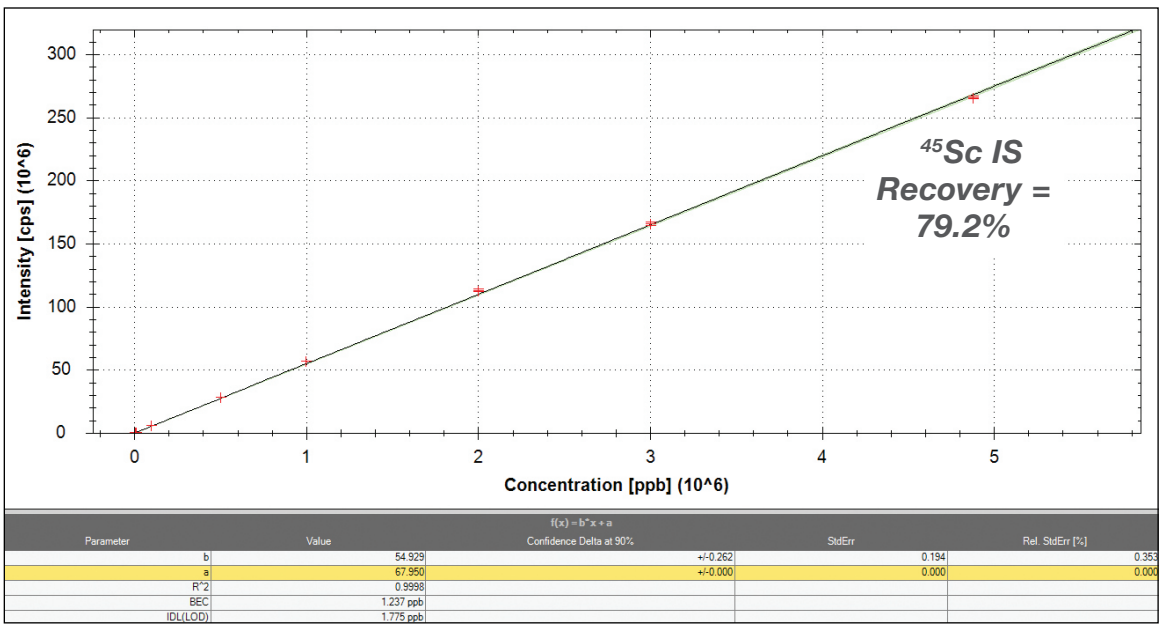
Compared to ^{23}Na, ^{43}Ca is a low abundance isotope (naturally occurring at 0.14%), so a 0.5% Ca standard gives a much lower ICP-MS response. Even with the 4.5 mm skimmer cone insert, however, the sensitivity is sufficient to provide a BEC of 1.2 ppb with a linear response up to 5000 ppm as shown by the R^2 of 0.9998. Internal Standard recovery of 79.2% for the 5000 ppm Ca standard again highlights the robustness of the interface and the ability of the 4.5 mm insert to reduce matrix suppression effects in 0.5% TDS samples. Furthermore, the reduced dilution requirement and elimination of additional analysis settings, (such as a gas dilution method set-up), improves laboratory productivity and running costs.



f(x) = b*x + a

Parameter	Value	Confidence Delta at 90%	StdErr	Rel. StdErr [%]
b	553.768	+/-4.092	3.001	0.542
a	3,739.379	+/-0.000	0.000	0.000
R^2	0.9995			
BEC	6.753 ppb			
IDL(LOD)	1.120 ppb			

Figure 3. 5 – 5000 mg·L^{-1} calibration for ^{23}Na.



f(x) = b*x + a

Parameter	Value	Confidence Delta at 90%	StdErr	Rel. StdErr [%]
b	54.929	+/-0.262	0.194	0.353
a	67.950	+/-0.000	0.000	0.000
R^2	0.9998			
BEC	1.237 ppb			
IDL(LOD)	1.775 ppb			

Figure 4. 5 – 5000 mg·L^{-1} calibration for ^{43}Ca.

Software controlled analysis modes

Each analysis mode has its own unique autotune and performance validation

1. Standard Mode offers high sensitivity that, when combined with very low detector background noise (<0.5 cps), delivers sub ng·L^{-1} detection limits for many elements; however, depending on the matrix, polyatomic and isobaric interferences may compromise the data by increasing the background at the isotope being measured. The interferences may be mathematically corrected, but the accuracy of the data will be compromised if the interference count rates are high relative to the analyte e.g. $^{40}Ar^{35}Cl$ interferes significantly with ^{75}As.

2. He Mode, together with the very low detector background count rate, is the preferred mode of data acquisition when some interferences are expected since most of the common polyatomic interferences are efficiently eliminated using a 4 to 6 mL·min^{-1} Helium gas flow in the QCell.

   He KED Mode attenuates the low to mid mass range and enables calibration to higher concentration levels whilst maintaining detection limits well within the ng·L^{-1} range.

3. On-the-Fly Resolution Switching allows data for each isotope in the method to be collected in the most sensitive Normal Resolution mode or attenuated using High Resolution Mode (0.3 amu) to shift the LDR to higher concentrations (Figure 5). The accuracy of the mass calibration allows single point data acquisition at the peak maximum to optimize counting statistics and results in highly efficient data acquisition in both resolutions.

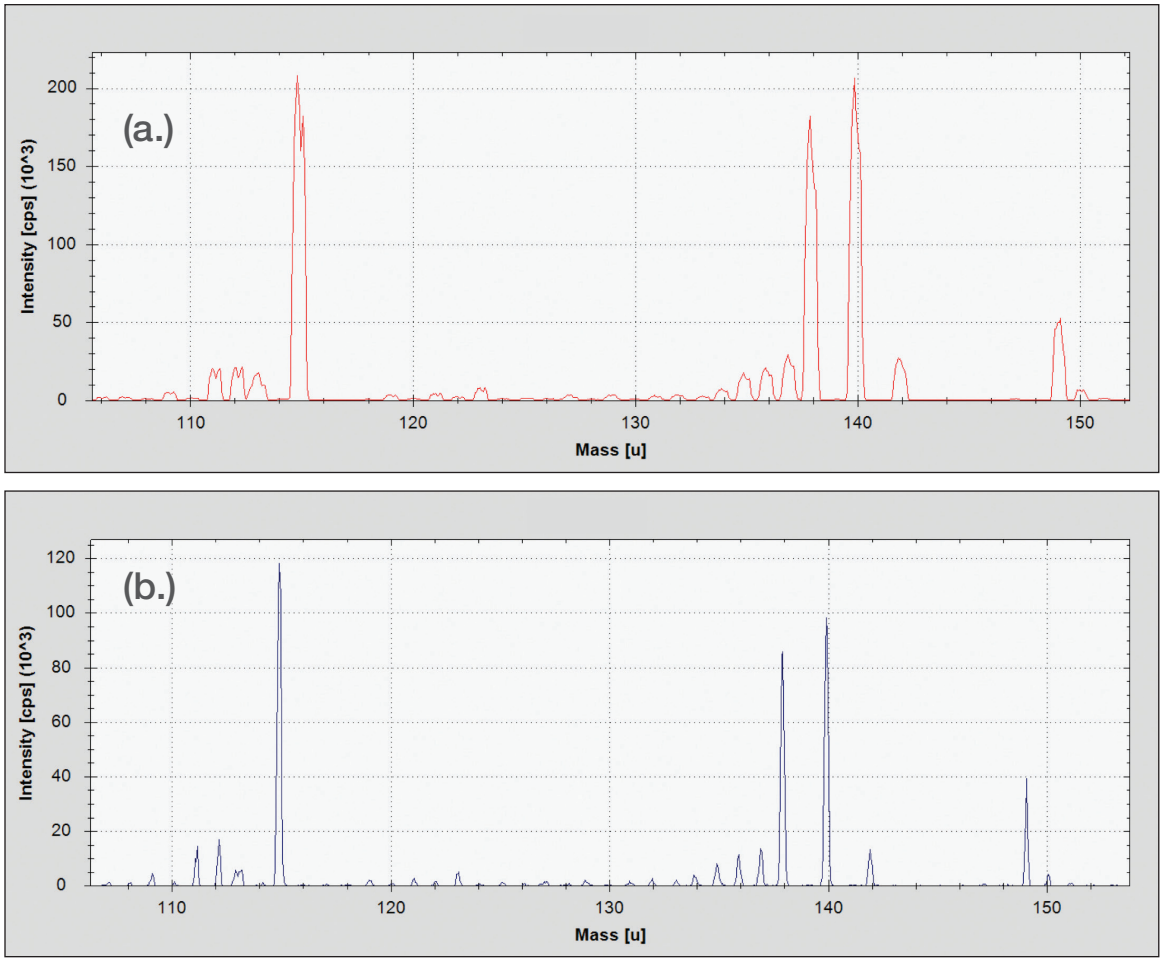


Figure 5. Mass spectra of the iCAP RQ ICP-MS 1 ppb tune solution in the mass range 105 to 155 amu in (a.) normal resolution, (b.) high resolution.

4. CCT Mode may be selectively applied to isotopes that have no interferences in order to improve sensitivity by 'collisional focusing' with a typical He gas flow range of 7 to 10 mL·L^{-1}. This is particularly useful for low level ^{9}Be analysis and Uranium isotope ratios.

5. Alternative isotopes of multi-isotopic elements may be used for quantitation to extend the dynamic range. Since the relative abundance of each isotope of a naturally occurring element is unique, choosing a low abundance isotope will enable calibration of a higher concentration range. Qtegra ISDS Software allows the use of more than one isotope per element such that the dynamic range may be further extended e.g. by a factor of 6 if using both ^{60}Ni (26.1%) and ^{62}Ni (3.9%).

Conclusion

The iCAP Qnova series ICP-MS combines:

- Over 10 orders linear dynamic range for one-shot analysis.
- Very low background counts for excellent detection limits.
- Easily interchangeable skimmer inserts to tailor the instrument to the application requirements.
- Wide choice of isotope specific data acquisition modes for optimum data acquisition.

The hardware and software works seamlessly together to provide the user with the ideal system for quantifying all of the elements in many types of samples using a single data acquisition method under optimum conditions for each element.

The unique combination of hardware and software make the iCAP Qnova series ICP-MS extremely versatile, able to meet the most challenging applications in trace elemental analysis.

Find out more at **thermofisher.com/ICP-MS**

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