

Thermo Scientific iCAP Qnova series ICP-MS

– Mass stability

Keywords

Calibration, KED, Mass accuracy, Mass stability

Introduction

Mass stability with quadrupole ICP-MS instruments is very important for accurate and reliable analytical measurements. When making ICP-MS measurements there are generally two approaches – scanning and peak jumping. Scanning involves taking number of measurements across a number of channels over the peak profile whereas peak jumping measures a single point which is usually the peak maximum.

In routine ICP-MS measurements when the lowest detection limits are required the typical approach is to use single point peak jumping at the peak maximum and not waste valuable analytical time on the sides of the peak where the signal to noise is poorer. To carry out peak jumping at a single point it is essential that the mass stability of the quadrupole is good enough to reproducibly go to the same mass point each time. The best detection limits for a given integration time will always be achieved if good mass stability can be guaranteed.

One of the main factors that will affect mass stability in ICP-MS is temperature. Thermal stability of the quadrupole power supply is a factor and relates directly to the laboratory environment where the ICP-MS instrument is installed. The Thermo Scientific™ iCAP™ Qnova series ICP-MS instruments are designed to operate at laboratory temperatures of 15 to 35 °C with an optimum operation temperature of 18 to 21 °C.

Many standardised analytical methods including US FDA and US EPA require that the ICP-MS instrument is checked for mass calibration and resolution to make sure that the peaks are in the correct position and of the correct width. US EPA methods state that specific criteria should be met prior to any analytical samples being measured. These criteria include the mass calibration not differing by more than 0.1 amu from the true value and that the resolution must be verified to less than 0.9 amu full width at 10% peak height.

This document details how the Thermo Scientific™ iCAP™ RQ ICP-MS and the Thermo Scientific™ iCAP™ TQ ICP-MS meet the specifications for mass calibration stability and how the Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution (ISDS) Software allows for these mass calibration tests to be performed automatically within a performance report to ensure the system is suitable for method compliant measurements.

Sample Analysis

All data acquisition was acquired with an iCAP RQ ICP-MS with default sample introduction system and interface. Equivalent function and performance is also provided for the iCAP TQ ICP-MS. Performance reports are supplied with Qtegra ISDS Software and are automatically associated to the measurement mode being used for data acquisition. For this work, performance reports were acquired in standard mode, no gas (STD) and He mode with kinetic energy discrimination (KED) using the default 1 ppb tune solution that contains Ba, Bi, Ce, Co, In, Li and U in 2% HNO₃ and 0.5% HCl.

Mass stability data was acquired by running consecutive performance reports over a period of 48 hrs and compiling the data from the reports into a time based excel plot.

⁷Li

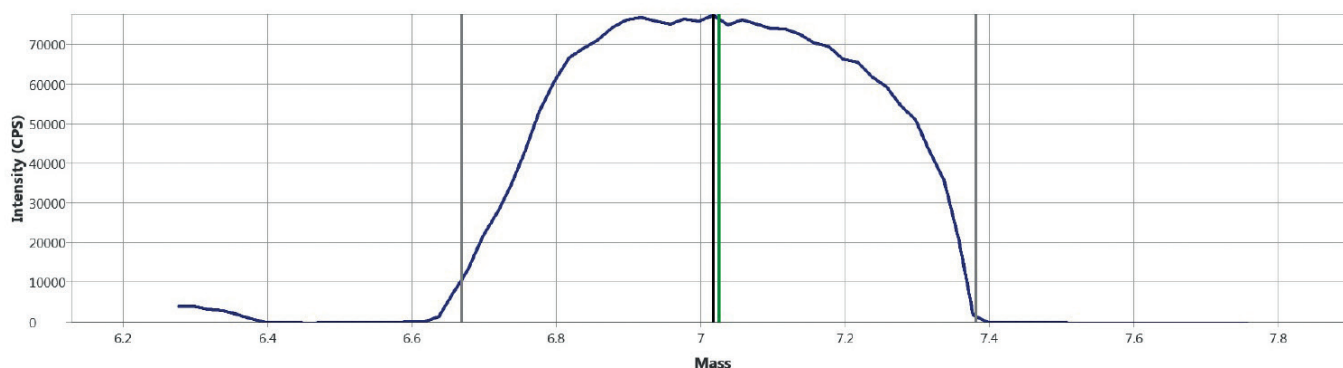


Figure 2. Peak profile for ⁷Li from the Qtegra ISDS Software performance report.

Results

Performance reports acquired using iCAP RQ ICP-MS and iCAP TQ ICP-MS instruments run a series of tests to validate the instrument performance prior to acquiring analytical data.

The measurement protocol includes a mass calibration check, sensitivity and background checks alongside oxide and doubly charged ion formation checks. The short term stability over a series of measurements is also monitored and reported.

A typical mass calibration test is shown in Figure 1 below measured at 4 masses across the mass range acquired using the standard performance report within Qtegra ISDS Software. The peak offset is recorded and the full width at 10% peak height to comply with current legislative methods.

Mass Calibration Test

Result	Channels	Dwell	MeasureWidth	PointSpacing	Sweeps
Passed	75	0.04	1.5	0.02	5

Analyte	Result	Centroid	Offset	Peak Width	Peak Width Min	Peak Width Max
⁷ Li	Passed	7.0241	0.0081	0.714	0.650	0.850
⁵⁹ Co	Passed	58.9284	0.0048	0.718	0.650	0.850
¹¹⁵ In	Passed	114.8815	0.0224	0.745	0.650	0.850
²³⁸ U	Passed	238.0581	0.0073	0.693	0.650	0.850

Figure 1. Mass calibration test from the Qtegra ISDS Software performance report.

It is shown in the tables that the measured offset is significantly below the 0.1 amu set out in EPA standards and that the peak width is below 0.9 amu across the mass range.

The peak profiles for the 4 measured masses are also displayed in the report showing the true and measured peak position (Figures 2-5)

⁵⁹Co

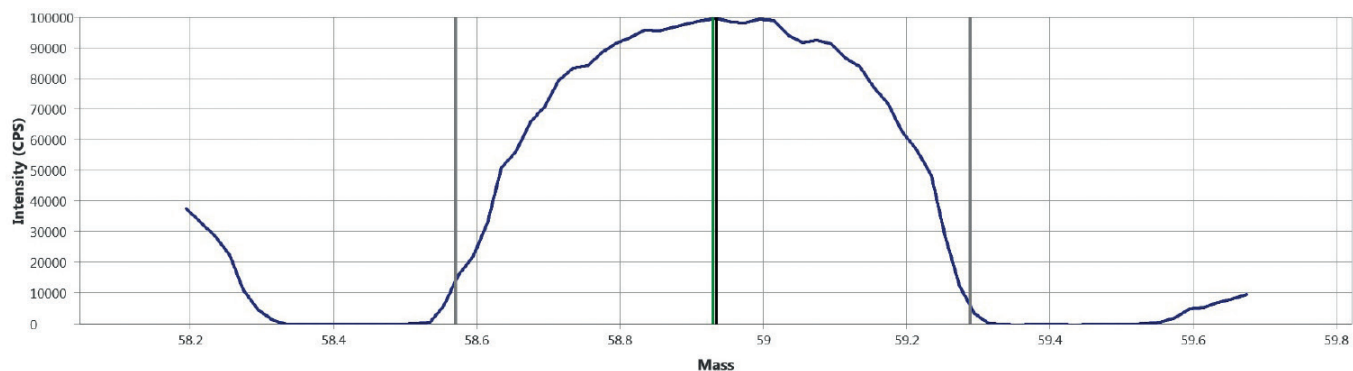


Figure 3. Peak profile for ⁵⁹Co from the Qtegra ISDS Software performance report.

¹¹⁵In

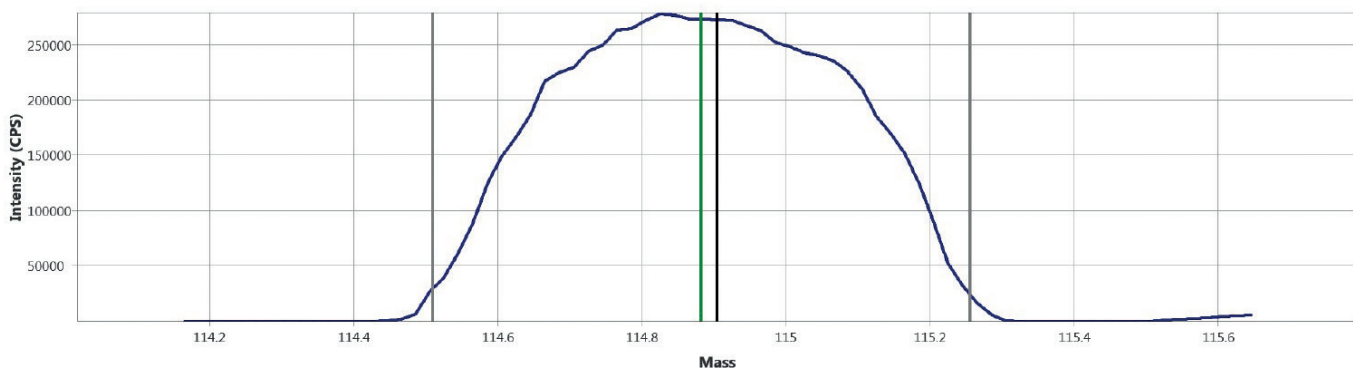


Figure 4. Peak profile for ¹¹⁵In from the Qtegra ISDS Software performance report.

²³⁸U

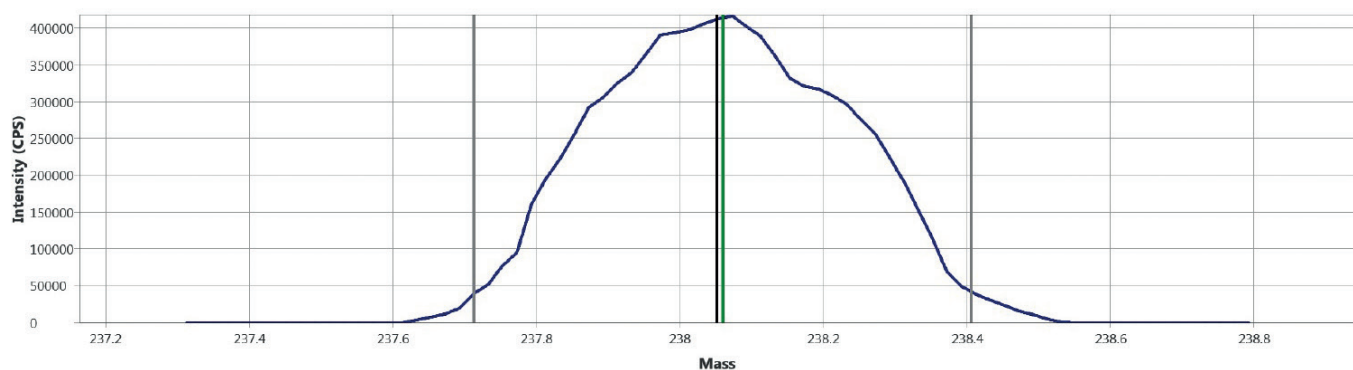


Figure 5. Peak profile for ²³⁸U from the Qtegra ISDS Software performance report.

The performance reports are automatically stored within Qtegra ISDS Software along with all the instrument settings to demonstrate that the instrument is suitable for analytical measurements. This information can easily be recalled and viewed for validation of analytical measurements.

To determine long term mass stability for an iCAP RQ ICP-MS instrument, performance reports were acquired in STD and KED mode over a 48 hour period and the data collated (Figures 6-12).

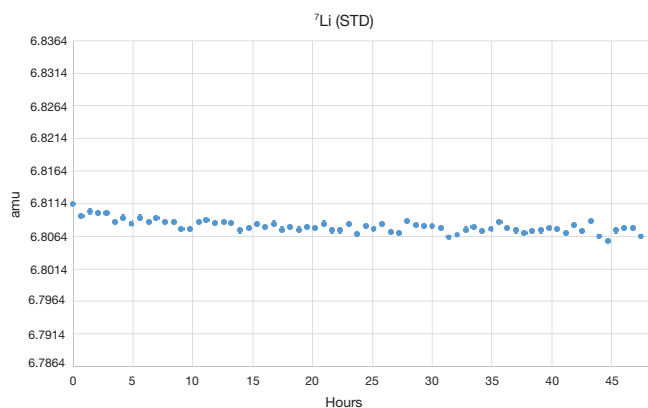


Figure 6. Mass stability over 48 hours for ${}^7\text{Li}$ (STD).

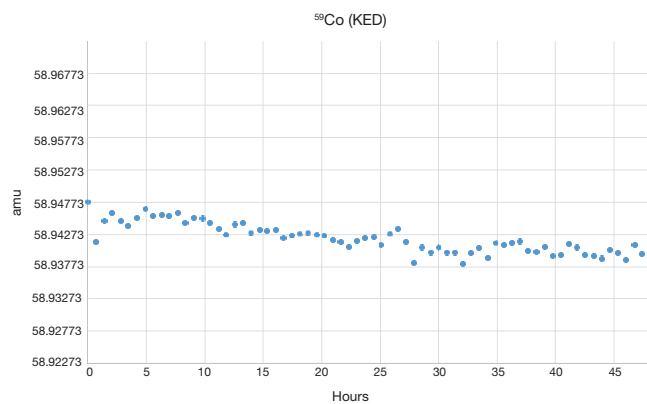


Figure 10. Mass stability over 48 hours for ${}^{59}\text{Co}$ (KED).

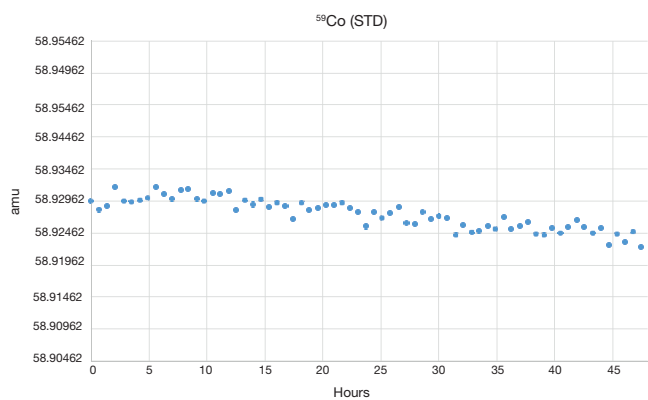


Figure 7. Mass stability over 48 hours for ${}^{59}\text{Co}$ (STD).

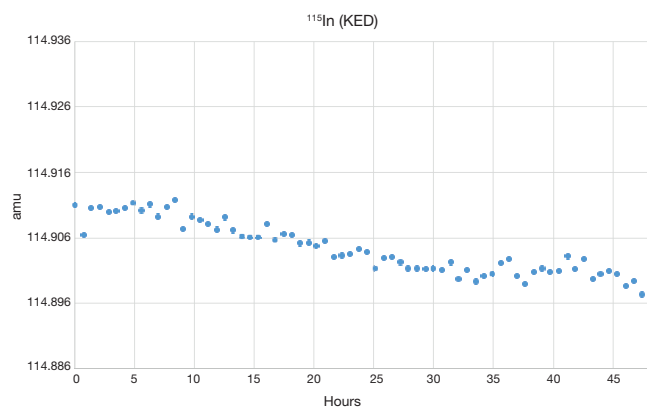


Figure 11. Mass stability over 48 hours for ${}^{115}\text{In}$ (KED).

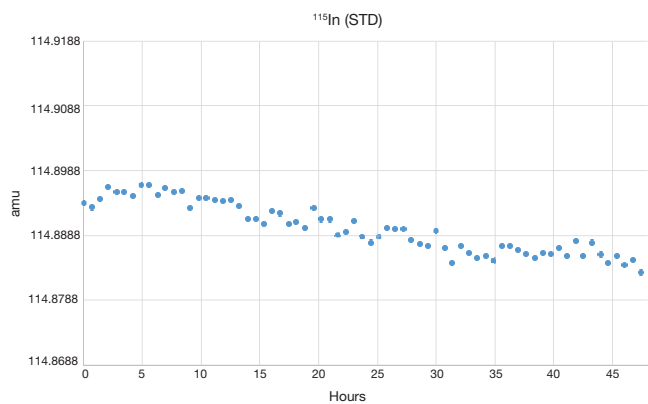


Figure 8. Mass stability over 48 hours for ${}^{115}\text{In}$ (STD).

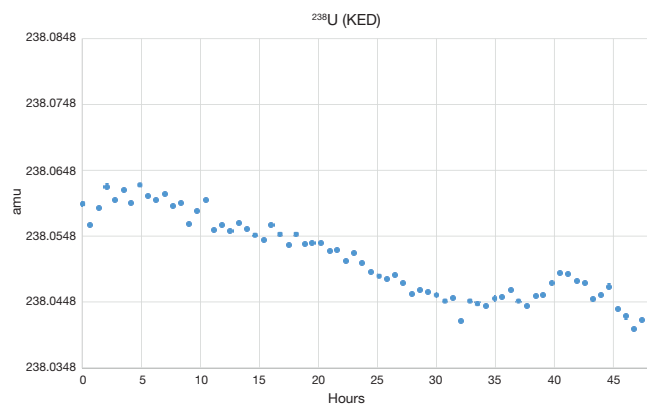


Figure 12. Mass stability over 48 hours for ${}^{238}\text{U}$ (KED).

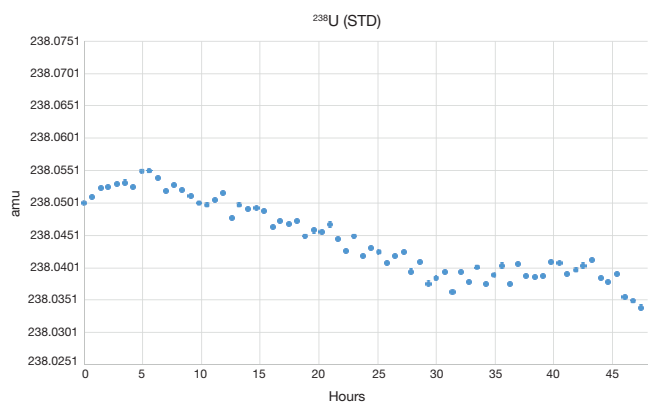


Figure 9. Mass stability over 48 hours for ${}^{238}\text{U}$ (STD).

The vertical axis of each of the graphs has been scaled to the specification limit of the iCAP RQ ICP-MS at ± 0.025 amu per 24 hr and these show clearly that in both STD and KED modes of operation all of the masses fall well inside of the required stability limits over a period of 48 hr. This demonstrates the excellent mass stability over extended time periods.

Conclusion

Mass stability is extremely important when making ICP-MS measurements particularly when operating in routine single point peak jumping mode to acquire data. The iCAP RQ ICP-MS and the iCAP TQ ICP-MS have a mass stability specification of ± 0.025 amu per 24 hours. The mass stability shown in this document for both STD and KED modes over a 48 hour period across the mass range shows the instrument exceeds this requirement. The performance reports that can be acquired automatically within Qtegra ISDS Software assist the user in monitoring and validating the mass calibration for routine use. Excellent mass stability equates to good long term analytical performance and compliance to legislative methods.

Find out more at thermofisher.com/ICP-MS