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Simplified workflows for the Thermo Scientific iCAP TQ ICP-MS

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Introduction

A mass spectrometer is a highly complex instrument with many parameters, for example, the large number of isotopes for analysis, the different measurement modes and even the wide range of peripherals. All of these can add complexity to method development. Choosing the right setup to maximize data quality and turning sample receipt into meaningful results has become increasingly challenging. However, through implementation of advanced hardware design and software solutions, these challenges can be minimized.

The Thermo Scientific™ iCAP™ TQ ICP-MS has been developed with ease of use features that simplify daily tasks and increase productivity. Common operator procedures such as sample introduction system maintenance are easier and faster with a drop-down door for simple cone maintenance and a bayonet style fully demountable torch system. Intuitive workflows and the Reaction Finder method development assistant within Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software simplify operation to make the iCAP TQ ICP-MS as easy to use as a single quadrupole (SQ) instrument.

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Triple Quadrupole ICP-MS

With ever decreasing limit of detection requirements, interference elimination on specific analytes is becoming more important. Removal of most of the common interferences can be efficiently achieved with high resolution ICP-MS; however, budget limitations means this technology is not accessible to all laboratories.

Quadrupole ICP-MS systems have both speed and fairly comprehensive interference removal capability. Systems fitted with collision/reaction cells (CRCs) are able to reduce polyatomic interferences on analyte signals using collisions with helium and Kinetic Energy Discrimination (KED) to give good quality data; however, this mode is not effective for isobaric interferences (i.e. interference between isotopes of the same mass, such as ^{48}Ti and ^{48}Ca).

Reaction gases can be used to mass shift the analyte away from the isobaric interference, but this is dependent on the new product ion mass also being interference free, as the sample matrix may contain an element with an overlapping mass. To continue the example, reacting ^{48}Ti with NH_3 produces the clustered product ion $^{114}Ti(NH_3)_3NH$, which has potential interferences of ^{114}Cd or ^{114}Sn.

Triple quadrupole (TQ) technology adds a third quadrupole in front of the CRC to pre-filter the ion beam and limit the masses entering the CRC. If the mass shift reaction creates a product ion at the same mass as an existing matrix component, the matrix component is filtered out so that the analyte can be measured interference free, e.g. ^{114}Cd and ^{114}Sn will be filtered out so that $^{114}Ti(NH_3)_3NH$ can be measured with a clean background.

Adding the third quadrupole enhances the existing capabilities of quadrupole ICP-MS and additionally creates new possibilities for advanced analysis. However, this brings with it multiple layers of complexity. The choices include the first quadrupole setting, the reaction gas to use, which product ion should be measured, and which internal standards to use. Having this variety of options available has the potential to make method development challenging and time consuming.

Setting up the instrument with Get Ready

Before any analysis can be done, the hardware needs to be inspected to ensure optimum performance. The drop-down door common to the Thermo Scientific™ iCAP Qnova™ Series ICP-MS allows the user quick and unhindered access to the cones and extraction lenses for easy inspection and maintenance if required. The sample introduction is equally accessible allowing the user to check and configure the torch, injector, spraychamber and nebulizer in a matter of minutes.

It is important that the daily performance of the system is stable over days and weeks to achieve reproducible results even when analyzing a variety of complex matrices. The ‘Get Ready’ feature guarantees this by automating daily tasks such as tuning the interface and lenses after a set stabilization time, and performing daily performance evaluations for traceability. This automated procedure extends to all of the different reaction modes installed in the system, and it is customizable for the greatest degree of flexibility. This one-click approach assures the laboratory user that any data gathered is of the highest quality.

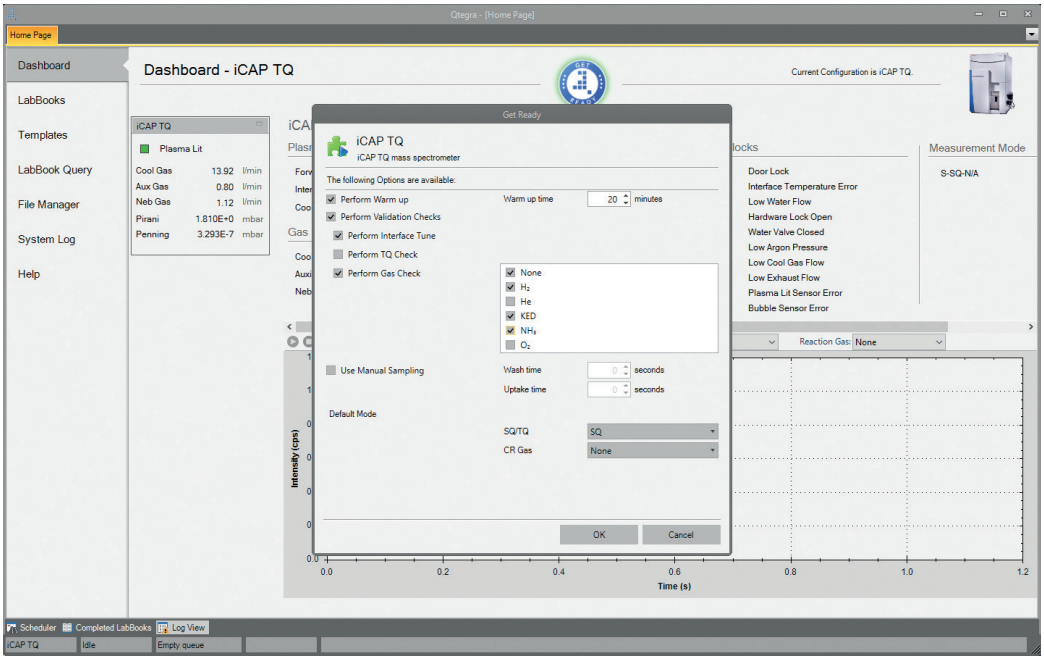

Figure 1. The 'Get Ready' feature of Qtegra ISDS Software allows you to perform daily startup routines with two clicks, with customizable warmup and tuning options.

Setting up the method with Reaction Finder

Qtegra ISDS Software simplifies LabBook setup by intelligently configuring the method according to the gases plumbed into the instrument and the analytes selected. Reaction Finder automatically chooses the optimum isotope for analysis, the CRC gas and mode that yields the best interference reduction, suggests the most appropriate internal standard for the analysis for selection and sets the Q3 analyte mass for the most reliable data. This does not mean, however, that the system is locked down. The operator is still free to override the Reaction Finder settings for exploring research applications if they wish to.

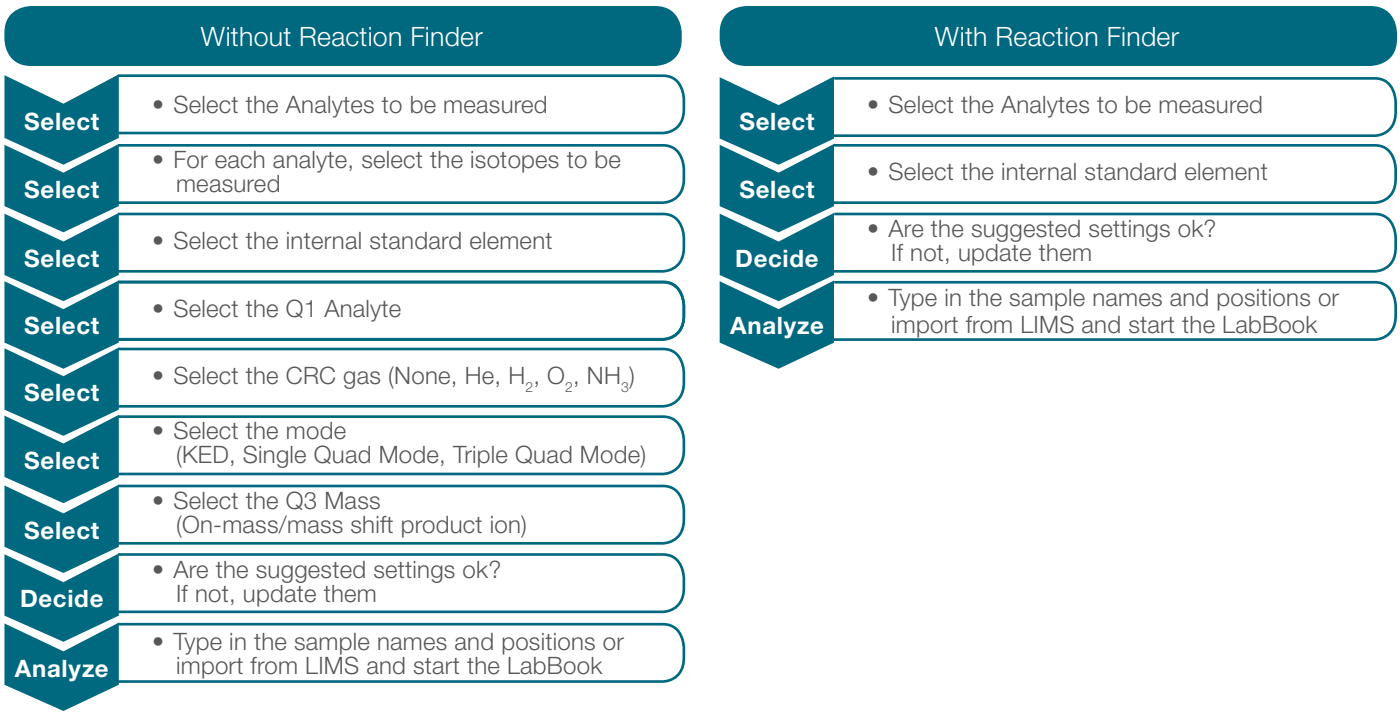

Figure 2. Comparison of Workflows between Manual Method Set up (without Reaction Finder) and Automated Method development with Reaction Finder.

In addition to the analytes, the suitable internal standard must also be selected, including again the question of whether the chosen internal standard should be measured on mass or mass shifted along with the analytes. Reaction Finder gives you the option to choose an appropriate internal standard from a pre-filtered list of elements so the complexity of internal standard selection based on the reaction modes and measurement modes used is removed.

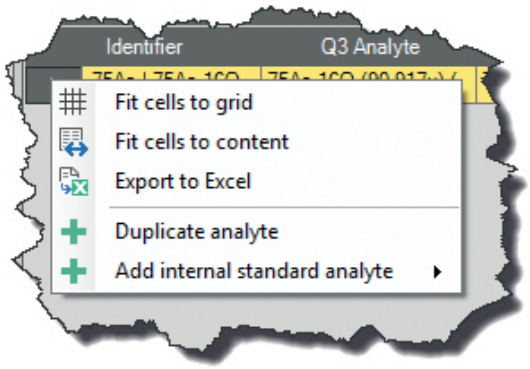

Figure 3. With a right mouse click on the analyte, Reaction Finder gives you the option to choose an appropriate internal standard from a pre-filtered list of elements.

Reaction Finder for Accurate Analysis of As in Co Matrix

The wrong choice of interference reduction method and associated parameters can lead to false results. This is demonstrated in Figure 4, which shows arsenic measured in varying concentrations of vitamin B12 from a series of nutritional supplements. Vitamin B12 contains cobalt, which easily forms the oxide $^{59}Co^{16}O$ at mass 75. Using a single quadrupole instrument, the best interference reduction method available is SQ-KED mode using the CRC to attenuate the polyatomic oxide signal.

This method also suppresses the true arsenic ion signal and has to be tuned carefully to maintain sufficient sensitivity at the same time. This usually means there is a compromise, and increasing concentrations of Co from vitamin B12 means the level of cobalt oxide eventually becomes too high for SQ-KED to effectively suppress.

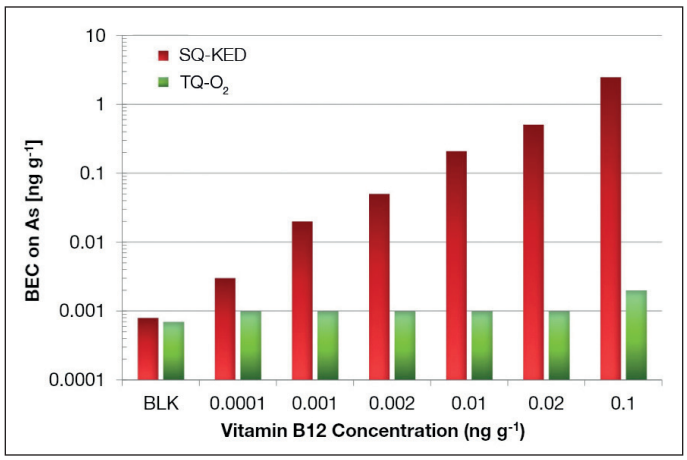

Figure 4. BECs on As in varying amounts of Vitamin B12 analyzed in SQ-KED and TQ-O_2 modes. The BECs in SQ-KED rise with vitamin B12 concentration as the mode fails to cope with increasing concentrations of CoO, whereas TQ-O_2 mode shifts the As to a clean portion of the mass spectrum to maintain the same reported As concentrations, regardless of the Co concentration.

Using the iCAP TQ ICP-MS equipped with oxygen as the CRC gas, the laboratory analyst simply chooses ^{75}As in the element selection list, and Qtegra ISDS Software automatically chooses TQ mass shift mode, pressurizing the CRC with oxygen and setting the Q3 analyte mass to *m/z* 91 to transmit the $^{75}As^{16}O$ product ion (Figure 5).

Identifier	Q3 Analyte	SQ / TQ	CR Gas	Dwell time (s)	Channels	Spacing (u)
75As | 75As.16O	75As.16O (90.917u) (default)	TQ	O_2	0.1	1	0.1

Figure 5. By clicking on an analyte, Reaction Finder automatically creates a method that yields the best LODs.

Using TQ mass shift mode, Q1 is set so that cobalt is filtered out of the ion beam (and cannot create any further oxide interference in the CRC), and ions at mass 91 (such as ^{91}Zr) are also filtered so that the product ion background is kept interference free. This mass shift method means that the arsenic is analyzed free from any possible Co- and Zr-based interferences, as illustrated in Figure 6 below.

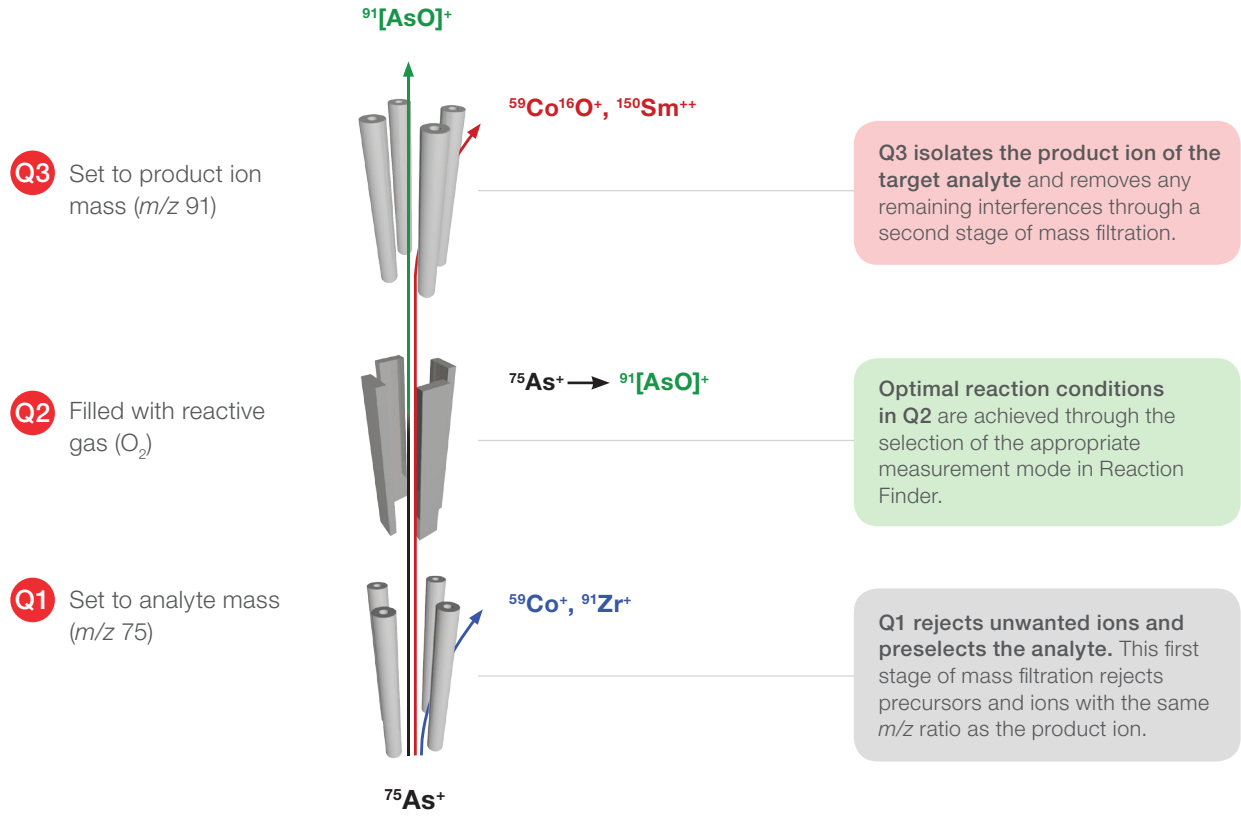

Figure 6. TQ mass shift mode for Arsenic.

Conclusion

The iCAP TQ ICP-MS is a fully featured triple quadrupole ICP-MS that is as easy to use as a single quadrupole ICP-MS. Hardware features from the iCAP Qnova Series ICP-MS Platform mean that regular inspection and maintenance is simple and hassle free. Qtegra ISDS Software workflows and Reaction Finder ensure that method development and data acquisition is simple, efficient and fast. The iCAP TQ ICP-MS reduces the complexity of TQ-ICP-MS to support laboratories in generating good quality, interference free data whilst maintaining the flexibility to analyze a host of different matrices for a range of challenging applications.

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

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