Product spotlight | 002969

Trace elemental analysis

Thermo Scientific iCAP MTX ICP-MS

Streamlined method development for triple quadrupole ICP-MS

The Thermo Scientific™ iCAP™ MTX ICP-MS instruments provide sensitive, accurate, and robust analysis of a wide variety of sample matrices. Designed with ease of use and intelligent solutions to time-consuming steps in the daily laboratory in mind, the Reaction Finder Method Development Assistant in the Thermo Scientific™ Qtegra™ ISDS™ Software removes the complexity from method development in triple quadrupole ICP-MS.

The accelerated adoption of triple quadrupole technology in ICP-MS, through its significant improvement in handling challenging interferences, has helped many laboratories to improve both data quality and productivity. However, method development is still often perceived as more complex compared with single quadrupole ICP-MS. To enable all laboratory personnel to fully leverage the superior interference removal that triple quadrupole technology offers, the Reaction Finder Method Development Assistant for Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software was developed.

The triple quadrupole technology used in the Thermo Scientific™ iCAP™ MTX ICP-MS achieves new levels of data quality and confidence in the result, with significant improvements for key elements. Interference removal based on triple quadrupole technology (also referred to as MS/MS) includes a mass filtration step before the collision/reaction cell (CRC), eliminating potential side reactions. Reactive gases such as oxygen, hydrogen, or ammonia are added to the CRC to induce highly selective ion-molecule reactions with either the analyte or the interfering ions, to eliminate interferences. A second mass filtration step in the analyzing quadrupole allows the target ion to be selected. The process of interference removal is illustrated in Figure 1.

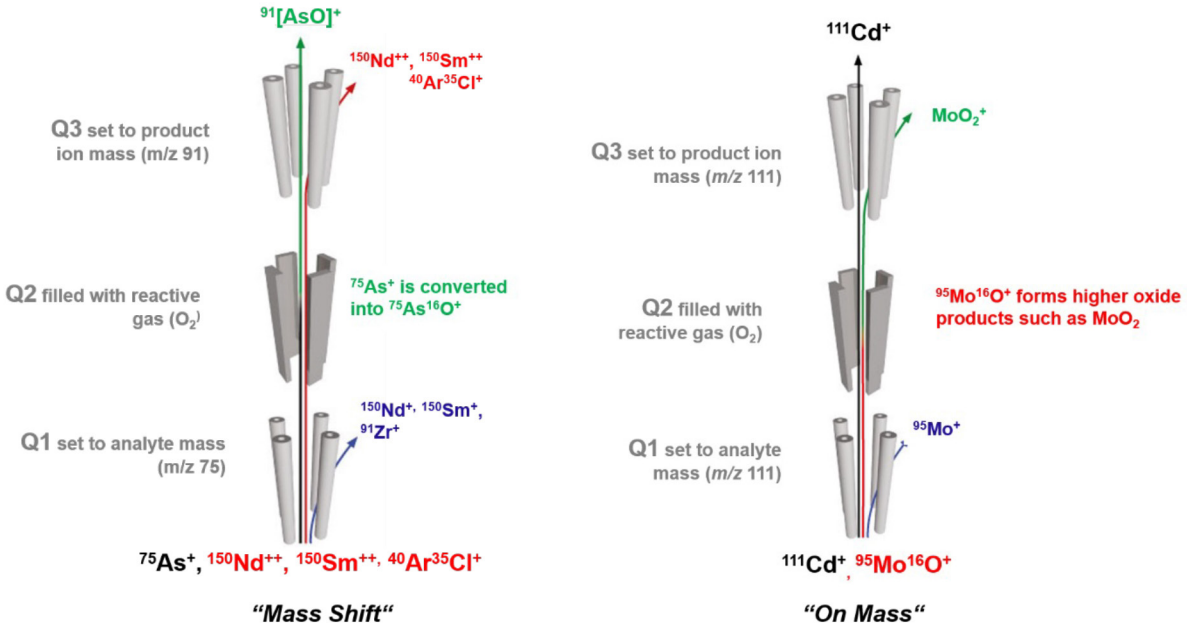


Figure 1. Possible reaction pathways in triple quadrupole ICP-MS

Whether a reaction inside the collision/reaction cell (CRC) leads to a change in the target analyte (a so-called "Mass Shift" reaction) or whether the interfering ions are removed (a so-called "On Mass" reaction) primarily depends on the respective analyte and the reactive gas used. In many cases, simple product ions, such as oxides are formed, but in other cases, more complex product ions result from the reactions. With triple quadrupole technology, selection of the default isotope to be selected for analysis may differ to a single quadrupole ICP-MS instrument due to the interference removal process.

Reaction Finder is a method development assistant for the iCAP MTX ICP-MS and is fully integrated in the Qtegra ISDS Software. Based on the user´s element selection, Reaction Finder identifies the most suitable isotope for analysis and then provides a complete set of measurement conditions, including the type of reaction if applicable ("Mass Shift" or "On Mass"), quadrupole scan settings, as well as the most suitable reaction gas. This process is displayed in Figure 2.

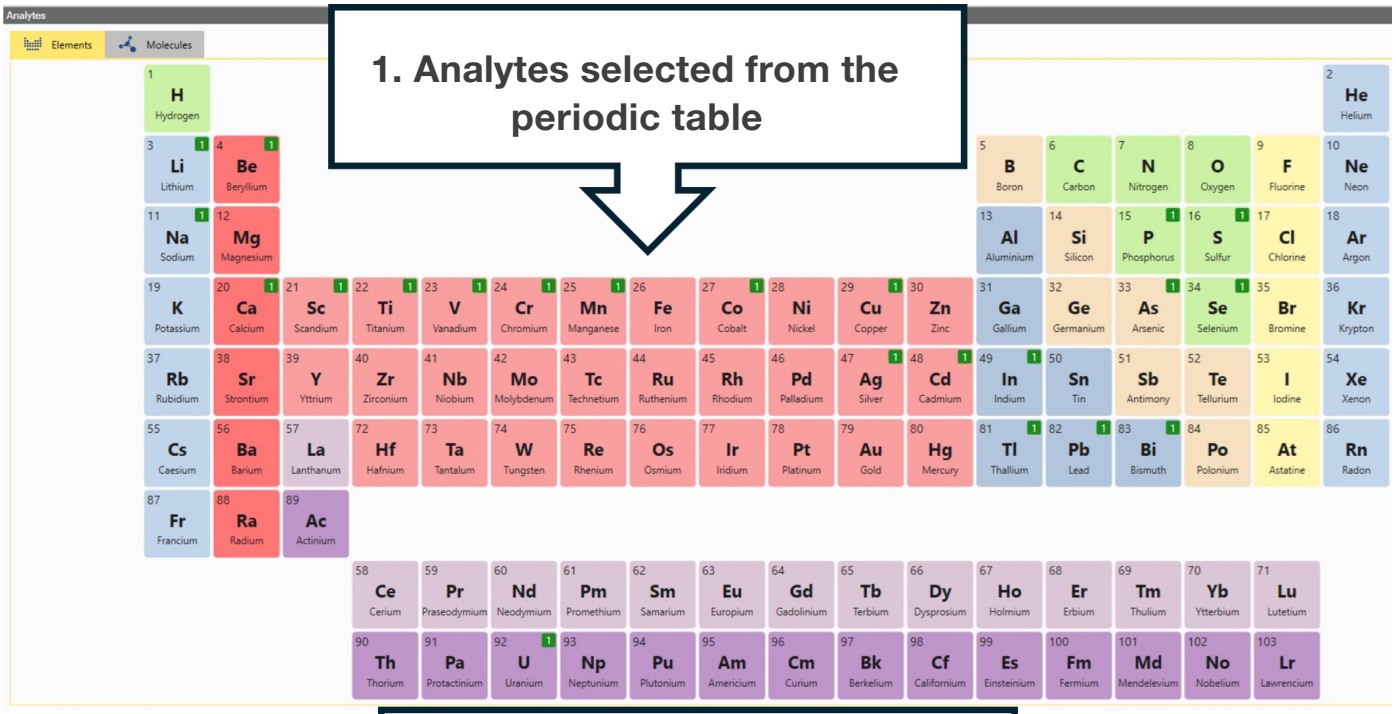
By default, Reaction Finder supports the following gases: helium (He), oxygen (O_2), ammonia (NH_3), and hydrogen (H_2). Other reactive gases, or reactive gases that leverage on mass reactions (i.e., reacting with the interference rather than the analyte), can be used as per the information provided in the Pre-Installation Requirement Guide of the instrument. One example is the use of nitrous oxide (N_2O), a gas which can been used as an alternative to O_2 to eliminate specific interferences.

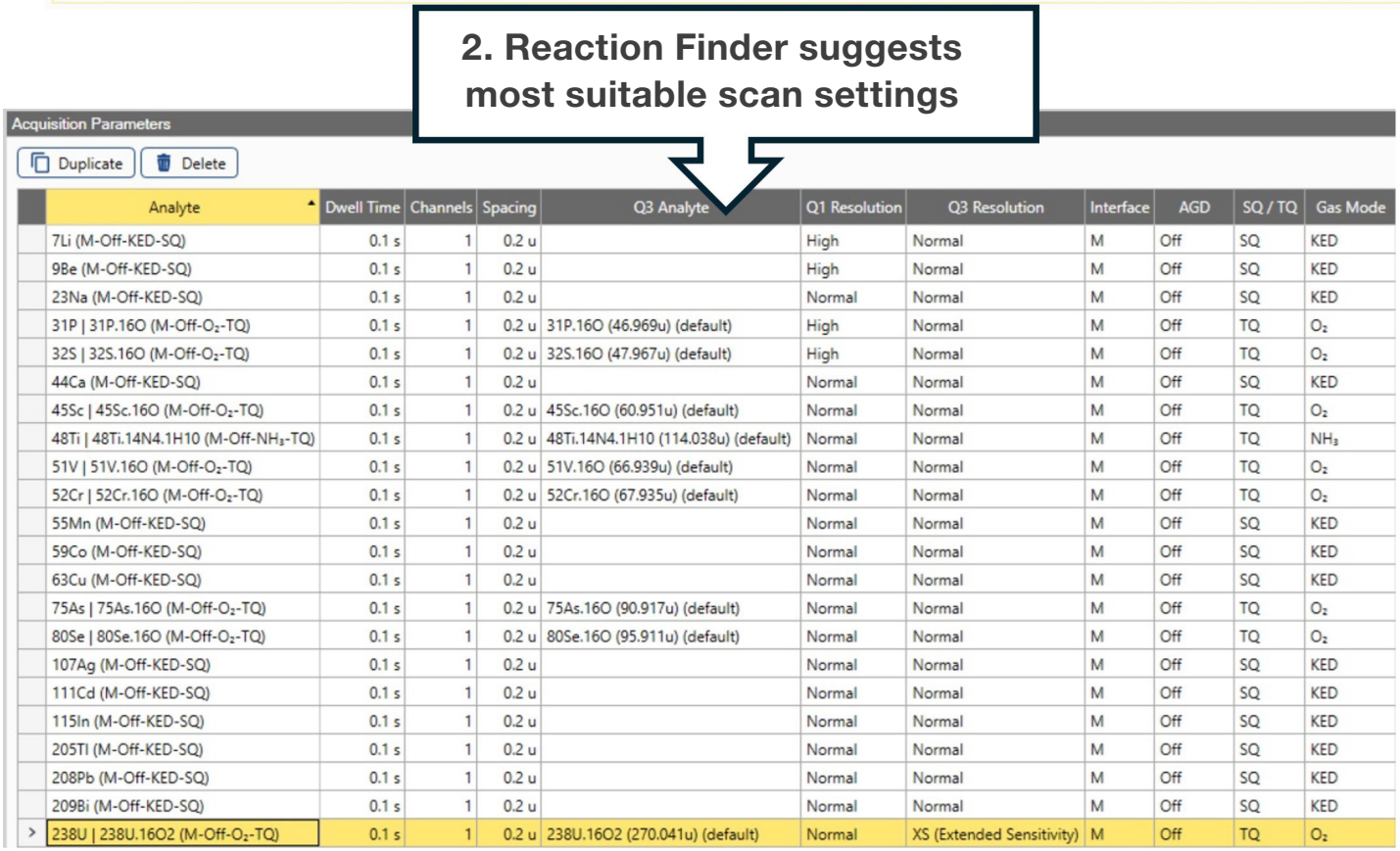
All settings in Reaction Finder can be modified by the user (e.g., addition of other measurement modes, selection of other reactive gases or product ions, etc.) so that the ability to perform method development is not restricted for experienced operators. To modify a Reaction Finder default setting, individual parameters can be edited using context menus, providing additional useful information. Multiple reaction options for the analysis of a given isotope are supported through a simple right mouse click.

The following adjustments are supported in Reaction Finder:

- Selection of single quadrupole/triple quadrupole scanning
- Selection of reactive gases for any analyte
- Selection of alternative product ions for each reactive gas
- Resolution settings for Q1 and Q3*

*Options include: intelligent Mass Selection (iMS) or High (less than 1 amu) for Q1, Normal (approx. 0.7 amu peak width), High (approx. 0.4 amu average peak width) for Q3; XS (Extended Sensitivity) only for single use instruments in the mass range above *m/z* 225





Analyte	Dwell Time	Channels	Spacing	Q3 Analyte	Q1 Resolution	Q3 Resolution	Interface	AGD	SQ / TQ	Gas Mode
7Li (M-Off-KED-SQ)	0.1 s	1	0.2 u		High	Normal	M	Off	SQ	KED
9Be (M-Off-KED-SQ)	0.1 s	1	0.2 u		High	Normal	M	Off	SQ	KED
23Na (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
31P | 31P.16O (M-Off-O_2-TQ)	0.1 s	1	0.2 u	31P.16O (46.969u) (default)	High	Normal	M	Off	TQ	O_2
32S | 32S.16O (M-Off-O_2-TQ)	0.1 s	1	0.2 u	32S.16O (47.967u) (default)	High	Normal	M	Off	TQ	O_2
44Ca (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
45Sc | 45Sc.16O (M-Off-O_2-TQ)	0.1 s	1	0.2 u	45Sc.16O (60.951u) (default)	Normal	Normal	M	Off	TQ	O_2
48Ti | 48Ti.14N4.1H10 (M-Off-NH_3-TQ)	0.1 s	1	0.2 u	48Ti.14N4.1H10 (114.038u) (default)	Normal	Normal	M	Off	TQ	NH_3
51V | 51V.16O (M-Off-O_2-TQ)	0.1 s	1	0.2 u	51V.16O (66.939u) (default)	Normal	Normal	M	Off	TQ	O_2
52Cr | 52Cr.16O (M-Off-O_2-TQ)	0.1 s	1	0.2 u	52Cr.16O (67.935u) (default)	Normal	Normal	M	Off	TQ	O_2
55Mn (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
59Co (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
63Cu (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
75As | 75As.16O (M-Off-O_2-TQ)	0.1 s	1	0.2 u	75As.16O (90.917u) (default)	Normal	Normal	M	Off	TQ	O_2
80Se | 80Se.16O (M-Off-O_2-TQ)	0.1 s	1	0.2 u	80Se.16O (95.911u) (default)	Normal	Normal	M	Off	TQ	O_2
107Ag (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
111Cd (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
115In (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
205Tl (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
208Pb (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
209Bi (M-Off-KED-SQ)	0.1 s	1	0.2 u		Normal	Normal	M	Off	SQ	KED
238U | 238U.16O2 (M-Off-O_2-TQ)	0.1 s	1	0.2 u	238U.16O2 (270.041u) (default)	Normal	XS (Extended Sensitivity)	M	Off	TQ	O_2

Figure 2. Overview of the Reaction Finder Method Development Assistant

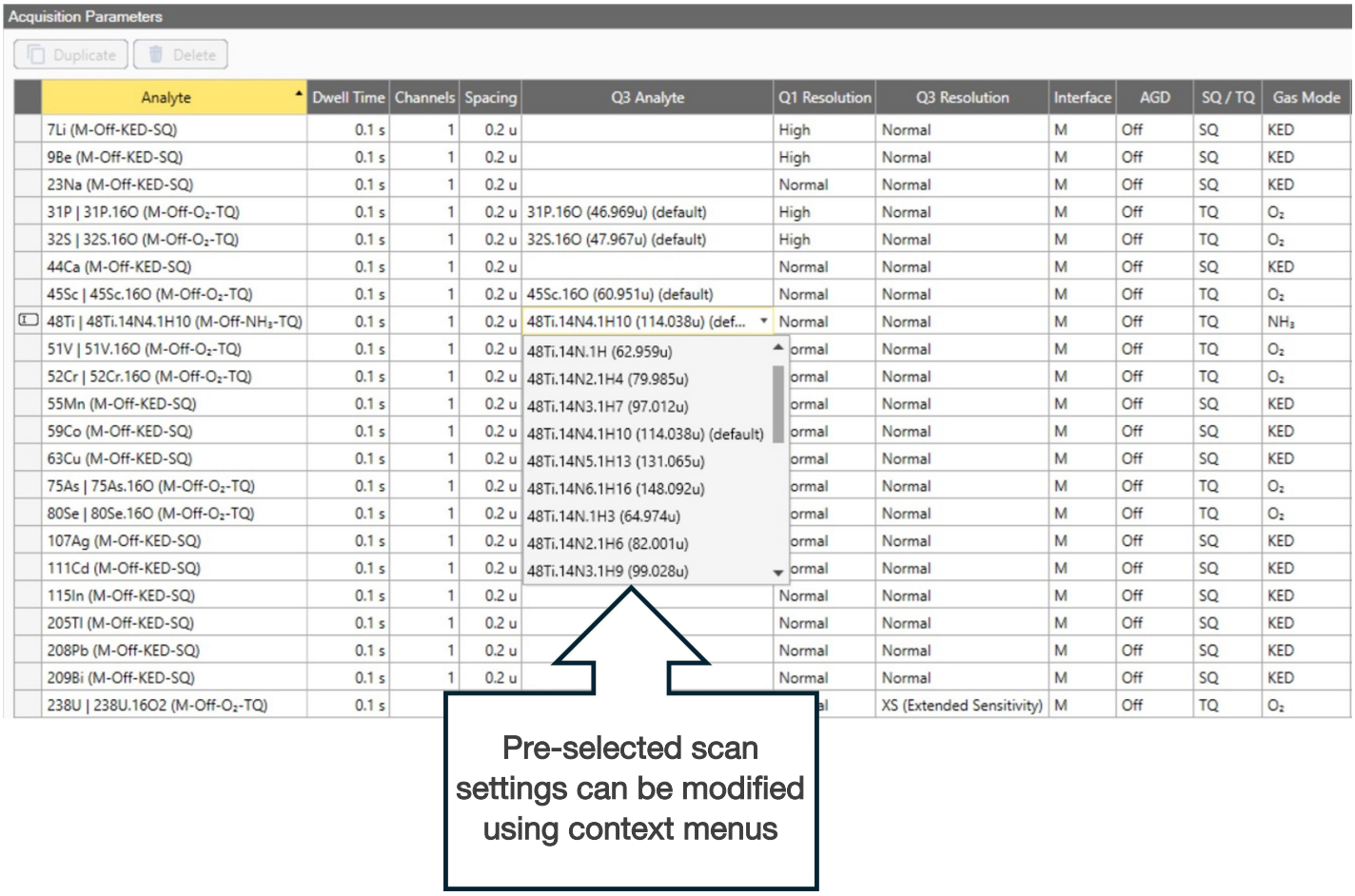


Figure 3. Modification of the Reaction Finder suggested settings

The Reaction Finder Method Development Assistant removes potential complexity from method development when using the iCAP MTX ICP-MS and allows all laboratories to benefit from superior interference removal. At the same time, it gives researchers the flexibility to test different reactive gases or product ions for specific applications.

- Based on the selection of elements to be measured, a set of measurement conditions is recommended for each analyte, ensuring interference removal and lowest detection limits.
- Defined settings can be user modified, and multiple settings can be tested for any given analyte to allow for comprehensive method development.
- Reaction Finder dynamically leverages adjustable quadrupole resolution to ensure optimum sensitivity with no sacrifice of interference removal.

Learn more at **thermofisher.com/icpms**

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