

# Interference Removal/Mitigation Utilizing ICP-MS/MS and Single Unit Mass Resolution

Agilent Technologies

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## Comparing Quadrupole ICP-MS Configurations

1 Quadrupole ICP-MS configurations; what they are and why it matters

2 Interference removal capabilities and other performance comparisons

*Comparing single quadrupole, bandpass, and MS/MS*

## Comparing Quadrupole ICP-MS Configurations

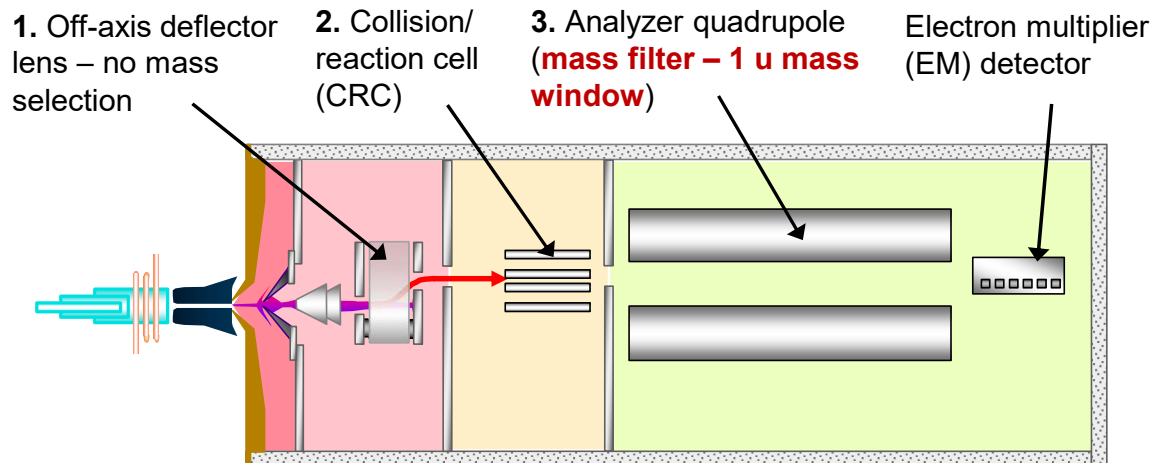
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***Comparing single quadrupole, bandpass, and MS/MS***

# Conventional (Single) Quadrupole ICP-MS

Simplest, lowest-cost solution for typical applications



A better way was needed to **control reaction chemistry**

The industry-standard ICP-MS layout:

1. Off-axis deflector lens to separate the ions from photons & neutrals
2. Collision/reaction cell (CRC)\*, and
3. **One quadrupole mass analyzer (a mass filter with a 1 u mass window)**

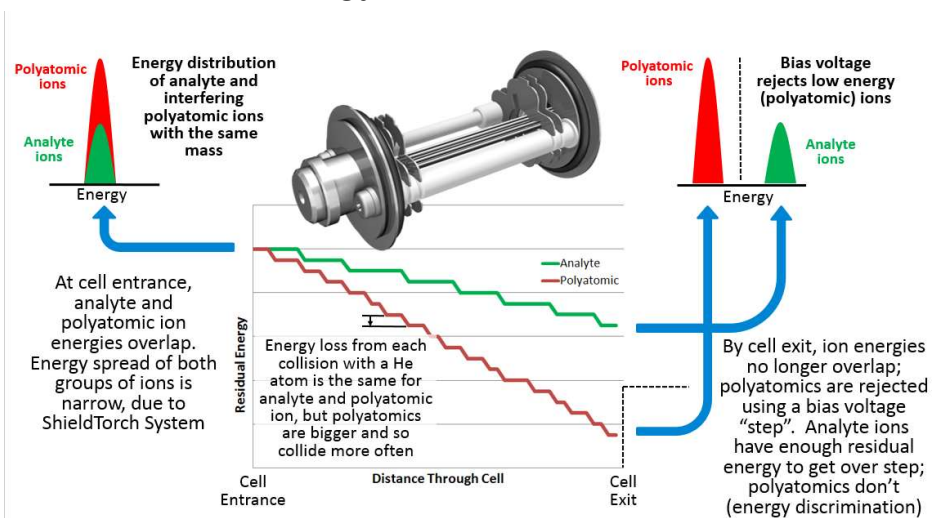
\* Since 1999 CRCs have been used to control spectral interferences in ICP-MS:

- Collision mode is well-established and widely used for typical analytes and applications
- Reaction mode is efficient and attractive, but can give errors due to **unwanted reactions** with other analytes and matrix elements

# Interference removal; Transitioning from ICP-SQMS to ICP-MSMS

- Modes of Interference Removal:

- Collision Mode
- He Gas
- Kinetic Energy Discrimination



Isotope	Principal Interfering Species (mixed matrix)
<sup>45</sup> Sc	<sup>13</sup> C <sup>16</sup> O <sub>2</sub> , <sup>12</sup> C <sup>16</sup> O <sub>2</sub> H, <sup>44</sup> CaH, <sup>32</sup> S <sup>12</sup> CH, <sup>32</sup> S <sup>13</sup> C, <sup>33</sup> S <sup>12</sup> C
<sup>47</sup> Ti	<sup>31</sup> P <sup>16</sup> O, <sup>48</sup> CaH, <sup>35</sup> Cl <sup>12</sup> C, <sup>32</sup> S <sup>14</sup> NH, <sup>33</sup> S <sup>14</sup> N
<sup>49</sup> Ti	<sup>31</sup> P <sup>18</sup> O, <sup>48</sup> CaH, <sup>35</sup> Cl <sup>14</sup> N, <sup>37</sup> Cl <sup>12</sup> C, <sup>32</sup> S <sup>16</sup> OH, <sup>33</sup> S <sup>16</sup> O
<sup>50</sup> Ti	<sup>34</sup> S <sup>16</sup> O, <sup>32</sup> S <sup>18</sup> O, <sup>35</sup> Cl <sup>14</sup> NH, <sup>37</sup> Cl <sup>12</sup> CH
<sup>51</sup> V	<sup>35</sup> Cl <sup>16</sup> O, <sup>37</sup> Cl <sup>14</sup> N, <sup>34</sup> S <sup>16</sup> OH
<sup>52</sup> Cr	<sup>36</sup> Ar <sup>16</sup> O, <sup>40</sup> Ar <sup>12</sup> C, <sup>35</sup> Cl <sup>16</sup> OH, <sup>37</sup> Cl <sup>14</sup> NH, <sup>34</sup> S <sup>18</sup> O
<sup>53</sup> Cr	<sup>36</sup> Ar <sup>16</sup> OH, <sup>40</sup> Ar <sup>13</sup> C, <sup>37</sup> Cl <sup>16</sup> O, <sup>35</sup> Cl <sup>18</sup> O, <sup>40</sup> Ar <sup>12</sup> CH
<sup>54</sup> Fe	<sup>40</sup> Ar <sup>14</sup> N, <sup>40</sup> Ca <sup>14</sup> N, <sup>23</sup> Na <sup>31</sup> P
<sup>55</sup> Mn	<sup>37</sup> Cl <sup>18</sup> O, <sup>23</sup> Na <sup>32</sup> S, <sup>23</sup> Na <sup>31</sup> PH
<sup>56</sup> Fe	<sup>40</sup> Ar <sup>16</sup> O, <sup>40</sup> Ca <sup>16</sup> O
<sup>57</sup> Fe	<sup>40</sup> Ar <sup>16</sup> OH, <sup>40</sup> Ca <sup>16</sup> OH
<sup>58</sup> Ni	<sup>40</sup> Ar <sup>18</sup> O, <sup>40</sup> Ca <sup>18</sup> O, <sup>23</sup> Na <sup>35</sup> Cl
<sup>59</sup> Co	<sup>40</sup> Ar <sup>18</sup> OH, <sup>43</sup> Ca <sup>16</sup> O, <sup>23</sup> Na <sup>35</sup> ClH
<sup>60</sup> Ni	<sup>44</sup> Ca <sup>16</sup> O, <sup>23</sup> Na <sup>37</sup> Cl
<sup>61</sup> Ni	<sup>44</sup> Ca <sup>16</sup> OH, <sup>38</sup> Ar <sup>23</sup> Na, <sup>23</sup> Na <sup>37</sup> ClH
<sup>63</sup> Cu	<sup>40</sup> Ar <sup>23</sup> Na, <sup>12</sup> C <sup>16</sup> O <sup>35</sup> Cl, <sup>12</sup> C <sup>14</sup> N <sup>37</sup> Cl, <sup>31</sup> P <sup>32</sup> S, <sup>31</sup> P <sup>16</sup> O <sub>2</sub>
<sup>64</sup> Zn	<sup>32</sup> S <sup>16</sup> O <sub>2</sub> , <sup>32</sup> S <sub>2</sub> , <sup>36</sup> Ar <sup>12</sup> C <sup>16</sup> O, <sup>38</sup> Ar <sup>12</sup> C <sup>14</sup> N, <sup>48</sup> Ca <sup>16</sup> O
<sup>65</sup> Cu	<sup>32</sup> S <sup>16</sup> O <sub>2</sub> H, <sup>32</sup> S <sub>2</sub> H, <sup>14</sup> N <sup>16</sup> O <sup>35</sup> Cl, <sup>48</sup> Ca <sup>16</sup> OH
<sup>66</sup> Zn	<sup>34</sup> S <sup>16</sup> O <sub>2</sub> , <sup>32</sup> S <sup>34</sup> S, <sup>33</sup> S <sub>2</sub> , <sup>48</sup> Ca <sup>18</sup> O
<sup>67</sup> Zn	<sup>32</sup> S <sup>34</sup> SH, <sup>33</sup> S <sub>2</sub> H, <sup>48</sup> Ca <sup>18</sup> OH, <sup>14</sup> N <sup>16</sup> O <sup>37</sup> Cl, <sup>16</sup> O <sub>2</sub> <sup>35</sup> Cl
<sup>68</sup> Zn	<sup>32</sup> S <sup>18</sup> O <sub>2</sub> , <sup>34</sup> S <sub>2</sub>
<sup>69</sup> Ga	<sup>32</sup> S <sup>18</sup> O <sub>2</sub> H, <sup>34</sup> S <sub>2</sub> H, <sup>16</sup> O <sub>2</sub> <sup>37</sup> Cl
<sup>70</sup> Zn	<sup>34</sup> S <sup>18</sup> O <sub>2</sub> , <sup>35</sup> Cl <sub>2</sub>
<sup>71</sup> Ga	<sup>34</sup> S <sup>18</sup> O <sub>2</sub> H, <sup>35</sup> Cl <sub>2</sub> H, <sup>40</sup> Ar <sup>31</sup> P
<sup>72</sup> Ge	<sup>40</sup> Ar <sup>32</sup> S, <sup>35</sup> Cl <sup>37</sup> Cl, <sup>40</sup> Ar <sup>16</sup> O <sub>2</sub>
<sup>73</sup> Ge	<sup>40</sup> Ar <sup>32</sup> SH, <sup>40</sup> Ar <sup>33</sup> S, <sup>35</sup> Cl <sup>37</sup> ClH, <sup>40</sup> Ar <sup>16</sup> O <sub>2</sub> H
<sup>74</sup> Ge	<sup>40</sup> Ar <sup>34</sup> S, <sup>37</sup> Cl <sub>2</sub>
<sup>75</sup> As	<sup>40</sup> Ar <sup>34</sup> SH, <sup>40</sup> Ar <sup>35</sup> Cl, <sup>40</sup> Ca <sup>35</sup> Cl, <sup>37</sup> Cl <sub>2</sub> H
<sup>77</sup> Se	<sup>40</sup> Ar <sup>37</sup> Cl, <sup>40</sup> Ca <sup>37</sup> Cl
<sup>78</sup> Se	<sup>40</sup> Ar <sup>38</sup> Ar
<sup>80</sup> Se	<sup>40</sup> Ar <sub>2</sub> , <sup>40</sup> Ca <sub>2</sub> , <sup>40</sup> Ar <sup>40</sup> Ca, <sup>32</sup> S <sub>2</sub> <sup>16</sup> O, <sup>32</sup> S <sup>16</sup> O <sub>3</sub>

## The Solution to Controlling Reaction Chemistry in the CRC?

### Triple Quadrupole ICP-MS (ICP-QQQ):

- Uses an **additional mass filter before** the CRC in a “tandem” mass spec configuration (MS/MS)
- First quadrupole (Q1) selects the **specific mass** of the ions that can enter the cell. Ensures that reaction chemistry is predictable and reliable
- Second quadrupole (Q2) selects the **specific mass** of the ions/product ions that are passed to the detector
- MS/MS allows reaction gas methods to be applied to normal applications and variable, real-world samples, with confidence in the results

MS/MS requires **two fully functioning mass filters**. Each mass spectrometer must be able to select **individual mass to charge values ( $m/z$ )**

First commercial ICP-QQQ instrument (Agilent 8800) in 2012. Superseded by the Agilent 8900 (below) in 2016



**MS/MS releases the full potential of reaction mode**

# ICP-MSMS; Unsurpassed Interference Removal Capabilities

Plasma-source mass spectrometer

- High ionization efficiency

Full-size quad before reaction cell

- Unit mass resolution (MS/MS)

Octopole Reaction System (ORS)

- High transmission efficiency cell

5-stage vacuum system

Full-size quad after reaction cell

High speed 11-order detector

- Wide dynamic range
- Fast acquisition for nano



## IUPAC Definitions – For Reference

### Taken from IUPAC 2013 Recommendations:

**Triple quadrupole mass spectrometer (Term 528):** *“Tandem mass spectrometer comprising two transmission quadrupole mass spectrometers in series with a (non-selecting) RF-only quadrupole (or other multipole) between them to act as a collision cell”*

**Transmission quadrupole mass spectrometer (Term 536)** is defined as consisting of *“an array of 4 parallel rod electrodes... [that allows] ...ions in a particular mass to charge range [to] be transmitted...”*

**Mass spectrometer (Term 318)** is defined as an *“Instrument that measures the **m/z values**... of gas-phase ions”*

*Pure Appl. Chem.*, Vol. 85, No. 7, pp. 1515–1609, 2013.  
<http://dx.doi.org/10.1351/PAC-REC-06-04-06>  
© 2013 IUPAC, Publication date (Web): 6 June 2013

#### Definitions of terms relating to mass spectrometry (IUPAC Recommendations 2013)\*

Kermit K. Murray<sup>1,‡</sup>, Robert K. Boyd<sup>2</sup>, Marcos N. Eberlin<sup>3</sup>,  
G. John Langlely<sup>4</sup>, Liang Li<sup>5</sup>, and Yasuhide Naito<sup>6</sup>

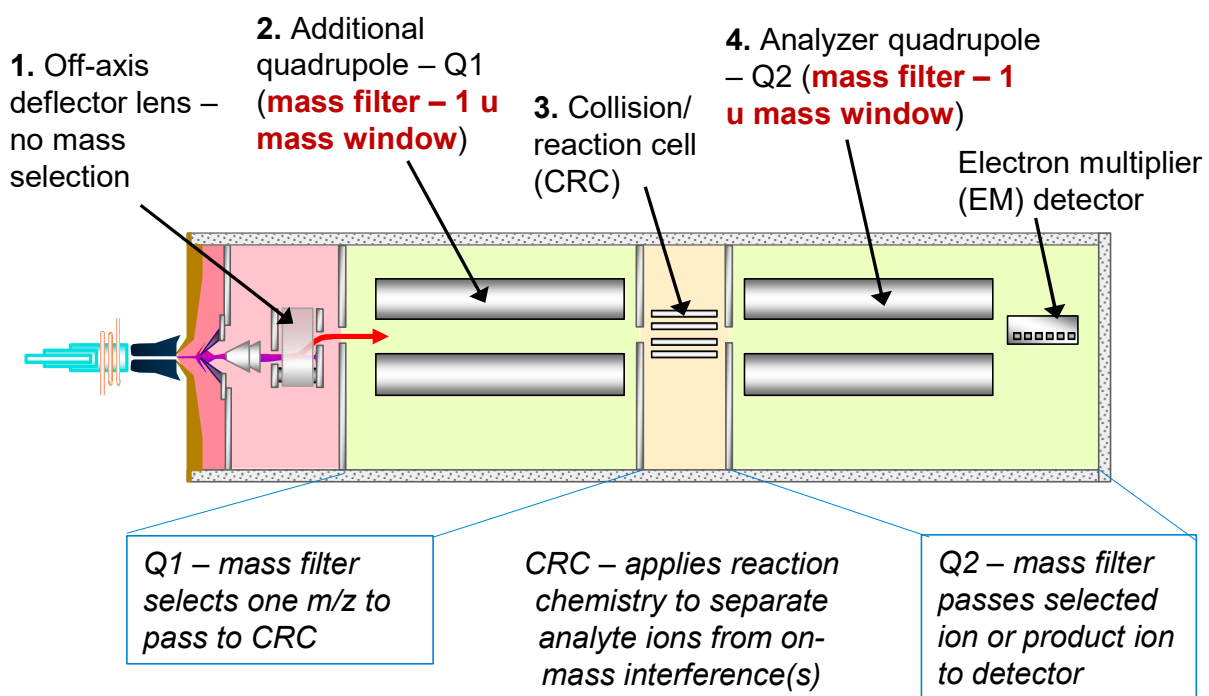
<sup>1</sup>Department of Chemistry, Louisiana State University, Baton Rouge, LA, USA;  
<sup>2</sup>Institute for National Measurement Standards, National Research Council, Ottawa, Ontario, Canada; <sup>3</sup>Department of Chemistry, University of Campinas, Campinas, Brazil; <sup>4</sup>Chemistry, Faculty of Natural and Environmental Sciences, University of Southampton, Southampton, UK; <sup>5</sup>Department of Chemistry, University of Alberta, Edmonton, Alberta, Canada; <sup>6</sup>Graduate School for the Creation of New Photonics Industries, Hamamatsu, Japan

From the IUPAC definitions, it's clear that a “mass spectrometer” must be capable of selecting ions of **specific m/z values** one mass at a time – i.e. unit (1 u) mass resolution

A Triple Quadrupole MS must have two such mass filters, each capable of 1 u resolution



## Tandem MS Instrument Layout: Unique to Agilent 8900 ICP-QQQ



Triple quadrupole ICP-MS layout, with:

1. An off-axis deflector lens to separate the ions from photons & neutrals
2. A **first quadrupole mass analyzer Q1** (a mass filter with a 1 u mass window) **before** the CRC
3. A collision/reaction cell capable of collision or reaction mode, and
4. A **second quadrupole mass analyzer Q2** (a mass filter with a 1 u mass window)

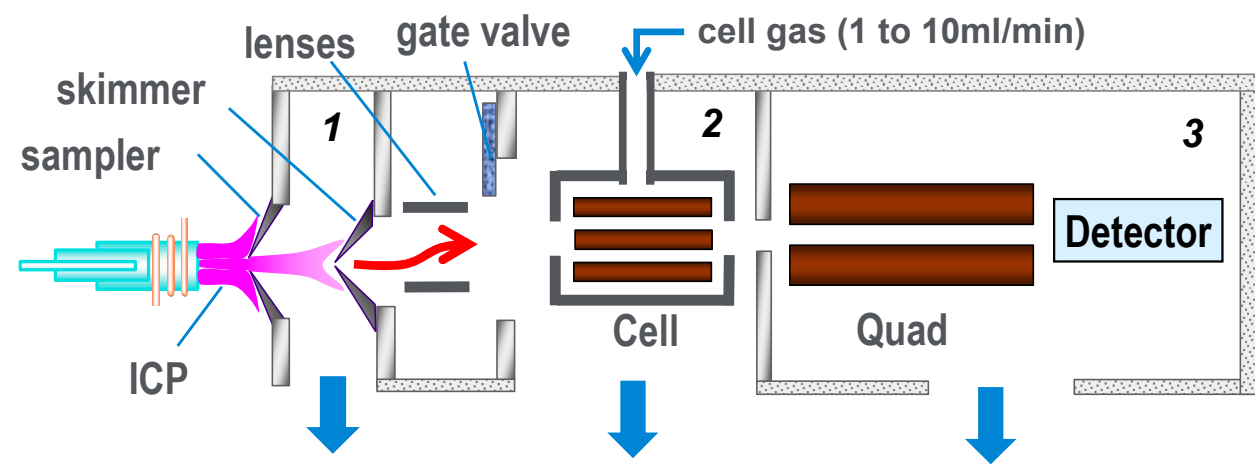
This configuration is unique to the 8900

The highest performance, most flexible configuration; the only solution that allows **complete control in reaction mode**

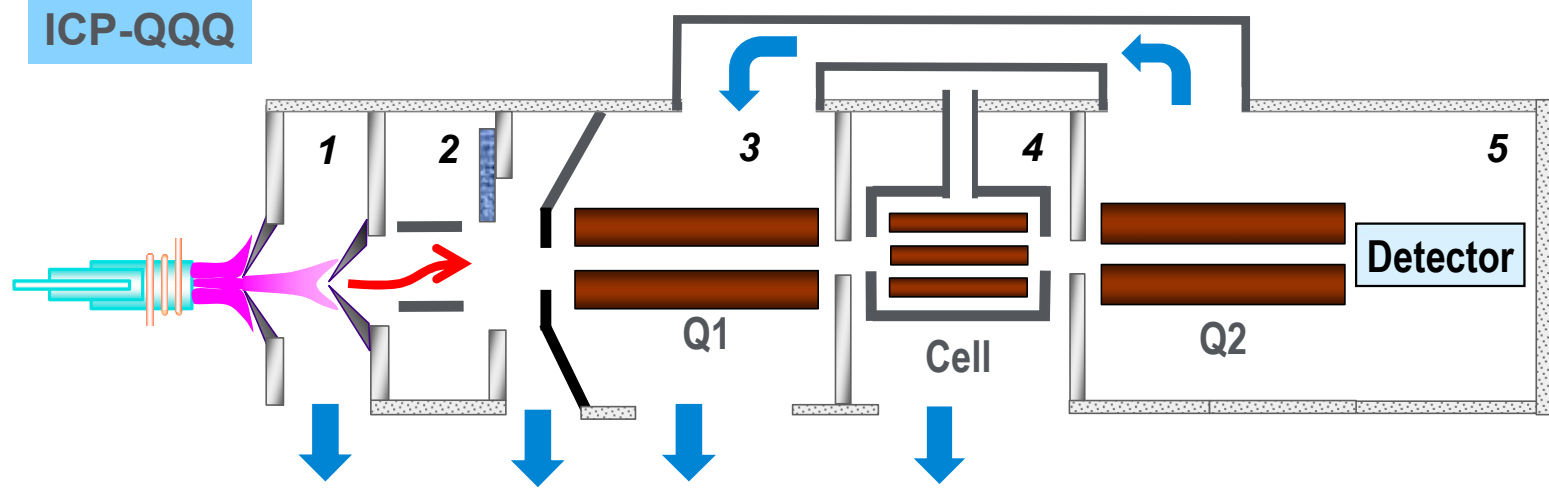
Agilent 8900 (MS/MS) system performs well in either collision or reaction mode – without restrictions

# Vacuum Consideration

ICP-MS SQ



ICP-QQQ



# Agilent Patented Vacuum System

US Patent 2013/0175442 A1

## High Selectivity

Q1 and Q3 must be under high vacuum in order to achieve single mass resolution filtering.



## High Sensitivity

Additional turbo pump required to accommodate longer ion flight path and ensure high ion transmission

# What Does MS/MS Mean for Your Analysis

## Comparing Single Quad (and Bandpass) vs Triple Quad

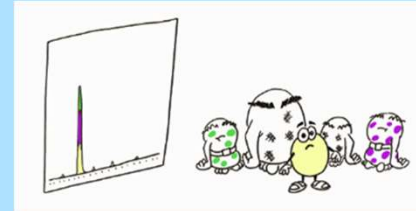
Single Quad and Bandpass ICP-MS. Single true mass filter, after the cell

**No mass filter (or Bandpass filter) before cell; ALL (or MANY) ions enter cell and can react**

12



Many ions can pass through cell or react to form new product ions



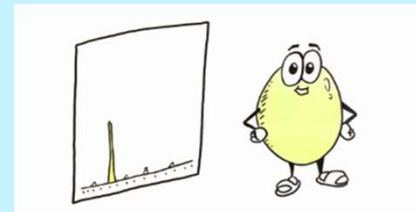
Many different ions can contribute to the measured signal

Triple Quadrupole ICP-MS (ICP-QQQ). Two true mass filters, before/after cell

**Mass filter before cell; Q1 rejects all masses except target ion  $m/z$ . ONLY target analyte and on-mass interferences enter cell. Overlaps at product ion mass are eliminated**



Analyte and on-mass interference separated by reaction chemistry



Only the target analyte ions contribute to the measured signal

## Single Quad ICP-MS with bandpass filter in or before the cell.

What do you want to analyze?



What elements enter the cell?



This excluding the polyatomics !

## ICP-MS/MS with Unit Mass Resolution Before the Cell

What do you want to analyze?



What elements enter the cell?



True MS/MS with unit mass resolution before the cell... when you must have Trusted Answers!

## Single Quad ICP-MS with bandpass filter in or before the cell.

Element of Interest	Isotopes entering the Cell
Ti-50, V-50, Cr-50	Sc-45, Ca-46, Ti-46, Ti-47, Ca-48, Ti-48, Ti-50, V-50, Cr-50, V-51, V-51, Cr-52, Cr-53, Cr-54, Fe-54 and Mn-55
V-51	Ca-46, Ti-46, Ti-47, Ca-48, Ti-48, Ti-49, V-51, Cr-52, Cr-52, Cr-53, Cr-54, Fe-54, Mn-55 and Fe-56
Cr-52	Ti-47, Ca-48, Ti-48, Ti-49, Ti-50, V-50, Cr-50, Cr-52, Cr-53, Cr-53, Cr-54, Fe-54, Mn-55, Fe-56 and Fe-57
Cr-53	Ca-48, Ti-48, Ti-49, Ti-50, V-50, Cr-50, V-51, Cr-53, Cr-54, Fe-54, Cr-54, Fe-54, Mn-55, Fe-56, Fe-57, Fe-58 and Ni-58
Cr-54, Fe-54	Ti-49, Ti-50, V-50, Cr-50, V-51, Cr-52, Cr-54, Fe-54, Mn-55, Mn-55, Fe-56, Fe-57, Fe-58, Ni-58 and Co-59
Mn-55	Ti-50, V-50, Cr-50, V-51, Cr-52, Cr-53, Mn-55, Fe-56, Fe-56, Fe-57, Fe-58, Ni-58, Co-59 and Ni-60
Fe-56	V-51, Cr-52, Cr-53, Cr-54, Fe-54, Fe-56, Fe-57, Fe-57, Fe-58, Ni-58, Co-59, Ni-60 and Ni-61
Fe-57	Cr-52, Cr-53, Cr-54, Fe-54, Mn-55, Fe-57, Fe-58, Ni-58, Fe-58, Ni-58, Co-59, Ni-60, Ni-61 and Ni-62
Fe-58, Ni-58	Cr-53, Cr-54, Fe-54, Mn-55, Fe-56, Fe-58, Ni-58, Co-59, Co-59, Ni-60, Ni-61, Ni-62 and Cu-63
Co-59	Cr-54, Fe-54, Mn-55, Fe-56, Fe-57, Co-59, Ni-60, Ni-60, Ni-61, Ni-62, Cu-63, Ni-64 and Zn-64
Ni-60	Mn-55, Fe-56, Fe-57, Fe-58, Ni-58, Ni-60, Ni-61, Ni-61, Ni-62, Cu-63, Ni-64, Zn-64 and Cu-65
Ni-61	Fe-56, Fe-57, Fe-58, Ni-58, Co-59, Ni-61, Ni-62, Ni-62, Cu-63, Ni-64, Zn-64, Cu-65 and Zn-66
Ni-62	Fe-57, Fe-58, Ni-58, Co-59, Ni-60, Ni-62, Cu-63, Cu-63, Ni-64, Zn-64, Cu-65, Zn-66 and Zn-67
Cu-63	Fe-58, Ni-58, Co-59, Ni-60, Ni-61, Cu-63, Ni-64, Zn-64, Ni-64, Zn-64, Cu-65, Zn-66, Zn-67 and Zn-68
Ni-64, Zn-64	Co-59, Ni-60, Ni-61, Ni-62, Ni-64, Zn-64, Cu-65, Cu-65, Zn-66, Zn-67, Zn-68 and Ga-69
Cu-65	Ni-60, Ni-61, Ni-62, Cu-63, Cu-65, Zn-66, Zn-66, Zn-67, Zn-68, Ga-69, Zn-70 and Ge-70
Zn-66	Ni-61, Ni-62, Cu-63, Ni-64, Zn-64, Zn-66, Zn-67, Zn-67, Zn-68, Ga-69, Zn-70, Ge-70 and Ga-71
Zn-67	Ni-62, Cu-63, Ni-64, Zn-64, Cu-65, Zn-67, Zn-68, Zn-68, Ga-69, Zn-70, Ge-70, Ga-71 and Ge-72
Zn-68	Cu-63, Ni-64, Zn-64, Cu-65, Zn-66, Zn-68, Ga-69, Ga-69, Zn-70, Ge-70, Ga-71, Ge-72 and Ge-73
Ga-69	Ni-64, Zn-64, Cu-65, Zn-66, Zn-67, Ga-69, Zn-70, Ge-70, Zn-70, Ge-70, Ga-71, Ge-72, Ge-73, Ge-74 and Se-74
Zn-70, Ge-70	Cu-65, Zn-66, Zn-67, Zn-68, Zn-70, Ge-70, Ga-71, Ga-71, Ge-72, Ge-73, Ge-74, Se-74 and As-75

# ICP-MS/MS with Unit Mass Resolution Before the Cell

Element of Interest	Isotopes entering the Cell
Ti-50, V-50, Cr-50	Ti-50, V-50, Cr-50
V-51	V-51
Cr-52	Cr-52
Cr-53	Cr-53
Cr-54, Fe-54	Cr-54, Fe-54
Mn-55	Mn-55
Fe-56	Fe-56
Fe-57	Fe-57
Fe-58, Ni-58	Fe-58, Ni-58
Co-59	Co-59
Ni-60	Ni-60
Ni-61	Ni-61
Ni-62	Ni-62
Cu-63	Cu-63
Ni-64, Zn-64	Ni-64, Zn-64
Cu-65	Cu-65
Zn-66	Zn-66
Zn-67	Zn-67
Zn-68	Zn-68
Ga-69	Ga-69
Zn-70, Ge-70	Zn-70, Ge-70

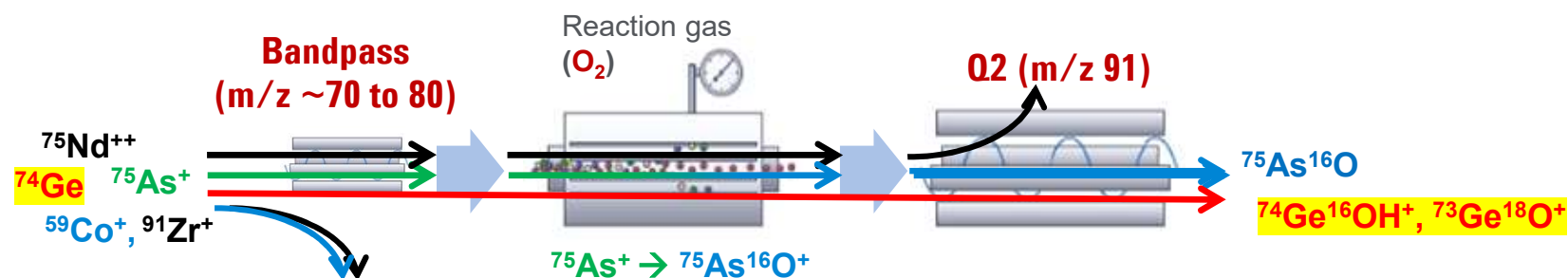
## What Does Bandpass MS Offer That Single Quad Can't?

### SOME control of reaction chemistry

Bandpass filter can reject SOME co-existing (analyte or matrix) ions that could appear at the same mass as the target analyte product ion, and SOME ions that might form reaction product ion overlaps on the target analyte ion, e.g. arsenic measured as  $\text{AsO}^+$  at  $m/z$  91 with  $\text{O}_2$  cell gas

- $^{75}\text{As}^{16}\text{O}^+$  product ion measured at  $m/z$  91 suffers overlap from  $^{91}\text{Zr}^+$ . Bandpass filter set to  $m/z$  75 to pass the  $\text{As}^+$  precursor ion. Zr at  $m/z$  91 is far enough away from  $m/z$  75 and so is outside the bandpass mass window and can be rejected from the ion beam
- In samples with high cobalt, Co ( $m/z$  59) forms  $\text{CoO}_2^+$  in the cell, overlapping the  $\text{AsO}^+$  product ion at  $m/z$  91. Bandpass filter (set to  $m/z$  75) rejects Co and stops formation of  $\text{CoO}_2^+$  in the cell

However, **bandpass filter CANNOT reject ions within ~ a 10 u window** around the analyte precursor ion ( $m/z$  75). Includes  $^{72}\text{Ge}$ ,  $^{73}\text{Ge}$ ,  $^{74}\text{Ge}$ ... which can form  $\text{GeO}$  &  $\text{GeOH}$  at  $m/z$  91



**ICP-QQQ with MS/MS** passes ONLY  $m/z$  75 to the cell, so Ge is rejected; **no GeO/GeOH overlaps**

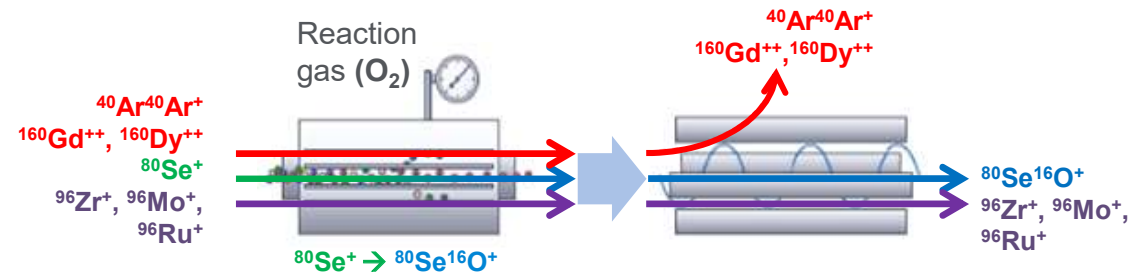


## Application Example: Analysis of Selenium Mass-shift with oxygen (O<sub>2</sub>) Reaction Gas on ICP-QMS

Se measured as SeO<sup>+</sup>, to avoid <sup>40</sup>Ar<sub>2</sub><sup>+</sup> & <sup>160</sup>Gd<sup>++</sup>/<sup>160</sup>Dy<sup>++</sup> overlaps on <sup>80</sup>Se<sup>+</sup>



**BUT** SeO<sup>+</sup> product ion at m/z 96 can be overlapped by <sup>96</sup>Zr<sup>+</sup>, <sup>96</sup>Mo<sup>+</sup>, <sup>96</sup>Ru<sup>+</sup>



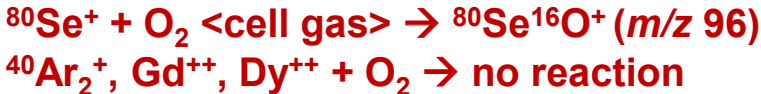
No Q1 - all ions  
enter the cell

Quad (m/z 96) – allows  
through all ions at m/z 96

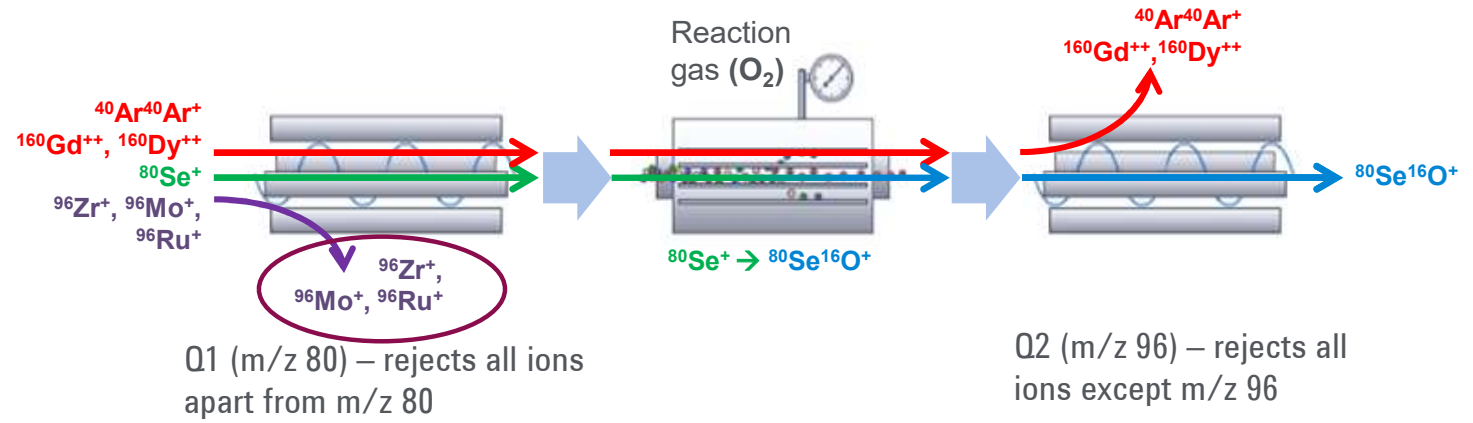
Conventional ICP-QMS has no mass filter before the cell, so cannot reject existing interferences that overlap cell-formed analyte reaction product ions

# Se by ICP-QQQ - MS/MS Mass-Shift with O<sub>2</sub> Cell Gas

Same reaction with O<sub>2</sub> cell gas for Se on 8900 ICP-QQQ with MS/MS:



In MS/MS, Q1 rejects any ions (Zr<sup>+</sup>, Mo<sup>+</sup>, Ru<sup>+</sup>) that could overlap SeO<sup>+</sup> product ion at mass 96



Allows measurement of SeO<sup>+</sup> at product ion mass, after removal of original Ar<sub>2</sub><sup>+</sup>/REE<sup>++</sup> interference, and existing ions at SeO<sup>+</sup> product ion mass

## Comparing Quadrupole ICP-MS Configurations

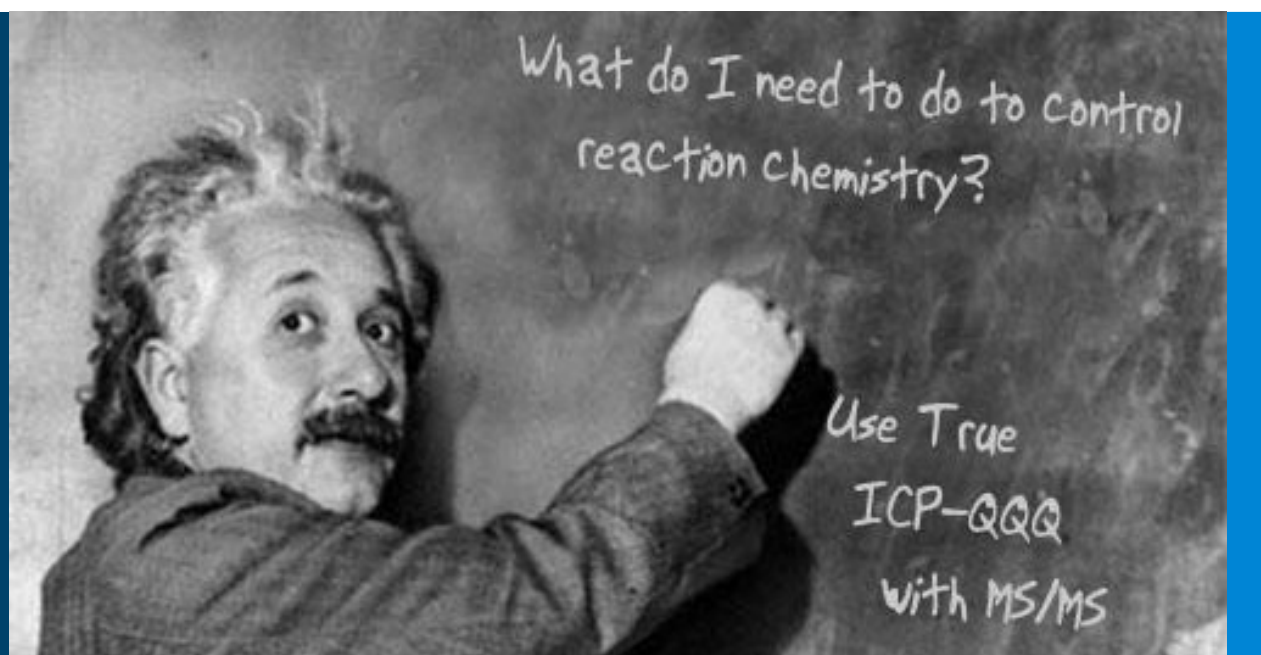
1 Quadrupole ICP-MS configurations; what they are and why it matters

2 Interference removal capabilities and other performance comparisons

***Comparing Bandpass MS and MS/MS***

## What Difference Does MS/MS Really Make to Reaction Mode Results

The key factor is the extra true mass filter (Q1) before the CRC

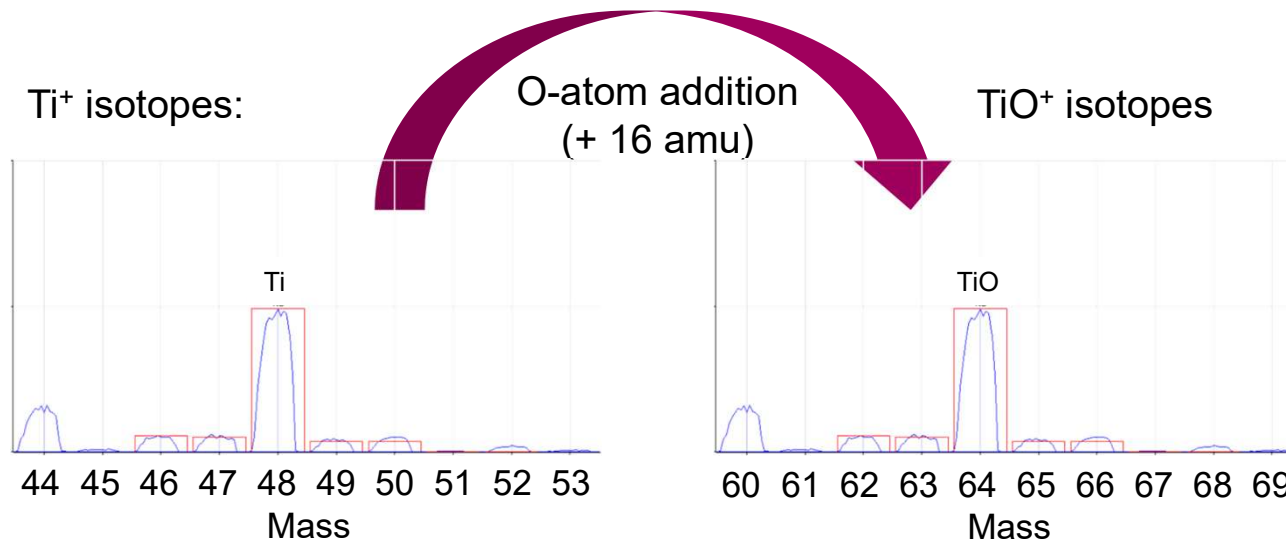


## Demonstration of MS/MS Mass-Shift in Practice Ti Analysis With O<sub>2</sub> Reaction Cell Gas

Many elements can be measured as MO<sup>+</sup> product ions with O<sub>2</sub> cell gas.

Reaction process used is O-atom addition:

Ti<sup>+</sup> **precursor** ions react with O<sub>2</sub> cell gas to form TiO<sup>+</sup> **product** ions:



## Comparison of Single Quad vs MS/MS Operation TiO<sup>+</sup> Product Ions with O<sub>2</sub> Cell Gas

O<sub>2</sub> reaction chemistry works in conventional ICP-QMS or ICP-QQQ cell

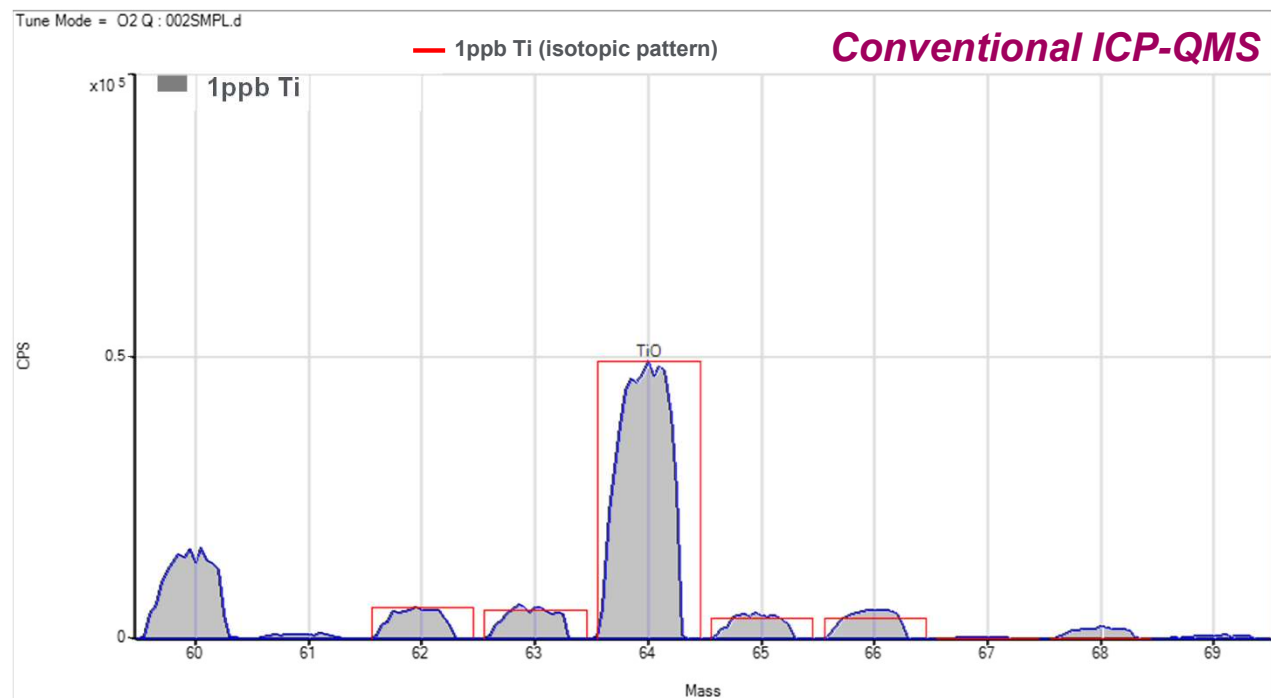
**BUT ICP-QMS can't control the ions that enter the cell**, so TiO<sup>+</sup> product ions can be overlapped by other analyte ions (or product ions).

	Precursor Ion (Q1)	Product Ion (Q2)	Potential Overlaps from other analytes		
<sup>46</sup> TiO <sup>+</sup> (mass 62) is overlapped by <sup>62</sup> Ni	Ti	TiO	Ni	Cu	Zn
<sup>47</sup> TiO <sup>+</sup> (mass 63) is overlapped by <sup>63</sup> Cu	46	62	<sup>62</sup> Ni		
<sup>48</sup> TiO <sup>+</sup> (mass 64) is overlapped by <sup>64</sup> Zn	47	63		<sup>63</sup> Cu	
<sup>49</sup> TiO <sup>+</sup> (mass 65) is overlapped by <sup>65</sup> Cu	48	64			<sup>64</sup> Zn
<sup>50</sup> TiO <sup>+</sup> (mass 66) is overlapped by <sup>66</sup> Zn	49	65		<sup>65</sup> Cu	
	50	66			<sup>66</sup> Zn

These overlapping ions cannot be rejected by a bandpass cell, because **they are at the same masses as the TiO<sup>+</sup> product ions being measured**

# TiO<sup>+</sup> Analysis by Conventional ICP-QMS

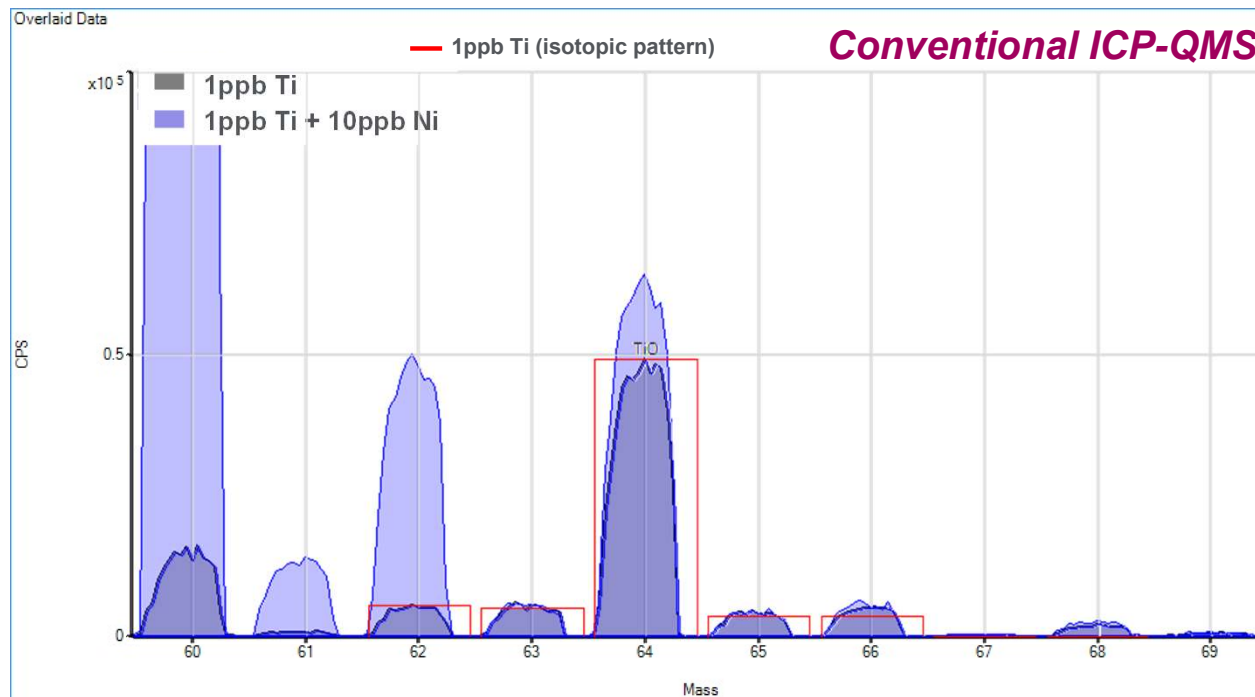
TiO<sup>+</sup> product ions in simple, single-element standard



**1 ppb Ti standard – TiO<sup>+</sup> peaks match theoretical isotopic abundances**

## TiO<sup>+</sup> by ICP-QMS; Other Elements Present

In mixed matrix, TiO<sup>+</sup> product ions are overlapped by other analyte (or matrix) ions. Ti (1 ppb) with Ni (10 ppb) shown below

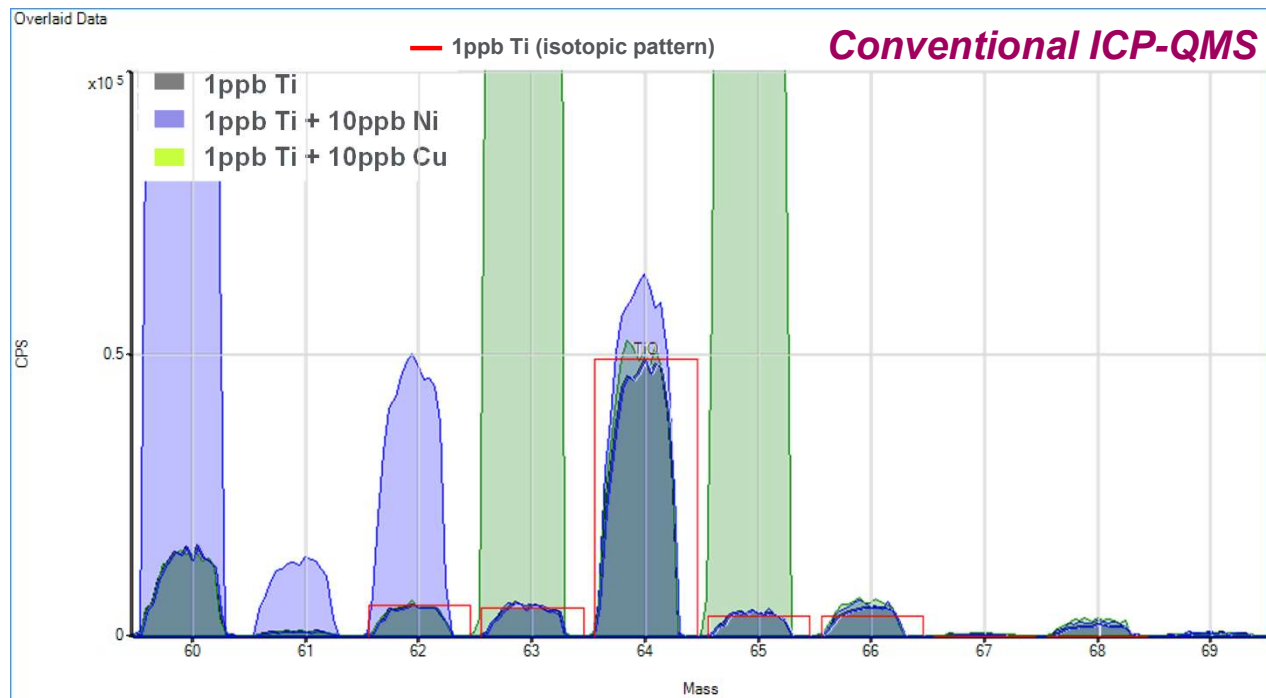


**1 ppb Ti overlaid with 1 ppb Ti + 10 ppb Ni (Ni<sup>+</sup> overlaps TiO<sup>+</sup>)**



## TiO<sup>+</sup> by ICP-QMS; Other Elements Present

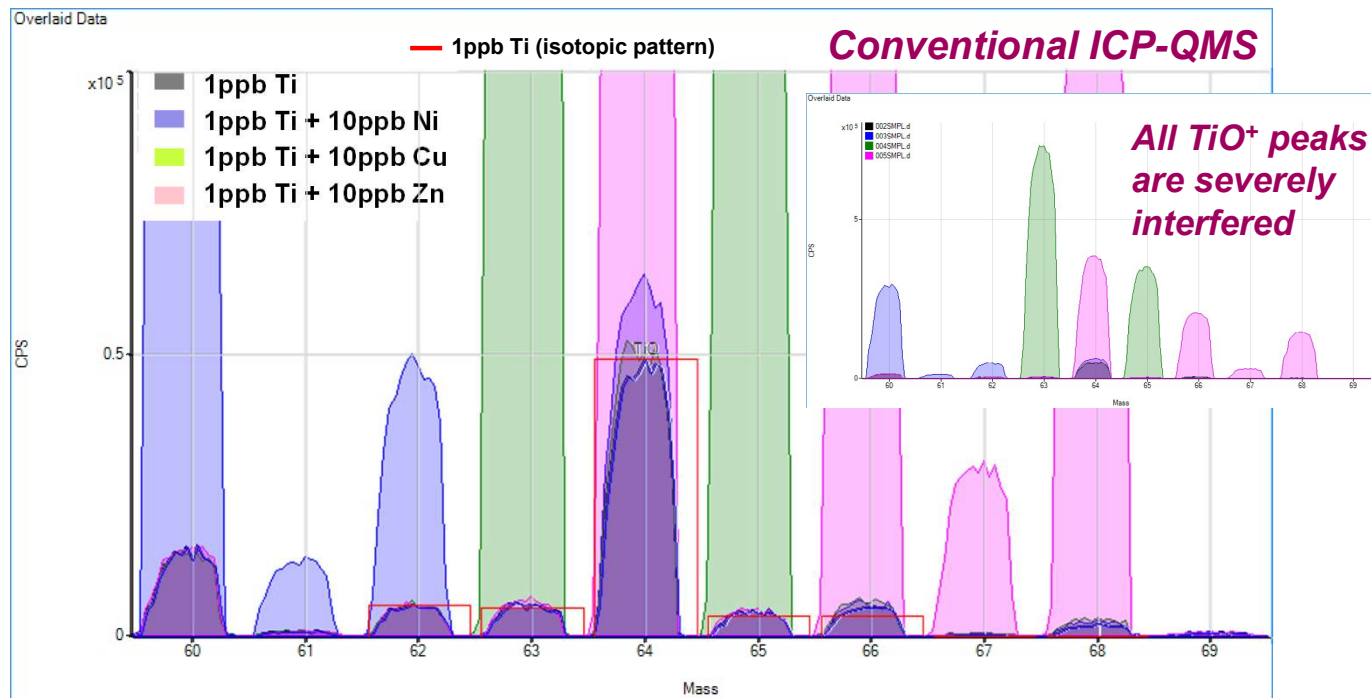
Further analyte (or matrix) ions give further overlaps. Ti (1 ppb) with Ni & Cu (10 ppb) shown below



**1 ppb Ti overlaid with 1 ppb Ti + 10 ppb Ni & Cu (Ni<sup>+</sup> & Cu<sup>+</sup> overlap TiO<sup>+</sup>)**

# TiO<sup>+</sup> by ICP-QMS; Other Elements Present

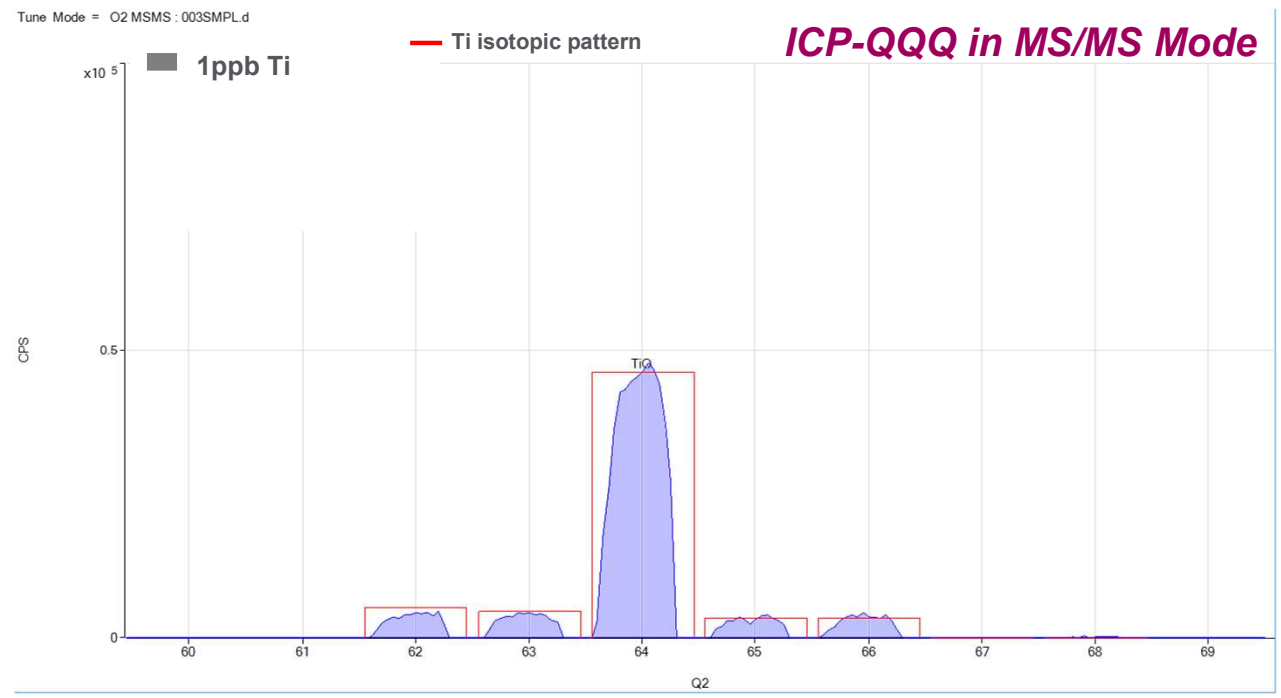
Even in a simple mix of common analytes, all the TiO<sup>+</sup> product ion isotopes are overlapped when conventional reaction cell ICP-QMS is used



**1 ppb Ti overlaid with 1 ppb Ti + 10 ppb Ni, Cu, Zn (Ni<sup>+</sup>, Cu<sup>+</sup>, Zn<sup>+</sup> overlap TiO<sup>+</sup>)**

# TiO<sup>+</sup> Analysis by ICP-QQQ (MS/MS)

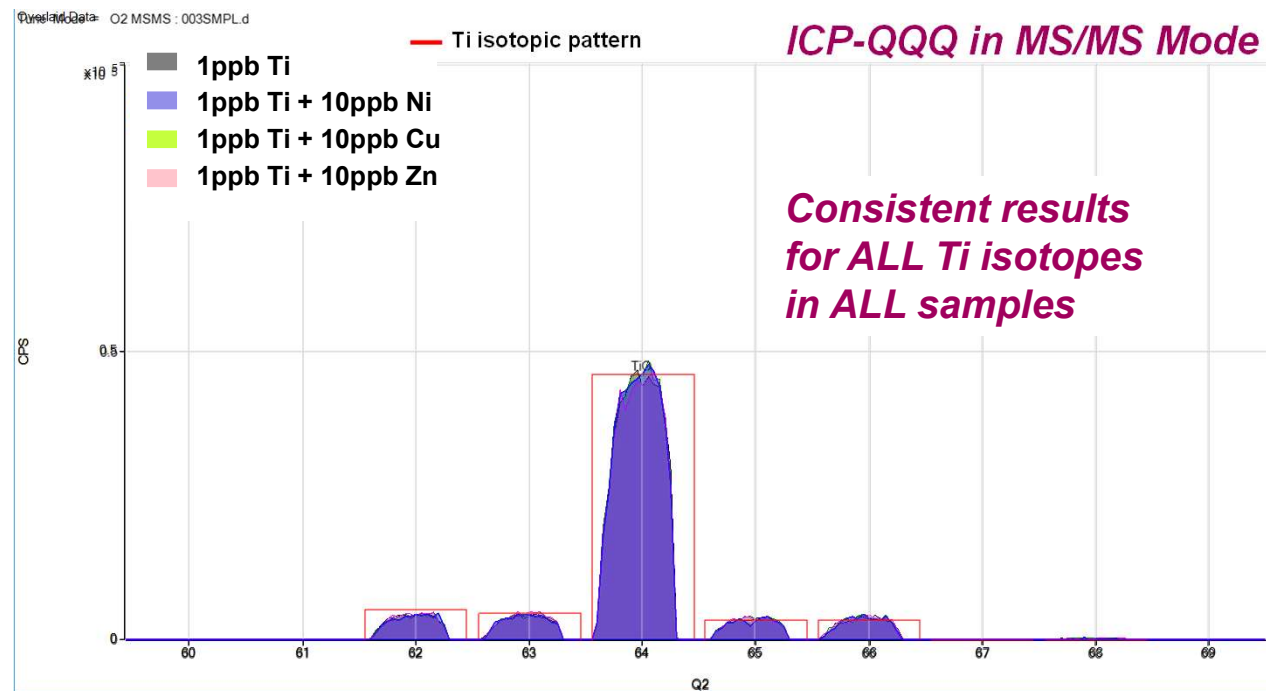
TiO<sup>+</sup> product ions in simple, single-element standard



**1 ppb Ti. Ti<sup>+</sup> is converted to TiO<sup>+</sup> with O<sub>2</sub> cell gas – perfect template match**

## TiO<sup>+</sup> by ICP-QQQ; Other Elements Present

TiO<sup>+</sup> product ions are consistent in all 4 samples; all the Ni, Cu and Zn overlaps are eliminated with the 8900 ICP-QQQ with MS/MS



**MS/MS mode - Q1 rejects all pre-existing ions at TiO<sup>+</sup> product ion masses, so there are no overlaps from Ni, Cu, Zn**

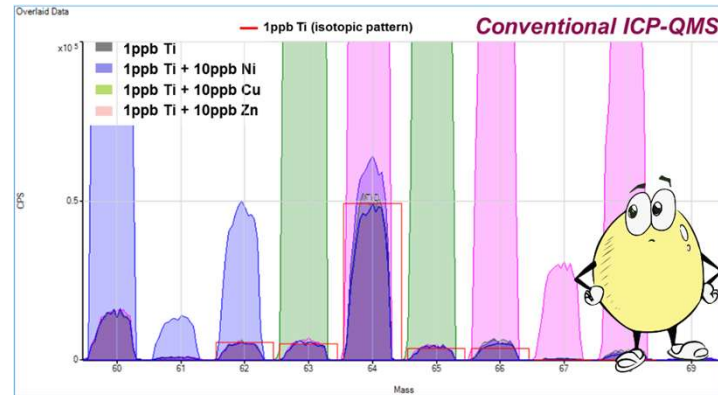
# ICP-QQQ; The Benefit of MS/MS is Clear

## Comparison of $\text{TiO}^+$ spectrum with ICP-QMS and ICP-QQQ

### Top – “Single-Quad” Bandpass Mode

All masses between ~ 30 amu and 80 amu enter the cell, so other ions ( $\text{Ni}^+$ ,  $\text{Cu}^+$ ,  $\text{Zn}^+$ ) contribute to signal at  $\text{TiO}^+$  isotope masses.

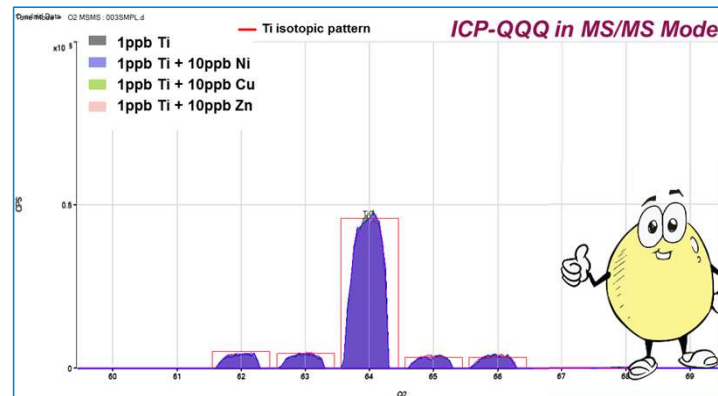
Results are unreliable; ALL Ti isotopes are interfered, and the interferences on the different Ti isotopes are matrix-dependent



### Bottom – Agilent ICP-QQQ in MS/MS Mode

$\text{TiO}^+$  peaks match the theoretical isotope abundance template in all samples.

All Ti isotopes are interference-free; secondary isotopes can be used for confirmation, or for isotopic analysis (isotope ratio or isotope dilution)



## Application Example: Sulfur Analysis

Previously difficult element for quadrupole ICP-MS

Sulfur analysis is of interest in many research and commercial laboratories

- Pharma and biopharma (sulfur-containing drugs)
- Life sciences research (protein/peptide quantification)
- Petroleum (fuels) and petrochemicals industry
- Environment (soil, plants, water, air quality)
- Food (preservatives, flavor/fragrance)

Reaction process is O-atom addition: S measured as  $\text{SO}^+$  product ions, i.e.  $^{32}\text{S}$  measured as  $^{32}\text{S}^{16}\text{O}^+$  at m/z 48

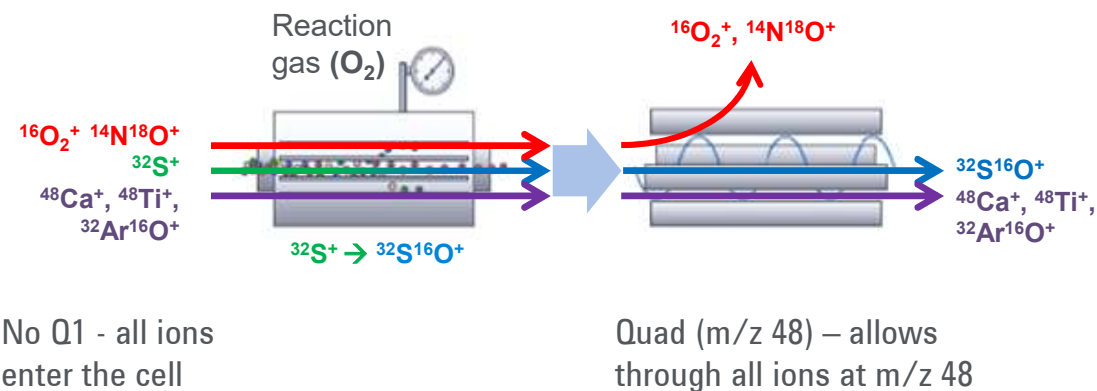
## Application Example: Analysis of Sulfur by ICP-QMS Mass-Shift with O<sub>2</sub> Reaction Gas

Sulfur is measured as SO<sup>+</sup> using oxygen (O<sub>2</sub>) cell gas with ICP-QMS.

O<sub>2</sub> reaction mode can avoid <sup>16</sup>O<sub>2</sub><sup>+</sup> and <sup>14</sup>N<sup>18</sup>O<sup>+</sup> overlaps on <sup>32</sup>S<sup>+</sup>:



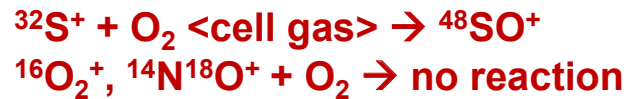
but SO<sup>+</sup> product ion at m/z 48 can be overlapped by <sup>48</sup>Ca<sup>+</sup>, <sup>48</sup>Ti<sup>+</sup>, <sup>36</sup>Ar<sup>12</sup>C<sup>+</sup>



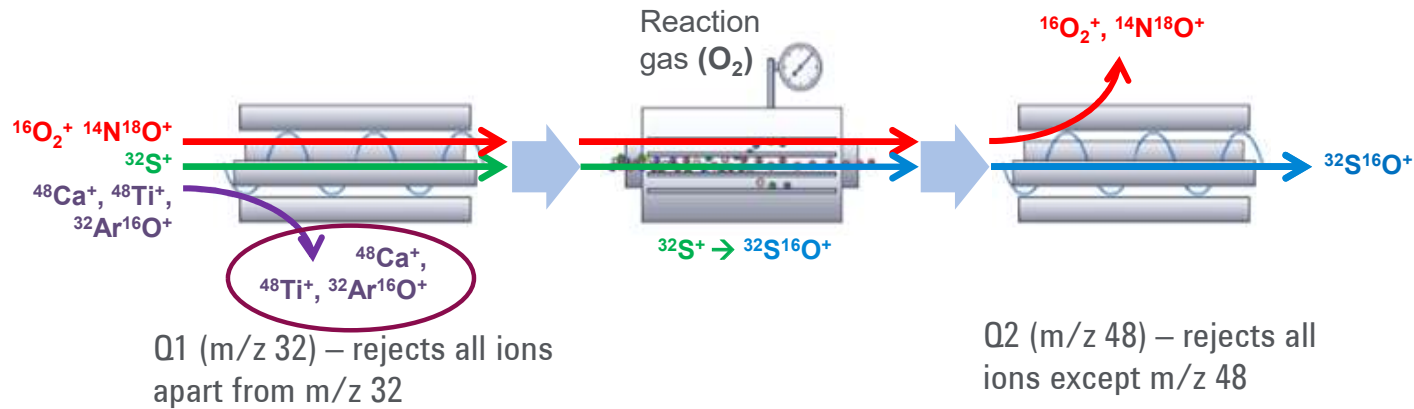
Conventional ICP-QMS has no mass filter before the cell, so cannot reject existing interferences that overlap cell-formed analyte reaction product ions

## Application Example: Analysis of Sulfur by ICP-QQQ MS/MS Mass-Shift with O<sub>2</sub> Reaction Gas

Same reaction with O<sub>2</sub> cell gas for S on 8900 ICP-QQQ with MS/MS:



***BUT*** Q1 of 8900 rejects any ions (Ca<sup>+</sup>, Ti<sup>+</sup>, ArC<sup>+</sup>) that could overlap SO<sup>+</sup> product ion at mass 48

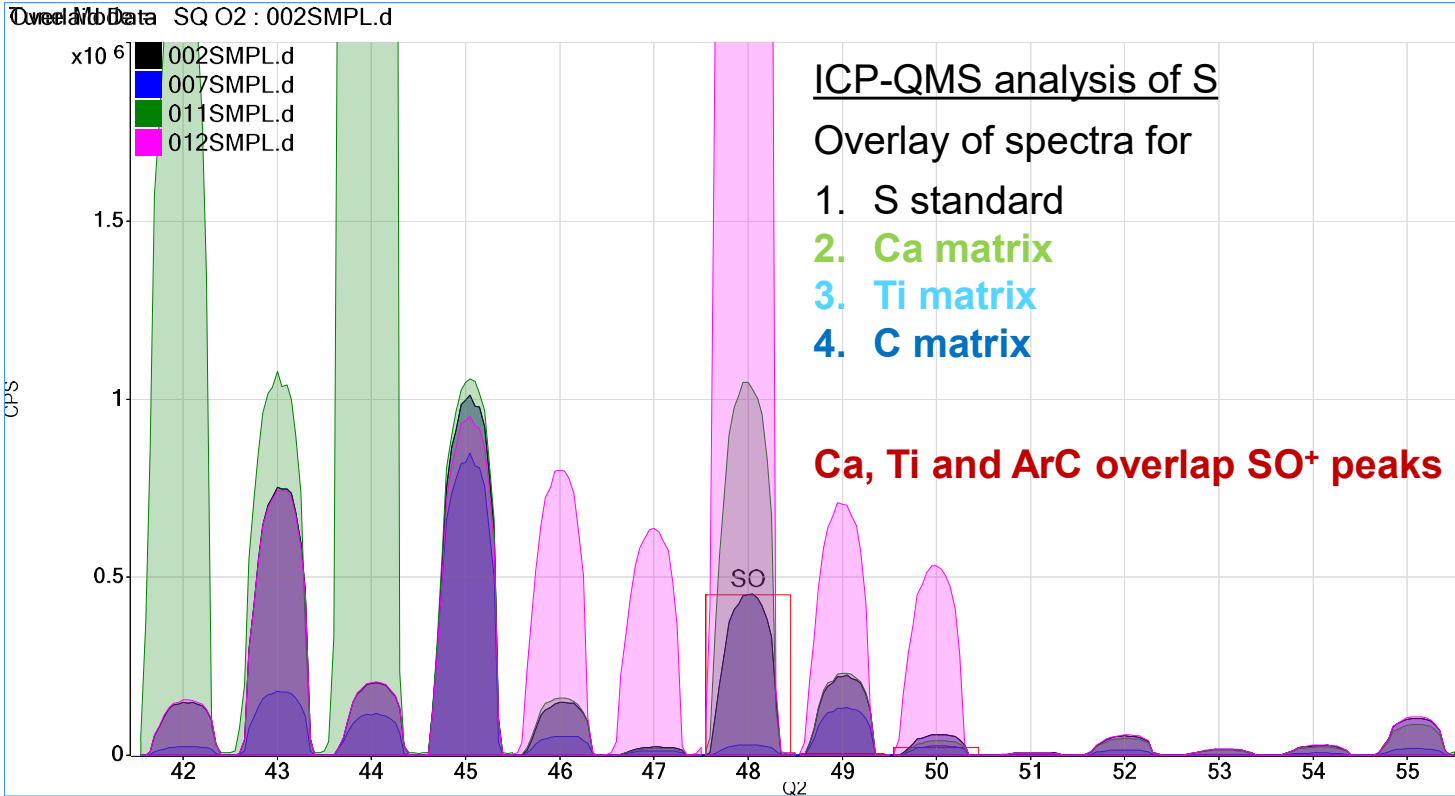


Allows measurement of SO<sup>+</sup> at product ion mass, after removal of original O<sub>2</sub><sup>+</sup>/NO<sup>+</sup> interference, and existing ions at SO<sup>+</sup> product ion mass



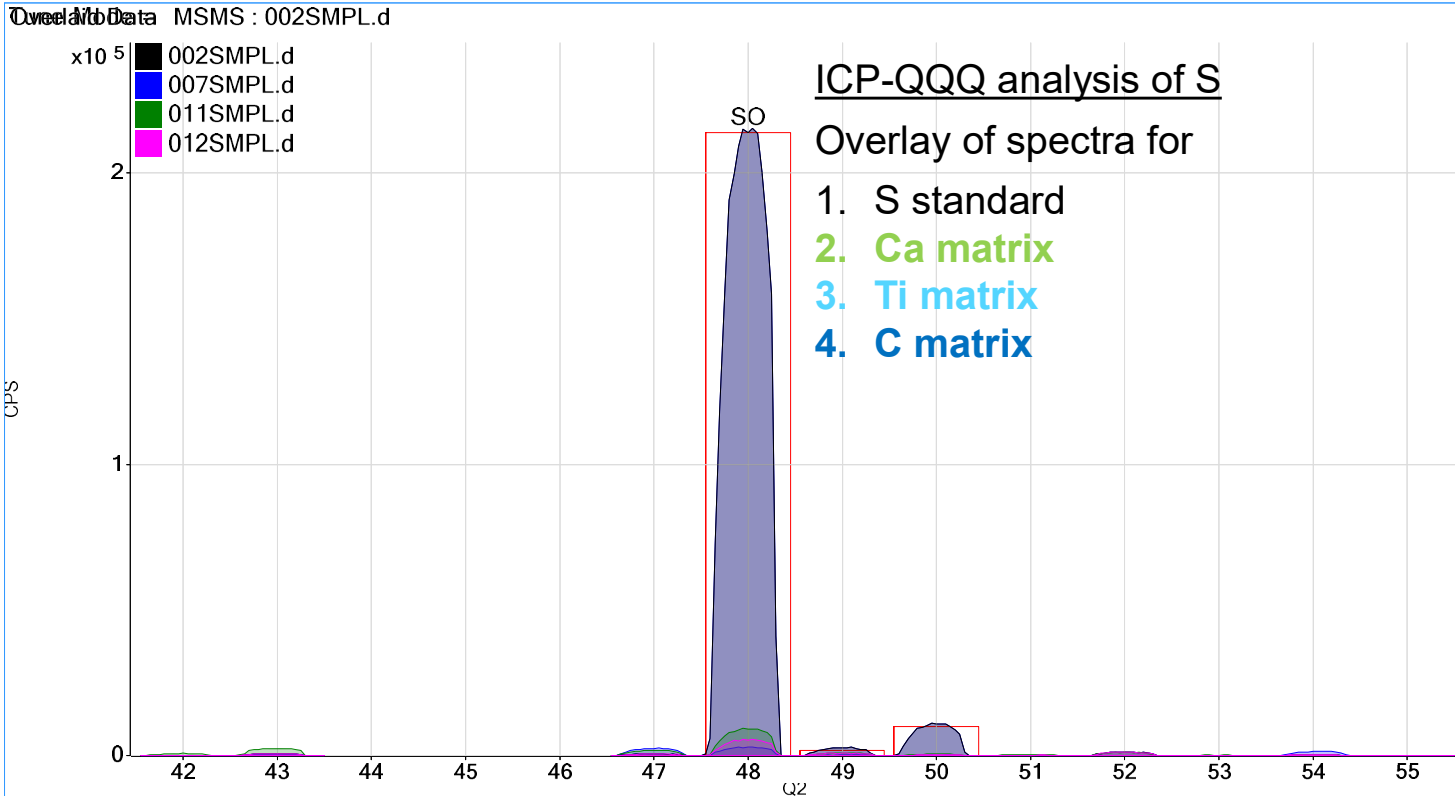
# Measurement of Sulfur by ICP-QMS

## S standard overlaid with Ca, Ti and C matrix



# Measurement of Sulfur by ICP-QQQ

S standard overlaid with Ca, Ti and C matrix



## Summary: Agilent ICP-MS and ICP-QQQ Enable You to:

Perform routine, typical applications cost-effectively using helium collision mode

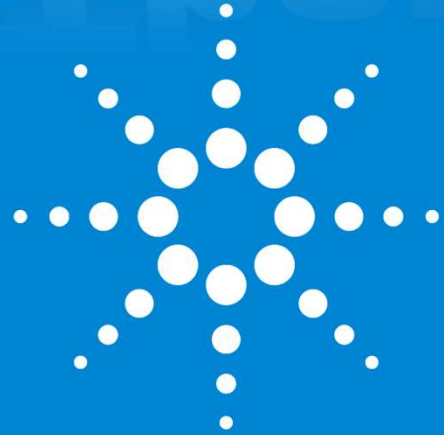
Use reactive cell gases to improve performance, access difficult/unusual applications, or undertake leading-edge research with the power of true ICP-QQQ with MS/MS



Agilent's ORS cell on the 7850/7900 is the **best way** to perform He mode

Agilent's 8900 ICP-QQQ is the **only way** to be sure of your results in reaction mode – address applications that SQ can't do

# Thank You



# Agilent

Trusted Answers