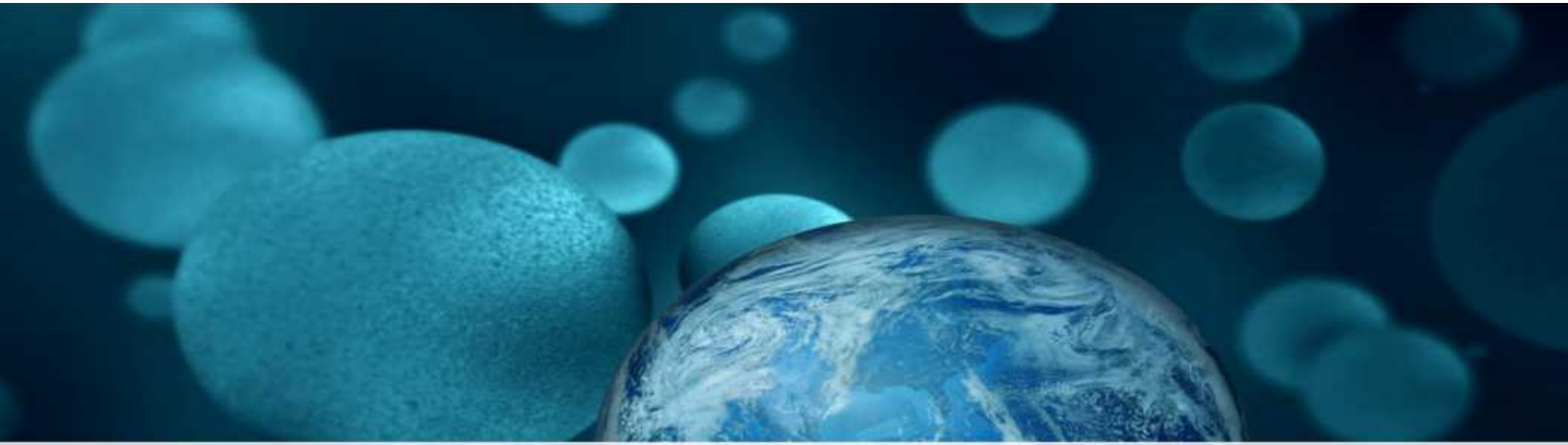


ThermoFisher SCIENTIFIC

All the Capability, None of the Limits: Routine and Research Trace Elemental Analysis

Matthew Cassap

Trace Elemental Analysis – low level detection of elements

- **BEA (Bulk Elemental Analysis)**
  - **5PPM to Percent Levels**
  - Arc/Spark OES (Optical Emission Spectrometer)
    - Metal composition (Iron/Steel making)
  - XRD/XRF (X-ray Diffraction/X-ray Flourescence)
    - Mining ore/Scrap Metal Sceening
- 1% = 10,000 ppm
- 1% = 10, 000 million ppt

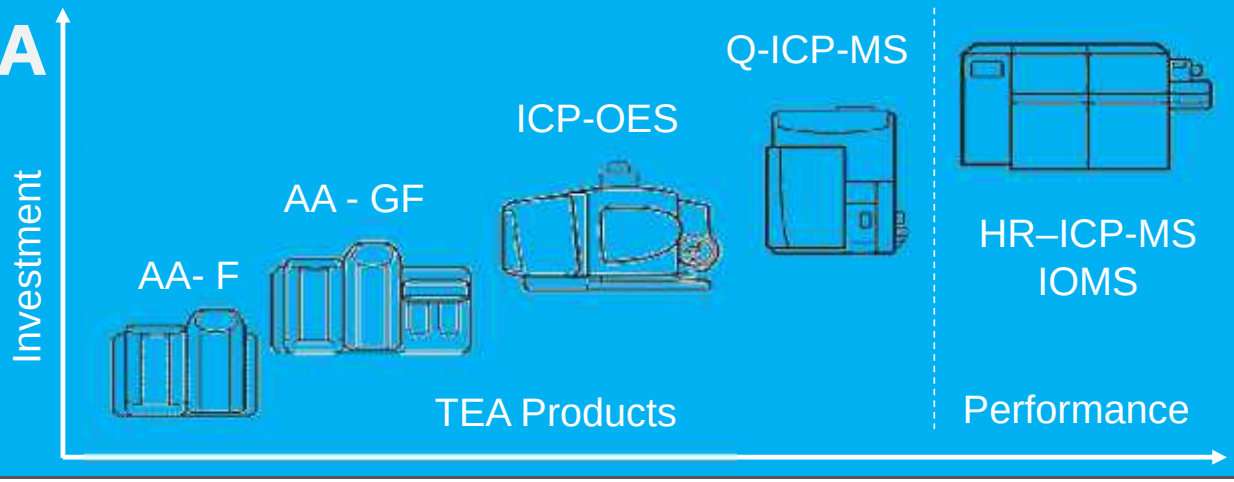
- **TEA (Trace Elemental Analysis)**
  - **PPM, PPB, PPT**
  - Atomic Absorption spectrometers (AA)
    - General lab analyzer – food, clinical
  - Inductively Coupled Plasma Optical Emmision Spectroscopy (ICP-OES)
    - High matrix samples – Soils, Used Oils
  - Inductively Coupled Plasma Mass Spec (ICPMS)
    - Low level – Drinking water, Semicon, Research
- 1 ppt = 0.000000000001% - very, very small
- 1 ppt = finding 1 person in the whole world

Trace Element Analysis

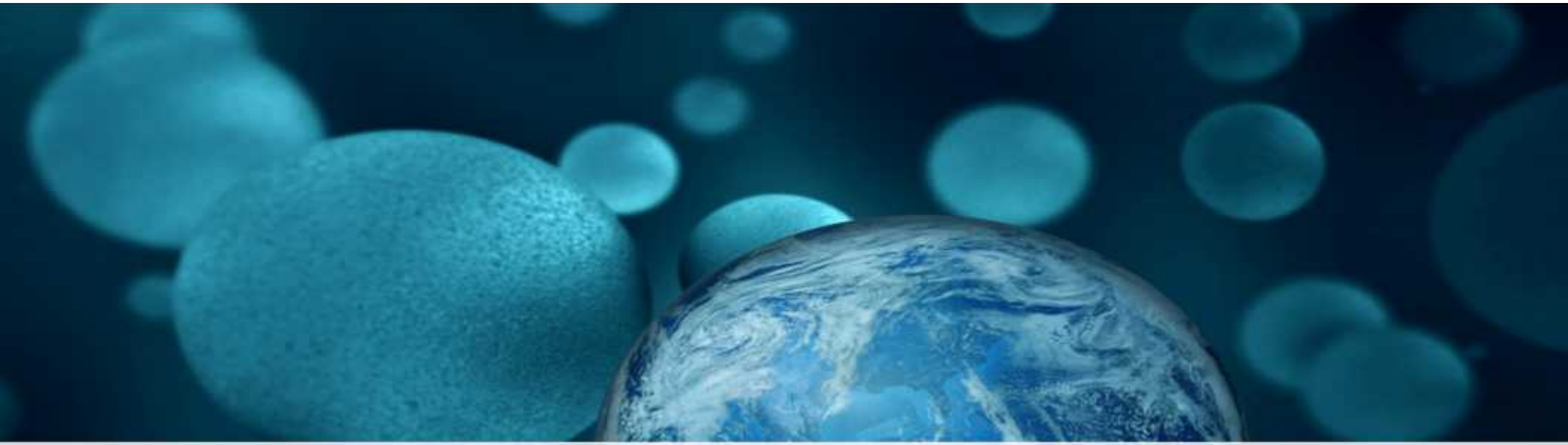
- Routine : Monitoring for QC/QC and human and environmental health
- Research : Tomorrow's routine analysis

Thermo Scientific TEA

- Over 50 year history
- Experience and Knowledge
- Complete Portfolio



ThermoFisher SCIENTIFIC



ThermoFisher SCIENTIFIC

iCE 3000 Series ICP-OES

The world leader in serving science

Product Range

iCE 3300

iCE 3300 GF

iCE 3400

iCE 3500

Graphite Furnace and Autosamplers

- To achieve to ppb detection limits
- For iCE 3300
  - GFS33
- For iCE 3400
  - GFS35Z
- For iCE 3500
  - GFS35 or GFS35Z
- Zeeman furnaces available with Rhodium plated centre block

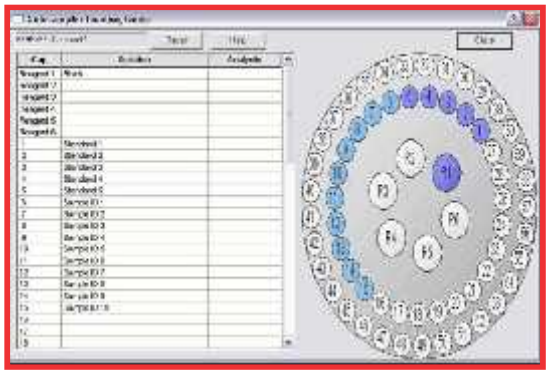
ThermoFisher SCIENTIFIC

Product Range – Graphite Furnace Modules

- Standard and Zeeman available
- Self-aligning cuvettes, easy to exchange
- Internal and external gas flow around cuvette
  - Protection of cuvette from air oxidation
  - Removal of vapours from inside cuvette
- Fast heating rates
- Voltage temperature control system
- Accurate heating regardless of cuvette life

Product Range – Furnace Auto-Sampler

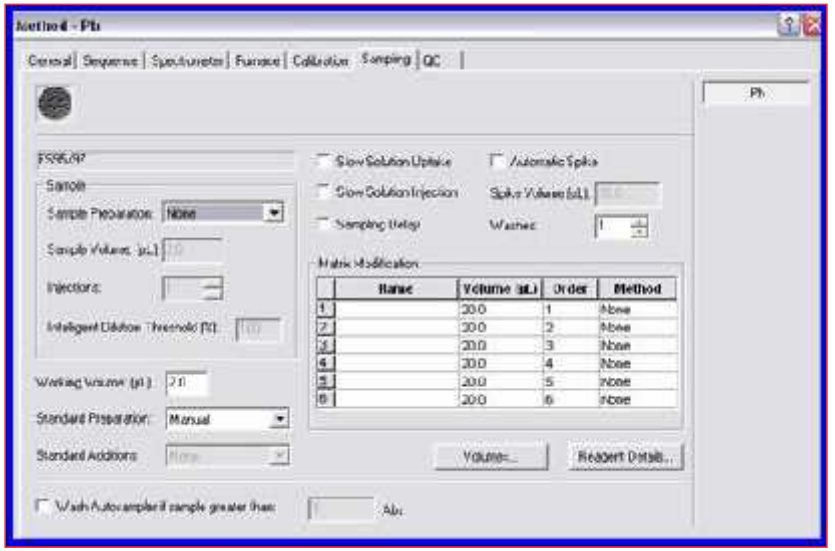
- Included with all furnace modules!!
- Replaces inaccurate and time consuming manual injection
- Invaluable for repeatable sample injection
- Fast furnace operation
- All functions programmed via software
- Fully configurable auto-sampler



ThermoFisher SCIENTIFIC

Product Range – Furnace Auto-Sampler

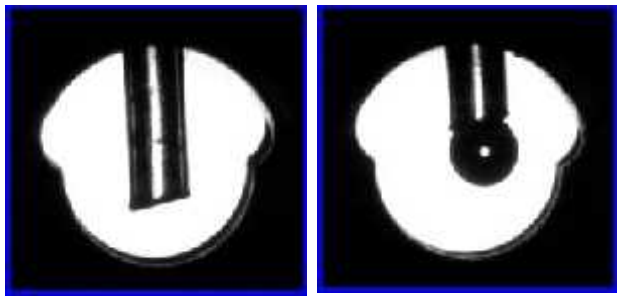
- More than just an auto-sampler
- Capable of:
  - Standard preparation
  - Matrix modification
  - Intelligent dilution
  - Standard additions
  - Slow uptake and injection
  - Wet, dry and pre-mix modifiers
- On board wash facilities

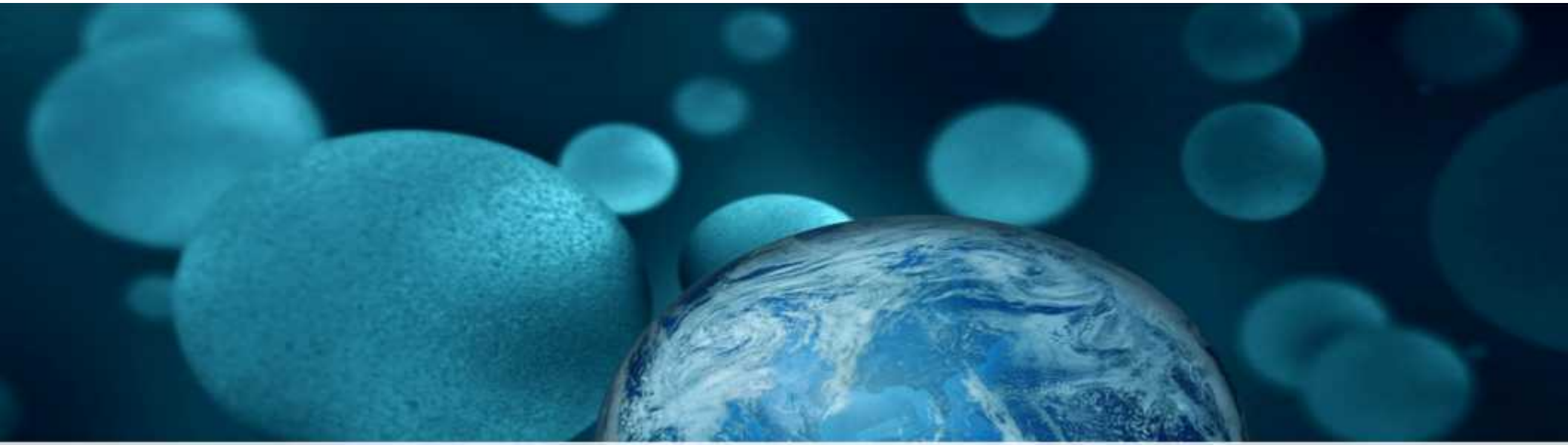


ThermoFisher SCIENTIFIC

- ***Open your eyes to furnace analysis***

- Valuable option on iCE 3300
- High definition images
- Colour graphics available
- Integrated into software





ThermoFisher SCIENTIFIC

iCAP 7000 Plus Series ICP-OES

The world leader in serving science

iCAP 7200 ICP-OES - Entry level, cost-effective analysis

Entry level, cost-effective analysis for low sample thru-put requirements.

Perfect analytical solution for restricted budgets or user moving up from AA

Simple Pre-optimised sample introduction

- Duo plasma viewing
- Pre-set 1150W plasma power
- Manual (pressure regulated) gas flow controls

Powerful Performance

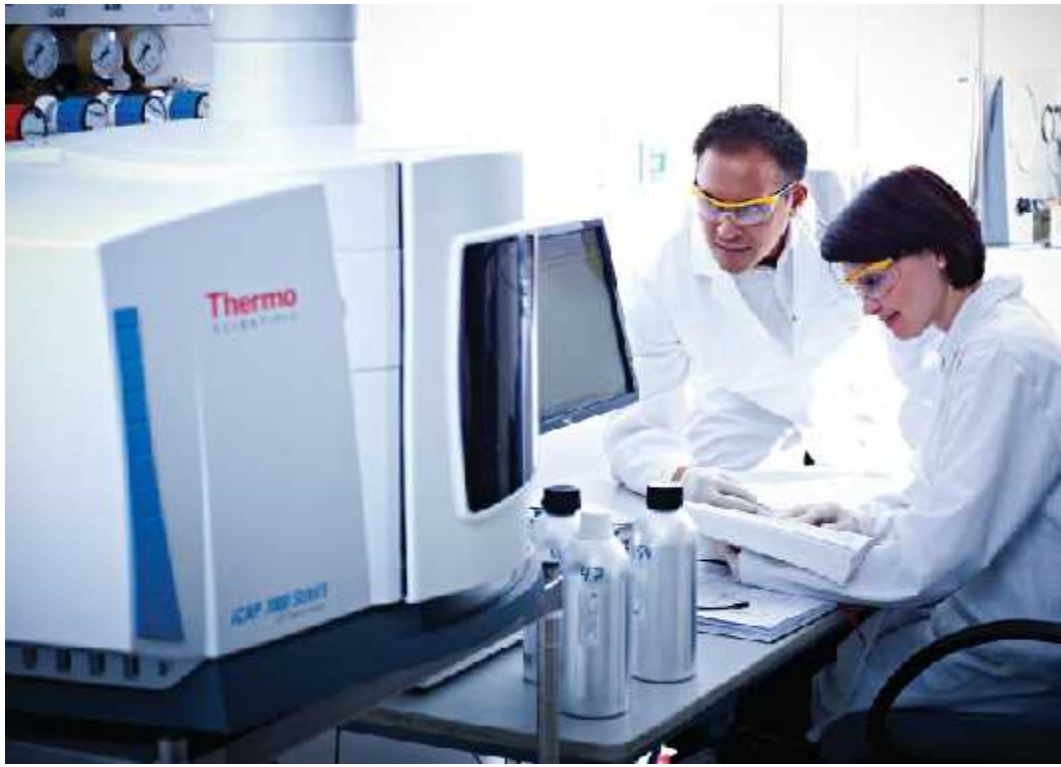
- Powerful resolution and DLs from iCAP 7000 Series ICP-OES
- Optimized productivity for small sample batches (≤ 100 samples per day)
  - Approximately 4 minutes per sample for a 15 element method (faster than AA)
  - Pre-loaded methods
  - ***Wavelength range 175-847 nm***
  - Access to most sensitive As, P, Hg, Tl, Sn and I wavelengths

iCAP 7400 ICP-OES - Entry level, cost-effective analysis

For routine analysis requirements and mid-range sample thru-put.

Ideal for QA/QC laboratories that require highest sensitivity from full wavelength coverage

- Powerful analytical detection & resolution
- Choice of plasma orientation to enable enhanced application suitability
- Intelligent software for powerful auto-optimization of the sample intro system



ThermoFisher SCIENTIFIC

iCAP 7600 ICP-OES – highest throughput ICP-OES

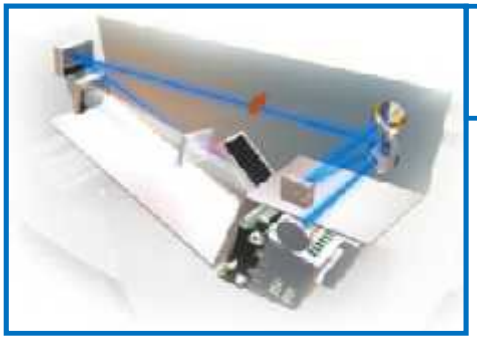
Highest productivity and maximum sample thru-put with advanced sprint valve sample introduction

Best solution for laboratories experiencing the most challenging analytical demands, such as large contract, or R&D facilities

- Powerful analytical detection & resolution
- Choice of plasma orientation to enable enhanced application suitability
- Intelligent software for powerful auto-optimization of the sample intro system
- Advanced data acquisition including ‘Sprint’ modes for ultimate productivity & versatility
- Comprehensive accessory compatibility

ThermoFisher SCIENTIFIC

The iCAP 7000 Series ICP-OES Core Technologies

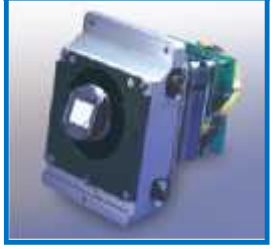


Optical design

EMT torch & Duo viewing

Clip-in sample intro systems

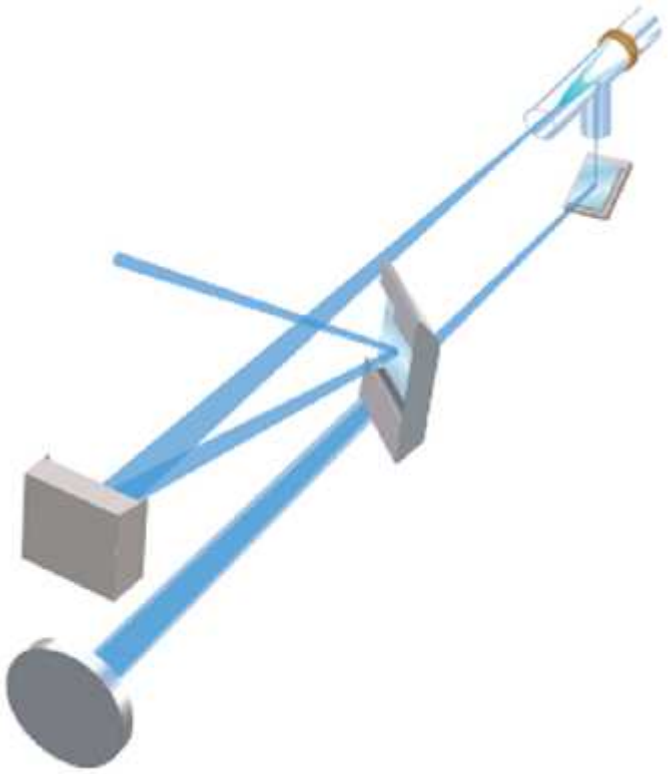
CID detector



Drain sensor

ThermoFisher SCIENTIFIC

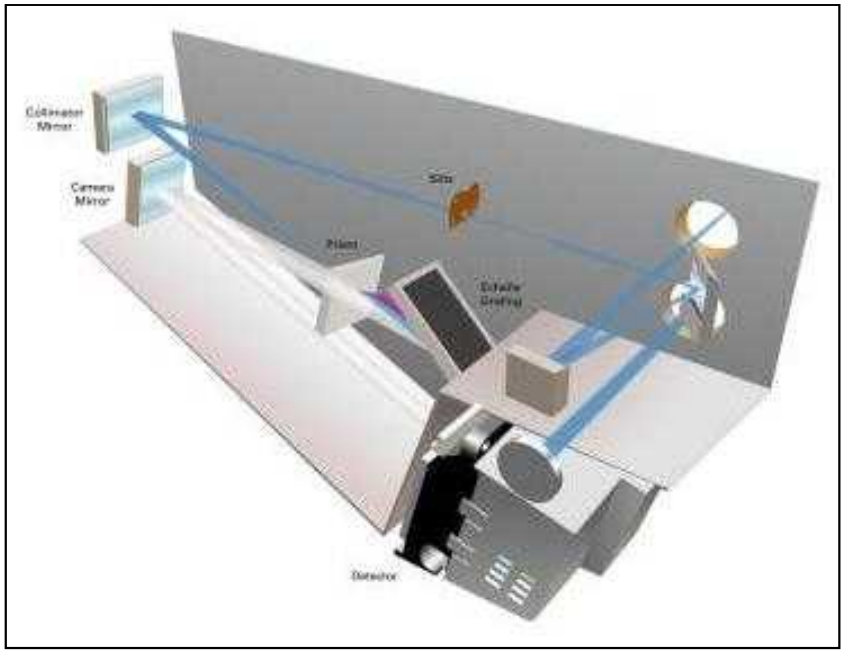
iCAP 7000 Series ICP-OES Optics – Fore Optics



- Duo View & Radial View Options
- Telephoto system (concave & convex mirror)
  - *Low aberrations (efficient collection of light)*
- Convex mirror (before slit) steerable in 2 directions
  - *selects view (in Duo)*
  - *allows peaking of plasma view (in Radial)*

iCAP 7000 Series ICP-OES Optical Design – Echelle Polychromator

- High optical stability & accuracy
  - *Compact optical design (thermally insulated with heater control to 0.1 ^{0}C)*
  - *Automated optical correction on GetReady*
  - *New wavelength calibration – accurate to <1 pixel*
- High resolution and image quality
  - *7 pm @ 200nm*
  - *Aberration compensation over whole chip*
  - *Reduced stray light effects*
  - *Anamorphic magnification focuses all lines on the chip*
- High sensitivity
  - *Compact design with reduced optical surfaces*
  - *Shorter integration times for faster analysis*
  - *UV & Vis slits for optimized light transmission*
- Low running costs
  - *Compact design allows fast purge & reduced gas consumption*

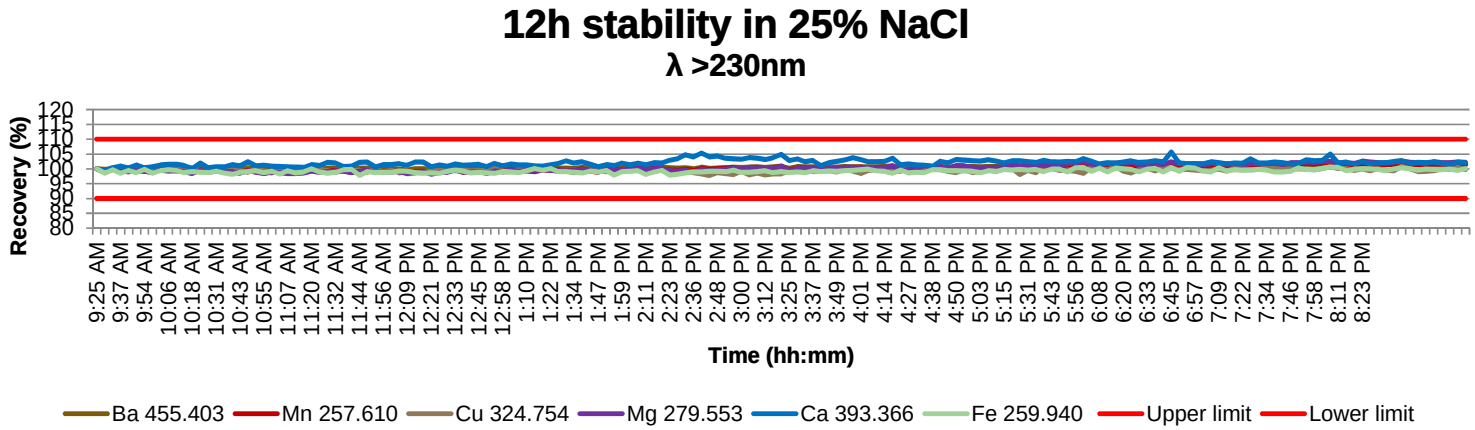


Sheath Gas for 7400 and 7600 Radial

- Sheath Gas improves the long term stability of instrument when running high salt applications
- Isolates the sample aerosol and prevents build up of salt crystals in the torch / Injector
- Allows customers to run for longer
- **Requires additional gas MFC (7400)**

Sheath Gas off

Sheath Gas on



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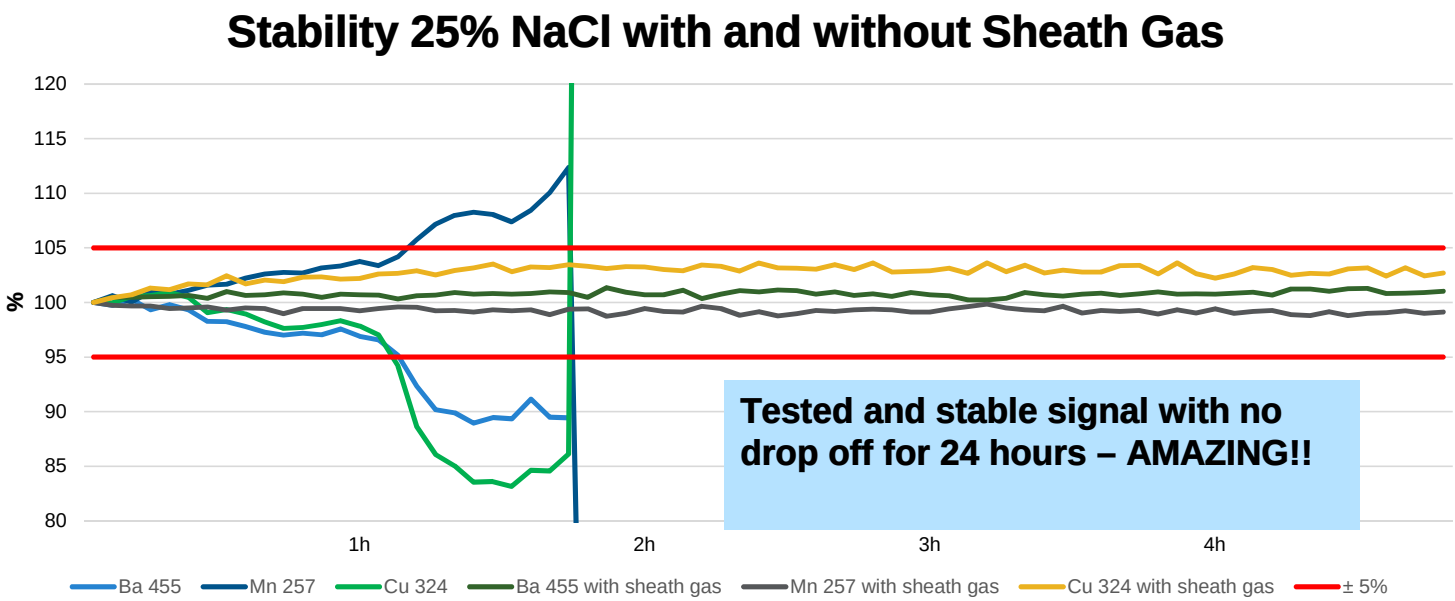
Stability data comparison with and without Sheath Gas



Tested and stable signal with no drop off for 24 hours – AMAZING!!

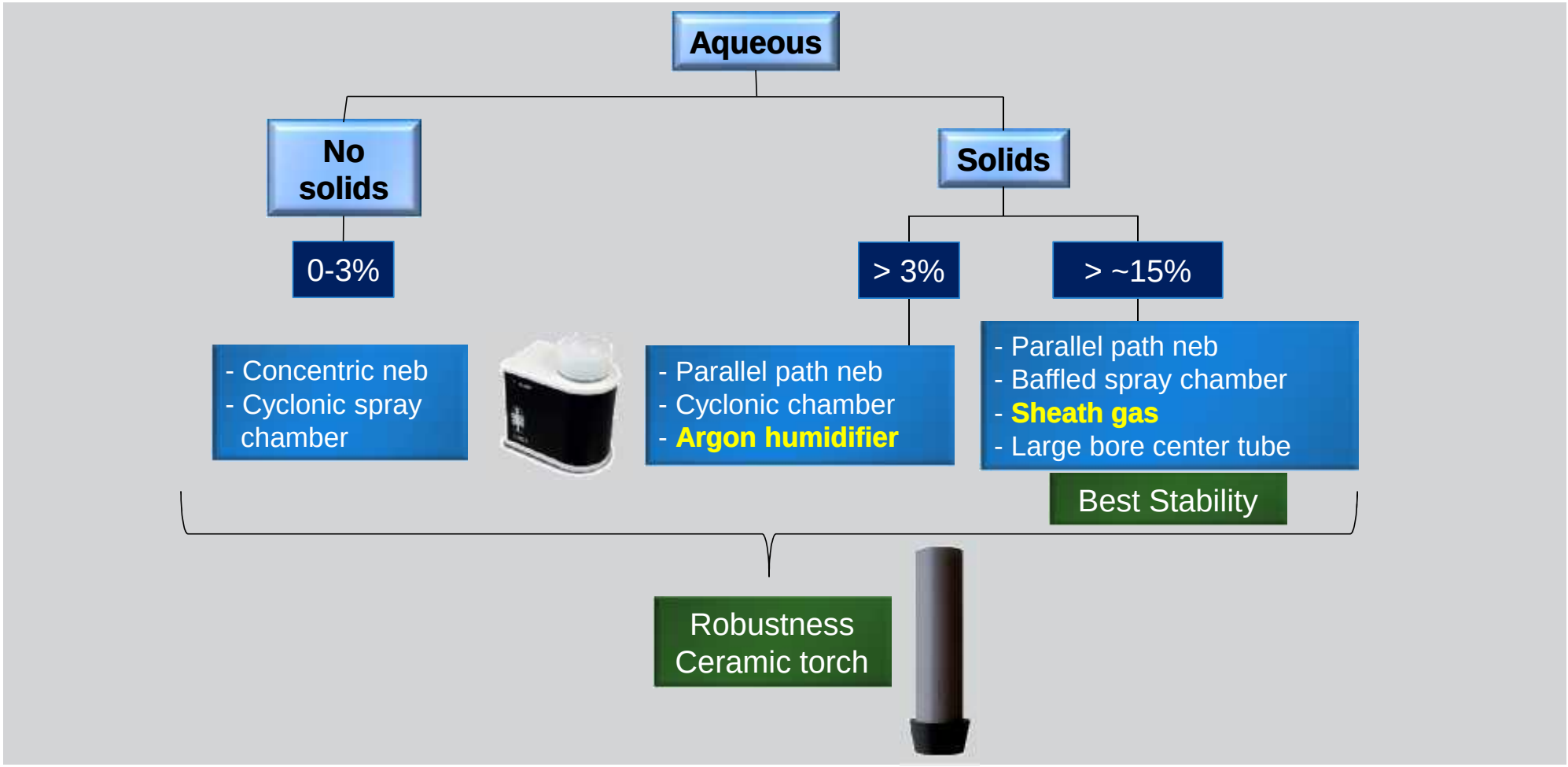
- This is now an option for the iCAP 7400 and iCAP 7600
- Greater robustness for extend periods of time

- Minimal sample preparation – less or no dilution of samples

Best ever performance OPTION for high matrix on 7400/7600 Radial

ThermoFisher SCIENTIFIC

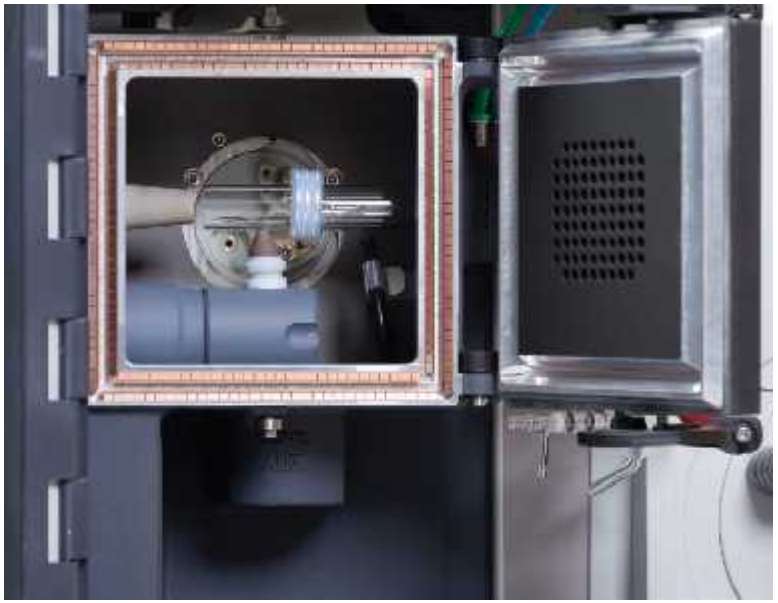
Argon Humidifier or Sheath Gas



ThermoFisher SCIENTIFIC

Performance – New Purged optical path plasma interfaces

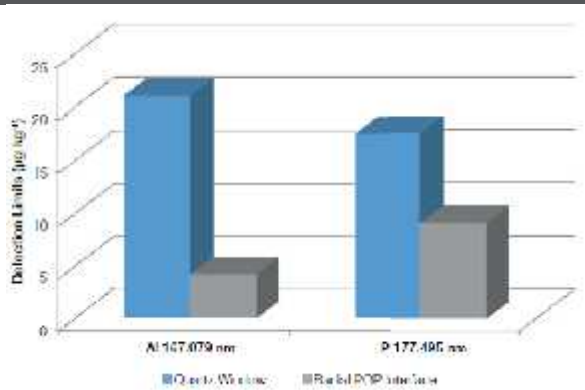
- As an option on all Duo instruments (72/74/7600)
- Ideal for heavy matrix customer measuring radial
  - Enviro (high P), Metals (Fe ore), Geochem (borate fusions)

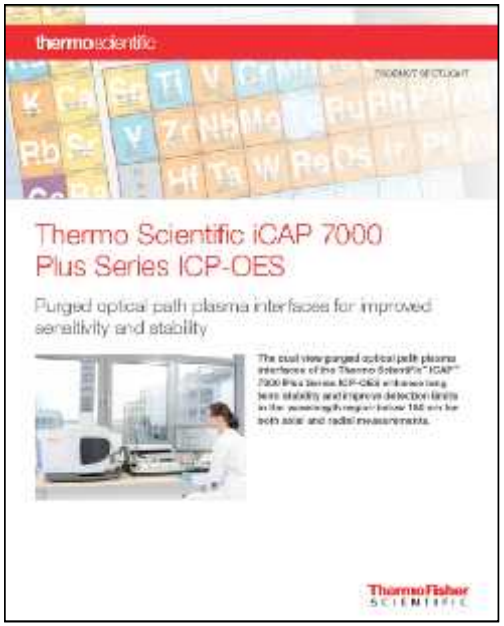


- Box contains:
  - 1x POP interface
  - 2x glass window
  - 2x O-ring
  - 1x alignment tool

Benefits of the POP Interface

- Improved sensitivity and stability
- Reduced need for user maintenance
- Improved UV detection limits through purged light path
- Long term stability of high matrix analysis





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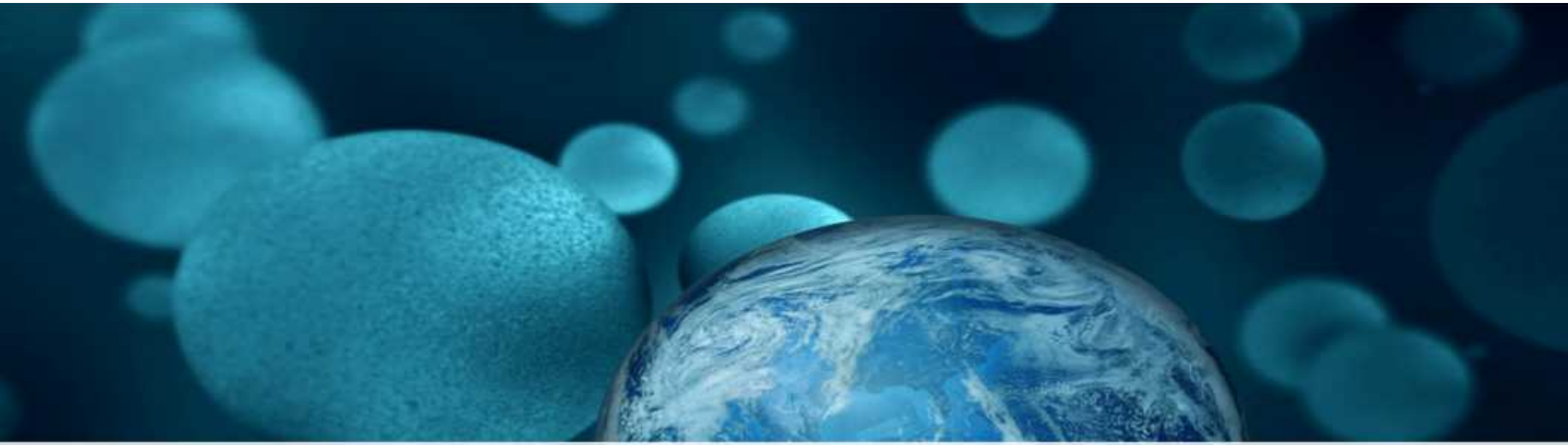


ThermoFisher SCIENTIFIC

Thermo Scientific iCAP RQ ICP-MS

The world leader in serving science

Advances in ICP-MS to Boost Simplicity and Accelerate Productivity

- Intuitive ‘hardware’ design
  - Designed with the operator in mind
- Simplified, yet powerful interference removal
  - KED with Qcell simplifies analysis
- Improved sample handling and automation
  - Automated plug-ins
- Larger dynamic range for real samples
- Minimal user intervention over prolonged analysis
- User-friendly software and workflows – Qtegra ISDS

ThermoFisher SCIENTIFIC

A Typical ICP-MS Standard Operating Procedure (SOP)

Instrument checks

- Interface and cones
- Sample Introduction System

Visual check to ensure correct installation and cleanliness

Getting operational

- Turn on plasma and check performance

Getting the ICP-MS ready for analysis, verify performance

Running samples

- Set up sequence of analysis
- Add QC and run samples
- Report/export data

Entering information into software to run samples and obtain results

Winning with Simplicity – User Friendly Operation

- Quick Connect Sample Introduction Svstem

- Simple torch assembly with no-nonsense gas connectivitv

- Unique drop-down door

- Unique flatapole with low mass cut-off

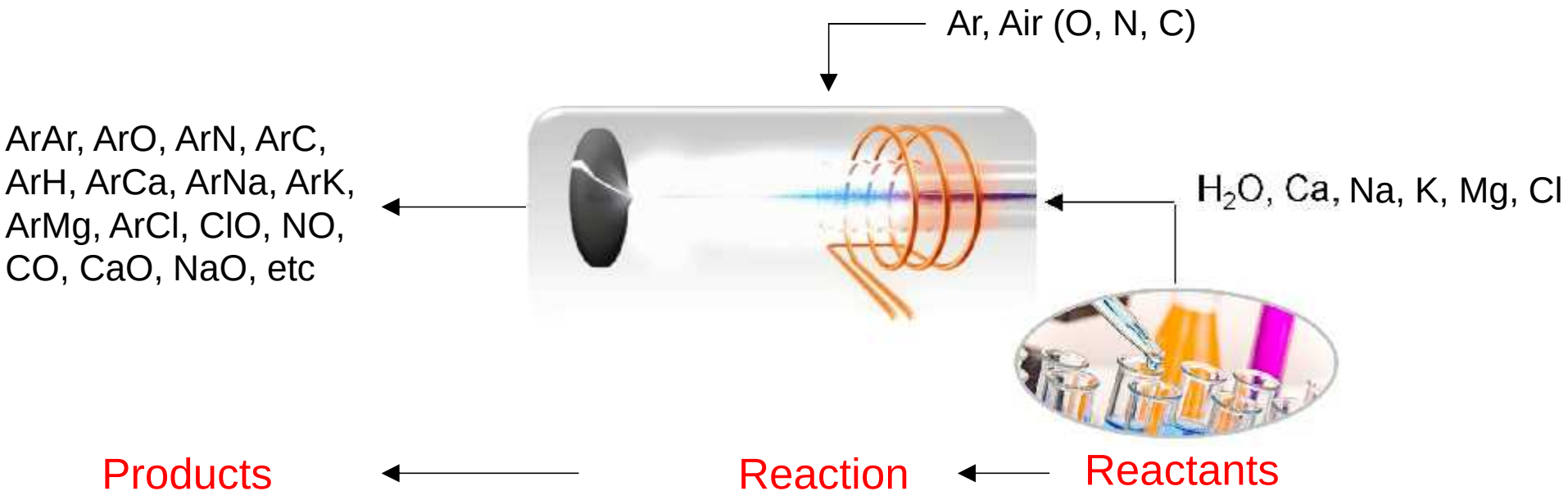
Quick Connect SIS	Fast, easy assembly	Minimal downtime
Simple torch assembly	Fool proof assembly	Consistent analysis
Drop down door	Easy access to cones & EL	Minimal downtime
QCell CRC	Single Mode He KED	No method development

Interferences – Spectral

Spectral Interferences – ICP-MS

- 2 most common types: isobaric and polyatomic

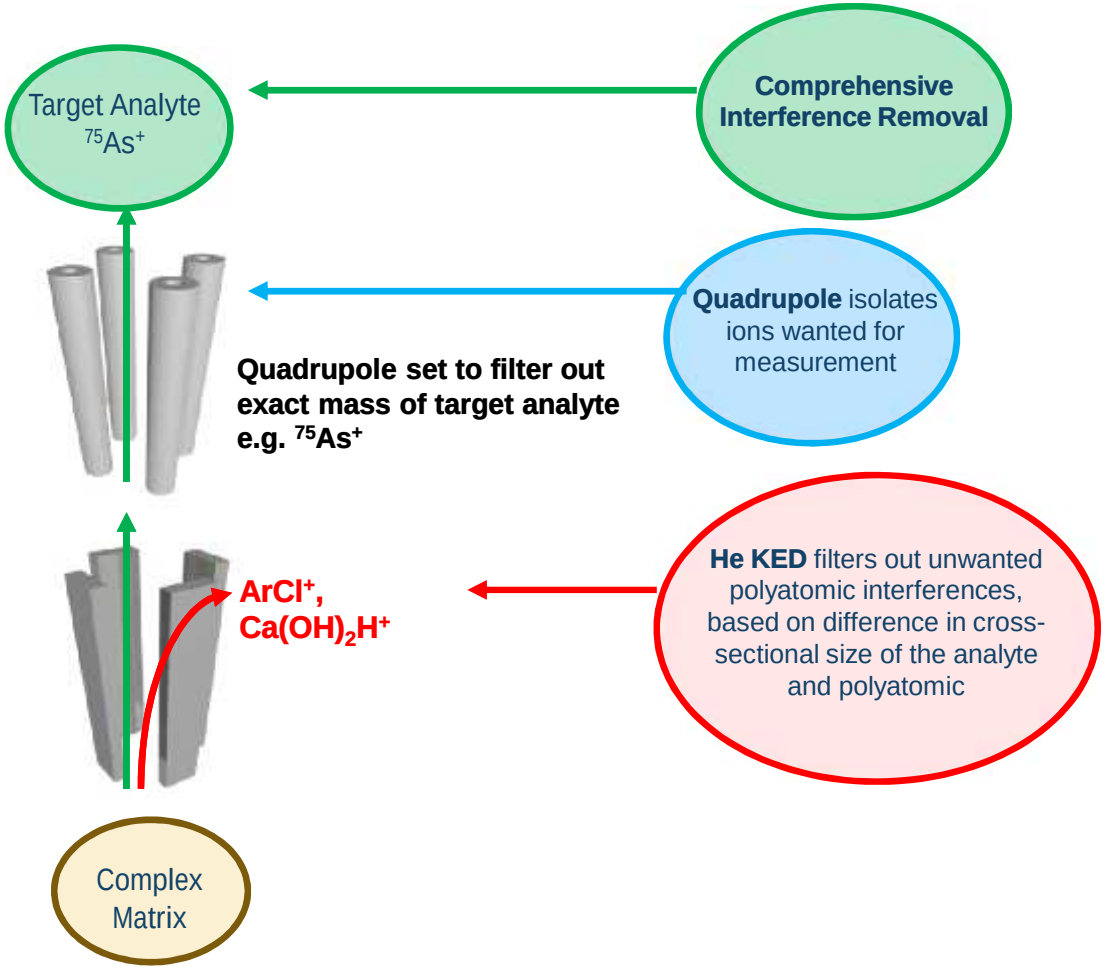
- Polyatomic Interferences
  - Produced when 2 or more isotopes combine to form a species with the same m/z as that of the analyte ion



Handling Interferences – QCell He KED Interference Removal

KED = Kinetic Energy Discrimination

- He KED filters out unwanted polyatomic interferences
- High transmission enables analysis of even low mass analytes in He KED mode
- Single measurement mode for all analytes in analytical method

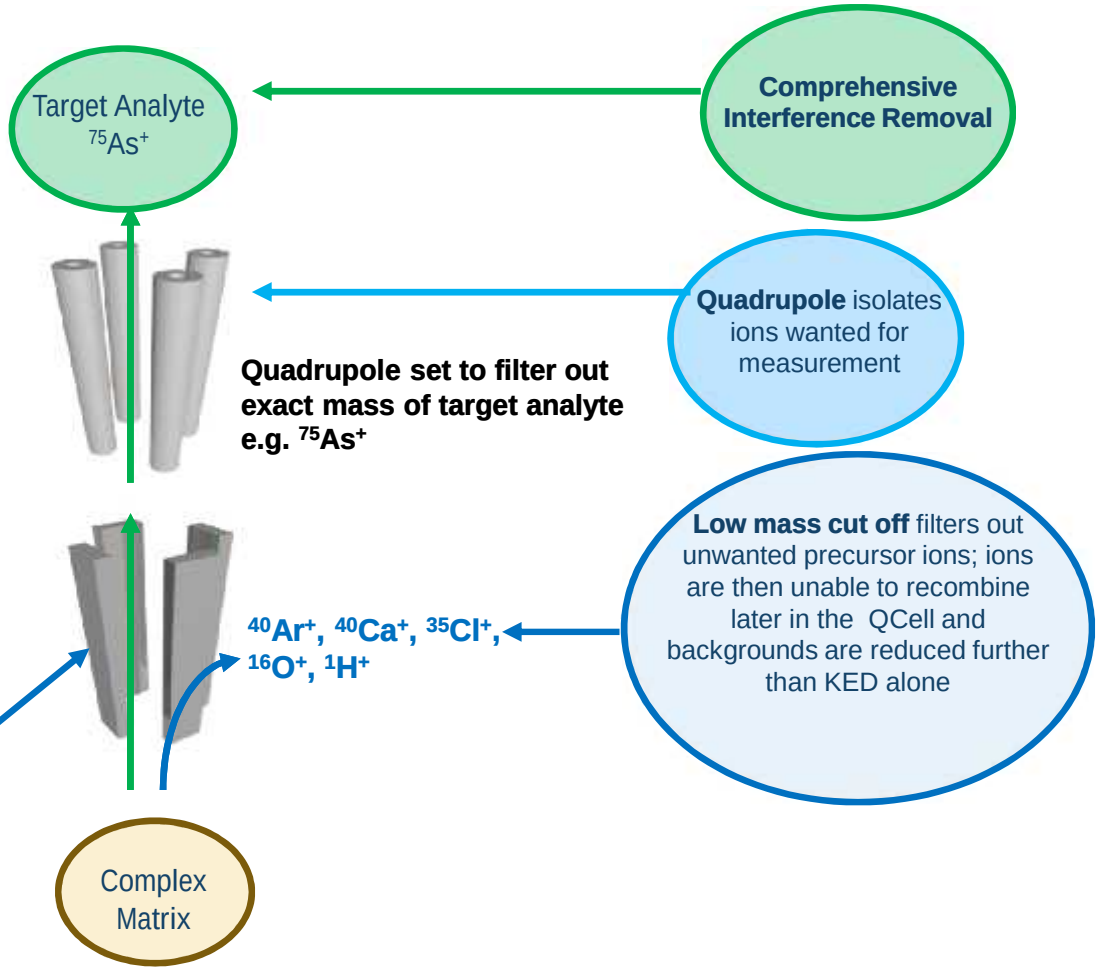


Handling Interferences – QCell Low Mass Cut-off

- QCell flatapole dynamically applies Low Mass Cut Off (LMCO) relative to target analyte

Anal	LMCO	Interferences	Precursors
^{51}V	35	$^{35}Cl^{16}O$, $^{37}Cl^{14}N$, $^{34}S^{16}OH$	H, N, O, S, Cl
^{56}Fe	39	$^{40}Ar^{16}O$, $^{40}Ca^{16}O$	O, Ar, Ca
^{63}Cu	45	$^{40}Ar^{23}Na$, $^{12}C^{16}O^{35}Cl$, $^{31}P^{32}S$	C, N, O, Na, P, S, Cl, Ar
^{75}As	47	$^{40}Ar^{35}Cl$, $^{40}Ca^{35}Cl$, $^{40}Ar^{34}SH$, $^{37}Cl_2H$	H, S, Cl, Ca, Ar

QCell (collision cell) flatapole design



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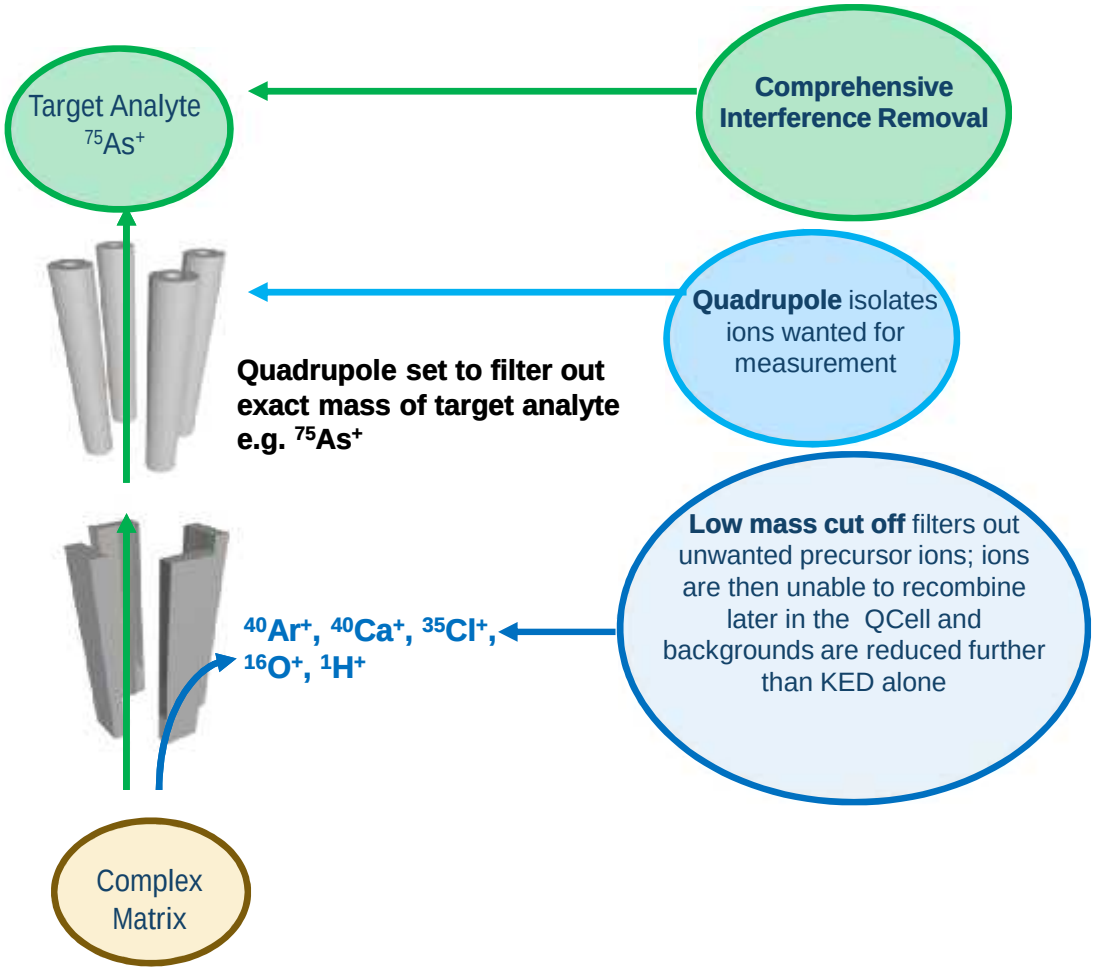
^{75}As	47	$^{40}Ar^{35}Cl$, $^{40}Ca^{35}Cl$, $^{40}Ar^{34}SH$, $^{37}Cl_2H$	H, S, Cl, Ca, Ar

- All unwanted precursors that contribute to intereferences are eliminated
- Easy and effective interference removal



Simplicity and Productivity - Single Measurement Mode

- **QCell collision/reaction cell enables analysis of all analytes in He KED mode**, including Li, Be at low mass and Pb, U at high mass

- Single measurement mode for all analytes in analytical method

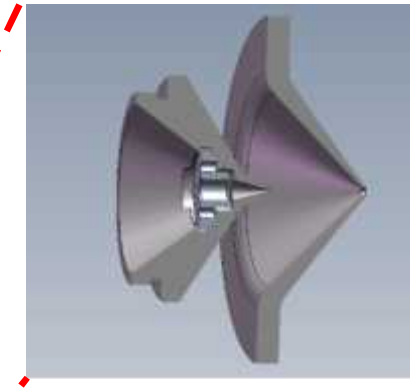
- Gas switching (10 – 20 s) is eliminated – that's a saving of 10 - 20 s per sample!

- Selection of 1 measurement mode effectively eliminates method development!

Acquisition Parameters

Identifier	Dwell time (s)	Channels	Spacing (u)	Measurement mode
7Li (KED)	0.01	1	0.1	KED
9Be (KED)	0.02	1	0.1	KED
23Na (KED)	0.01	1	0.1	KED
24Mg (KED)	0.01	1	0.1	KED
27Al (KED)	0.02	1	0.1	KED
39K (KED)	0.01	1	0.1	KED
44Ca (KED)	0.01	1	0.1	KED
45Sc (KED)	0.01	1	0.1	KED
51V (KED)	0.01	1	0.1	KED
52Cr (KED)	0.01	1	0.1	KED
55Mn (KED)	0.01	1	0.1	KED
57Fe (KED)	0.01	1	0.1	KED
59Co (KED)	0.01	1	0.1	KED
60Ni (KED)	0.01	1	0.1	KED
63Cu (KED)	0.01	1	0.1	KED
66Zn (KED)	0.02	1	0.1	KED
75As (KED)	0.05	1	0.1	KED
78Se (KED)	0.05	1	0.1	KED
89Y (KED)	0.01	1	0.1	KED
103Rh (KED)	0.01	1	0.1	KED
107Ag (KED)	0.01	1	0.1	KED
111Cd (KED)	0.01	1	0.1	KED
115In (KED)	0.01	1	0.1	KED
121Sb (KED)	0.01	1	0.1	KED
137Ba (KED)	0.01	1	0.1	KED
175Lu (KED)	0.01	1	0.1	KED
205Tl (KED)	0.01	1	0.1	KED
208Pb (KED)	0.01	1	0.1	KED
209Bi (KED)	0.01	1	0.1	KED
238U (KED)	0.01	1	0.1	KED

Handling Matrix – Customized Interfaces for Maximum Flexibility



Unique interface designed for maximum coverage of sensitivity and dynamic range:

		
Robust 4.5 mm	High Matrix 3.5 mm	High Sensitivity 2.8 mm

DRIVEN BY OTEGRA ISDS

STDR	**STD**	**STDS**
KEDR	KED	KEDS
CCTR	CCT	CCTS

Easily implemented through dedicated grouping and autotunes in the software

Handling Matrix – Customized Interfaces for Maximum Flexibility

4.5 mm

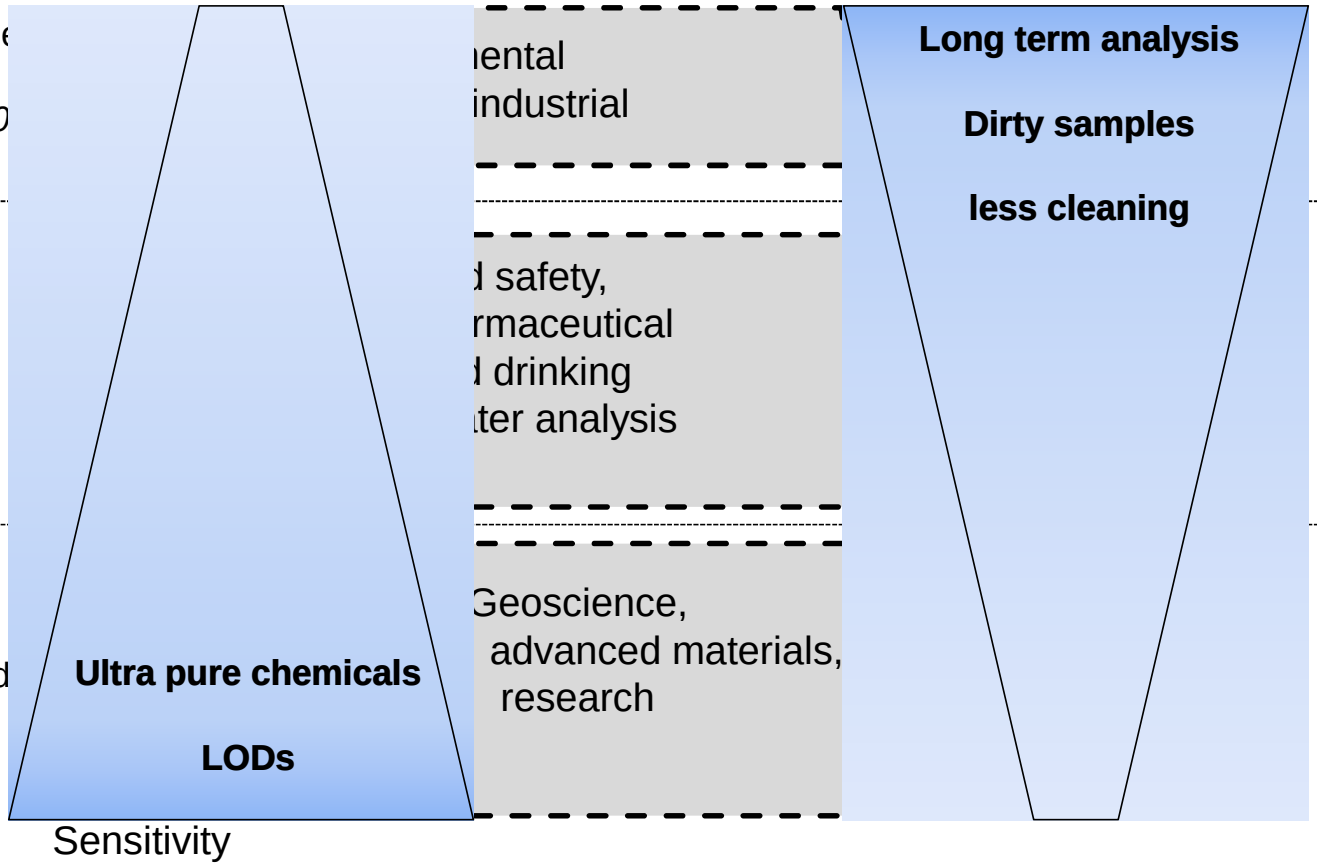
Minimal drift and reduced use
maintenance
- *Calibration Range (>2000*

3.5 mm

Best balance for sensitivity
and matrix tolerance

2.8 mm

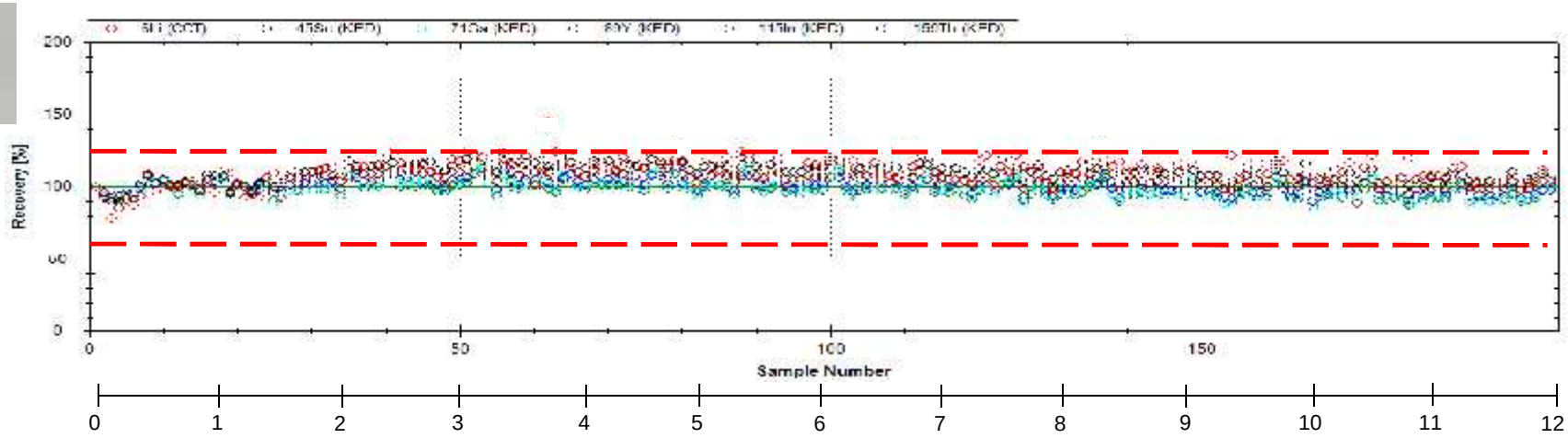
Best signal to noise ratio and
lowest detection
- *Sub-ppt analysis*



ThermoFisher SCIENTIFIC

Matrix Handling – US EPA 200.8 for Water Analysis

4.5 mm insert



Time/hours

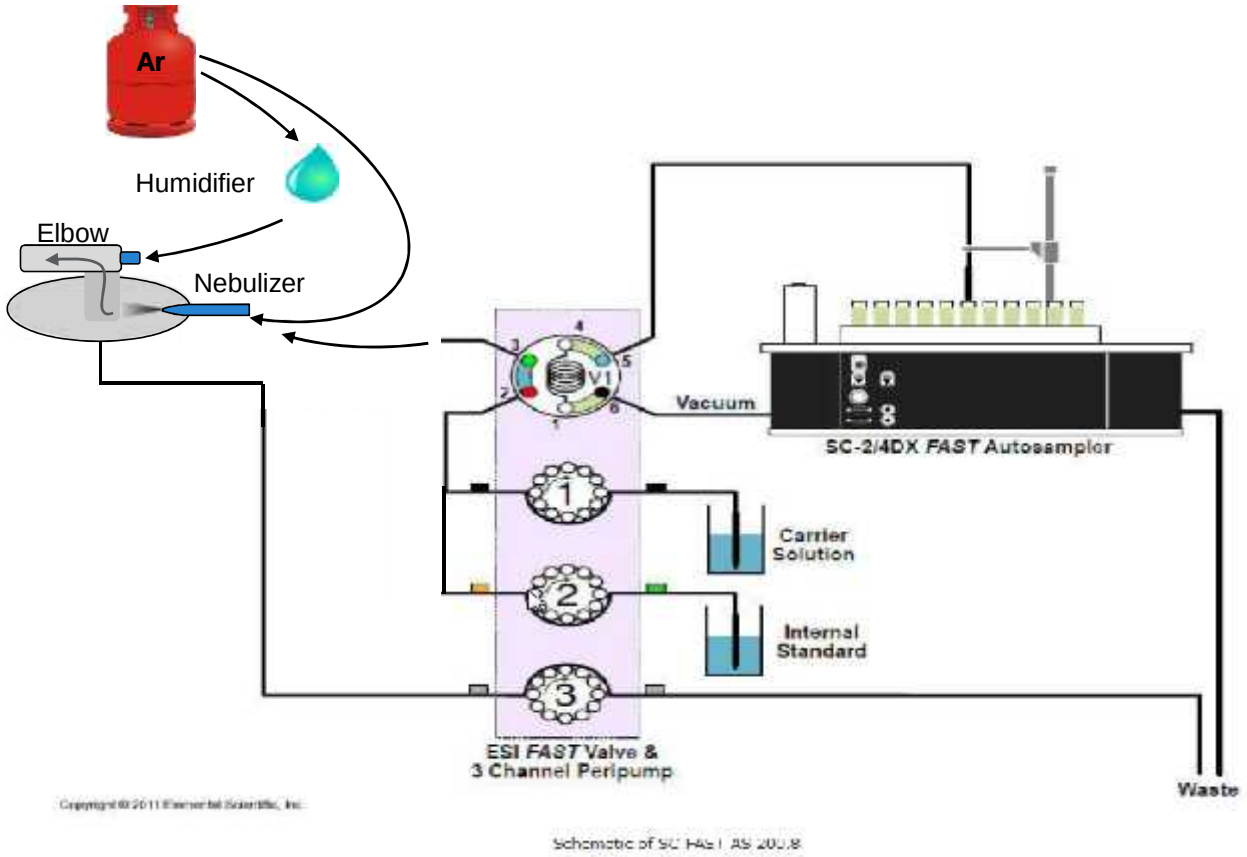
Internal Standard Test enabled

Low Warning Limit (%)	70	Low Failure Limit (%)	60
High Warning Limit (%)	120	High Failure Limit (%)	125

ThermoFisher SCIENTIFIC

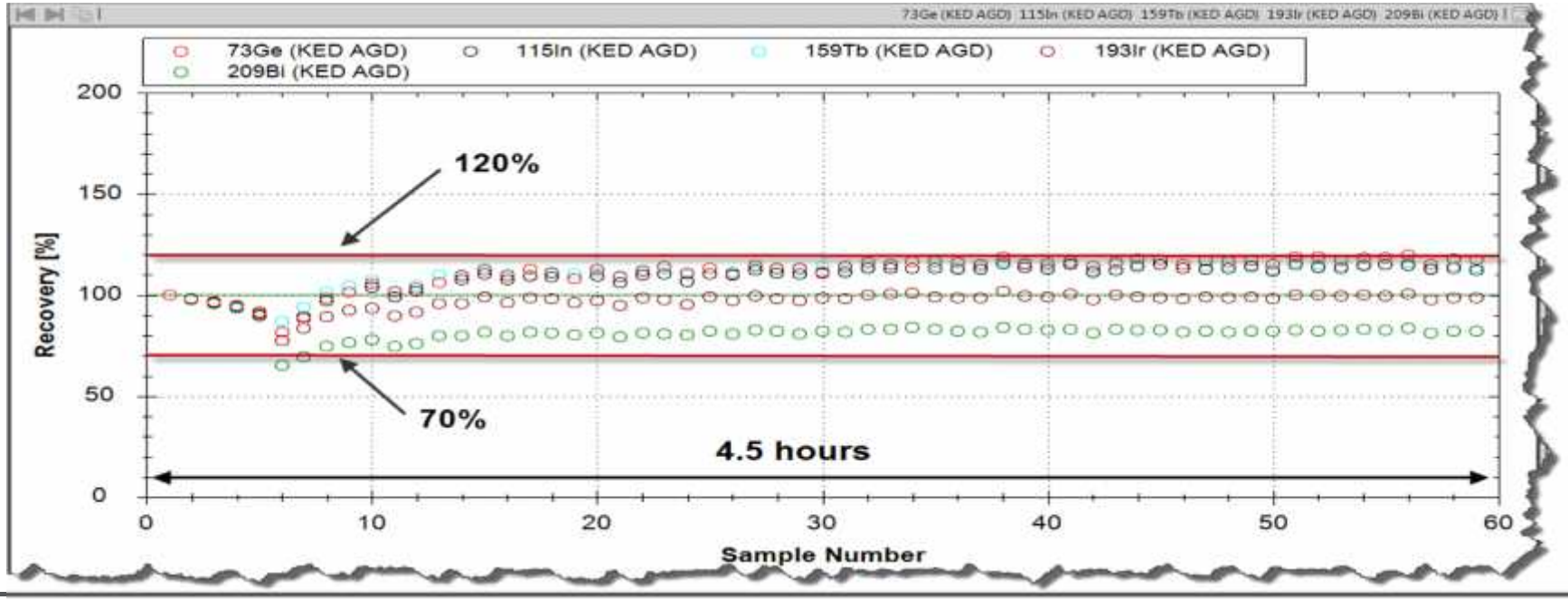
Robustness – Argon Gas Dilution (AGD) – good for similar sample types

- Simple and cost effective solution for direct analysis of high matrix samples
- Combination of **AGD** and ***Fast* system** from Elemental Scientific Inc**.** (ESI) for discrete sampling of high matrix samples



Robustness – Argon Gas Dilution (AGD)

- Samples contained 25% NaCl
- Outstanding stability
- Spike Recoveries between 85-116%
  for more than 4.5 hours



ThermoFisher SCIENTIFIC

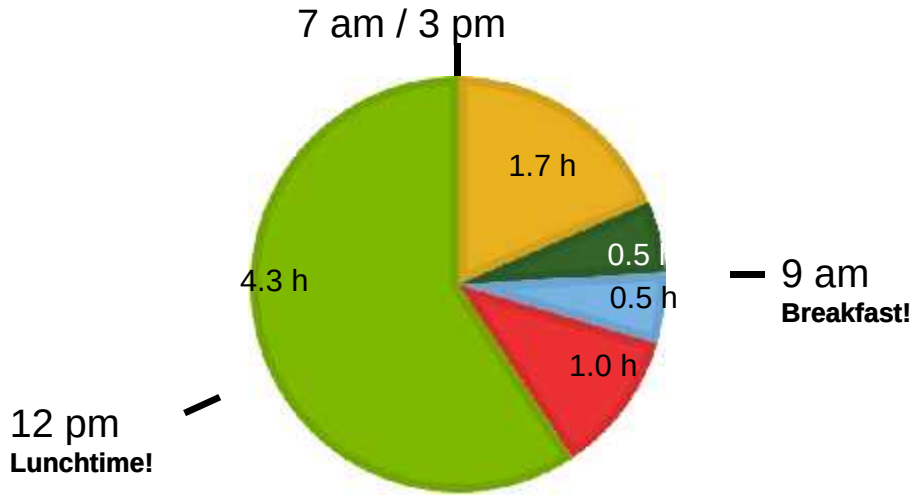
Matrix Handling – Autodilution

- Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ (ISDS) Software provides complete software control of the ESI prep*FAST*:

- Automated ***prescriptive*** dilution for preparation of:
  - Samples
  - Standards
- Automated ***intelligent*** dilution:
  - Internal standard range auto-dilution
  - Over calibration range auto-dilution

- Close coupling of the discrete sampling valves to ICP for minimized uptake and washout – increases throughput and reduces contamination

A Typical Day in the Busy Lab without Autodilution

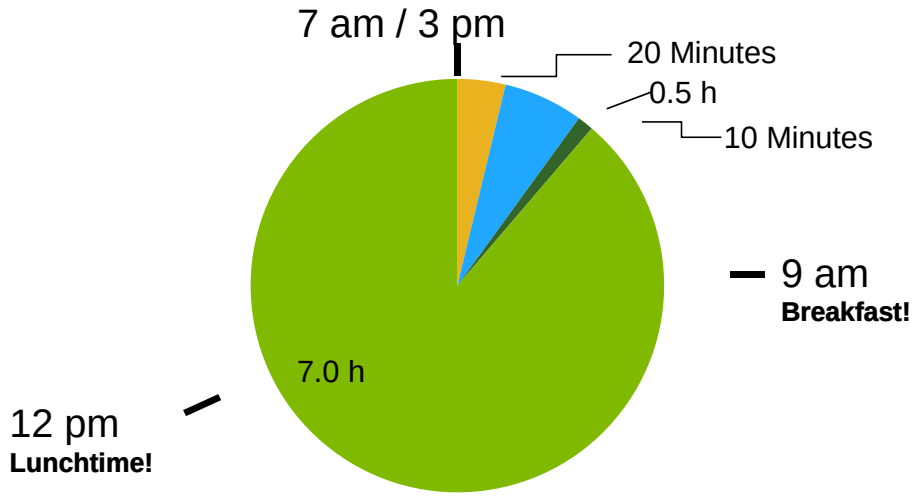


Action	Time	#	Total
Dilution	20s / sample	300	1.7 h
Preparation of Calibration/QC solutions	30 Minutes		0.5 h
Performance Verification	30 Minutes		0.5 h
Re-run failed samples	2 minutes	10%	1.0 h
Remaining Time			4.3 h

Improvement Opportunities:

- Operator time wasted for simple tasks
- Risk of contamination
- Manual interaction may be error prone

A Typical Day in the Busy Lab with Autodilution



Action	Time	#	Total
Dilution	20s / sample	300	20 Minutes
Preparation of Calibration/QC solutions	30 Minutes		10 Minutes
Performance Verification	30 Minutes		0.5 h
Re-run failed samples	2 minutes	10%	0
Remaining Time			7.5 h

Advantages:

- Completely integrated
- Optimized flow paths
- Prescriptive Autodilution
- Intelligent Autodilution
  - → Calibrated Range
  - → Internal Standard Recovery

Gain:

- 3 h Operator time per day!

Thermo Scientific iCAP RQ ICP-MS

Simplicity

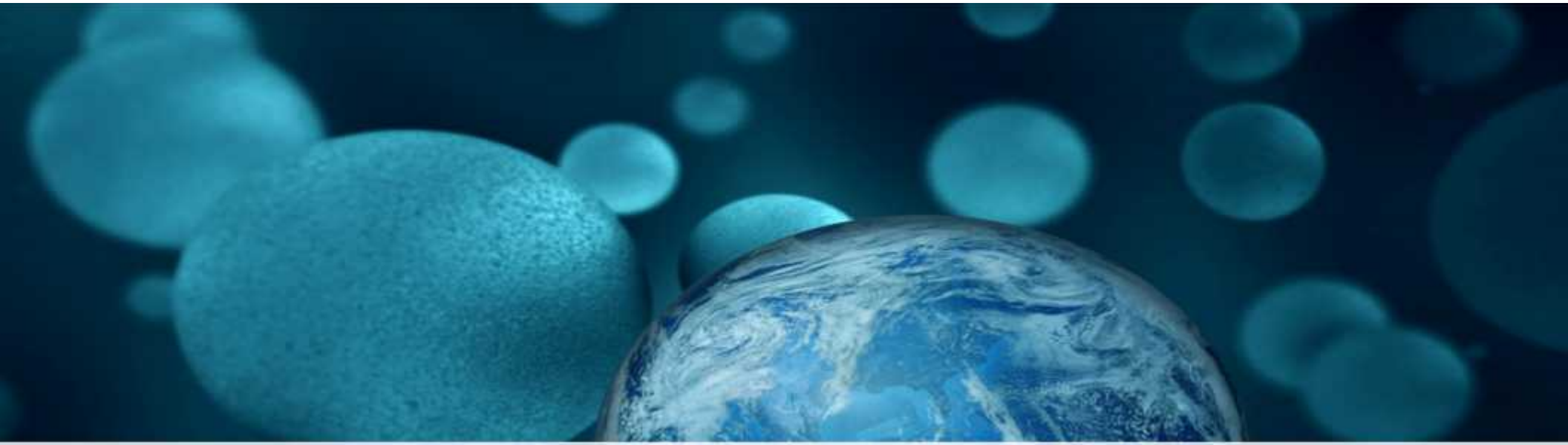
- Built in Simplicity for user-friendly operation and easy installation
- Qtegra ISDS for plug-ins, easy workflow and compliance

Productivity

- The most productive ICP-MS on the market
  - Single measurement mode, integrated sampling valves
- Best interference removal Q-ICP-MS:
  - Unique QCell flatapole technology with low mass cut-off + He KED mode

Robustness

- New interface design configured for the application
  - Robust interface (4.5mm), everyday interface (3.5 mm), high sensitivity interface (2.8 mm)
- New robust and reliable design for low maintenance and service costs
  - 2 years parts warranty as standard



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Thermo Scientific iCAP TQ ICP-MS

The world leader in serving science

iCAP TQ ICP-MS – TQ as easy to use as a SQ

Robust and reliable

Completely re-designed electronics

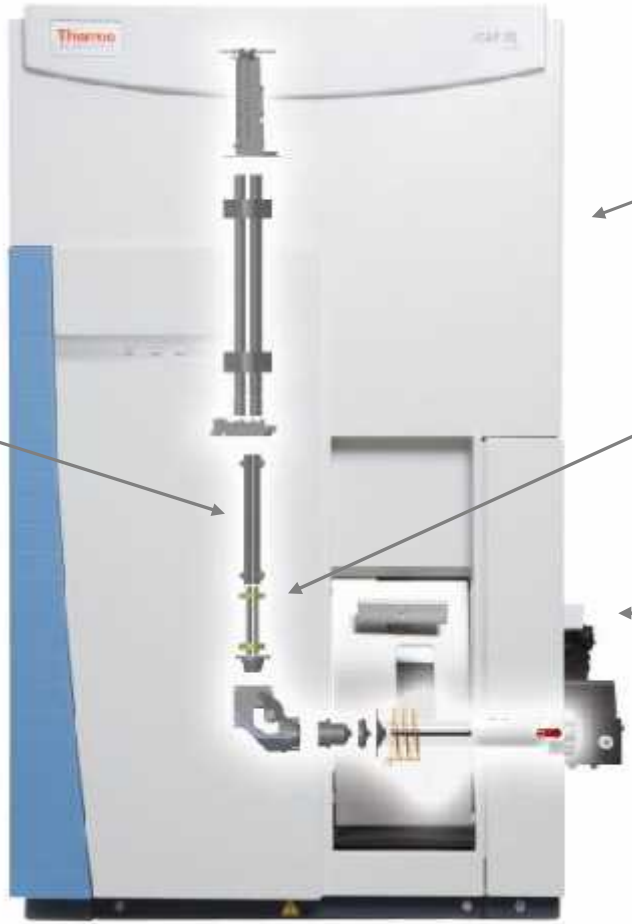
New RF-generator

QCell CRC for SQ & TQ

4 MFCs as standard for max. flexibility - Safe use of reactive, pure gases

Integrated automation, advanced applications and qualification

Easier to install and service



Qtegra ISDS software v2.8

Ease of Use and Simplicity

Highest data accuracy in challenging samples

Maintains small footprint

and intuitive handling

Zero user maintenance beyond the interface

What's the difference between a SQ and TQ-ICP-MS

iCAP RQ ICP-MS

iCAP TQ ICP-MS

Additional Q1 mass filter quadrupole

Additional electronics

Additional gases

Enhanced software

Same platform but there are more differences than you think!

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Safe Use of Reactive Gases

- The collision/reaction cell can be used with inert collision gases or pure reactive gases
  - He, H_2, O_2, NH_3
- Pure reactive gases can cause laboratory safety issues:
  - H_2 – flammable
  - NH_3 – toxic and corrosive
- Gas distribution module has safety features built-in:
  - Valve restriction modules to stop gas flows if the instrument is powered off or if vacuum system fails
  - Active ventilation inside the instrument housing

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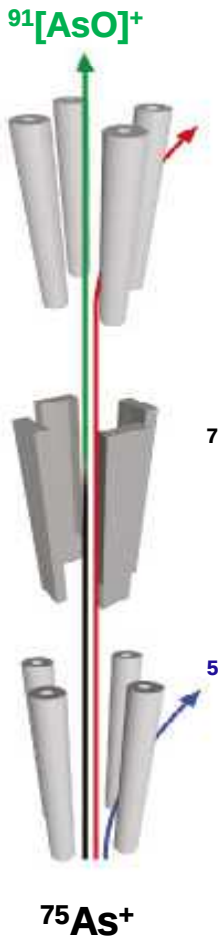
Thermo Scientific iCAP TQ ICP-MS – How it Works

Q3 set to product ion mass (*m/z* 91)

Q2 filled with reactive gas (O_2)

Q1 set to analyte mass (*m/z* 75)



Q3 isolates the product ion of the analyte and removes any remaining interferences through a second stage of mass filtration

Optimal reaction conditions in Q2 are achieved through the selection of the appropriate measurement mode in Reaction Finder

Q1 rejects unwanted ions and preselects the analyte. This first stage of mass filtration rejects precursors and ions with the same m/z ratio as the product ion.

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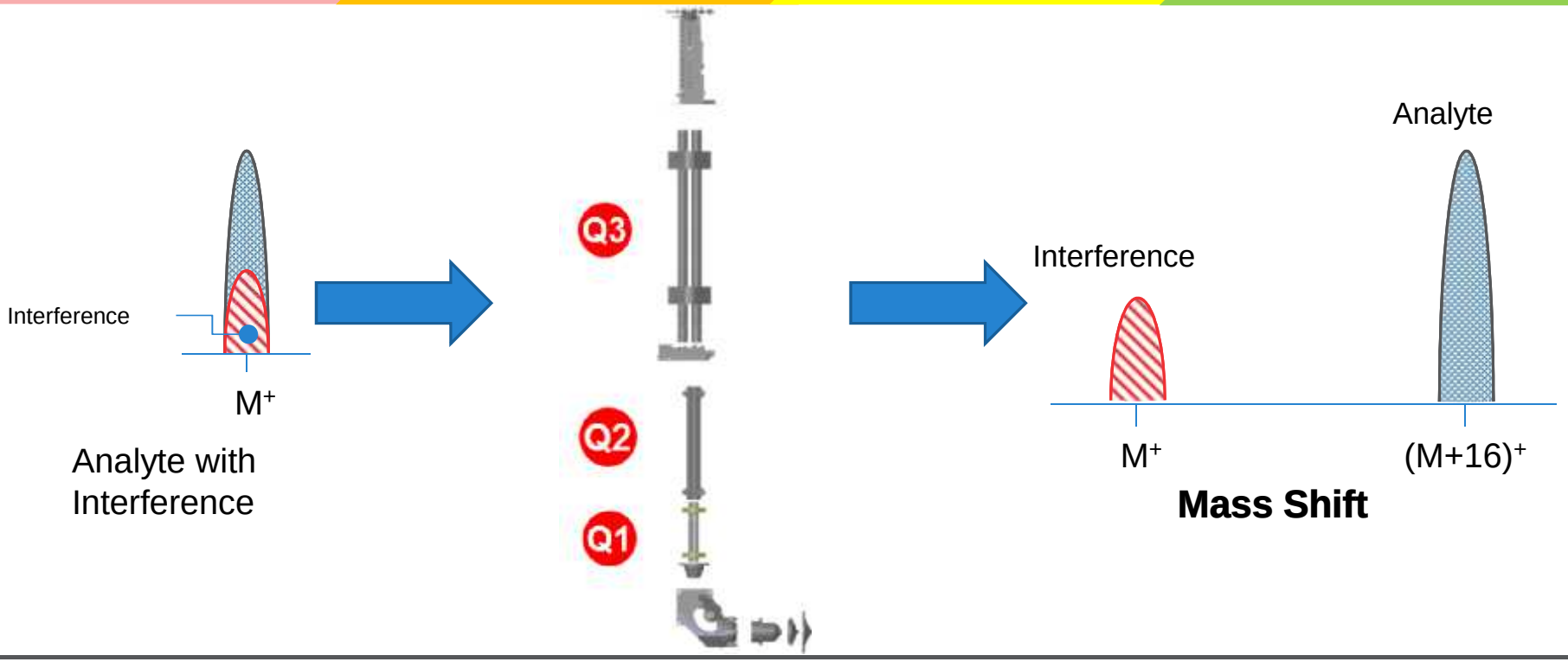
Thermo Scientific iCAP TQ ICP-MS

Problem	Feature	Benefit	Value
Interference removal still major challenge in ICP-MS	TQ technology dramatically improves interference removal	Measure more accurately and with lower LOD	Meet requirements of challenging applications



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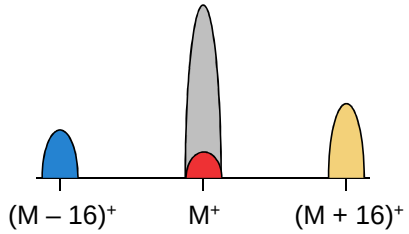
Interference removal using TQ Reaction Chemistry (with O_2)

Precursor Ion

Isobaric Interference

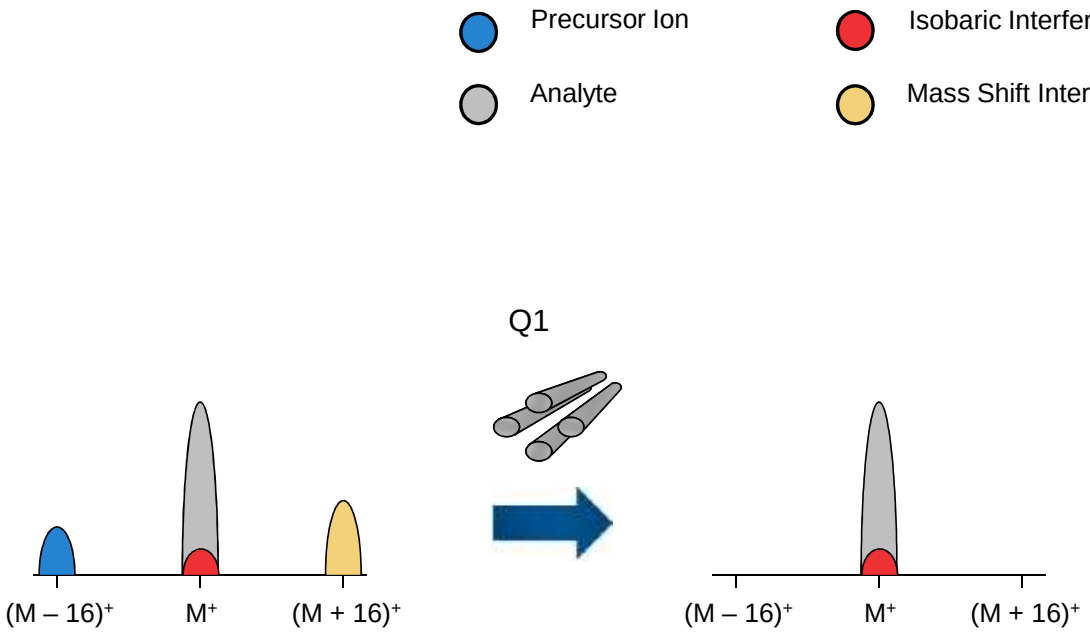
Analyte

Mass Shift Interference



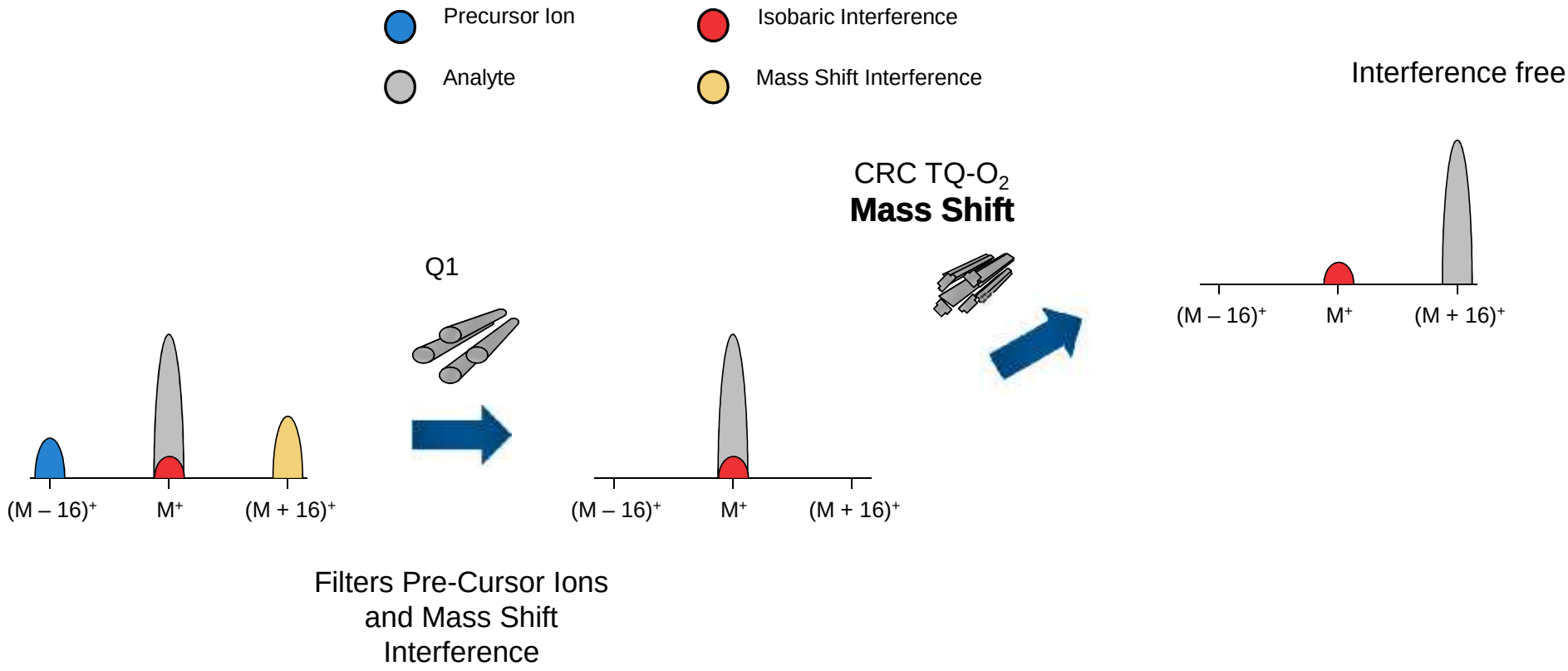
Mixture of analytes and interferences

Interference removal using TQ Reaction Chemistry (with O_2)



Filters Pre-Cursor Ions and Mass Shift Interference

Interference removal using TQ Reaction Chemistry (with O_2)



Filters Pre-Cursor Ions and Mass Shift Interference

Interference removal using TQ Reaction Chemistry (with O_2)

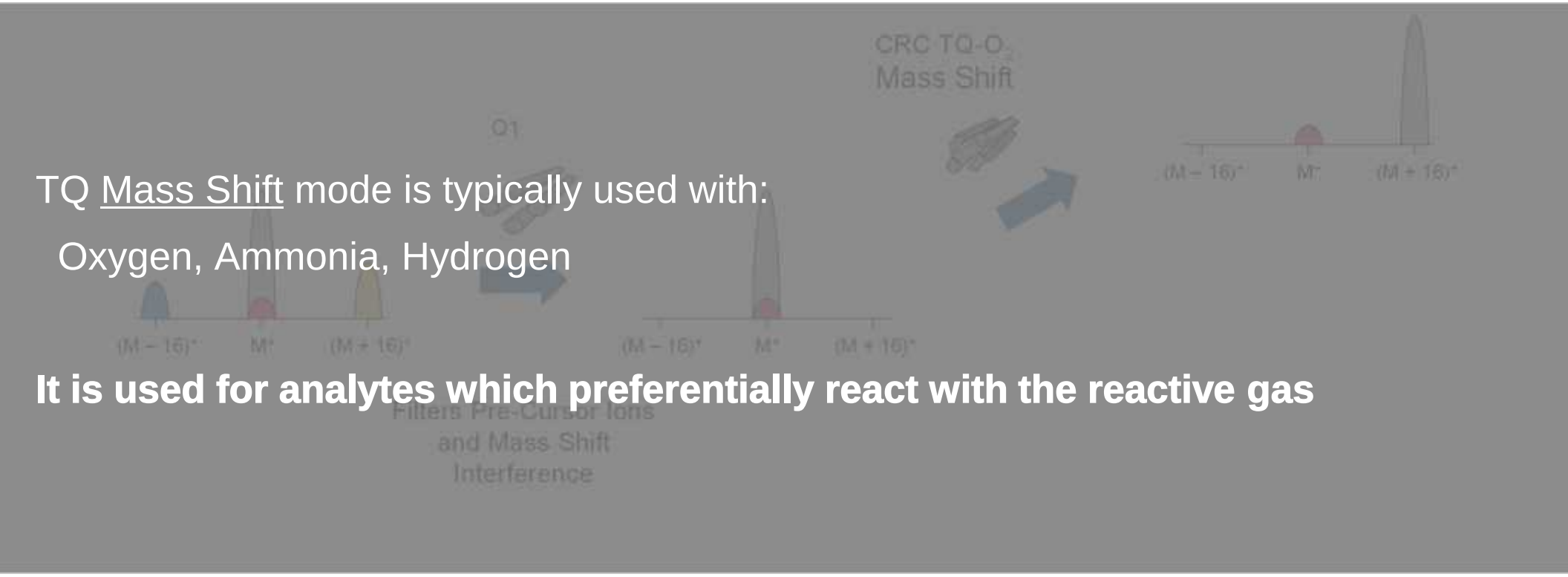
Precursor Ion

Isobaric Interference

Analyte

Mass Shift Interference

Interference free

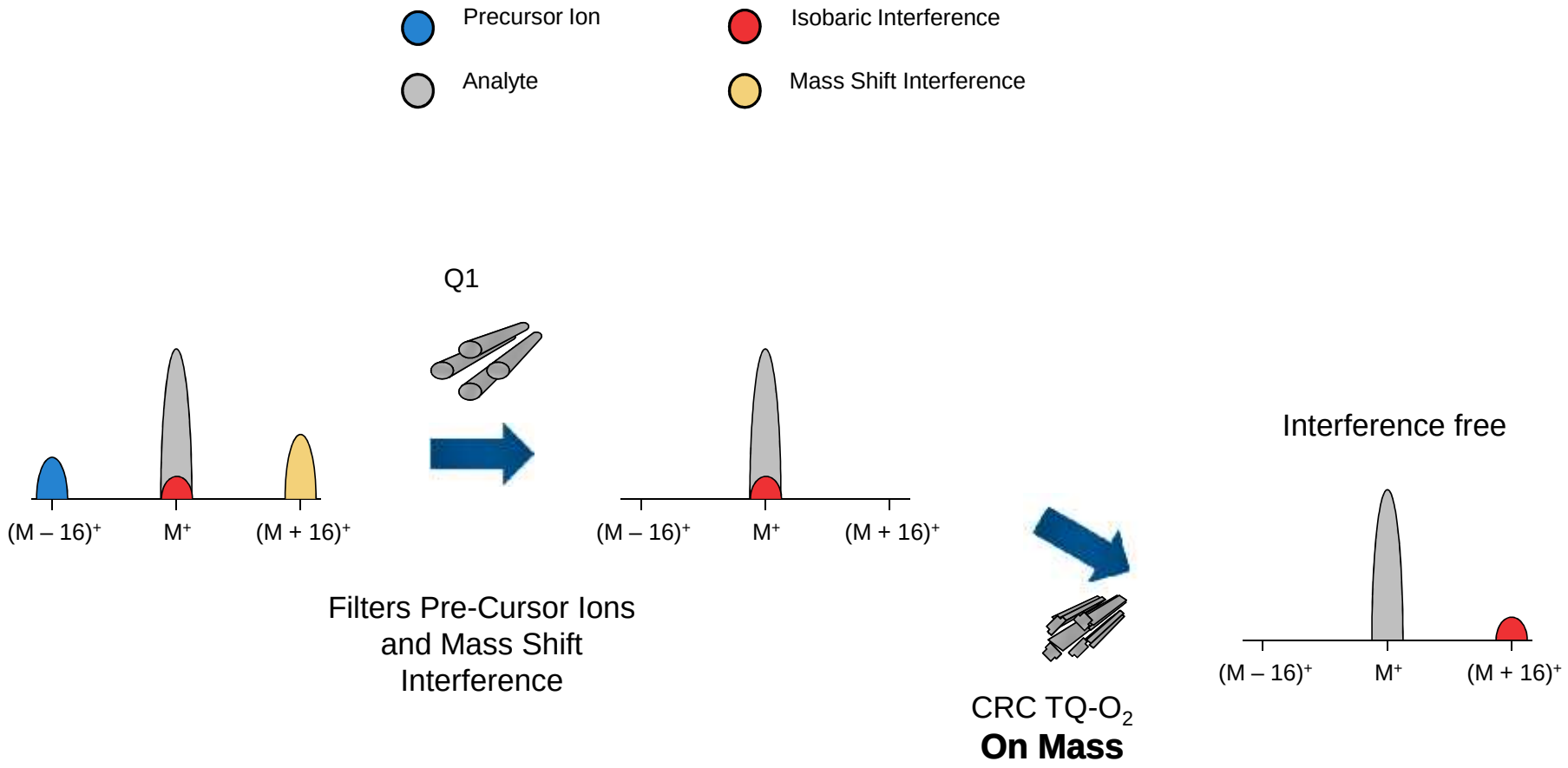


TQ <u>Mass Shift</u> mode is typically used with:

Oxygen, Ammonia, Hydrogen

It is used for analytes which preferentially react with the reactive gas

Interference removal using TQ Reaction Chemistry (with O_2)



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Interference removal using TQ Reaction Chemistry (with O_2)

Precursor Ion

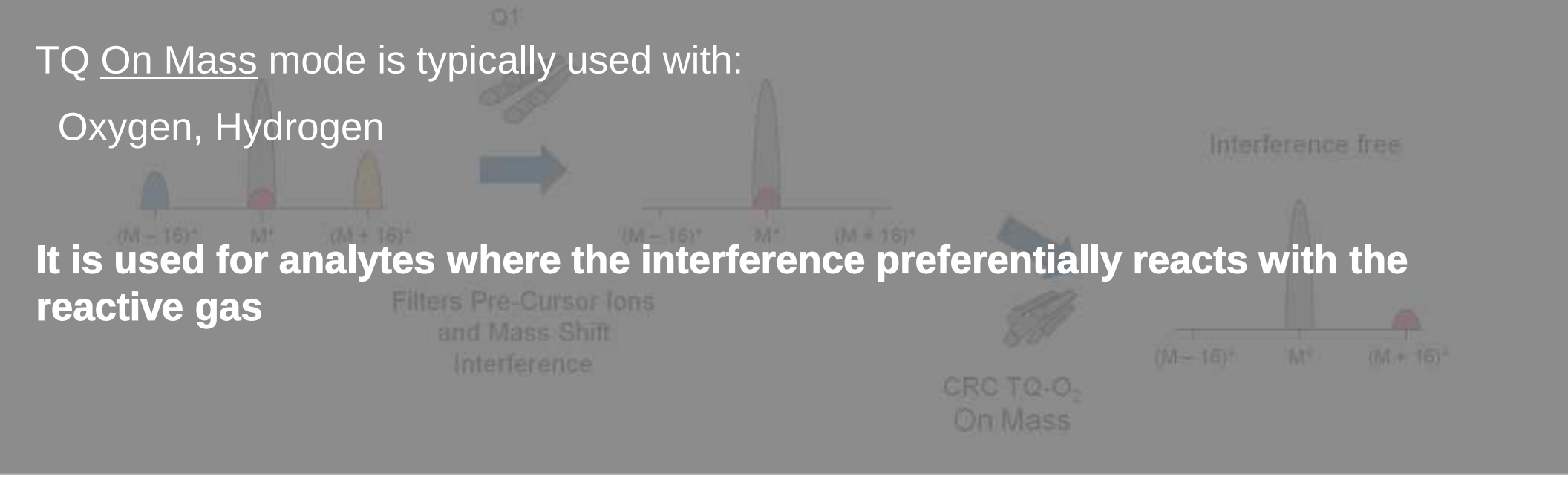
Isobaric Interference

Analyte

Mass Shift Interference

TQ <u>On Mass</u> mode is typically used with:

Oxygen, Hydrogen



It is used for analytes where the interference preferentially reacts with the reactive gas

The Power of Triple Quadrupole Technology

- **Problem:** the possibilities are endless!
- Collision cell operation:
  - Standard mode, collision (KED) mode, reaction mode, or a combination?
  - If reaction mode, which reaction gas/es?
  - Collision mode: what gas flow rate?
  - Reaction mode: what gas flow rate/s?
  - Collision cell voltage setting?
  - Do you measure the analyte on mass or on mass-shift?
- Quadrupole 1:
  - Voltage setting?
- Quadrupole 3:
  - Voltage setting?
- Sample intro settings (RF power, plasma gases, spray chamber temperature)

Eliminate the Complexity of Triple Quadrupole ICP-MS

- Reaction Finder for Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution™ Software

Step 1: Select your element/s or isotope/s

Step 2: You're done!

- **Reaction Finder proposes the most appropriate gas/scan settings**
- **Settings for both single quad mode and triple quad mode are suggested, for reference**

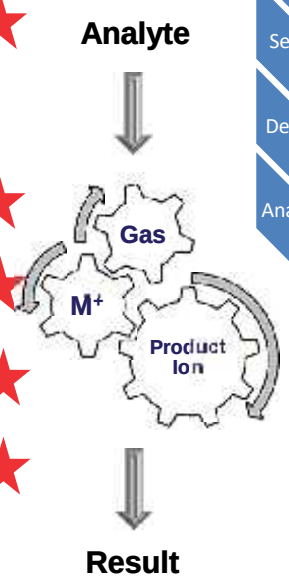
Identifier	Q3 Analyte	SQ / TQ	CR Gas	Dwell time (s)	Channels	Spacing (u)	
78Se | 78Se.16O	78Se.16O (93.912	TQ	O_2	0.1	1	0.1	Normal
80Se | 80Se.16O	80Se.16O	TQ	O_2	0.1	1	0.1	Normal

Redefining triple quadrupole technology with unique ease of use

Reaction Finder Method Development Assistant

Without Reaction Finder

- Select: • Select the Analytes to be measured
- Select: • For each analyte, select the isotopes to be measured ★
- Select: • Select the internal standard element
- Select: • Select the Q1 Analyte ★
- Select: • Select the CRC gas (None, He, H_2, O_2, NH_3) ★
- Select: • Select the mode (KED, Single Quad Mode, Triple Quad Mode) ★
- Select: • Select the Q3 Mass (On-mass/mass shift product ion) ★
- Decide: • Are the suggested settings ok? If not, update them
- Analyze: • Enter sample names and positions or import from LIMS and start the LabBook



With Reaction Finder

- Select: • Select the Analytes to be measured
- Select: • Select the internal standard element
- Decide: • Are the suggested settings ok? If not, update them
- Analyze: • Enter sample names and positions or import from LIMS and start the LabBook

Less than 20 Minutes until a method is set up and the samples are queued to run!

★ Operator knowledge and understanding essential

Redefining Trace Elemental Analysis with Triple Quadrupole ICP-MS

Meeting human health, environmental challenges

- **Clinical Research : S, Ti**
- **Metallopharmaceuticals: Se, P**
- **Environmental and Food Safety: As, Se**

Advancing development in metals, materials, chemicals

- **Materials analysis: Cd, Zr**
- **Advanced Alloys: Se, Ni**
- **Semiconductor impurities: Ca, Zn**

Our Product Portfolio with Qtegra Software

- iCAP™ …**I**nductively **C**oupled **A**rgon **P**lasma
- Over 8000 ICP-OES Installed (> 800 in 2017 alone)
- Over 2500 ICP-MS Installed

iCAP 7000 Plus Series

iCAP RQ

iCAP TQ

Qtegra Software

- Intuitive, and easy workflow
- Compliant
- Accessory Plug-ins for Automation
- Advanced Application Plug-ins

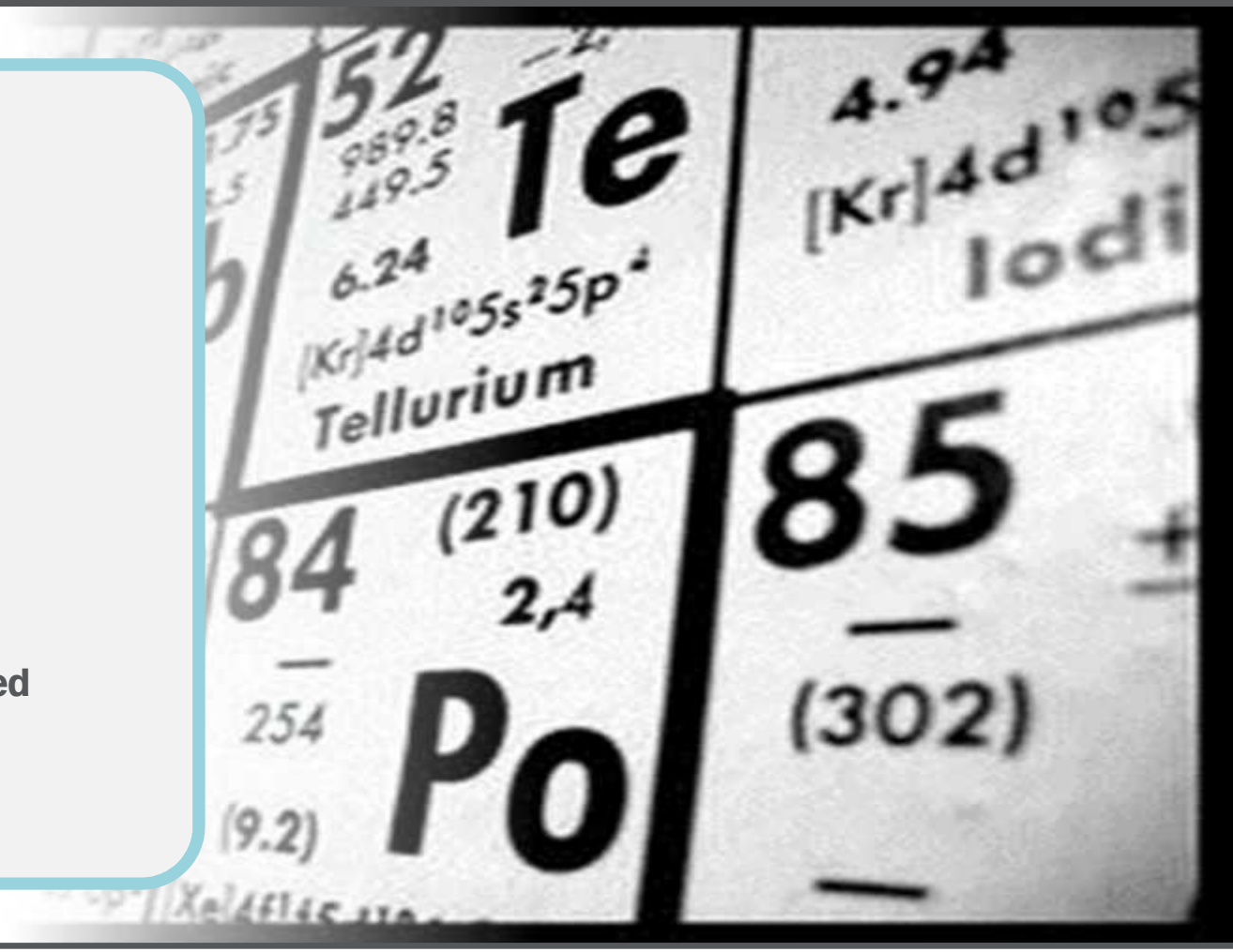
Qtegra ChromControl with Chromeleon Plug-in for speciation

Qtegra NpQuant for Nanoparticle Analysis

Thermo Scientific and Trace Elemental Analysis

A Company to work with

- **Experience …….Long History**
- **Innovation ……..Performance**
- **Routine……Rugged/Reliable**
- **Software……..Easy, and integrated**
- **Large Portfolio……Right Solution**



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Thank You!

Questions?