

# Elemental and isotopic analysis: solutions for food authenticity, quality and safety

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Sales representative Inorganic Mass Spectrometry

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RAFA 2022

 The world leader in serving science



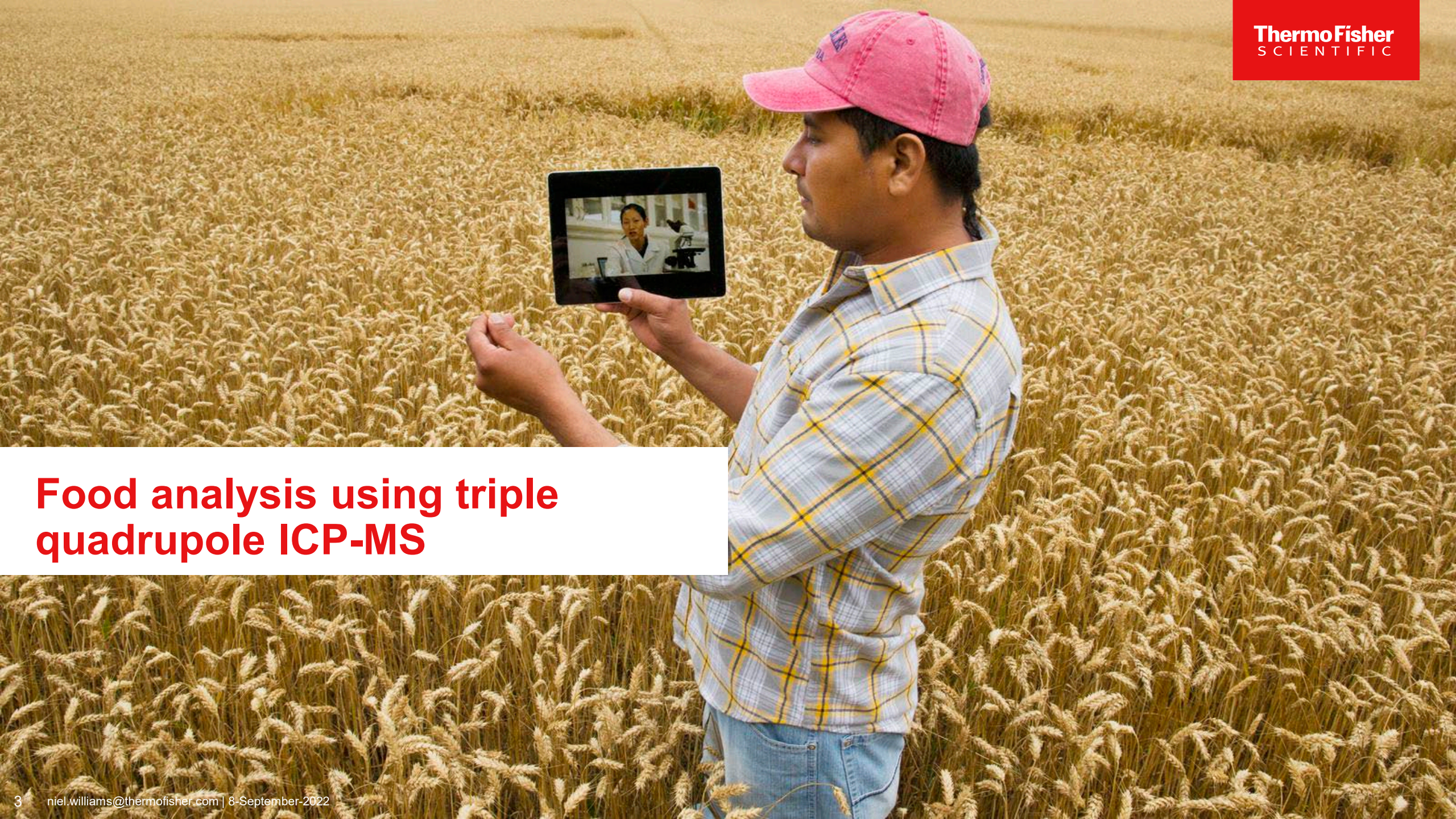
# Agenda

1 Food analysis using triple quadrupole ICP-MS

2 Elemental analysis workflow

2 Isotope analysis workflow





## Food analysis using triple quadrupole ICP-MS

# Regulatory limits

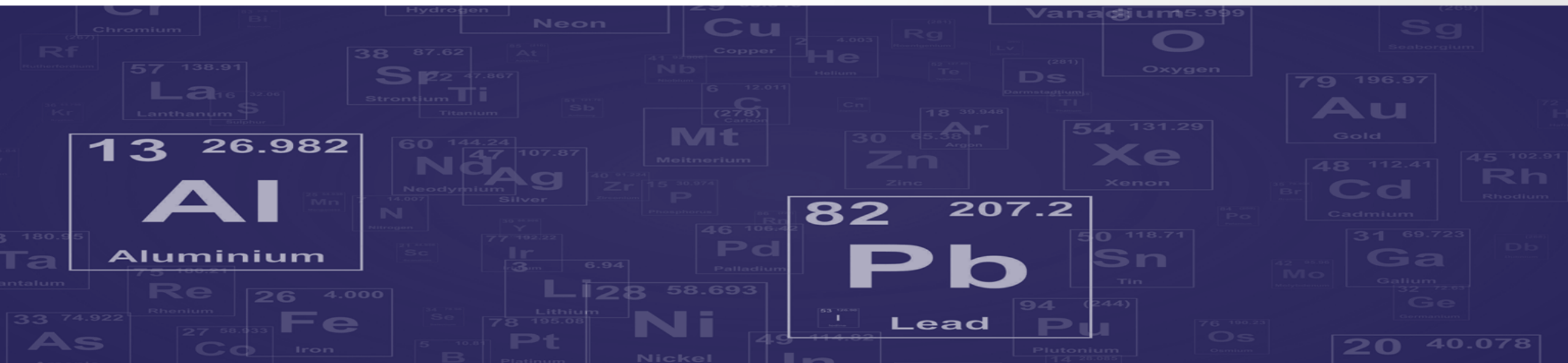
- Regulations for nutritional and toxic elements in baby foods vary globally
- Toxic elements low limits – subject to regular amendments!
- The Baby Food Safety Act introduced on 25<sup>th</sup> March 2021 in US reduces low limits for heavy metals in baby foods e.g., Hg → **2  $\mu\text{g}\cdot\text{kg}^{-1}$**

Toxic element	Lowest limit value globally ( $\mu\text{g}\cdot\text{kg}^{-1}$ )	Target conc. = 30% of the limit ~MLOQ ( $\mu\text{g}\cdot\text{kg}^{-1}$ )
As	10	3.0
Cd	5	1.5
Hg	2	0.6
Pb	5	1.5
Sn	5000	1500

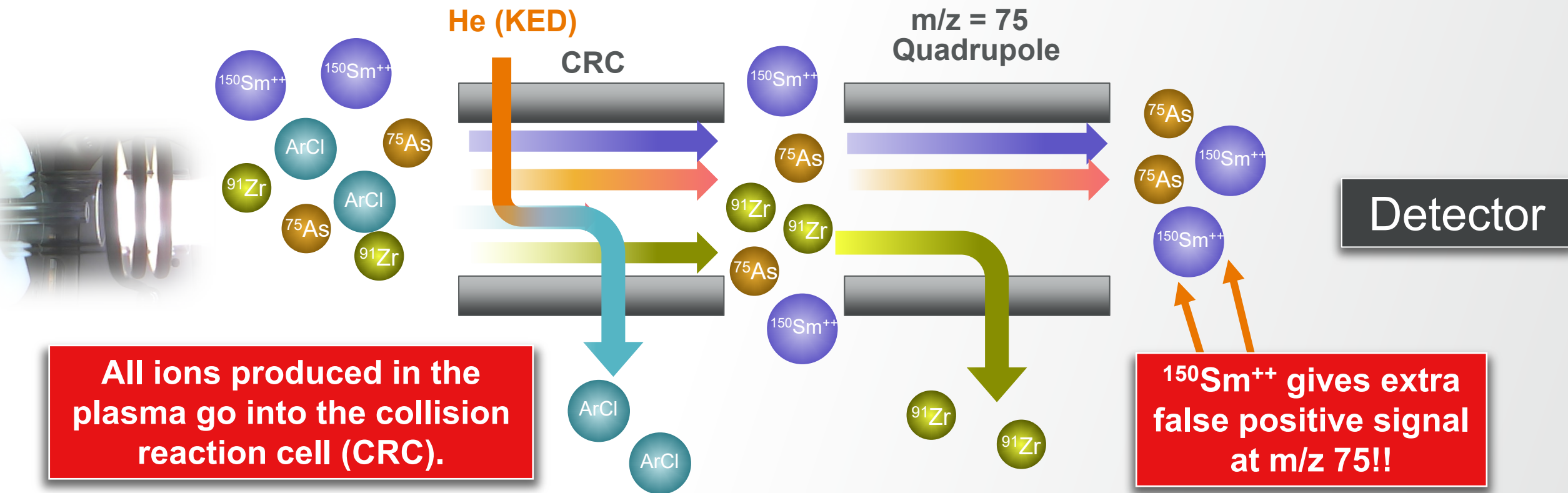


# Regulatory limits – How can interferences bias?

Toxic element	Lowest limit value globally ( $\mu\text{g}\cdot\text{kg}^{-1}$ )	Target conc. = 30% of the limit $\sim$ MLOQ ( $\mu\text{g}\cdot\text{kg}^{-1}$ )	Commonly analyzed isotope	Potential interferences
As	10	3.0	$^{75}\text{As}^+$	$^{150}\text{Nd}^{++}$ , $^{150}\text{Sm}^{++}$
Cd	5	1.5	$^{111}\text{Cd}^+$	$^{95}\text{Mo}^{16}\text{O}^+$
Hg	2	0.6	$^{202}\text{Hg}^+$	$^{186}\text{W}^{16}\text{O}^+$
Pb	5	1.5	$^{206-208}\text{Pb}^+$	-
Sn	5000	1500	$^{118}\text{Sn}^+$	-



# As determination using SQ ICP-MS with KED mode

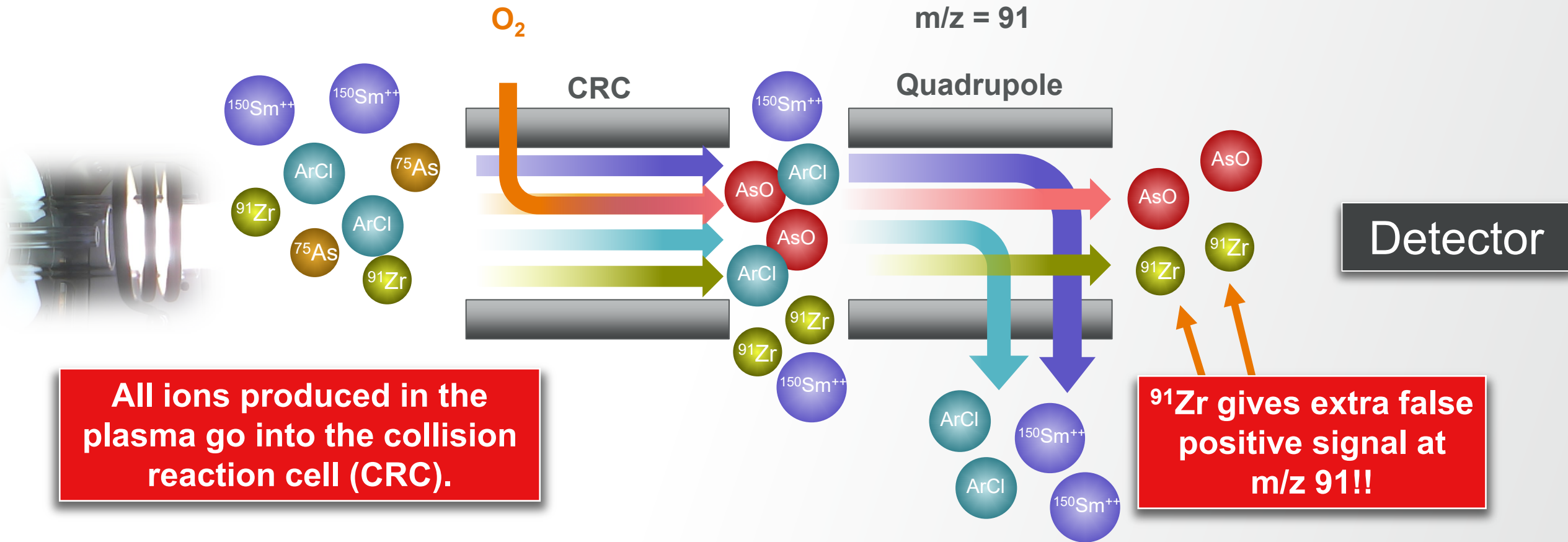


All ions produced in the plasma go into the collision reaction cell (CRC).

$^{150}\text{Sm}^{++}$  gives extra false positive signal at  $m/z$  75!!

What happens if we use a reactive gas?

# As determination using SQ ICP-MS with O<sub>2</sub> mode



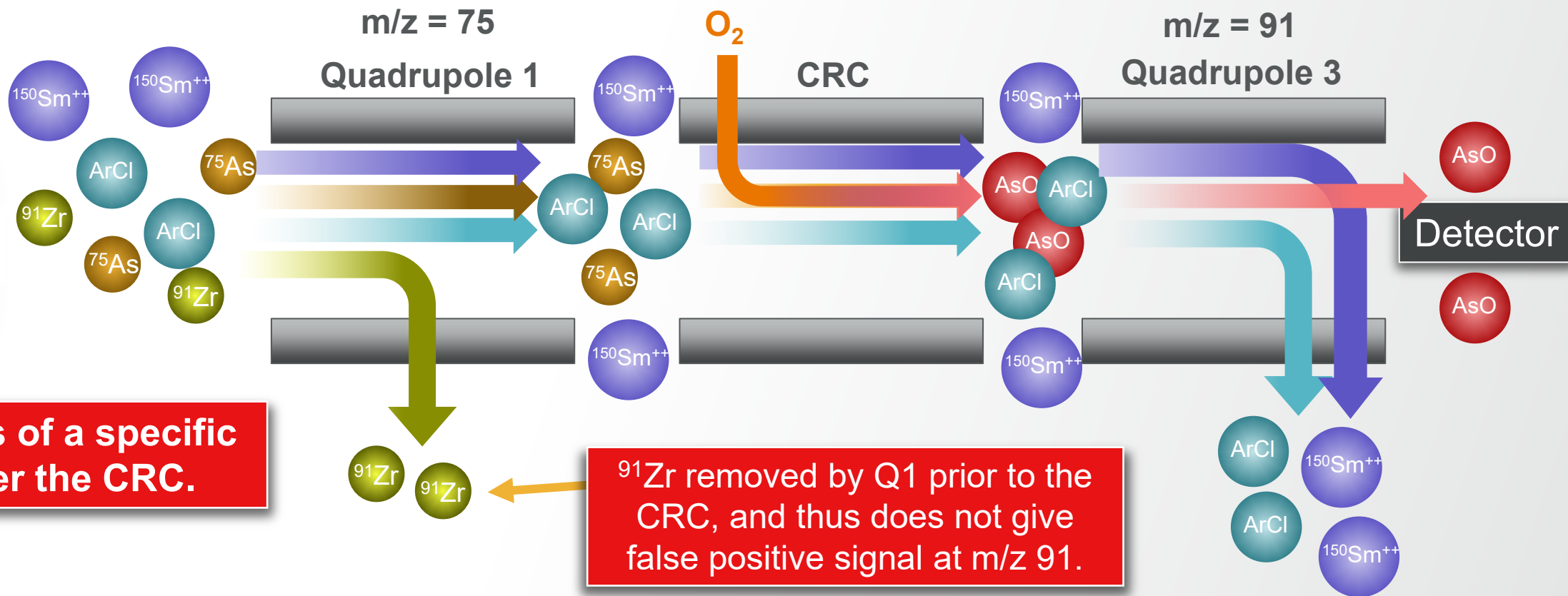
All ions produced in the plasma go into the collision reaction cell (CRC).

<sup>91</sup>Zr gives extra false positive signal at m/z 91!!

What happens when we add an extra quadrupole?

# Why do we need another quadrupole?

Consider analysis of As using TQ-ICP-MS with Collision/Reaction Cell – O<sub>2</sub> mode



**ONLY** ions of a specific m/z enter the CRC.

<sup>91</sup>Zr removed by Q1 prior to the CRC, and thus does not give false positive signal at m/z 91.

Interference free analysis with iCAP TQe ICP-MS system



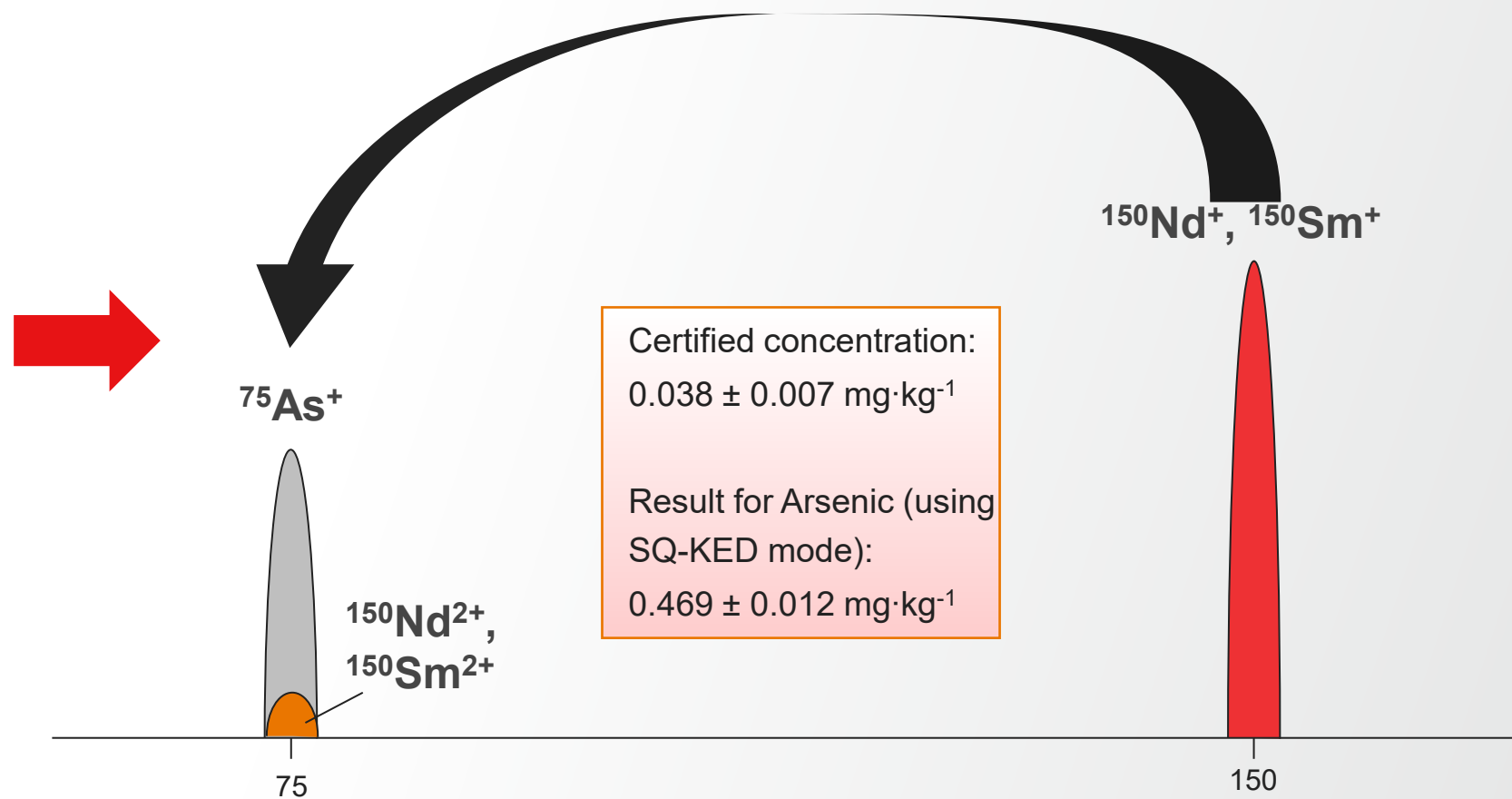
# Impact of interferences

National Institute of Standards and Technology (NIST) CRM 1515 – Apple Leaves

Table 2. Information Mass Fraction Values for Elements in SRM 1515

	Mass Fraction (mg/kg)
Nitrogen (N) <sup>(a)</sup>	23100
Sulfur (S)	1800
Antimony (Sb)	0.013
Bromine (Br)	1.8
Cerium (Ce)	3
Chromium (Cr)	0.3
Cobalt (Co)	0.09
Europium (Eu)	0.2
Gadolinium (Gd)	3
Gold (Au)	0.001
Iodine (I)	0.3
Lanthanum (La)	20
Neodymium (Nd)	17
Samarium (Sm)	3
Scandium (Sc)	0.03
Terbium (Tb)	0.4
Thorium (Th)	0.03
Tungsten (W)	0.007
Uranium (U)	0.006
Ytterbium (Yb)	0.3

ough total nitrogen is certified, nitrogen determined by the Kjeldahl procedure is n



**Doubly charged interferences cause enhancement effects**

# Which type of ICP-MS should be used?

## Single Quad ICP-MS

Thermo Scientific™ iCAP™  
RQ ICP-MS



Compact footprint

Quick connect and push-fit sample intro components

Innovative QCell Collision Cell

### Interference Removal

**KED**

Polyatomic



Isobaric

X

Doubly charged

X

## Triple Quad ICP-MS

Thermo Scientific™ iCAP™  
TQe ICP-MS



Additional quadrupole for superior interference removal

Built-in safety for handling reactive gases

2 mass flow controllers with optimized flow rates

### Interference Removal

Polyatomic

Isobaric

Doubly charged

Thermo Scientific™ iCAP™  
TQ ICP-MS



Additional quadrupole for superior interference removal

Built-in safety for handling reactive gases

4 mass flow controllers with optimized flow rates

### KED, Reactive Gas



# Analysis of Baby food

## Instrument configuration

- iCAP TQe ICP-MS
- ASX560 with ASXPRESS<sup>®</sup> PLUS (Teledyne Cetac Technologies)
- O<sub>2</sub> mode utilized for all analysis
- 1 minute 19 seconds analysis time

## Sample Preparation

- $0.4 \pm 0.05$  g of dry sample or 2.0 g of wet sample + 5 ml HNO<sub>3</sub> + 1 ml HCl
- Closed vessel microwave digestion for 20 mins at 1200 W
- Dilution factors – 125x for dry samples, 25x for wet samples



# Thermo Scientific™ iCAP™ TQe Instrument Parameters

ThermoFisher  
SCIENTIFIC

**Footprint** – Smallest footprint of any ICP-MS

**1 SEM**– with improved lifetime

**2 Quadrupole** – Dwell times - 0.2 s for As, Hg, Se; 0.1 s for Cd, Fe, Pb, Sb, Sn; 0.05 s for others. 5 sweeps, 3 main runs

**3 QCell** – O<sub>2</sub> mode only

**4 Additional 'Q1'** quadrupole for best interference removal

**5 Interface settings** - RF power 1550 W Nebulizer : Borosilicate glass micromist, 400  $\mu\text{L}\cdot\text{min}^{-1}$  at Ar flow rate 1.13  $\text{L}\cdot\text{min}^{-1}$

**6 MFC** – 100% O<sub>2</sub>, 0.34  $\text{mL}\cdot\text{min}^{-1}$  or 0.7  $\text{mL}\cdot\text{min}^{-1}$  (analyte dependent)



**Robust and innovative design for greater ease of use**

# Detection limits

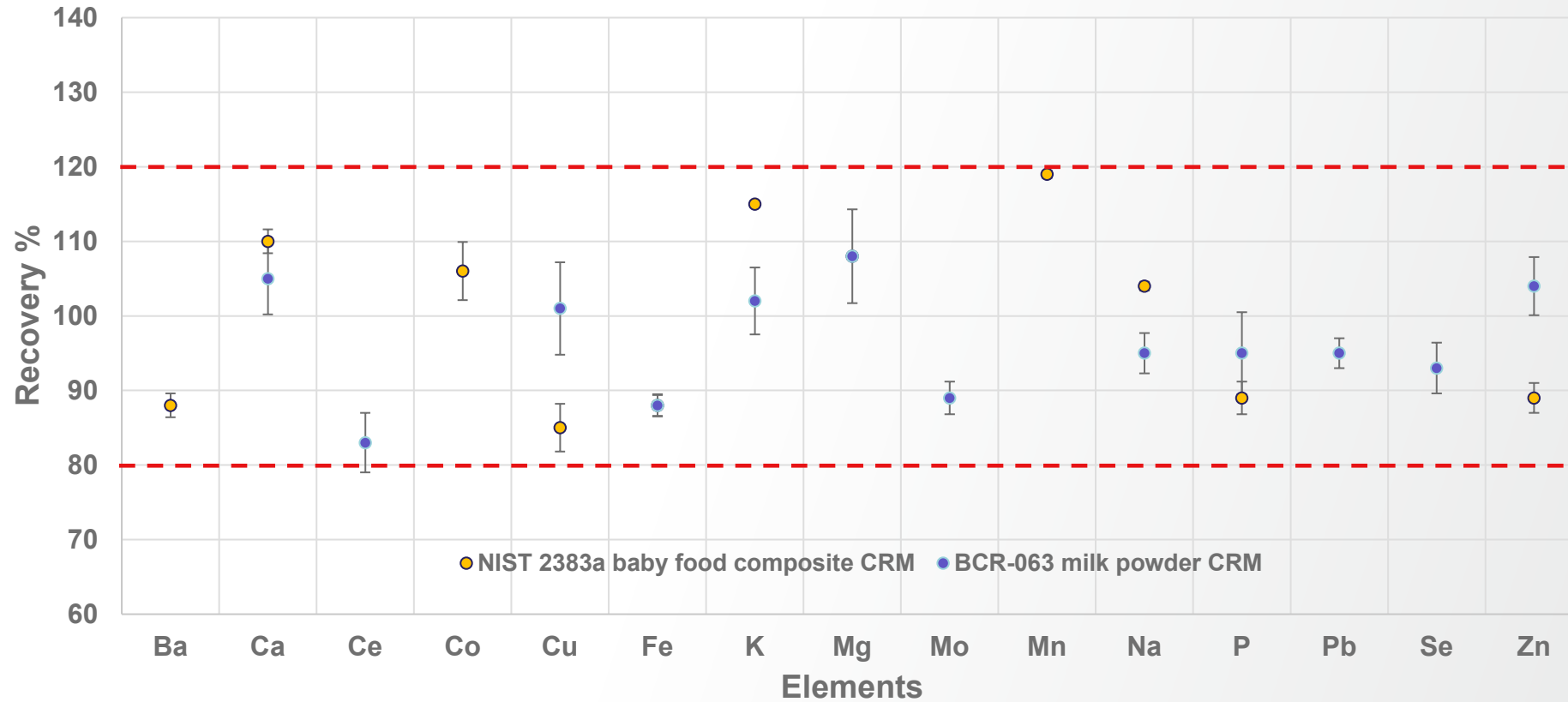
- Instrument detection limit (IDL) based on standard deviation of blank concentrations
- Instrumental limit of quantification (ILOQ) in solution
  - 3 x IDL
- Method LOQ in baby food samples (MLOQ)
  - 125 x LOQ for powders
  - 25 x LOQ for purees

## Toxic elements

Element	R <sup>2</sup>	BEC (µg·L <sup>-1</sup> )	IDL (µg·L <sup>-1</sup> )	ILOQ = 3 x IDL (µg·L <sup>-1</sup> )	MLOQ in dry samples (125 x LOQ) (µg·kg <sup>-1</sup> )	MLOQ in puree or wet samples (25 x LOQ) (µg·kg <sup>-1</sup> )
<sup>75</sup> As	0.9995	0.002	0.004	0.012	1.44	0.29
<sup>9</sup> Be	0.9994	0.024	0.126	0.377	47.1	9.4
<sup>111</sup> Cd	> 0.9999	0.007	0.003	0.009	1.09	0.22
<sup>59</sup> Co	> 0.9999	0.001	0.001	0.004	0.49	0.10
<sup>52</sup> Cr	0.9993	0.028	0.032	0.096	12.0	2.4
<sup>63</sup> Cu	0.9996	0.024	0.013	0.040	5.0	1.0
<sup>56</sup> Fe	0.9993	0.190	0.058	0.174	21.8	4.4
<sup>202</sup> Hg	> 0.9999	0.002	0.0003	0.001	0.11	0.02
<sup>60</sup> Ni	0.9993	0.060	0.033	0.099	12.4	2.5
<sup>208</sup> Pb	> 0.9999	0.006	0.001	0.004	0.45	0.09
<sup>78</sup> Se	0.9999	0.005	0.010	0.030	3.7	0.7
<sup>118</sup> Sn	0.9998	0.015	0.003	0.009	1.11	0.22
<sup>51</sup> V	0.9995	0.059	0.021	0.064	8.0	1.6

Data for more elements can be found in AN 00209

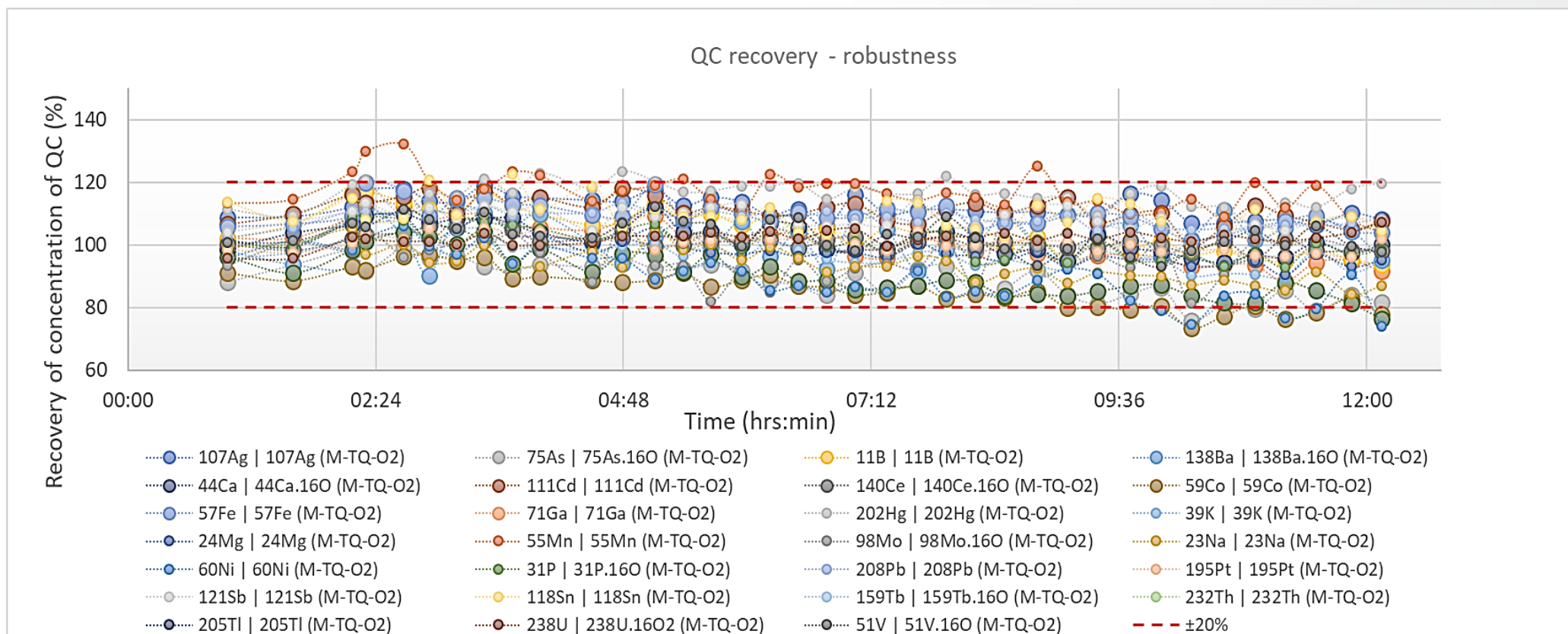
# Accuracy – analysis of certified reference materials



Excellent agreement with certified values achieved

# Robustness – QC standard recovery

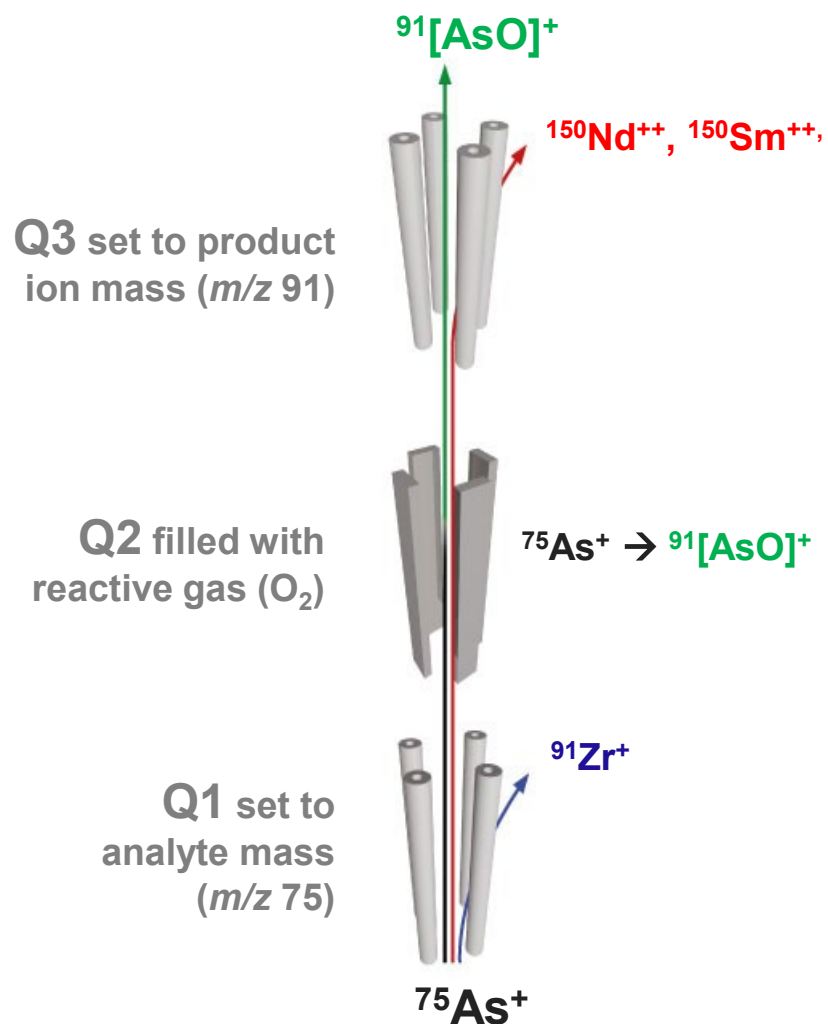
- QC standard concentration –  $0.1 \mu\text{g}\cdot\text{kg}^{-1}$  Hg,  $1 \mu\text{g}\cdot\text{kg}^{-1}$  other traces,  $20 \text{mg}\cdot\text{kg}^{-1}$  major elements



**Consistent QC recovery obtained throughout the entire measurement time**

# Analysis of arsenic

## iCAP TQe – O<sub>2</sub> mass shift



### 75As (M-SQ-KED)

		$^{75}As$ [ $\mu g \cdot kg^{-1}$ ]
Kinetic Energy Discrimination (KED)	Original Sample	$0.034 \pm 0.06$
	Sample + 20 $\mu g \cdot L^{-1}$ REE	<b><math>1.00 \pm 0.02</math></b>
	Sample + 50 $\mu g \cdot L^{-1}$ REE	<b><math>2.44 \pm 0.1</math></b>

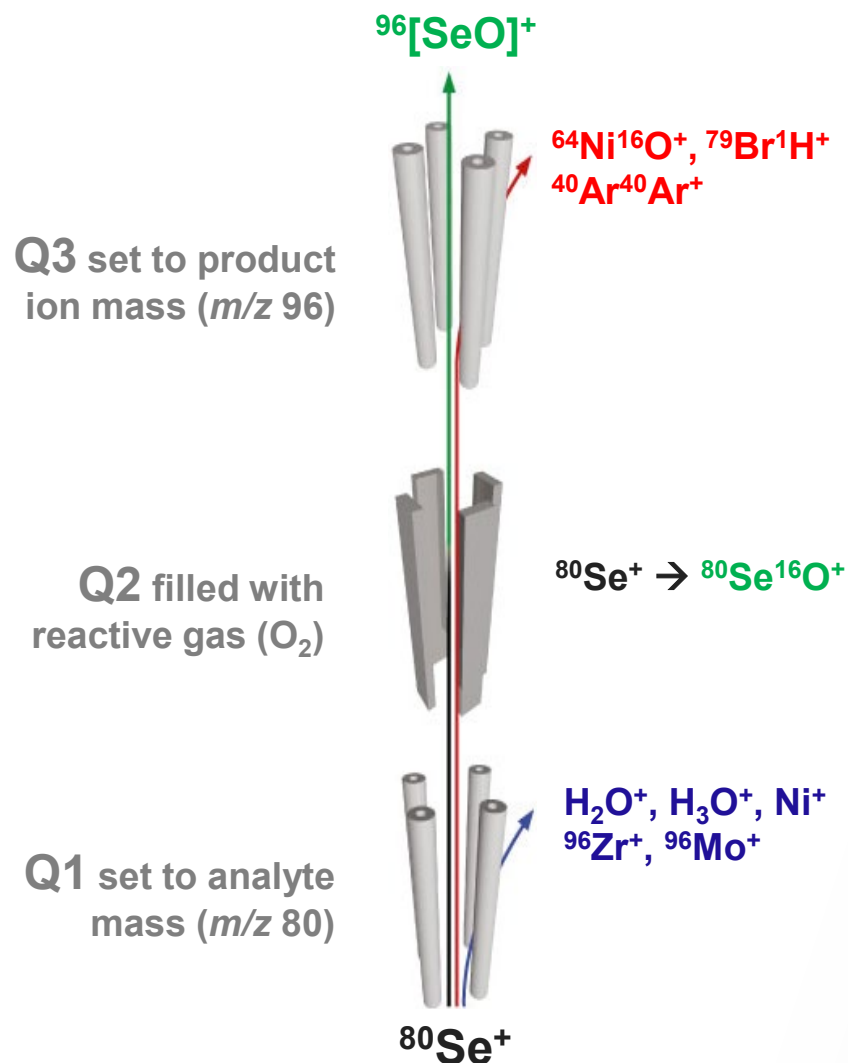
### 75As | 75As.16O (M-TQ-O2)

		$^{75}As$ [ $\mu g \cdot kg^{-1}$ ]
TQ-O <sub>2</sub> mode	Original Sample	$0.028 \pm 0.003$
	Sample + 20 $\mu g \cdot L^{-1}$ REE	$0.027 \pm 0.004$
	Sample + 50 $\mu g \cdot L^{-1}$ REE	$0.034 \pm 0.003$



# Analysis of selenium

## iCAP TQe – O<sub>2</sub> mass shift



### 78Se (M-SQ-KED)

		$^{78}\text{Se}$ [ $\mu\text{g}\cdot\text{kg}^{-1}$ ]
<b>Kinetic Energy Discrimination (KED)</b>	Original Sample	$0.029 \pm 0.01$
	Sample + 20 $\mu\text{g}\cdot\text{L}^{-1}$ REE	$6.46 \pm 0.2$
	Sample + 50 $\mu\text{g}\cdot\text{L}^{-1}$ REE	$16.22 \pm 0.5$

### 80Se | 80Se.16O (M-TQ-O2)

		$^{80}\text{Se}$ [ $\mu\text{g}\cdot\text{kg}^{-1}$ ]
<b>TQ-O<sub>2</sub> mode</b>	Original Sample	$0.015 \pm 0.009$
	Sample + 20 $\mu\text{g}\cdot\text{L}^{-1}$ REE	$0.015 \pm 0.004$
	Sample + 50 $\mu\text{g}\cdot\text{L}^{-1}$ REE	$0.021 \pm 0.007$

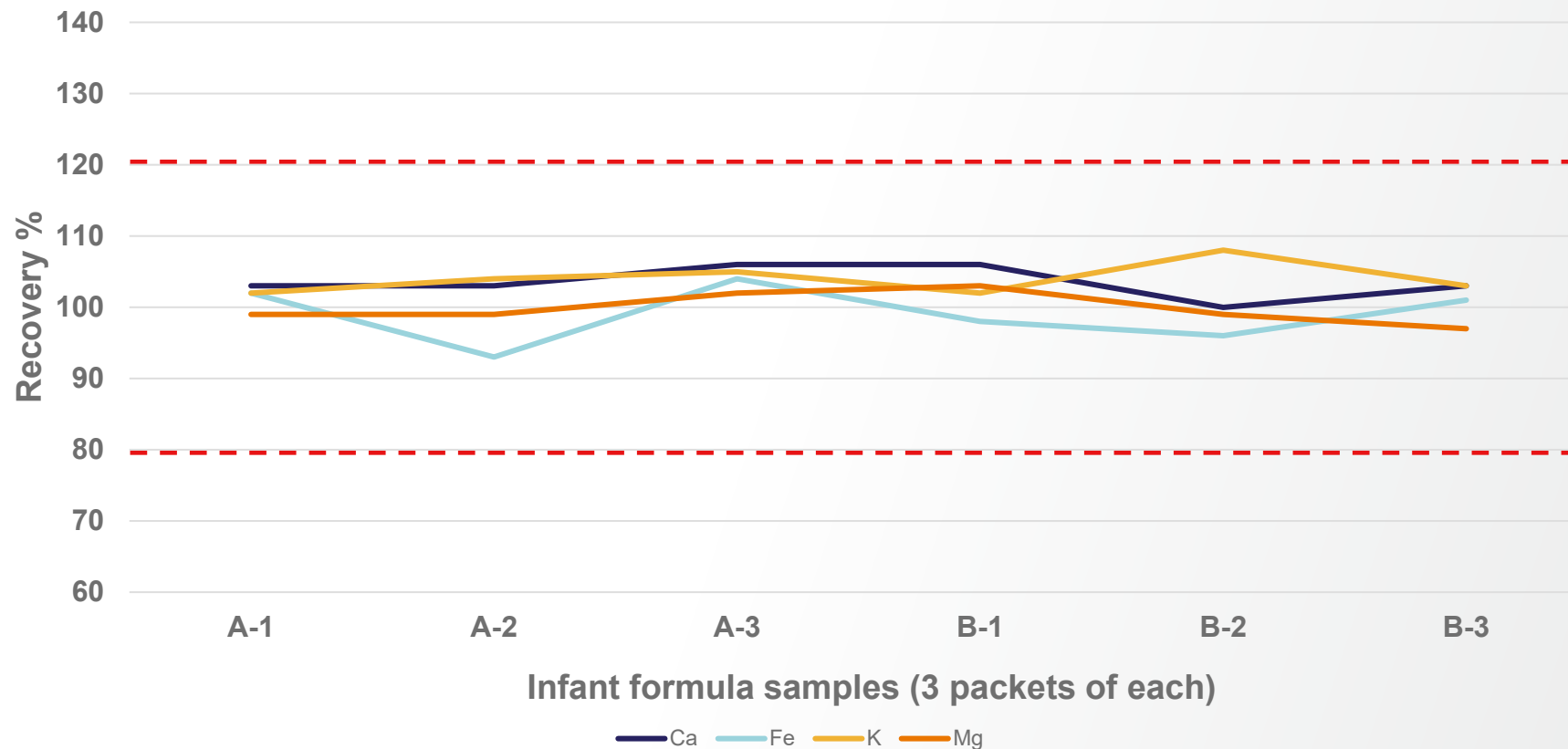
# Food Nutrition & Safety Measurements Quality Assurance Program (FNSQAP) organized by National Institute of Standards and Technology (NIST)

	Dates	Samples	Nutritional Elements	Toxic Elements
<b>FNSQAP Exercise 1 - Spring 2021</b>	Samples received: April 10, 2021	Infant Formula A	Na, K, Ca, Mg	-
		Infant Formula B		
		Baby Food A	-	As, Cd, Hg, Pb
		Baby Food B		
<b>FNSQAP Exercise 2 - Spring 2022</b>	Samples received: May 10, 2022	Infant Formula B	Cr, Mo, Se	-
		Infant Formula C		
		Cocoa Powder	-	Cd, Pb
		Chocolate Drinking Mix		

- Three packets of each sample provided → three results for each analyte required

# FNSQAP Ex-1, NIST

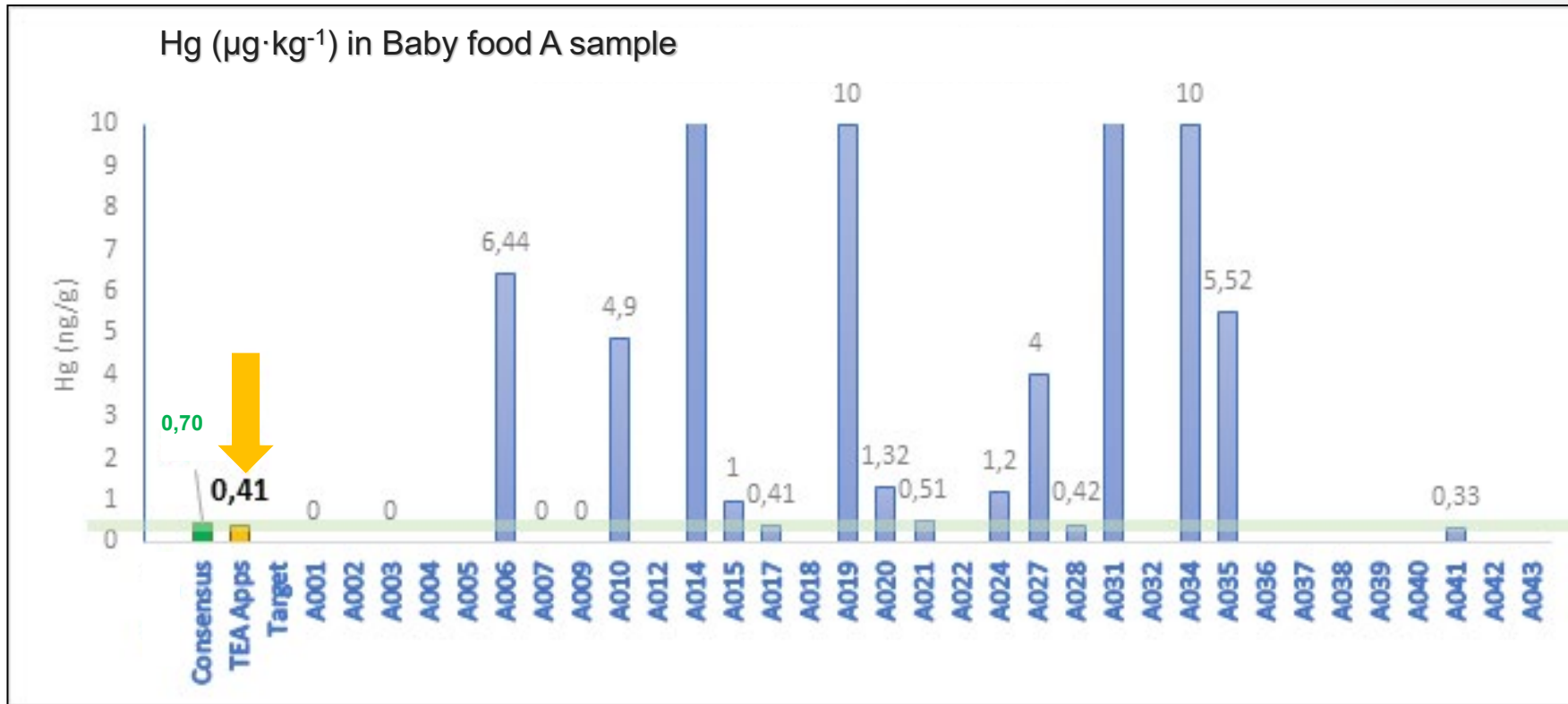
Results - Major elements in Infant formula samples



**Excellent agreement with certified values achieved**

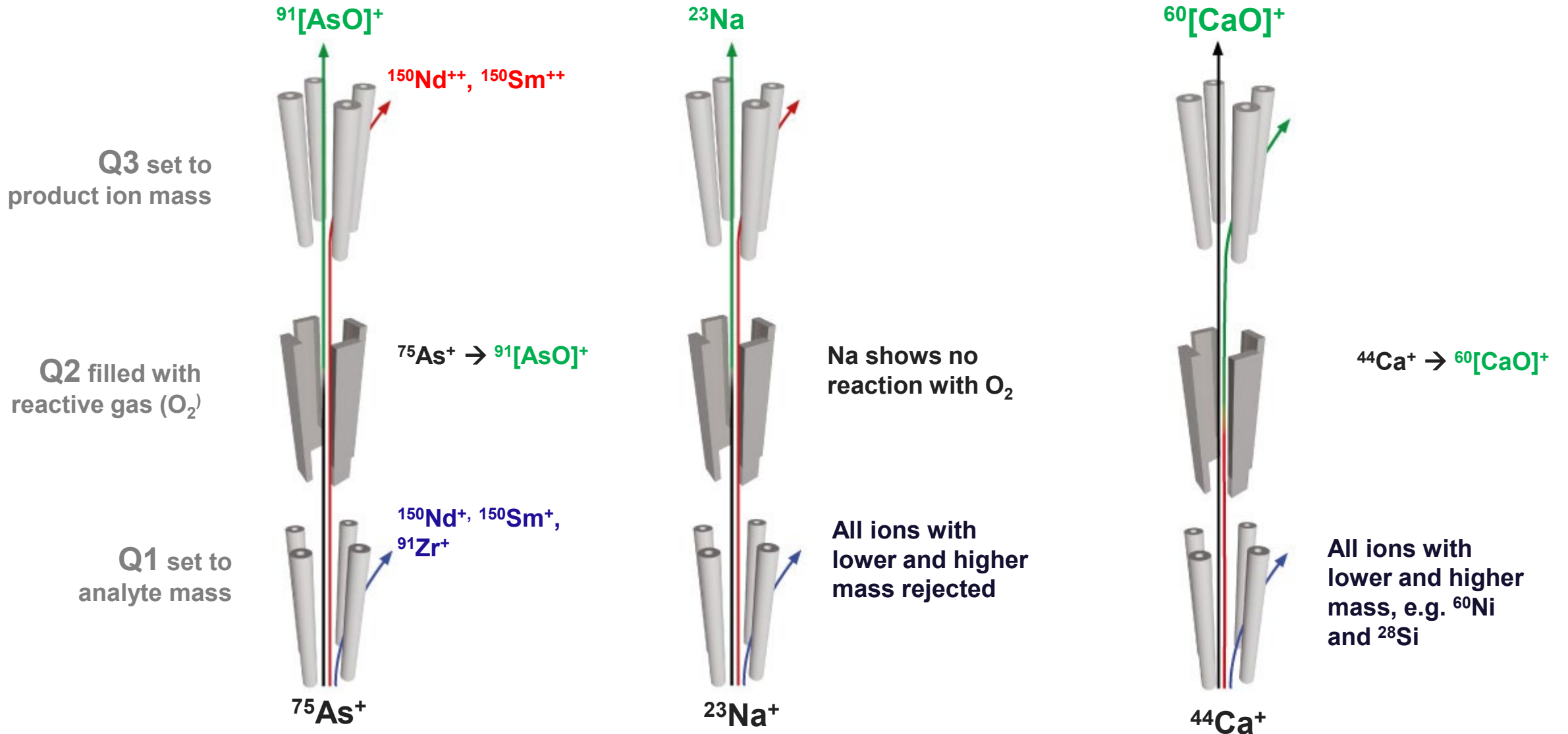
# FNSQAP Ex-1, NIST

Results - Mercury in provided samples, our data point in yellow



- Only 18 reported values for mercury out of 33 participants
- Many reported values extremely high – false positives?
- Single mode iCAP Tqe ICP-MS analysis was able to provide accurate values close to LOQ level for mercury!

# Even easier method development: single mode analysis



# Even easier method development: single mode analysis

## Single mode analysis using just TQ-O<sub>2</sub> mode

- Very straightforward method development – one mode for all elements
- Improved interference removal for key analytes (e.g. V, As, Se, Cd, Hg) eliminates false positive results

### Advantages:

- Reduced method runtime enables increased laboratory productivity



Reduced sample  
turnaround times

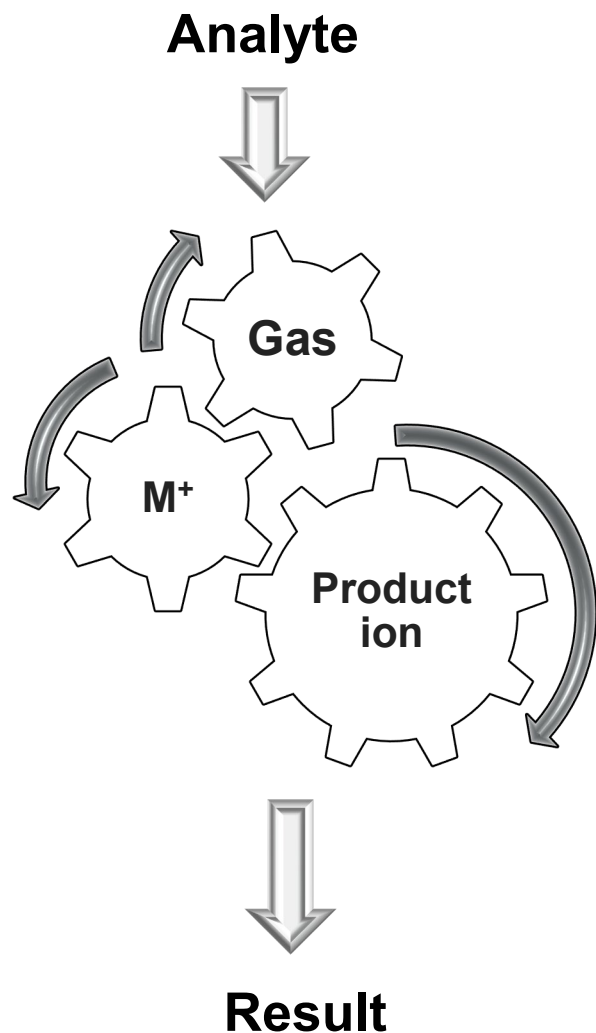


Increased  
throughput

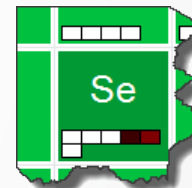


Improved return  
on investment

# 'Reaction Finder' - method development assistant



- Select Element/Isotope of interest



- Reaction Finder proposes most appropriate gas/scan setting combination

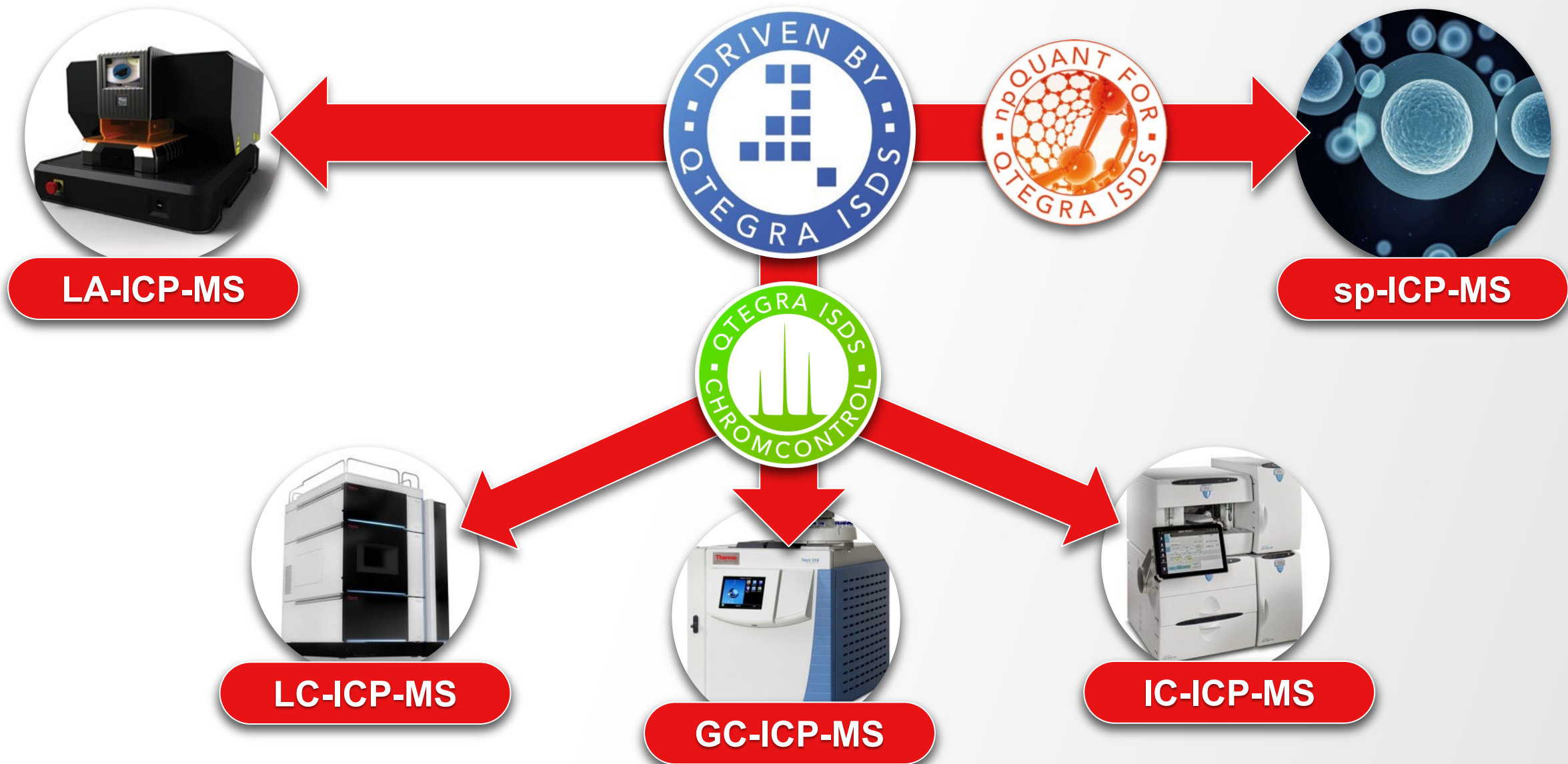
Identifier	Q3 Analyte	SQ / TQ	CR Gas	Dwell time (s)	Channels	Spacing (u)	
78Se   78Se.160	78Se.160 (93.912)	TQ	O <sub>2</sub>	0.1	1	0.1	Normal
80Se   80Se.160	80Se.160	TQ	O <sub>2</sub>	0.1	1	0.1	Normal

- Choose from list of Internal Standards

Identifier	Q3 Analyte	SQ / TQ	CR Gas	Dwell time (s)	Channels	Spacing (u)
7Li (S-SQ-KED)		SQ	KED	0.1	1	0.1
55Mn (S-SQ-KED)		SQ	KED	0.1	1	0.1
65Cu   65Cu.14N	65Cu.14N2.1H6	TQ	NH <sub>3</sub>	0.1	1	0.1
51V   51V.16D (S)	51V.16D	TQ	O <sub>2</sub>	0.1	1	0.1
48Ti   48Ti.14N4	48Ti.14N4.1H10	TQ	NH <sub>3</sub>	0.1	1	0.1
Fit cells to grid		SQ	KED	0.1	1	0.1
Fit cells to content		SQ	KED	0.1	1	0.1
Export to Excel		SQ	KED	0.1	1	0.1
Duplicate analyte		SQ	KED	0.1	1	0.1
Add internal standard analyte						
			59Co			
			115In			
			209Bi			

Redefining triple quadrupole ICP-MS with unique ease of use

# Options for transient signals analysis in Qtegra ISDS with Thermo Scientific™ iCAP™ TQ ICP-MS





# Elemental analysis workflow

# Food cycle quality control



# Why run elemental analysis in food?

# N

Nitrogen

- Monitoring protein content

# Protein

- Determination of the nutritional quality of the products
- Transparent labelling - nutritional, health, safety and economical point of view
- Price definition and quality comparison enablement based on % protein declarations

# S

Sulfur

- Of essential importance for synthesis of amino acids and vitamins
- Cattle – good regeneration of the udder during lactation
- Horse – essential for healthy hoof growth
- Brewery – preserving the shelf life of beer and securing the safety of the raw materials and final products

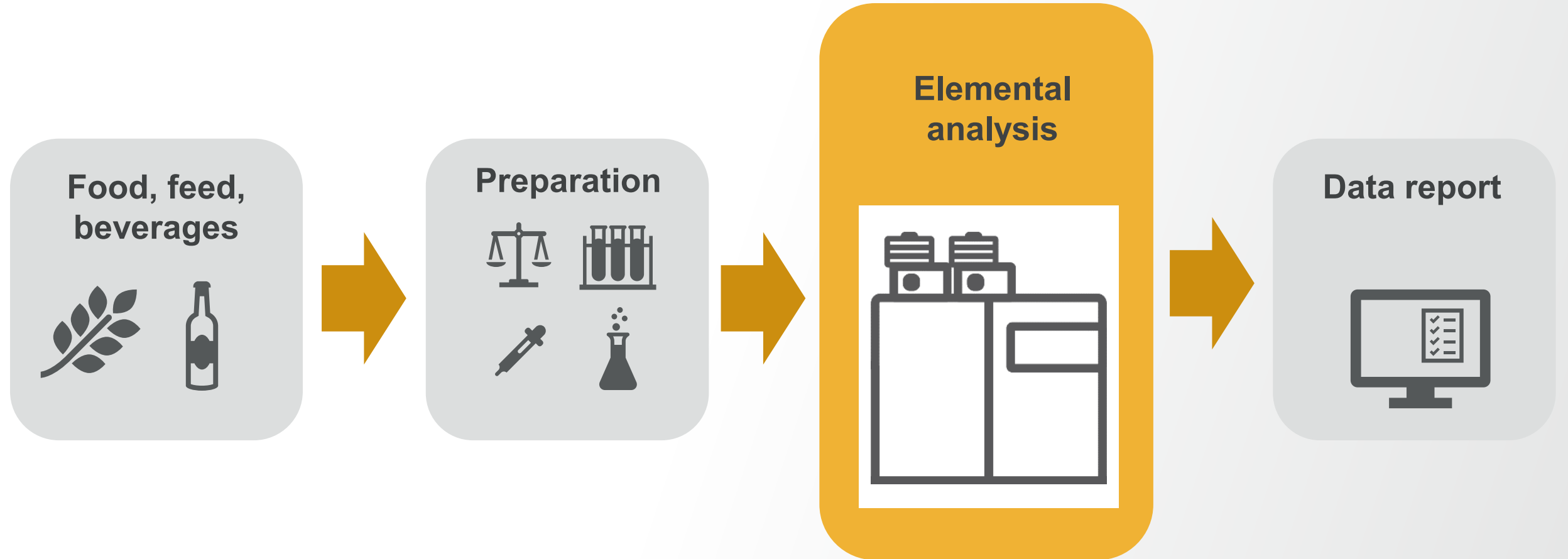
# Official methods

## Interlaboratory data standardization

- Dumas (combustion) methods for N/Protein determination as the alternative to the Kjeldahl method

Application	Official Association	Official Method		
	<b>AACC</b> (American Association of Cereal Chemists)	Crude Protein in Cereal, 46-30, 1999		<b>ASBC</b> (American Society of Brewing Chemists) Official Method 1996. Nitrogen Determination in Barley
	<b>AOAC</b> (Association of Official Analytical Chemists)	Official Method 990.03. Protein (crude) in Animal Feed 4.2.08		<b>ASBC</b> (American Society of Brewing Chemists) Total Nitrogen in Wort and Beer by Combustion Method. Report of Subcommittee, 1994
	<b>AOAC</b> (Association of Official Analytical Chemists)	Official Method 992.15. Crude Protein in Meat and Meat Products including Pet Foods 39.1.16		<b>DIN, EN, ISO 16634-1, 2008</b> (International Organization for Standardization) Food Products – Determination of the Total Nitrogen Content by Combustion According to the Dumas Principle and Calculation of the Crude Protein Content. Part 1: Oil Seeds and Animal Feeding Stuffs
	<b>AOAC</b> (Association of Official Analytical Chemists)	Official Method 992.23. Crude Protein in Cereals, Grain and Oilseeds 32.2.02		<b>DIN, EN, ISO 16634 – 2</b> (International Organization for Standardization) Food Products – Determination of the Total Nitrogen Content by Combustion According to the Dumas Principle and Calculation of the Crude Protein Content. Part 2: Cereals, Pulses and Milled Cereal Products
	<b>AOAC</b> (Association of Official Analytical Chemists)	Official Method 997.09 Nitrogen in Beer, Wort, and Brewing Grains Protein (Total) by Calculation (Combustion Method)		<b>IFFO</b> (International Fishmeal and Fish Oil Organization Ltd.) Nitrogen Determination in Fish Meal by Combustion Method
	<b>AOAC</b> (Association of Official Analytical Chemists)	Official Method 972.43 Microchemical Determination of Carbon, Hydrogen and Nitrogen		<b>ISO 14891 (International Organization for Standardization)</b> <b>FIL 185 (International Dairy Federation)</b> Nitrogen Determination in Dairy Products by Combustion Method
	<b>AOCS</b> (American Oil Chemists Society)	Official Method Ba 4e-93 (revised 1995). Combustion Method for Determination of Crude Protein		<b>Office International de la Vigne et du Vin</b> Resolution OENO 13/2002 Quantification of Total Nitrogen by Dumas Method (Must and Wines) Quantification de l'Azote Total Selon la Methode de Dumas (Mouts et Vins)

# Elemental analysis workflow



Sample prep

Homogenization

Sample intro

Elemental  
analysis

Data report

# FlashSmart Elemental Analyzer

## What is the Thermo Scientific™ FlashSmart™ EA?

- An elemental analyzer which operates with the dynamic flash combustion (modified Dumas method) with the Thermal Conductivity Detector (TCD).

## What is FlashSmart EA measuring?

- Carbon, hydrogen, nitrogen, sulfur and oxygen

## How is the sample introduced in the system?

- Thermo Scientific™ MAS Plus Autosampler for solids, viscous and liquids (weighed in containers)
- Thermo Scientific™ AI/AS 1310 Liquid Autosamplers



# Data report

The screenshot displays the 'Edit Method' window with the following settings:

- Report parameters 5 | Report stripchart 6 | Operator I.D./Info 7
- Method title 1 | Detection parameters 2 | Integration parameters 3 | Calculation parameters 4
- Calibration: Calibration method: K-Factor
- Heat Value: Calculation: Solids
- Heat Value: CO2 Emission Trade: Both
- Protein:  Protein calculation

The 'Sample table' below shows a list of samples with columns for Sample name, Filename, Type, Standard name, Weight (mg), Protein F., and Category. A yellow box highlights the 'Protein F.' column, and an arrow points from the 'Protein calculation' checkbox to this column.

A	Sample name	Filename	Type	Standard name	Weight (mg)	Protein F.	Category
1	Blank	NProtein test 001	Blank				
2	Bypass	NProtein test 002	Bypass				
3	std1	NProtein test 003	Std	Aspartic acid	50.472		
4	std2	NProtein test 004	Std	Aspartic acid	69.02		
5	std3	NProtein test 005	Std	Aspartic acid	85.366		
6	std4	NProtein test 006	Std	Nicotinamide	51.028		
7	std5	NProtein test 007	Std	Nicotinamide	66.287		
8	std6	NProtein test 008	Std	Nicotinamide	78.768		
9	unk 1	NProtein test 009	Unk		62.53	6.25	
10	unk 2	NProtein test 010	Unk		55.411	6.25	
11	Sample 1	NProtein test 011	Unk		151.442	6.25	
12	Sample 1	NProtein test 012	Unk		159.92	6.25	
13	Sample 1	NProtein test 013	Unk		129.703	6.25	
14	Sample 1	NProtein test 014	Unk		151.96	6.25	

- Specific factors for the conversion of nitrogen content to protein content (FAO)
- **Acquired data:**
  - Nitrogen
  - N/Protein
  - Sulfur
- Personalized reports

Thermo Scientific™ EagerSmart™ Data  
Handling Software

# All-in-one analyzer

## FlashSmart EA applications





- Cereals and beans are the main component of the human diet and of feeding stock for domestic animals
- In addition to its dietary importance, protein content has become a quality guideline for some cereal trade transactions



Sample	N%	Protein %	RSD%
Corn	1.14	7.10	0.74
Bran	2.27	14.19	0.81
Wheat	1.74	10.89	0.30
Rice	1.10	6.27	0.83
Soy	6.21	38.81	0.55
Lentils	3.84	23.99	0.55
Beans	3.54	22.15	0.69
Peas	4.46	27.89	0.40
Green beans	3.90	24.40	0.53

# Dairy products

- Solid, liquid and viscous dairy products
- Nitrogen/Protein determination for food quality control and R&D purposes
- Protein content and labeling requirements enable consumers to compare price and quality



Sample	N%	Protein %	RSD%
Raw milk	0.476	3.04	0.61
Pasteurized milk	0.510	3.25	0.68
UHT milk	0.529	3.38	0.56
Milk powder	5.46	34.83	0.30
Emmental	3.38	21.07	0.88
Parmesan	5.21	33.25	0.80
Provolone	4.35	27.77	0.67
Spread cheese	3.36	20.99	0.99
Yoghurt	0.515	3.28	0.95

# Meat products

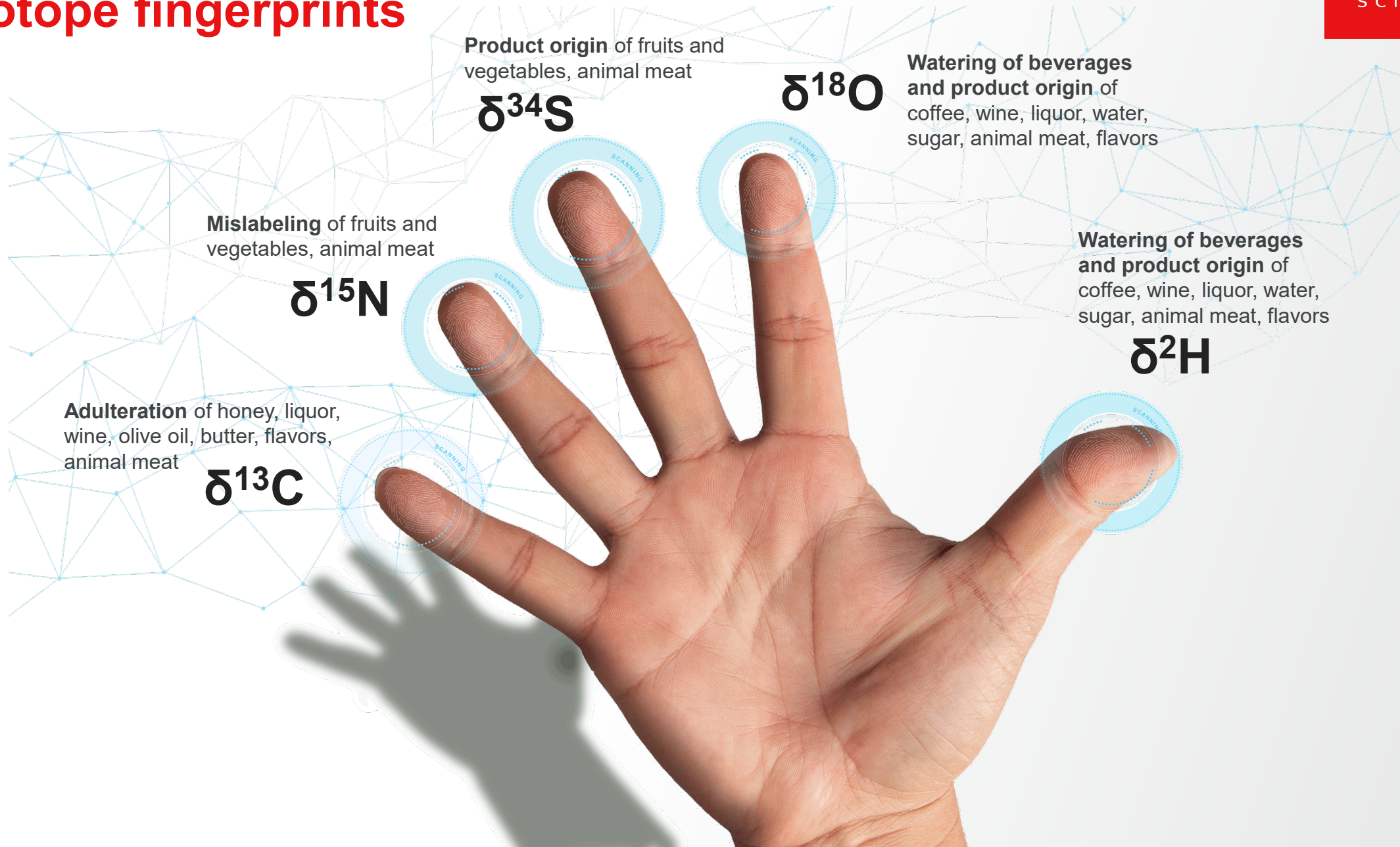
- Meat products require homogenization
- Nitrogen/Protein determination for food quality control



Sample	N%	Protein %	RSD%
Cured ham	4.51	28.19	0.35
Coppa	4.34	27.12	0.71
Beef sausage	2.99	18.69	1.54
Wurstel	2.42	15.15	0.83
Salame	3.18	19.87	0.49
Bacon	2.75	17.19	1.15
Mortadella Bologna	3.27	20.44	1.32

## Isotope analysis workflow

# Isotope fingerprints

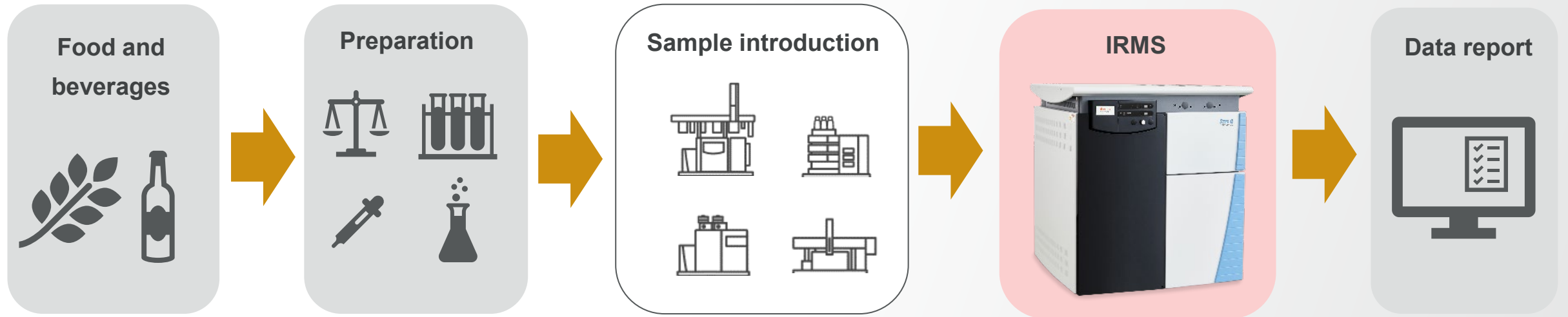


# Official methods in food integrity applications

- CODEX ALIMENTARIUS INTERNATIONAL FOOD STANDARDS (FAO/WHO)
  - Recommended methods of analysis and sampling CXS 234-1999
- CEN Technical Committee 460 'Food Authenticity' Working Group 6 - IRMS

Product	Official method	Isotope fingerprint	Sample	What does it address?	Analytical solution
<b>Wine</b>					
	OIV-MA-AS2-12	$\delta^{18}\text{O}$	Water	Adulteration, Geographical origin, Year of vintage	Thermo Scientific™ GasBench II System, Thermo Scientific™ Dual Inlet
	OIV-MA-AS312-06	$\delta^{13}\text{C}$	Ethanol, Wine must, Grape sugar	Adulteration, origin	Thermo Scientific™ EA IsoLink™ IRMS System, Thermo Scientific™ GC IsoLink II™ Interface for GC-IRMS
	OIV-AS312-07	$\delta^{13}\text{C}$	Glycerol in wines	Adulteration by addition of glycerol from C4 maize or Fossil sources	GC IsoLink II Interface for GC-IRMS, Thermo Scientific™ LC IsoLink™ Interface for IRM-LC/MS
	OIV-OENO 510-2013	$\delta^{13}\text{C}$	Acetic acid in wine, vinegar		GC IsoLink II Interface for GC-IRMS, EA IsoLink IRMS System
	OIV-OENO 510-2013	$\delta^{18}\text{O}$	Water in wine, vinegar	Adulteration, Geographical Origin, Year of Vintage	Thermo Scientific™ GasBench II System, Dual Inlet
<b>Sparkling wine</b>					
	OIV-MA-AS314-03	$\delta^{13}\text{C}$	CO <sub>2</sub> in sparkling wine	Origin and authenticity of sparkling wine	GasBench II System, EA IsoLink IRMS System, GC IsoLink, Dual Inlet
<b>Spirits</b>					
	OIV-AS312-07	$\delta^{13}\text{C}$	Glycerol in spirits	Adulteration by addition of glycerol from C4 maize or Fossil sources	GC IsoLink II Interface for GC-IRMS, LC IsoLink Interface for IRM-LC/MS
<b>Fruit Juice</b>					
	EU – CEN 1995	$\delta^{13}\text{C}$	Sugars	Adulteration	GasBench II System, LC IsoLink Interface for IRM-LC/MS, GC IsoLink II Interface
	USA – AOAC 1981	$\delta^{13}\text{C}$	Sugars	Adulteration	GasBench II System, LC IsoLink Interface for IRM-LC/MS, GC IsoLink II Interface
	EU – CEN 1998	$\delta^{13}\text{C}$	Sugars and pulp	Adulteration	GasBench II System, LC IsoLink Interface for IRM-LC/MS, GC IsoLink II Interface
	EU – CEN 1995	$\delta^2\text{H}$ and $\delta^{18}\text{O}$	Water	Adulteration	GasBench II System, LC IsoLink Interface for IRM-LC/MS, GC IsoLink II Interface
	AOAC method 2004.01	$\delta^{13}\text{C}$	Ethanol (From Fermentation)	Adulteration	GasBench II System, LC IsoLink Interface for IRM-LC/MS, GC IsoLink II Interface
<b>Fruit Juice (Concentrate)</b>					
	AOAC 1992	$\delta^{18}\text{O}$	Water	Adulteration	GasBench II System, LC IsoLink Interface for IRM-LC/MS, EA IsoLink IRMS System
<b>Honey</b>					
	AOAC method 991.41	$\delta^{13}\text{C}$	C-4 plant sugars at concentration >7%	Adulteration of honey	EA IsoLink IRMS System
	AOAC method 998.12	$\delta^{13}\text{C}$	C-4 plant sugars at concentration >7%	Adulteration of honey	EA IsoLink IRMS System
<b>Cheese</b>					
	EU Reg 548/2011	$\delta^{13}\text{C}$	PDO	PDO Grana Padano	EA IsoLink IRMS System

# Isotope analysis workflow



Sample prep

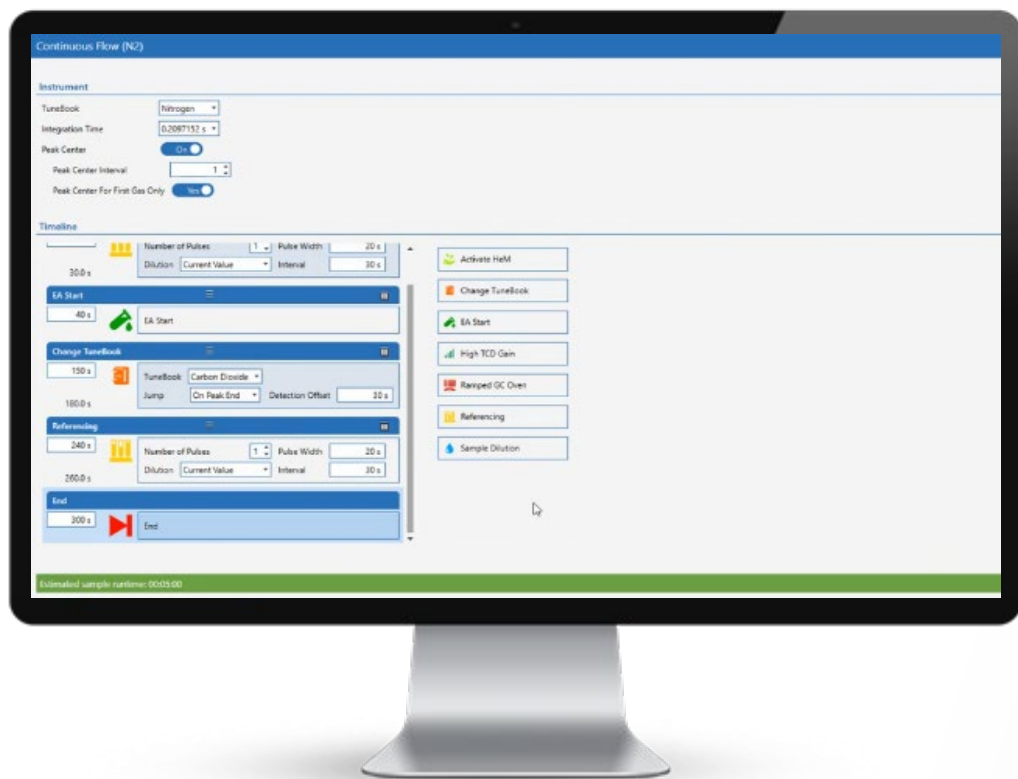
Sample intro

Conversion

IRMS analysis

Data report

Driven by Thermo Scientific™ Qtegra™ Intelligent Scientific Data Solution (ISDS) Software



## Why Qtegra ISDS Software?

- Automate workflows
- Simplify your experience
- Improve efficiency

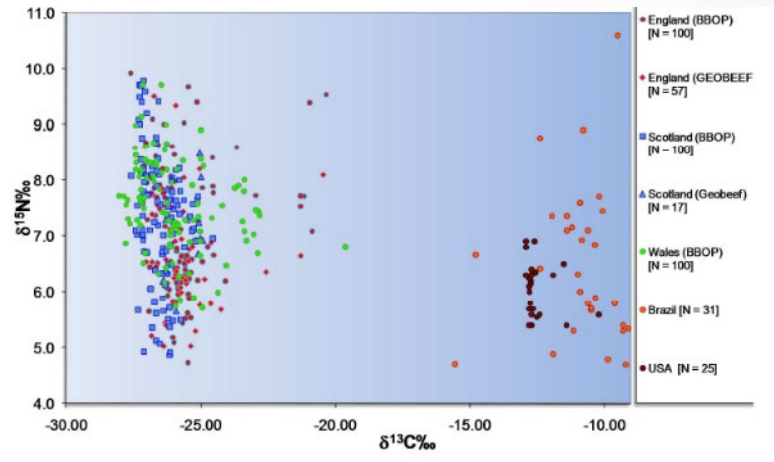




# Where does my beef come from?



Thermo Scientific™ EA IsoLink™ IRMS System



Heaton et al., 2008

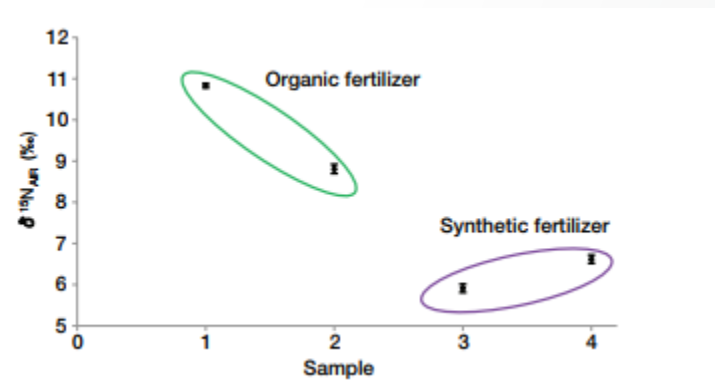
- Carbon and Nitrogen isotope fingerprint
- Pasture varies between C3 and C4 plant groups, which result in difference in animal (i.e., dietary differences)
- UK cattle reared on C3 diet, whilst Brazilian cattle reared on C4 diet



# Was my produce organically grown?



Thermo Scientific™ EA IsoLink™ IRMS System



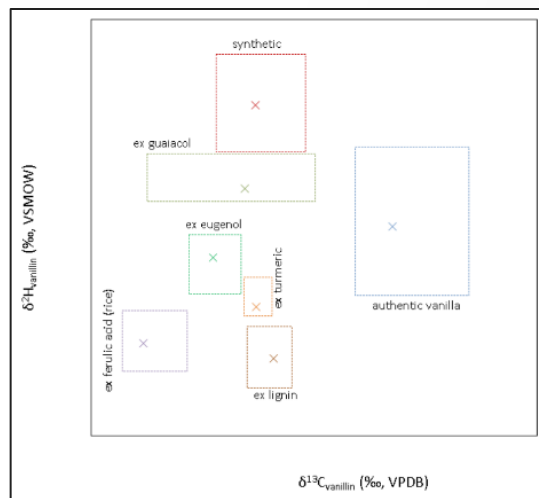
- Nitrogen isotope fingerprint
- Differentiation of nitrogen isotopes in plants and soils due to ammonia volatilization, denitrification, nitrification, etc.
- Organic (+8‰ to +20‰) versus synthetic fertilization (+3‰ to +6‰)



# What is in my ice cream?



Thermo Scientific™ GC IsoLink II™ IRMS System



Courtesy D. Psomiadis, Imprint Analytics

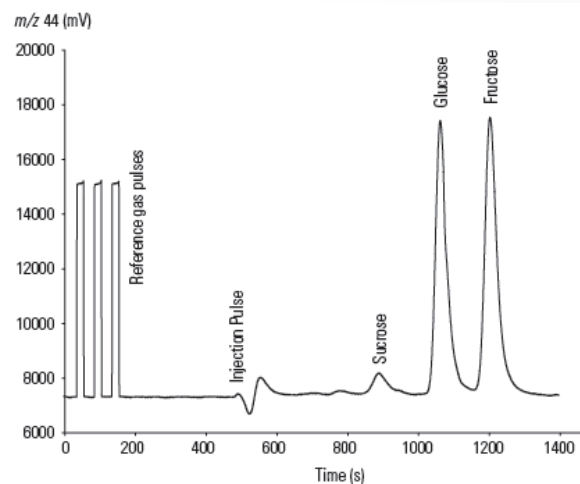
- Carbon and Hydrogen isotope fingerprint
- Investigation the origin of vanillin in ice cream, cakes, cookies
- Natural (vanilla pods) vs. synthetic (e.g. wood, petroleum) vs. biosynthetic (e.g. cloves, rice, corn)



# Was my honey sweetened?



Thermo Scientific™ LC IsoLink™ IRMS System



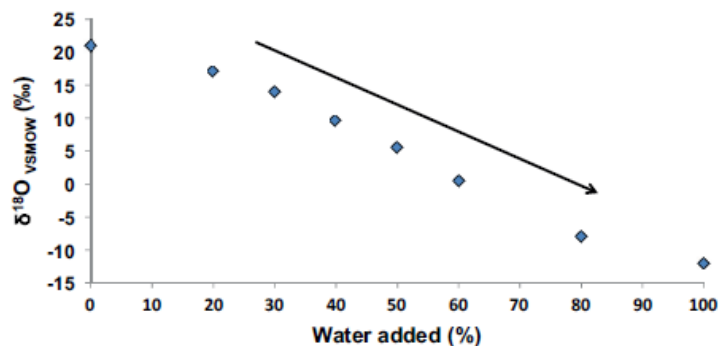
- Carbon isotope fingerprint
- Honey adulteration by addition of exogenous sugars
- Official method AOAC 998.12 (detection limit 7% sugar from C4 plant source) by EA-IRMS
- Compound specific analysis of individual sugars by LC-IRMS



# Was my wine watered down?



Thermo Scientific™ GasBench Plus IRMS System



- Oxygen isotope fingerprint
- Geographical origin and adulteration OIV-MS-AS2-12
- Grapes have local-regional fingerprint associated with local-regional rainfall
- If adulterated by water or juices, the oxygen isotope fingerprint changes



# Summary and Conclusion

- **Triple Quad ICP-MS** – Single method
  - 30 elements – Toxic and nutritional
  - Excellent interference removal
- **Elemental Analysis** – C,N,O,S and H
  - Nitrogen/Protein determination
  - All in one analysis of liquid and solid samples
- **Isotopic analysis**– origin and authenticity
  - Bulk and compound specific information
  - Fully integrated peripherals



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# Thank you

