

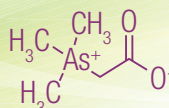
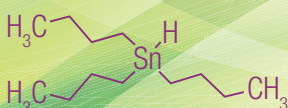
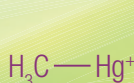
# A Guide to Trace Elemental Speciation

## What is elemental speciation?

**IUPAC Definition** – ‘the analytical activity of identifying and/or measuring the quantities of one or more individual chemical species in a sample’

**That means** – chemical species of an element are determined rather than the total element concentration

**Examples** – Methylmercury, tributyltin, arsenobetaine



## Why is speciation important?

Elemental speciation data can reveal valuable information in addition to total element concentrations such as:

Environmental Fate

Bioavailability

Mobility

Reactivity

Toxicity

Process Control  
Chemistry



## What sample types is speciation analysis applied to?

Speciation analysis is useful for a wide range of sample types, including foodstuffs and beverages, environmental samples, biological specimens and even petrochemicals. Key applications include As in rice and fruit juice and Cr in potable water.



## What instrumentation is used for elemental speciation?

Liquid chromatography (either HPLC or IC) connected to ICP-MS  
Used for e.g. As, Cr, Se and I speciation



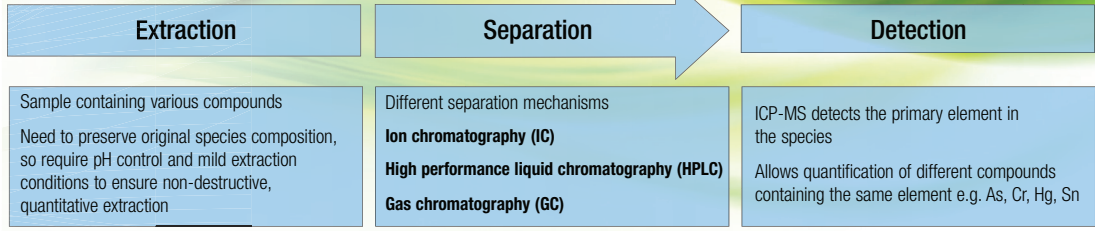
Thermo Scientific™ Dionex™ ICS-5000 IC coupled to the Thermo Scientific™ iCAP™ Q ICP-MS

Gas chromatography connected to ICP-MS  
Used for e.g. Hg, S and Sn speciation



Thermo Scientific™ Trace™ 1310 GC coupled to the Thermo Scientific™ iCAP™ Q ICP-MS

## What steps make up the speciation analysis workflow?



Speciation analysis performed together with total element concentration measurement – as a rule, the sum of the species should match this concentration

## Using IC-ICP-MS for elemental speciation

- Metal-free PEEK systems – lower backgrounds and better detection limits especially for Cr
- Sharp, well resolved peaks with short run times
- Reproducible and sensitive
- Reagent-Free Ion Chromatography Eluent Generation (RFIC-EG) – the ion chromatograph electrolytically creates the eluents and regenerants required for IC applications, as required

## Automating speciation analysis using IC-ICP-MS

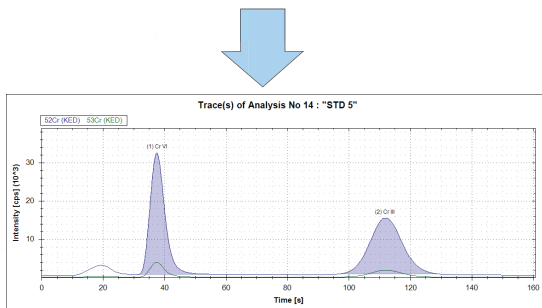
Requires fully integrated hardware and software system:

Thermo Scientific™ Qtegra™ ISDS drives the whole system and includes:  
Thermo Scientific™ Dionex™ Chromeleon™ plug-in drivers to control the IC or HPLC.

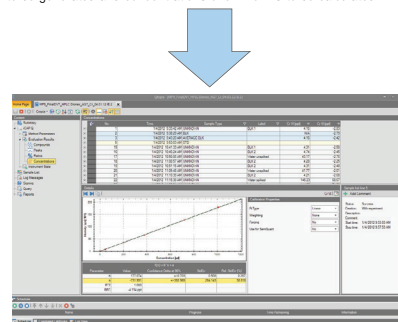
### Single control software

One software interface controls both the IC and the ICP-MS  
Simple hardware connection – inert tubing connection from the IC directly to the ICP-MS nebuliser

Transient chromatographic peaks captured by the Qtegra software



Peak search and integration capabilities allow species specific calibrations to be generated and concentrations of unknowns to be calculated



## Speciation resources

- [www.thermoscientific.com/dramatic](http://www.thermoscientific.com/dramatic) – iCAP Q Resource Centre
- [www.thermoscientific.com/HPLC](http://www.thermoscientific.com/HPLC) – High Pressure Ion Chromatography
- For more information on speciation analysis in general, visit The European Virtual Institute for Speciation Analysis (EVISA) web site at: <http://www.speciation.net>
- Commission Regulation (EU) 2015/1006 regarding maximum levels of inorganic arsenic in foodstuffs

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