Speciation Analysis
Solutions for LC-ICP-MS

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An Endress+Hauser Company

LC-ICP-MS: PQ LC and PlasmaQuant MS

Make more of your daily lab routine and discover the undiscovered. The combination of PQ LC and PlasmaQuant MS offers the perfect match for your requirements in speciation analysis.

The combination of PQ LC and PlasmaQuant MS (LC-ICP-MS) offers a versatile, robust, and highly sensitive solution for the determination of element species in various kinds of samples. The species or chemical form of elements determines their mobility, bioavailability, and toxicity. Since characteristics vary dramatically depending on the species in which an element is present, careful characterization of environmental, food, and agricultural samples and of consumer goods is required. Liquid chromatography or ion chromatography makes it possible to separate these species. The subsequent detection by inductively coupled plasma mass spectrometry provides a highly sensitive method for their quantification. Hence, LC-ICP-MS and IC-ICP-MS provide an essential tool for assessing benefits and/or risk of elements present in the sample.

Environmental
Elemental speciation plays an important role in respect to evaluating chemistry, geo-chemistry or bio-geo-chemistry of different pollutants as well as their bioavailability and toxicity towards organisms or their chemical and physical effects on natural cycles. Elements of interest in species identification are arsenic, selenium, chromium, mercury, cadmium, and many more.

Food and Agriculture
The quantification of major and trace elements, and of essential, nutritional, and potentially toxic elements is a common application in ICP-MS. Since an element can be essential or toxic just based on the oxidation state or compound in which it occurs, the determination of elemental species in foods and beverages is crucial for ensuring the safety of foodstuffs. LC-ICP-MS makes the determination of elemental species possible, for example in the analysis of food samples, such as sea fish, rice, chocolate, and apple juice for arsenic, selenium, or chromium.

Clinical and Pharma
Multiple regulations and standards describe quality control procedures to ensure the efficiency and harmlessness of pharmaceutical products . During production, pharmaceutical products may, for example, be contaminated with chromium. Therefore, the potential toxicity must be evaluated by identifying the species present according to defined standards.
In clinical analysis, element speciation plays a minor role. However, the identification of arsenic species in body fluids, such as whole blood, serum, or urine, gives insight for the risk assessment of workplaces.

PlasmaQuant MS

PQ LC
Solutions for LC-ICP-MS

LC-ICP-MS Is the Key to the World of Elemental Species

Make more of your daily lab routine. Choose workflows and solutions that provide more than just results. Use high efficiency, simplicity and flexibility – without compromising productivity, reliability, or precision.

PQ LC series for High Performance Liquid Chromatography
PQ LC is a series of modular chromatography systems, available as compact routine LC system for limited lab space or as fully equipped LC model with various upgrade options, such as temperature control for the sample injector, column oven, or UV/Vis detector. An ion chromatography option completes the portfolio.

An LC-ICP-MS interface kit allows quick connection to the ICP and minimizes dead volume for precise peak separation. The Chromatography Data Station (CDS), including full instrument control as well as data acquisition and processing drives all PQ LC models. The communication to HPLC and ICP-MS ensures safe operation. All results are handled by the CDS to provide the full power of data processing for easy and uncompromised characterization of elemental species in various sample types.

The PQ LC series offers three models for individual adaptation to your needs:

Your benefits
- Flexible system for individual adaptation to your requirements
- Variable modular design for easy upgrade
- Easy handling with up to four solvents for uncompromised method flexibility
- Interactive setup for seamless communication

- **PQ LC compact –** the routine HPLC system, metal free in PEEK
- **PQ LC –** available in stainless steel and PEEK with various upgrades
- **PQ IC –** the uncompromised ion chromatography solution

All systems of the PQ LC series are equipped with a sample-introduction system with variable volume injection, a quaternary gradient HPLC pump system with vacuum degasser, and a solvent tray for the safe storage of all solvents.

PQ LC compact

The PQ LC compact is a chromatography system for routine applications. With a small footprint and a metal-free configuration in PEEK, it allows for all applications in food and environmental characterization.
PQ LC compact can be upgraded with a UV/Vis detector.

Features:
- Metal-free system for flexible adaption to various applications
- Compact design for limited lab space
- Easy handling for routine applications in LC-ICP-MS

PQ LC

The PQ LC is the versatile system offering various options for a flexible configuration. It is available in stainless steel and PEEK. The basic system can be upgraded with a cooling and heating option for the sample-introduction system, a column oven for temperature stabilized column environment, and a UV/Vis detector for monitoring the chromatographic separation.

Features:
- Flexible system in stainless steel or PEEK
- Upgrade to a fully equipped HPLC system
- Easy handling for routine and advanced applications in LC-ICP-MS

PQ IC

The PQ IC system is the ion chromatography solution for routine applications that avoids matrix effects. In addition to the basic system available in PEEK it includes the ion chromatography module for reduction of background conductivity of the solvents.
The system can be further upgraded with a UV/Vis detector.

Features:
- Inert system in PEEK for flexible adaption to various applications
- Matrix suppression for reliable and precise detection
- Easy handling for routine applications in IC-ICP-MS

PQ LC series covering a standard LC system, a compact version and an IC solution

Reasons for Choosing PlasmaQuant MS and PQ LC

01

Simultaneous identification of major and trace species

- Reliable identification of trace species down to ultra-low detection limits thanks to outstanding sensitivity of the PlasmaQuant MS
- Wide linear operation range in all-digital detection (ADD[10] – ten orders of linear dynamic range)

02

High sample throughput and minimum downtime

- Quick and easy coupling of PlasmaQuant MS and PQ LC and short warm-up times
- Short analysis times thanks to high sensitivity and exceptional long-term robustness
- Flexible automation and connection of upgrade modules
- Ideal for unattended operation around the clock
- Low maintenance requirements

03

Simple handling and smooth workflows

- Intuitive handling and colored status indicator
- Straightforward access to all control parameters
- Fast change of applications thanks to the modular design of the PQ LC
- Seamless software connection to ICP-MS
- Easy to use with interactive and user-friendly software interface
- Automatic safety check, alarm function, and safety shutdown

04

Flexible configuration and individual adaptation to your needs

- Various upgrade modules, such as temperature control for the sample injector, column oven, or UV/Vis detector
- Quick and easy connection to ICP-MS for fast change of applications
- Flexible automation with variable vial racks and adaptors for microtiter plates
- Fits to smallest footprint, including autosampler and solvent tray

Carefree Solutions

A flexible software package helps you tackle all your tasks.

Chromatography Data System – CDS

The LC system and components are controlled by the Clarity Chromatography Software (DataApex). It also connects to the ASpect MS ICP-MS instrument software. Once the ICP-MS is running Clarity takes all control and processes all data handling. Constant status updates ensure seamless communication with a shutdown of all components in case of failure events. The Clarity software package also supports other manufacturers' LC systems for increased flexibility.

FDA 21 CFR Part 11 compliance

The Clarity Chromatography Software provides a variety of tools to configure the chromatography station to comply with the requirements of the FDA 21 CFR Part 11, including:

- Software Validation
- Installation and Operational Qualification
- Creation of user profiles and definition of individual user accounts
- Electronic Signatures and Audit Trail
- History of all methods and calibrations as part of chromatogram files
- System Suitability Test
- Method performance and system consistency monitoring
- Printed reports

Your benefits
- Seamless control of all components
- Flexible data handling with full CDS capability
- Higher flexibility through support of various HPLC systems
- Full support for GxP practices

Solutions for Your Needs

LC-ICP-MS provides a simple yet highly sensitive method for identifying and characterizing element species in diverse fields of application.

The PQ LC systems coupled to the PlasmaQuant MS offer excellent precision and accuracy with well-defined and clearly separated peaks. The combination of excellent chromatography and the high sensitivity of the PlasmaQuant MS allows for sub parts per trillion (<1 ng/kg) limits of detection for arsenic or chromium species.

Environmental
In environmental monitoring, various sample matrices, sources and parameters are investigated. Effluents and emission sources can contaminate the environment with various pollutants that undergo complex reactions and form new species or compounds. These can enter the food chain and pose a potential risk to organisms. But natural sources can also be a ause of contaminations in water, soil, or air. Monitoring as well as evaluating and investigating sources and natural cycles is thus crucial to health.

Food and Agriculture
LC-ICP-MS enables an easy identification of toxic and non-toxic element species in food and agricultural products, for example, in rice, fish, and beverages. Arsenic in particular occurs in food products in different species with varying toxicities. The inorganic trivalent arsenic (AsIII) and pentavalent arsenic (AsV), for example, are the most toxic arsenic forms, whereas the organic monomethyl arsenic (MMA) and dimethyl arsenic (DMA) have significantly reduced toxicities and arsenobetaine (AsB) is not toxic at all.

Table 1: Example for As species concentration in apple juice samples

	Concentration (µg/L)				
	AsIII	DMA	MMA	AsV	Total As
Juice 1	0.297	0.088	0.010	1.550	1.945
*Juice 2	0.052	0.037	0.007	0.102	0.198
Juice 3	0.186	0.084	0.007	0.430	0.707
Juice 4	1.172	0.220	0.006	0.197	1.595
Juice 5	0.331	0.051	0.000	1.847	2.229

* Juice 2 was an organically grown product and had the lowest concentration of arsenic. The total As content in all five juices did not exceed 3 µg/L.

Consumer goods

Consumer goods shape our daily lives. Textiles, plastics, and leather, as well as toys and other products for children, undergo complex production steps, including chemical reactions or treatment with chemicals. Contact with skin or oral uptake can lead to severe intoxication if toxic elements or species are present in the final product. The safety of toys and children's products is regulated within standards, such as the European Standard EN 71. This norm, for example, describes material categories, migration methods and limits to be monitored. In addition to toxic elements, such as As, Cd, Pb, and Sb, especially chromium is under observation since its hexavalent form (CrVI) is highly toxic to humans. LC-ICP-MS provides a simple yet highly reliable method for monitoring chromium species as well as other harmful components in consumer goods.
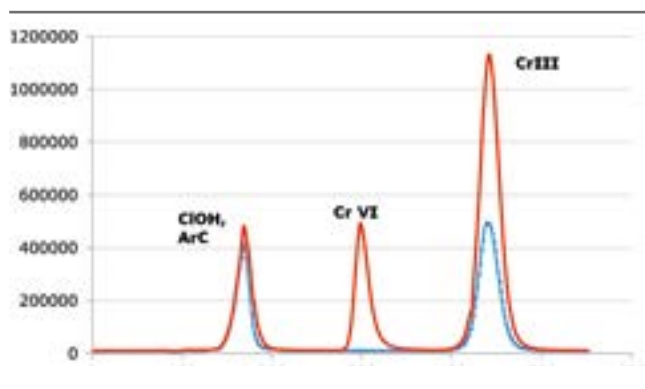

Fig. 1 Chromatograms showing an addition of 0.005 mg/kg (red) of Cr(III) and Cr(VI) on a toy sample (blue)

Figure 1 displays the overlaid chromatograms for a toy paint sample and the sample spiked with 0.1 µg/L (0.005 mg/kg) of Cr(III) and Cr(VI). The spike concentration represents the lowest limit for Cr(VI) out of the three categories.

Solutions for Your Needs

LC-ICP-MS provides a simple yet highly sensitive method for identifying and characterizing element species in diverse fields of application.

## Clinical and Pharma Applications

As toxicity, mobility, and bioavailability can vary significantly within the elemental species in which an element occurs, reporting of the total concentrations only can often be misleading. The monitoring of arsenic species in urine, for example, can greatly assist with risk-based toxicity assessments when elevated arsenic levels in urine are detected. Speciation analysis makes it easy to distinguish between harmful arsenic compounds that may come from contaminated working environments or non-toxic organic arsenic compounds caused by consumption of seafood.

An example for the speciation of arsenic in urine is shown in Table 2. The urine reference materials ClinCheck Urine Control Level I and II (Recipe, Germany) were characterized by LC-ICP-MS.

Table 2: Results for characterization of reference material

	ClinCheck level I [µg/L]		ClinCheck level II [µg/L]	
	Control range	Measured value	Control range	Measured value
AsB	12.6 – 21.0	16.4	23.0 – 34.6	27.9
As III	1.44 – 3.84	2.6	7.05 – 11.8	9.4
DMA	5.88 – 13.7	8.9	32.6 – 54.3	41.5
MMA	1.50 – 3.50	2.3	5.03 – 8.38	6.9
As V	2.10 – 4.90	3.6	18.9 – 31.5	25.8

With detection limits in the low ng/L range for the individual species in urine the LC-ICP-MS is an ideal tool for risk assessment in the manufacturing industry.
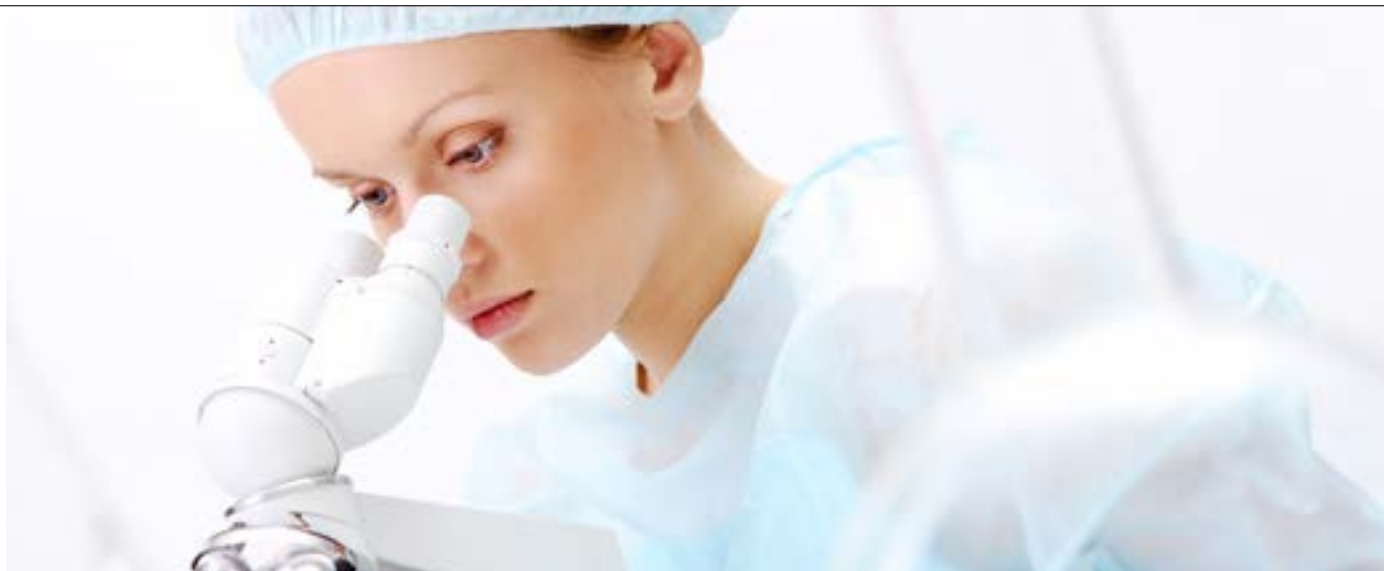
Academic & Research

In speciation analysis, the monitoring, as well as evaluation and investigation of sources, natural cycles, and metabolic pathways of element species is crucial for understanding their effect on organisms and or enabling a reliable risk assessment concerning toxicities.

In food analysis, for example, the routinely identified arsenic species are just a minority of more than 250 known species. Compounds from groups such as arsenolipids and arsenosugars that are widely found in marine organisms are a highly noticed field of research for learning more about their chemistry and metabolic pathways, as well as potential toxicity.

Another field of research supported by LC-ICP-MS is gadolinium complexes used in gadolinium-based magnetic resonance imaging (MRI) contrast agents. Some of these compounds have been found to increase the risk of nephrogenic systemic fibrosis with patients with chronic or severe kidney disease and acute kidney injury. For example, Gadoteric acid is considered harmless, whereas Gadopentetic acid should be strictly avoided for patients with kidney disease (Figure 2). Therefore, a clear understanding of the structure of the gadolinium-based agent is absolutely crucial. LC-ICP-MS is a tool to easily separate and identify the individual gadolinium compounds.
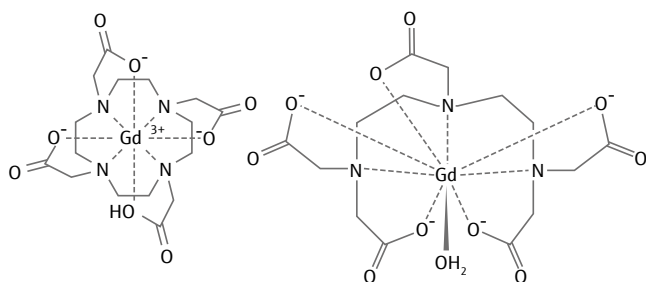
Other fields of application

In addition to the identification of different compounds and the chemical state of an element, other parameters are used to separate species, for example, the size of molecules. This is used in size exclusion chromatography. In combination with ICP-MS, it offers complementary information, such as the nature of the central atom or elements bound to molecular structures.

Figure 2 Chemical structure of gadoteric acid (Gadolinium-DOTA) (left) and Gadopentetic acid (right)

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