Product Specifications

Aqueous elemental speciation analysis is enabled easily by coupling HPLC to the open architecture of the XSERIES 2 ICP-MS sample introduction system. The Thermo Scientific PlasmaLab software and external trigger card facilities enable automated HPLC accessory control using bi-directional communications and intelligent peak integration facilities.

XSERIES 2 ICP-MS:

Coupling the Thermo Scientific XSERIES 2 Quadrupole ICP-MS with High Performance Liquid Chromatography for Elemental Speciation Analysis

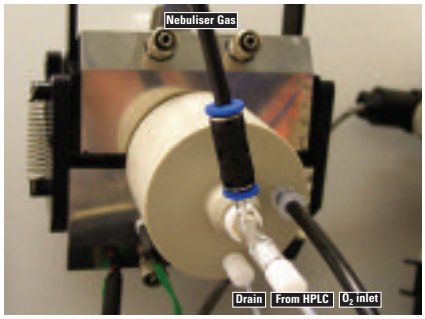
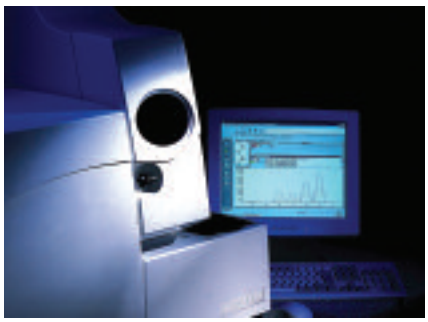


Figure 2: XSERIES 2 sample introduction and addition of oxygen to the plasma using the Organics Kit



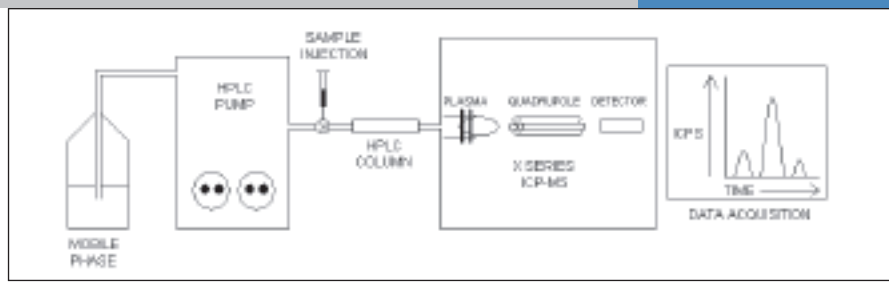


Figure 1: Block diagram of HPLC-ICP-MS setup

Introduction

ICP-MS is a rapid and highly sensitive multi-element analytical technique, used routinely for quantification of total analyte concentrations in environmental, clinical, geological, semi-conductor, nuclear and speciality chemical matrices. However, the measurement of total element concentrations provides no information about the chemical species of the elements in the sample. There is increasing interest in elemental speciation analysis because each elemental species exhibits unique physical properties such as solubility, boiling point, toxicity and metabolic pathways in living organisms.

An effective analytical approach to enable quantification of elemental species in liquid samples is to couple High Performance Liquid Chromatography (HPLC) with ICP-MS instrumentation and this is achieved by connecting the outlet from the HPLC directly to the nebuliser of the ICP-MS (Figure 1).

The two techniques are readily compatible because the liquid HPLC sample is delivered to the ICP-MS nebuliser in a flow of liquid mobile phase, which is pumped at a typical flow rate of 1.0-2.0 ml min^{-1} and element specific detection is provided by the ICP-MS detector. The HPLC system facilitates sample introduction and separation of dissolved inorganic ions, organometallic compounds, protein-metal complexes or other elemental species in accordance with their affinity for a mobile and stationary phase component and separated compounds are pumped to the nebuliser for introduction to the ICP-MS. The sample is processed in the plasma and concentrations of the elemental species constituents are quantified through the acquisition of transient time resolved signals.

HPLC-ICP-MS enables on-line separation of species in liquid samples with a high degree of specificity, and low detection limits are achieved by using ICP-MS analyte detection. The technique is increasingly favoured for elemental speciation analysis in both environmental and biological samples to assess direct toxicological risks to biota and to evaluate the extent of bio-transformations in living organisms, which may modify the potential for toxicity. Some example applications for this technique include the separation of

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Cr(VI) and Cr(III) species in contaminated waters and leachates and the separation of selected as species including arsenate, arsenite, arsenobetaine and arsenosugars in marine organisms and human foods.

Rapidly interchangeable HPLC-ICP-MS and ICP-MS coupling:

HPLC-ICP-MS coupling is easily achieved when using the XSERIES 2 ICP-MS because the open architecture sample introduction system (Figure 2) permits easy access to the ICP-MS nebuliser and allows the user to interchange rapidly and simply between ICP-MS and HPLC-ICP-MS configurations. The outlet of the chromatographic column is connected to the standard concentric nebuliser of the XSERIES 2 using PEEK tubing and an Ezyfit connector supplied in the Thermo Scientific HPLC-ICP-MS Coupling Pack (P/N 4600485). However, the Burgener MiraMist nebuliser (P/N 4600356) is recommended when using mobile phases containing 0.1-0.2 % total dissolved solids.

Mobile phases with organic solvent components may require the addition of oxygen to the plasma to prevent carbon deposits from blocking the Sampler and Skimmer cones and a Pt tipped sampler cone may be required to prevent rapid degradation of the cone orifice. (P/Ns 1600335 and 3201101 for Pt tipped Xi and HPI Sampler cones respectively). Oxygen can be supplied to the plasma through the ICP-MS nebuliser using a T-Piece adapter (P/N 1600374) or directly into an XSERIES 2 inert polypropylene spray chamber supplied with the XSERIES 2 Organics Kit (P/N 4600298) as shown in Figure 2.

Automated bi-directional accessory control for enhanced productivity

The XSERIES 2 PlasmaLab software will control any third party accessories which can give and/or receive contact closure signals or specific voltage change signals to allow a fully automated and productivity enhancing 'rack and run' analysis approach. Examples of such accessories include the Thermo Scientific Surveyor™ HPLC pump and autosampler (P/Ns 1600621 and 1600622 respectively). Third party accessory control is readily achieved by configuring the external trigger card in the XSERIES 2 ICP-MS PC to enable bi-directional communications between PlasmaLab and the required accessories. The external trigger card is supplied complete with all electrical connections in the HPLC-ICP-MS Coupling Pack (P/N 4600485). The resultant bi-directional communications provide a failsafe operation for the HPLC-ICP-MS instrumentation. For example, the HPLC pump and auto sampler can be triggered to abort the analytical run in the event of a hardware or software error to prevent the loss of precious samples and mobile phase.

Third party accessory functions are harmonised effectively with XSERIES 2 ICP-MS data acquisition using PlasmaLab Accessory Control Language (ACL) scripts. These scripts provide a flexible and readily adaptable approach to co-ordinate XSERIES 2 ICP-MS 'acquisition commands' and 'external trigger' commands. A typical PlasmaLab ACL script used to control a Finnigan HPLC is presented in Figure 3.

Flexible data acquisition and processing for Transient TRA

Transient TRA data can be acquired following analyte selection and definition of the required Acquisition Parameters within the Transient TRA experiment and analytical templates can be customised and stored within PlasmaLab for routine speciation analysis. The Acquisition Parameters tab allows individual analyte dwell times to be defined and the Sample List tab provides a simple format for defining analytical run times and sequencing automated sample analysis. Two modes of internal standardisation may also be used when acquiring Transient TRA data within the XSERIES 2 PlasmaLab software. Timeslice Internal Standards facility can be used to correct for changes in nebulisation efficiency when using gradient elution HPLC through post column introduction of internal standards and Transient TRA Internal Standards facility allows transient peaks to be quantified as internal standards for instrumental drift correction.

PlasmaLab Transient TRA timeslice data is automatically stored in the Numerical Results tab of the PlasmaLab software and the associated chromatographic data is plotted automatically in the Acquisition Parameters tab. An intelligent peak searching facility allows integration of the raw data within the PlasmaLab software and chromatographic peaks can be integrated and identified in accordance with user defined Peak Search windows. These search windows are superimposed over the raw analytical data to allow the user to check and re-integrate the analytical data as required (Figure 4).

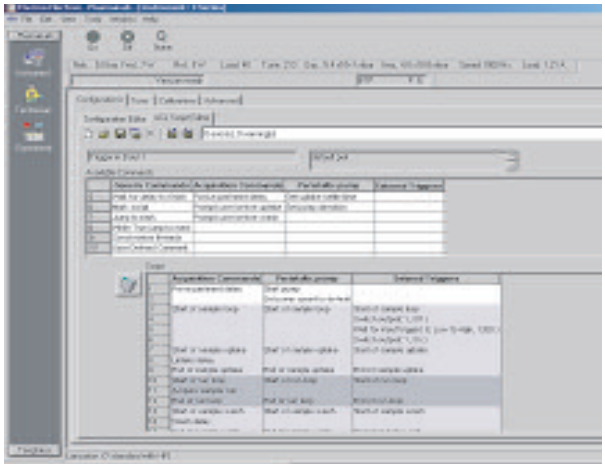

Figure 3: PlasmaLab ACL script for HPLC accessory control

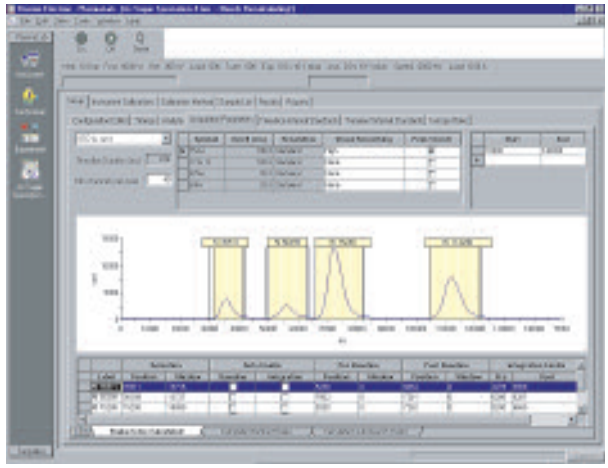

Figure 4: PlasmaLab acquisition parameters showing a chromatogram for As speciation

The Numerical Results tab automatically displays integrated counts per second (ICPS) for transient peaks following assignment of the peak integration parameters and unknown analyte concentrations can be quantified in PlasmaLab using fully quantitative calibration methods. Fully quantitative concentration data is displayed in the Numerical Results tab and some example calibration data is shown in Figure 5.

Reports

The XSERIES 2 PlasmaLab software provides a flexible approach towards data reporting and automatically presents transient TRA concentrations, integrated counts per peak and raw timeslice TRA data. Analytical results are displayed and printed in XML format to allow integration with LIMS systems and third party software packages and data can also be exported easily in CSV format if required.

Conclusions

Elemental speciation analysis is readily achieved by coupling HPLC systems such as the Surveyor to the XSERIES 2 ICP-MS. The open architecture sample introduction system of the XSERIES 2 facilitates rapid and simple interchangeability between ICP-MS and HPLC-ICP-MS configurations and both aqueous and organic mobile phases can be easily utilised for chromatographic separations. The XSERIES 2 PlasmaLab software enables automated control of HPLC accessories using bi-directional communication and flexible chromatographic peak integration facilities to enhance productivity and provide a routine analytical solution for elemental speciation.

Features

- Open architecture of XSERIES 2 ICP-MS for rapid HPLC-ICP-MS coupling.
- Flexible control of HPLC accessories using bi-directional communications.
- Integrated software facilities for chromatographic peak integration.
- Two internal standardisation modes to enable automated HPLC gradient drift correction (Timeslice Internal Standards) and monitoring of instrumental drift (Transient Internal Standards).
- Flexible reporting for raw timeslice and integrated peak data.

Parts List	P/N
HPLC-ICP-MS Coupling Pack -PEEK Tubing (x i.d) (2.0m) -Ezyfit Connector -Advantech PCI Trigger Card -7/02 Electrical Wire (2.0m) -37 Pin D-Type Male Connector -Peek T-piece (1/16")	4600485
Surveyor HPLC Pump	1600621
Surveyor HPLC Autosampler	1600622
Burgener MiraMist Nebuliser	4600356
4mm Nylon Tee-Piece	1600374
XSERIES 2 Organics Kit	4600298
Pt tipped Xi Sampler Cone	1600335
Pt tipped HPI Sampler Cone	3200262

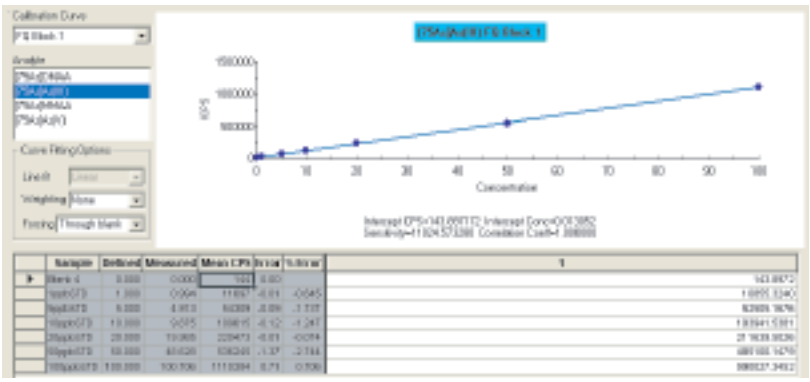

Figure 5: Fully quantitative calibration for As(III) using integrated PlasmaLab Transient TRA data

Plasma Capabilities from Thermo Fisher Scientific

The use of an Inductively Coupled Plasma source (ICP) is the accepted and most powerful technique for the analysis and quantification of trace elements in both solid and liquid samples. Its applications range from routine environmental analyses to the materials industry, geological applications to clinical research and from the food industry to the semiconductor industry.

Thermo Fisher Scientific is the only instrument manufacturer to offer the full range of Inductively Coupled Plasma Spectrometers (ICP, Quadrupole and Sector ICP-MS) to satisfy every aspect of plasma spectrometry from routine to highly demanding research applications.

Develop your lab from the easy-to-use iCAP ICP to the high performance XSERIES 2 Quadrupole ICP-MS and up to the ultra-sophisticated ELEMENT2 and NEPTUNE Sector ICP-MS instruments. Each instrument combines leading-edge technology, fit for purpose and affordability with a tradition of quality, longevity, accuracy and ease of use.

Thermo Scientific iCAP ICP

Thermo Scientific XSERIES 2 ICP-MS

Thermo Scientific ELEMENT2 HR-ICP-MS

Thermo Scientific NEPTUNE Multi-collector ICP-MS

Thermo Fisher Scientific (Bremen) GmbH is certified DIN EN ISO 9001:2000

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Africa +43 1 333 5034 127
Australia +61 2 8844 9500
Austria +43 1 333 50340
Belgium +32 2 482 30 30
Canada +1 800 530 8447
China +86 10 5850 3588
Denmark +45 70 23 62 60
Europe-Other +43 1 333 5034 127
France +33 1 60 92 48 00
Germany +49 6103 408 1014
India +91 22 6742 9434
Italy +39 02 950 591
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Sweden/Norway/Finland +46 8 556 468 00
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