Technical Features of the ICP-MS Plasma Chromatographic Software

Technique/Technology

Inductively Coupled Plasma Mass Spectrometry

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Abstract

The new Plasma Chrom software for the 7500 Inductively Coupled Plasma Mass Spectrometry ChemStation integrates chromatographic separation with inductively coupled plasma mass spectrometry detection. The combination makes speciation measurement a routine process.

Introduction

Trace element speciation measurement is one of the fastest growing areas in analytical chemistry. Chromatography coupled to inductively coupled plasma mass spectrometry (ICP-MS) is used increasingly to meet the needs of analysts around the world. The speed, sensitivity, and multi-element capability of the Agilent 7500 Series ICP-MS makes it the ideal detector for all chromatographic techniques including liquid chromatography (LC), gas chromatography (GC) and column electrophoresis (CE). Now, Plasma Chromatographic software (Plasma Chrom), from Agilent Technologies, provides seamless integration of the 7500 Series ICP-MS with chromatography instrumentation. Together, the software and hardware bring speciation measurement into the routine laboratory environment.

Plasma Chrom users can now perform fully automated, real time data analysis using chromatography ICP-MS. As a fully integrated component of the 7500 ICP-MS ChemStation software, Plasma Chrom features comprehensive data handling capabilities including powerful new integration, calibration, and compound or species identification routines.

Total System Integration

Plasma Chrom is based upon Agilent Technologies' industry standard GC/MS chromatography software and is fully integrated into the 7500 Series ICP-MS ChemStation software suite, allowing real-time chromatographic data analysis. In fact, the Agilent 7500 can perform automated analysis with any chromatographic system capable of sending an external start signal. Sample sequences can be created within the 7500 ChemStation or downloaded via a LAN connection. The software automatically performs calibration, sample analysis, and real time data reporting. Plasma Chrom provides users with full sample sequence editing, including the capability of inserting rush samples. Real time QC, such as retention time recalibration and the use of qualifier ions to ensure analytical accuracy is also fully supported.

Unrivaled Data Analysis Capability

Plasma Chrom provides for complete flexibility in data analysis including four different modes of peak integration:

- Auto-integration
- ChemStation integration
- Real time integration
- Manual integration

Auto-integration automatically sets all of the pertinent integration parameters, such as integrator sensitivity and peak smoothing criteria, based upon the current chromatogram. Alternatively, users can define up to 19 custom integration parameters. Once the integration criteria are selected, Plasma Chrom will draw the resultant chromatograms in real time indicating the identity, retention times and baselines of each detected peak (Figure 1).

There are five different calibration options available for peak quantification (Figure 2):

- Average of the response factors
- Linear regression
- Linear regression through zero
- Quadratic regression
- Quadratic regression through zero
- Weighting factors can also be used for improving the calibration accuracy over wide concentration ranges

In addition, Plasma Chrom supports the use of independent internal standards to correct for both changes in chromatographic and plasma conditions. And, since the ICP-MS Chromatographic software is seamlessly integrated, all calibrations, QC, and integration parameters are saved in a normal ICP-MS method file.

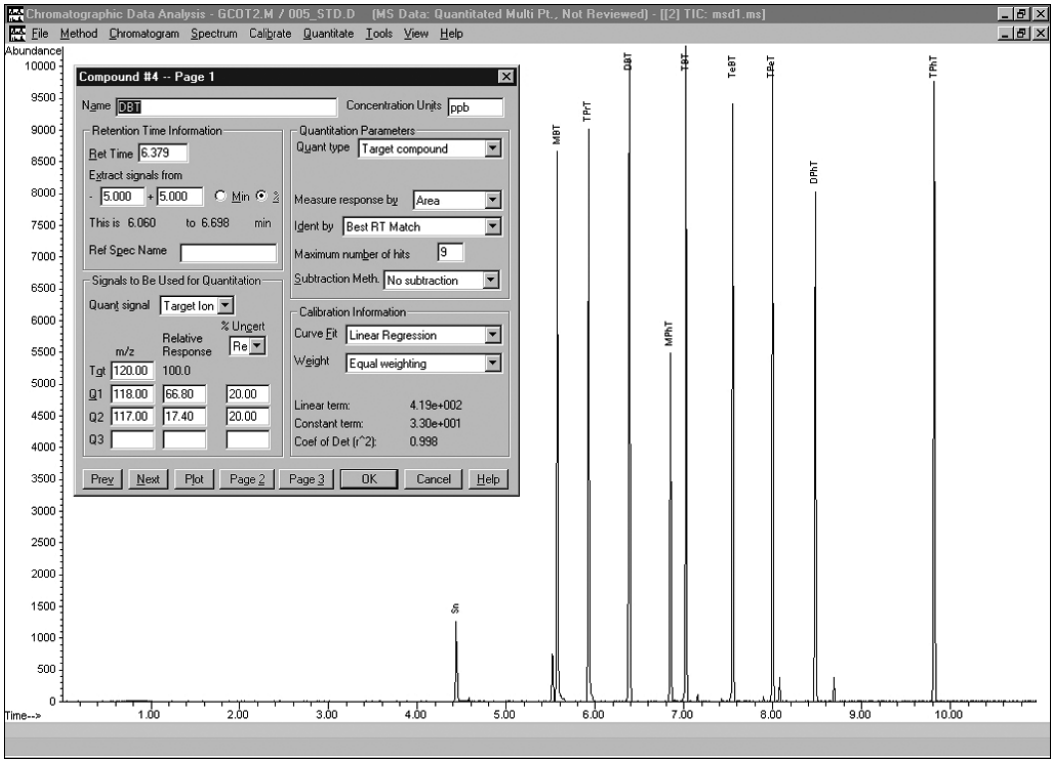

Figure 1: Plasma Chrom software window showing organotin chromatogram by GC-ICP-MS and interactive calibration setup.

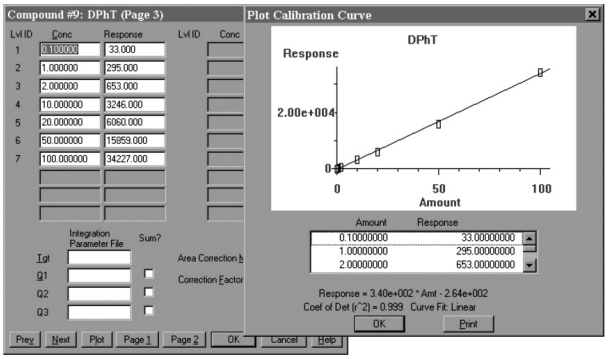

Figure 2: GC-ICP-MS Calibration Table and Calibration Plot.

Real Time QA/QC Capability

Plasma Chrom now features several powerful new real-time QA/QC protocols for chromatograph ICP-MS users. The automated identification and analysis of qualifier ions ensures accurate quantification for every sample.

The use of qualifier ions for QA/QC (Figure 3) is based upon the naturally occurring elemental isotope ratios. For any given analyte, one isotope is used as a quantitative mass and up to three other isotopes of the same element can be selected as qualifier ions. During real time data analysis, the isotopic ratio between the quantitative mass and the qualifier mass(es) are evaluated to ensure that the characteristic isotopic "fingerprint" for the analyte is correct. In this way, the use of qualifier ions is uniquely suited to identifying potential interferences that could otherwise result in false positive results.

Plasma Chromatography Software Features Include:

- Powerful graphics manipulation and display features
- Advanced integration routines including peak search, shoulder detection, and peak smoothing
- Range of quantitative features including weighting and internal standardization
- Automated qualifier ion identification for confirmation of target analyte
- Automatic synchronization of chromatograph and Agilent 7500 data acquisition
- Fully automated chromatography ICP-MS analysis with real time data analysis and output
- Real time QC with retention time calibration
- Full sample sequence editing capability, including insertion of rush samples

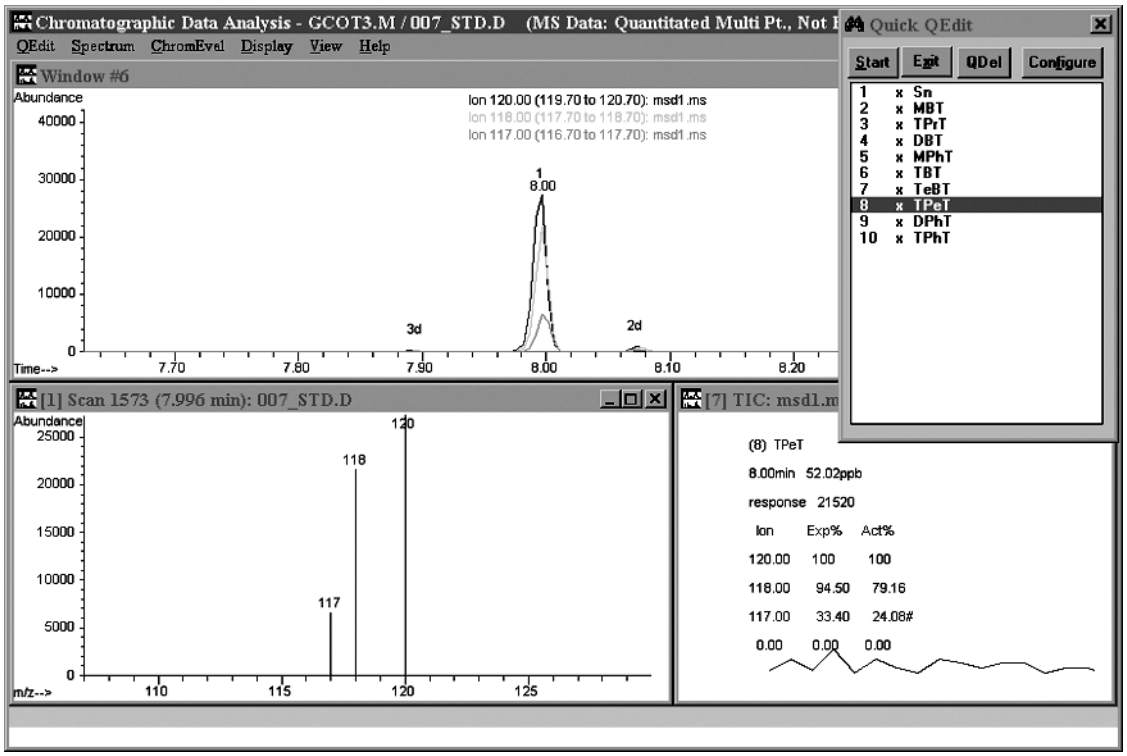

Figure 3. Plasma Chrom software window depicting manual quantitation review mode with qualifier ion ratios.

Plasma Chrom also supports retention time recalibration. This feature provides facilities for automatically resetting the calibration table and locking in new retention time or response factor values. This extremely useful feature corrects for any time variations, such as changes in chromatographic solvent strength, which may affect the analytical response. Retention times and response factors can be updated with a weighted average of the initial and current measured value, or by simply replacing the original value with that obtained in the current sample (Figure 4).

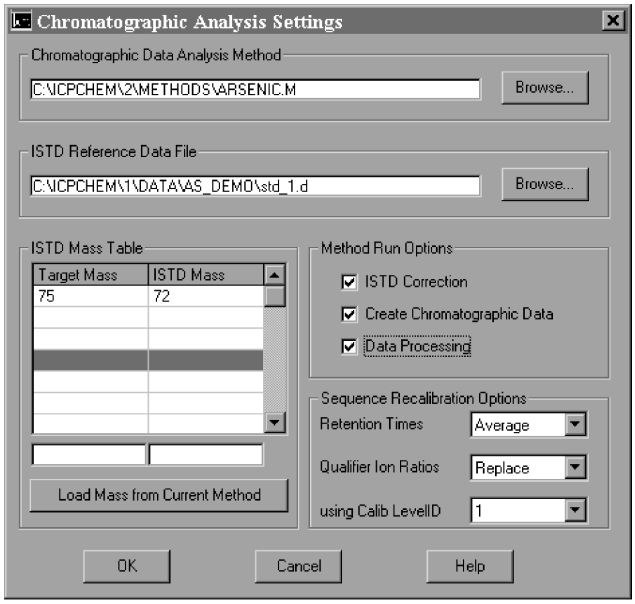

Figure 4. Chromatographic Settings Window linking Plasma Chrom Data Analysis to ICP-MS Data Acquisition. Note selection of plasma internal standard and sequence recalibration options.

Powerful Graphics Manipulation and Custom Reporting

Once the data has been collected, Plasma Chrom brings it all together with the most comprehensive graphics and editing package available featuring up to 30 separate windows for spectral displays. Mass spectra can be averaged together, added, subtracted, have the background spectra subtracted and much more! The results of these data manipulations are available in both graphical and tabular format. In addition, any of these graphical windows can be annotated for future use. In short, Plasma Chrom provides all of the flexibility and functionality one would expect from Agilent Technologies – the world leader in chromatographic and ICP-MS instrumentation.

For More Information

For more information on our products and services, you can visit our site on the World Wide Web at: **http://www.agilent.com/chem.**

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