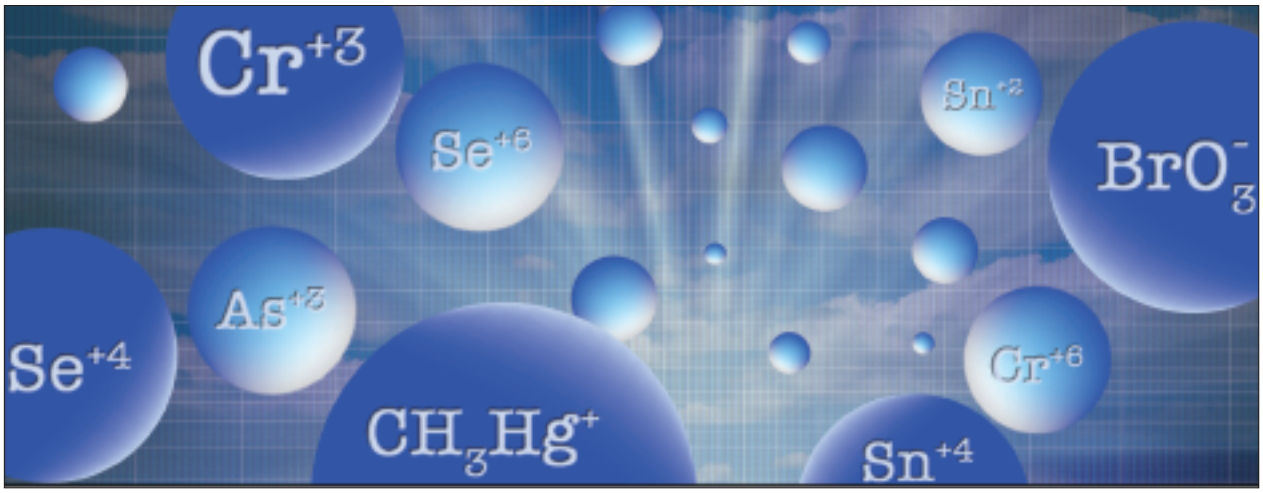
Chromera Software

The Right Tool for the Right Answer



The 21st century is providing some exciting new challenges for the analytical chemist that span traditional boundaries and conventional thinking on how analytical chemistry measurements are performed. In many cases, it is no longer a question of answering "how much" is in the sample but "what forms" of the species are present; for example, not how much arsenic, but how much dimethylarsinic acid is present. The correct answer is crucial as many inorganic forms are extremely toxic, while most other forms are not. The answer affects environmental impact assessments and guides remedial activities.

Why speciate?

Toxicity, bioavailability, metabolism and environmental mobility of elements are dependent on their form or species. Total element determination alone does not provide all the information. For example:

- Inorganic arsenic species are toxic. Organic species such as arsenobetaine are non-toxic.
- Chromium(VI) is more toxic while chromium(III) is an essential nutrient.
- Selenium species originate from different sources.

Environmental remediation depends on the species present.

Key Benefits

- Fully-integrated system with seamless operation
- Proven multielement analytical methodologies
- Efficient workflow tools
- Extensive reporting capabilities
- Complete control of all system components from a single PC
- Single source for instrumentation, expertise, installation, service and training

PerkinElmer® precisely.

Being a leader in separation technologies as well as the premier supplier of element-specific detection systems, PerkinElmer once again has recognized the needs of the analytical community. Need- and productivity-driven systems have been developed that seamlessly couple HPLC elemental separation and ultra-high sensitivity detection with the PerkinElmer® SCIEX™ ELAN® ICP-MS instruments into a fully integrated package called Chromera™ software.

Chromera software sets the standard

Due to our close working relationship with our customers, we recognized they were faced with the challenge of speciation measurements. Our discussions led to a clear understanding of their requirements for an integrated speciation measurement system including:

- Proven analytical methodologies
- Efficient workflow tools
- Extensive reporting capabilities
- Complete integrated control of all system components from a single PC
- Single source for instrumentation, expertise, installation, service and training

An application-specific tool for speciation analysis

Chromera software was designed by chemists for use in elemental speciation analysis. It presents a unified user interface that integrates and manages the ELAN ICP-MS and the Series 200 HPLC system. The tedium of having to switch between the ICP-MS and the HPLC to start the system or set up operating parameters is completely avoided. Chromera software sets a new standard for efficiency and optimized workflow.

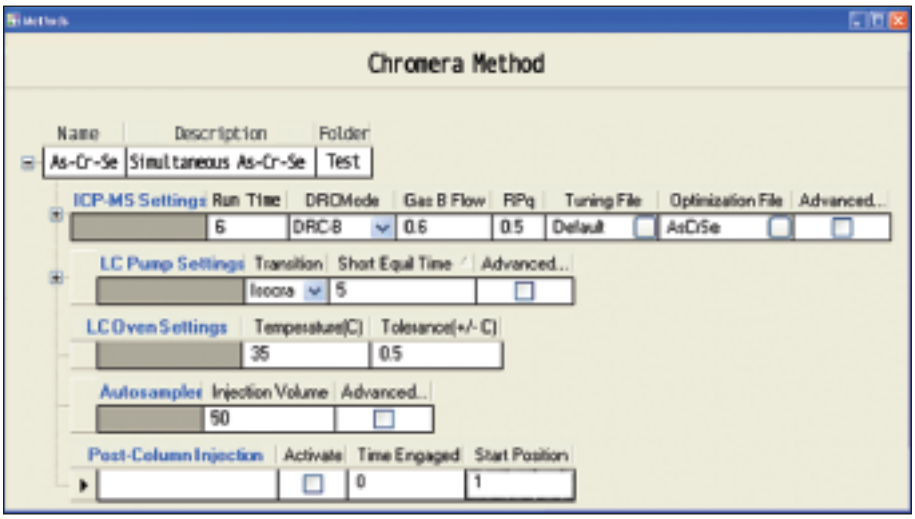


Figure 1. All analytical parameters for a complete speciation analysis are entered in a single window, including species labels, ICP-MS hardware and analytical settings, and HPLC settings.

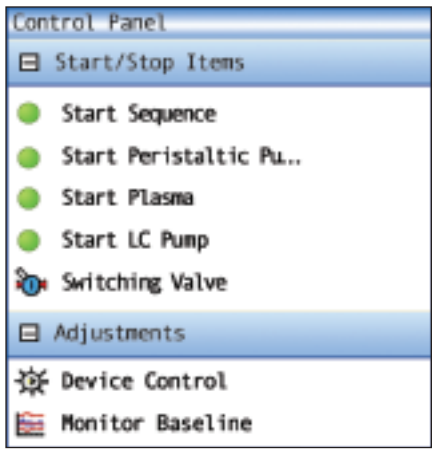


Figure 2. Control Panel gives direct control of hardware.

This type of analytical chemistry is broadly termed "elemental speciation". The IUPAC defines this as:

Speciation of an element; speciation. Distribution of an element amongst defined chemical species in a system

Speciation analysis. Analytical chemistry: analytical activities of identifying and/or measuring the quantities of one or more individual chemical species in a sample

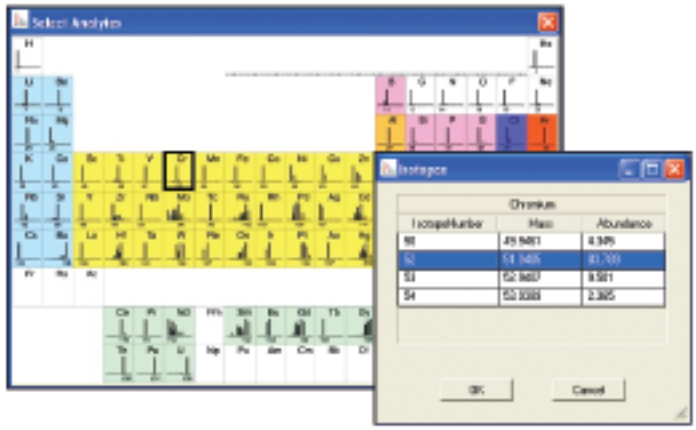


Figure 3. Isotope selection is facilitated by the availability of a pop-up periodic table.

Method development made simple

Chromera software visually puts method information pertaining to the ELAN ICP-MS and Series 200 HPLC at your fingertips. The interface contains all the information you want, visible or in the background – it is your decision.

Instrument status display

During the analysis, it is important to quickly check the status of the ELAN ICP-MS and Series 200 HPLC system. Chromera software makes this easy. The status of the HPLC or ELAN ICP-MS is always available through floating status bars. There is never a need to toggle to another program, as in some competitive systems.

Control of all hardware integrated into Chromera

Typical offerings for speciation require users to separately and manually control the ICP-MS and HPLC as these systems use separate, independent, "stand-alone" components from other applications. Chromera software was designed from the start to provide integrated control of the ELAN ICP-MS as well as the Series 200 HPLC system. This means that the user has no interaction with the HPLC system once samples are loaded into the autosampler tray.

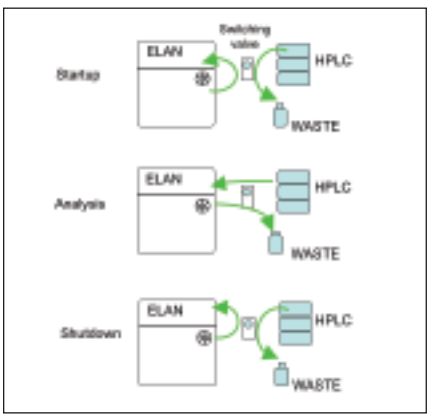


Figure 4. The automated switching valve is beneficial for HPLC column conditioning and cleaning, ELAN warm-up, optimization, and shut-down, and during a speciation analysis.

Chromera software starts and controls the entire system.

The Chromera system is unique in that it includes a controlled "by-pass" valve that integrates the HPLC and ELAN ICP-MS into a compatible system. The valve allows the user to decide which solution goes to the nebulizer: the HPLC eluent or the uptake from the ICP-MS peristaltic pump. This allows for daily optimizations of the ELAN ICP-MS, while conditioning the HPLC column. Chromera software provides automatic system shutdown capabilities in case of interlock error or at end of run.

With the by-pass valve, the column output can be directed to waste rather than entering the ELAN ICP-MS; instead, a flow of clean acid from the peristaltic pump can be pumped through the nebulizer. This is an important task if both systems are to operate correctly and reliably. The unique approach in Chromera software is to eliminate the need to make this connection manually.

The comfort of a real-time display

For reliable monitoring of analysis progress, it is essential to see data as it is acquired, rather than waiting until after the run is complete. This confidence builder has been a dream until now – Chromera software allows viewing of single or multiple curves while they are acquired with automatic real-time autoscaling. Not only can you watch the chromatography develop – you can see real-time peak identification and quantitation of your samples.

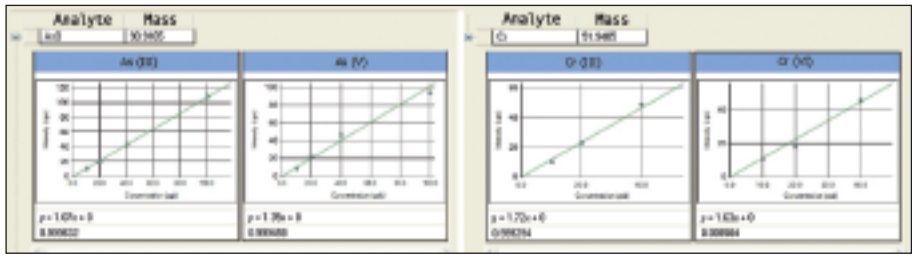


Figure 5. Calibration graphs and information for the various species can be viewed simultaneously.

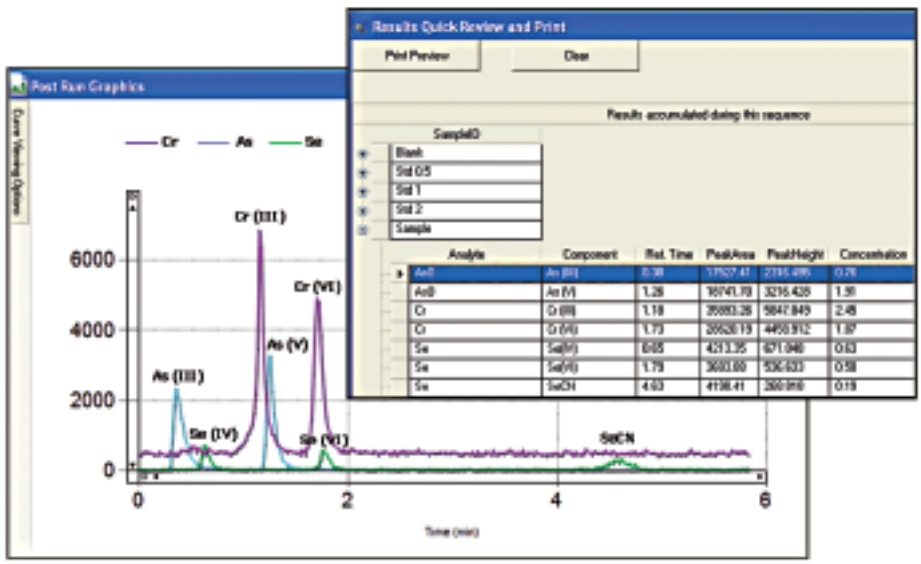


Figure 6. Post-run allows the user to adjust the axis range and display parameters, manage the printing of graphics data, perform post run calculations, control the colors used on the display and set the font and type size for titles and label text.

Getting the correct answer

The fundamental concern of every analytical measurement is to efficiently produce the best results possible. In the speciation arena, basic requirements are to precisely identify when a peak begins and ends, even in noisy data. Peak detection in Chromera software is accomplished using the proven and validated, industry-standard technology used in the PerkinElmer TotalChrom® chromatography data system for peak-detection algorithms.

The creation of species-specific calibrations is also an integral part of Chromera software. Calibration curves are always available for review, and errant standards can be identified and re-run. If necessary, questionable data can be eliminated from the calibration curve. Curves can be displayed and printed in either a single-curve detail or multi-curve summary formats.

Figure 7. Speciation analysis is accomplished with the Series 200 HPLC system performing the separation and the ELAN providing detection.

There is more: utility after the run

Chromera software fully supports post-run review and analysis of data. Adjustments can be made to the display range, font and graphics format of the report. Calculations can also be reviewed post-run and corrections implemented. These features add utility to the analysis, without re-running the sample.

Customizable

Chromera can be organized and set up to the preferences of the individual lab or user. The user-interface workspace includes the required screens for running samples and auxiliary screens are placed in the background. Screens can be "tacked" so they are always visible or "hidden". The presence of hidden screens is indicated by tabs, which, when pointed to, will cause them to reappear. For preparation of specific reports or scientific papers, data can be output in multiple formats including ASCII or XML.

Chromera software – making your life simpler

At last, a software tool that enables efficient and effective speciation measurements. Whether your challenge is routine or research, Chromera software will make your workflow and results efficient and reliable and your life easier.

Worldwide support

With over 60 years of experience and as a world leader in analytical instrumentation, PerkinElmer is the right partner for your industry. In concert with global distribution of instruments, turnkey systems, and consumables, we provide global factory-trained service and support.

PerkinElmer's OneSource® Laboratory Services provides you with a comprehensive worldwide service offering that lets you take care of business and set your sights on what matters most – results. With over 1000 factory-trained professionals serving more than 125 countries worldwide, PerkinElmer is your single source for instrument care and repair, validation services, software and hardware upgrades, education and more.

Join many of the world's leading speciation researchers in using our knowledge, products and comprehensive support. Together, we can solve your speciation needs.

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