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 elements are present. For example, “How much arsenic?” gives important information, but “How much dimethylarsinic acid is present?” is increasingly becoming more important. The correct answer is crucial as some forms of an element are toxic, while other forms are not. The answers affect health and environmental impact assessments and guide remedial activities.

**Chromera Speciation Software – The Right Tool for the Right Answer**

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.
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, while many organic forms are less- or non-toxic, such as arsenobetaine.
- Chromium(VI) is toxic, while chromium(III) is an essential nutrient.
- Selenium species originate from different sources, both natural and anthropogenic.

In many cases, health and environmental remediation depend on the species present.

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® NexION® and ELAN® ICP-MS instruments into a fully integrated package – Chromera® speciation 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 an 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

Chromera 2 incorporates many improvements based upon user feedback.

**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 PerkinElmer NexION and ELAN ICP-MS instruments and the Flexar™ and Series 200 HPLC systems. The complexity of having to switch between the ICP-MS and the HPLC to start the system or set up operating parameters is completely avoided: hardware control, methodology, and data processing are all included in Chromera, thereby setting a new standard for efficiency and optimized workflow.

![Chromera software](image)

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

![Chromera interface](image)

**Figure 1.** Chromera has a new look and feel which features environments to simply use, a tree control to quickly scroll through data, and updated Control and Status panels for more convenient interaction with the hardware. The screen in this figure shows a typical view during data acquisition while running a Sequence.

**Figure 2.** A single method now contains all analytical parameters required for speciation analysis: instrumental parameters, peak identification and detection, and calibration information.
Instrument status display

During the analysis, it is important to quickly check the status of the ICP-MS and HPLC system. Chromera software makes this easy with a customizable floating Status Panel—the user selects what parameters to display and the size of the Status Panel. There is never a need to toggle to another program—once you enter Chromera, everything is there.

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 ICP-MS as well as the HPLC system—Chromera software starts and controls the entire system.

The Chromera system is unique in that it includes a controlled switching valve that simplifies operation and decreases maintenance. 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 warming up and daily optimizations of the ICP-MS while equilibrating the HPLC column, thus decreasing the amount of time required before an analysis can begin. Chromera also provides automatic system shutdown capabilities in case of hardware problems or at the end of a run.

With the switching valve, the column eluent can be directed to waste rather than entering the ICP-MS during equilibration; instead, a flow of clean acid from the peristaltic pump can be pumped through the nebulizer. This is an important capability to maximize system uptime and limit ICP-MS maintenance.

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 the beginning and ending of peaks. Peak detection in Chromera software is accomplished using the proven and validated, industry-standard algorithms used in the PerkinElmer TotalChrom® chromatography data system.

The creation of species-specific calibrations is also an integral part of Chromera software. Calibration curves are 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 3. The Control Panel gives the user direct control over the LC and ICP-MS hardware, while the Status Panel allows the user to select which parameters to display and provides a quick, easy way to monitor the LC and ICP-MS.

Figure 4. The automated switching valve improves ease-of-use and allows more up-time for the system. While the ICP-MS is warming up and the daily optimizations are being performed, the LC column can be equilibrating, with the mobile phase being sent to waste instead of into the instrument. When the analysis starts, the LC flow is automatically sent to the ICP-MS; at the end of an analysis, the LC flow is diverted to waste.
There is more: utility after the run
Chromera software fully supports post-run review and data analysis. The Post Run environment displays the chromatograms and a scrolling list of results which updates after each sample is run. The chromatograms can be customized in a wide variety of ways to facilitate data analysis or incorporation into presentations or publications.

A new reporting package has been implemented in Chromera 2, along with a wizard to assist with report creation.

Simplified ease-of-use
To facilitate usability, work environments have been created and several wizards have been incorporated, as well as a number of other features designed to enhance the user experience, such as dictionary files, a data selector, and the ability to customize the graphical displays in a variety of ways.

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 increase the efficiency of your workflow and generate reliable results.

Figure 5. The Post Run environment allows the user to view the results of previously completed samples while a Sequence is being run; chromatograms are displayed in the upper part of the screen and quantitative results appear in the lower half. Samples can be quickly reviewed through the tree control. There are a variety of viewing options available, including overlaying chromatograms, displaying a matrix of chromatograms, and 3-D plots. In addition many of the characteristics of the upper half of the screen are user-customizable, allowing for flexibility when preparing figures for presentations or publications.

Figure 6. When opening data to display in Post Run, data selection is done through the Data Selector. To facilitate selecting the correct data, highlighting a row automatically displays the associated chromatogram for that sample.

Figure 7. Methods, Results, and Sequences can be quickly and easily transferred between systems using the Import and Export capabilities.

Figure 8. To increase productivity, two sessions can be opened at once: one for acquiring data and one for reviewing data which has been previously acquired.
The number one name in laboratory services

With over 70 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 and consumables, we provide global factory-trained service and support.

PerkinElmer’s OneSource® is the market leading laboratory asset management solution, pioneered more than a decade ago with more than 400,000 multivendor assets under its care. OneSource Laboratory Services goes beyond just maintenance and repair of instrumentation. OneSource incorporates laboratory asset management as part of our customer’s business equation – a partner with proven results in improving efficiencies, optimizing operations and providing cost certainty across the globe. The ONE you can count on.