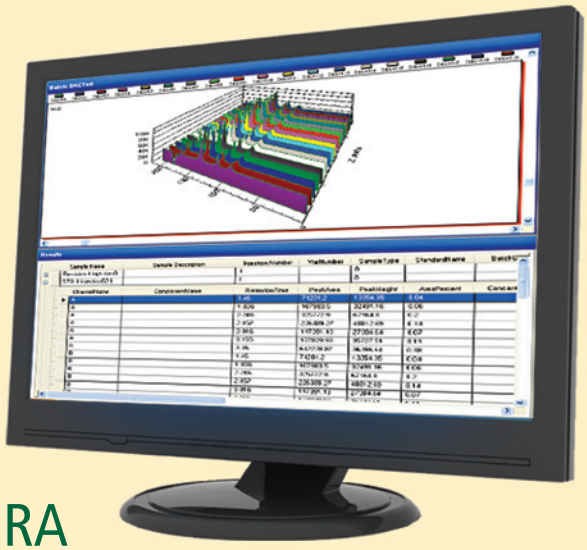
TECHNICAL NOTE

Liquid Chromatography



CHROMERA
CHROMATOGRAPHY DATA SYSTEMS

Key Benefits

- Add another dimension of confidence with spectral measurement
- Monitor progress of chromatographic separations with real-time 3-D data display
- Assure data quality by reporting peak purity and compound identification for each sample run
- Examine unknowns and annotate chromatograms using Peak Library Search function
- Confirm compound identification using Spectral Library Confirmation
- Develop more robust methods and identify co-eluting peaks by examining chromatographic peak purity
- Process spectra numerically or graphically; add, divide, subtract or perform derivative functions
- Learn and use quickly and easily – intuitive Outlook®-like user interface with functions only 1 or 2 clicks away

Verify with Confidence Using Chromera LC Photodiode Array Analysis

As the complexity of samples being analyzed using liquid chromatography increases, many chromatographers are turning to photodiode array (PDA) analysis for the added dimension of information-rich spectral analysis. Spectral data complementing chromatographic separation provides a deeper understanding of a sample, and allows a more confident identification of chromatographic peaks.

Chromera® is a powerfully-easy chromatography data system (CDS) for liquid chromatography continuing a rich and award-winning heritage of CDS design at PerkinElmer. Preserving the best functionality inherited from its predecessors, Chromera is a totally new application and 100% PerkinElmer, built from the ground up, using the latest technologies available.

Get up and running quickly. Based on an Outlook®-like user interface, Chromera's navigation provides the path of least resistance to powerful functions only 1 or 2 clicks away. It's familiar to most everyone and, therefore, very quick and easy to learn.

PerkinElmer®
For the Better

An Added Dimension of Spectral Confirmation

Spectral library matching

PDA spectra can be used to confirm the identity of chromatographic peaks. Chromera incorporates a spectral library function, allowing users to construct libraries of standard spectra taken under specific analytical conditions. These libraries can be used for automated spectral matching. A chromatogram, when collected or reprocessed, can be compared against the library – and each component's spectral profile analyzed to find the best match. The matching algorithm gives a "Hit Quality" rating, indicating the quality or confidence level in the match. This value can be used to automatically update the chromatographic method and can be included in the final analytical report, an ideal tool for laboratories working in method development.

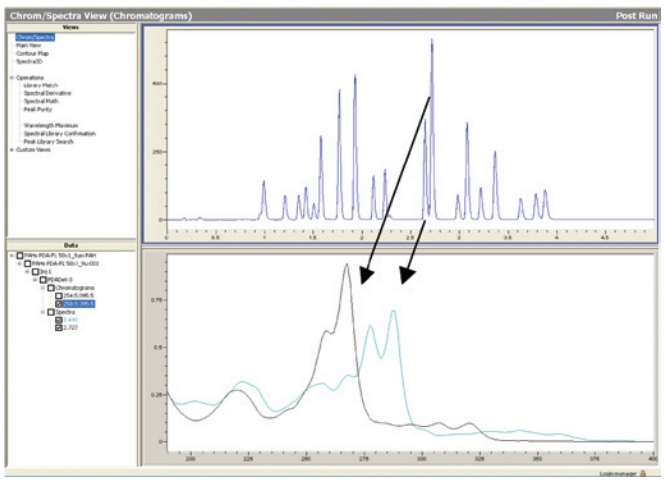
Interact with Your Data

Views

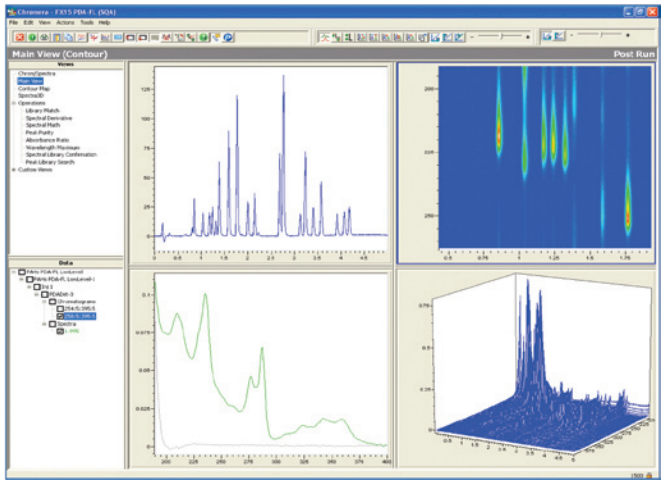
Chromera's Spectral Processing function supports a number of very convenient data views, putting valuable information about your sample and your chromatogram at your fingertips. Sweeping across chromatogram(s) or contour map(s), immediately displays corresponding spectra and chromatograms in adjacent windows, providing real-time interaction with your data.

Chromera has several built-in views but also allows the user to build their own customized view showing only what the user wants to see. Some of these views are:

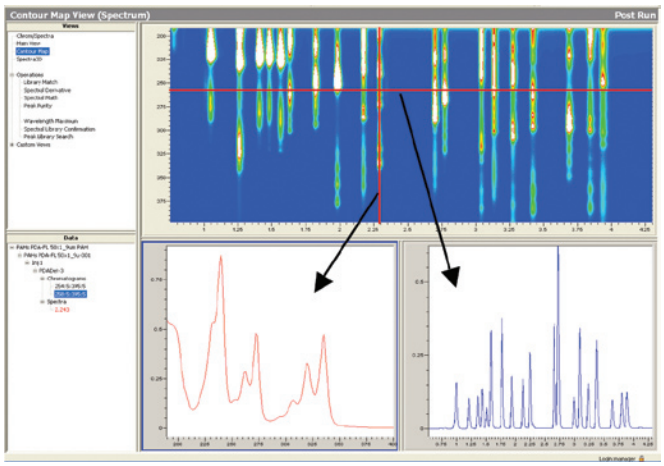
Chrom/Spectra View – View spectral peak profiles of chromatographic peaks in single or multiple chromatograms, either overlaid or stacked. Effective in quickly scanning and comparing spectral characteristics of chromatographic peaks, this view helps you rapidly identify or confirm your compounds. Build a spectral library including the apex spectra for all labeled components.



Main View – Offers the user the most all-encompassing, interactive viewing mode, including chromatograms, spectra, contour map and 3D plot.



Contour Map – The Contour Map is a powerful way to both quickly and critically evaluate your chromatography, especially if it contains unknown components. Define optimal absorbance regions, select the optimal reference wavelength or establish cursory peak purity evaluation.



Operations

Chromera's Spectral Processing application allows the user to more critically evaluate their chromatographic results. These operations can also be performed automatically, after each real-time run. Information such as peak purity, absorbance max and peak/spectral library confirmation can be reported as part of each and every report.

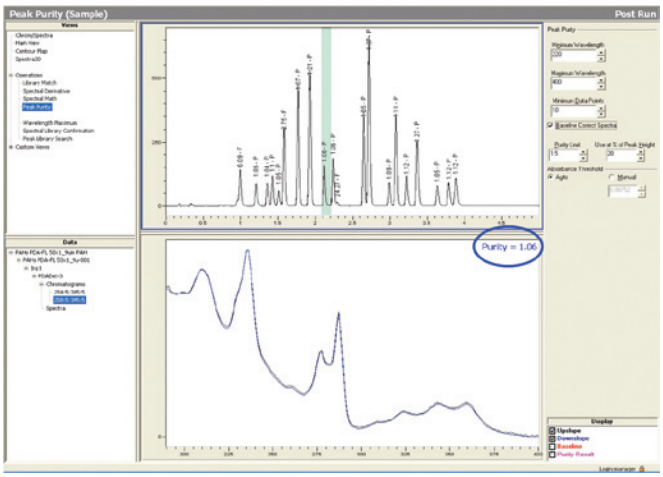
Some of the available operations include:

Library Match – Compare the spectra of the components in your chromatogram(s) to the spectra stored in one or more libraries.

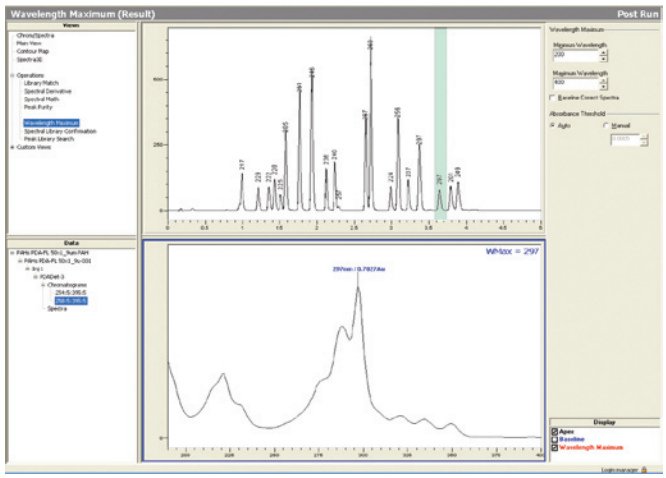
Spectral Derivative – View captured component spectra graphically as 1st through 4th order derivatives. This can be particularly helpful in discerning any spectral differences to those of other components in your chromatogram.

Spectral Math – Make graphical and numerical comparisons of any two spectra, comparing either two peaks in the chromatogram or two spectra taken at different points along a peak.

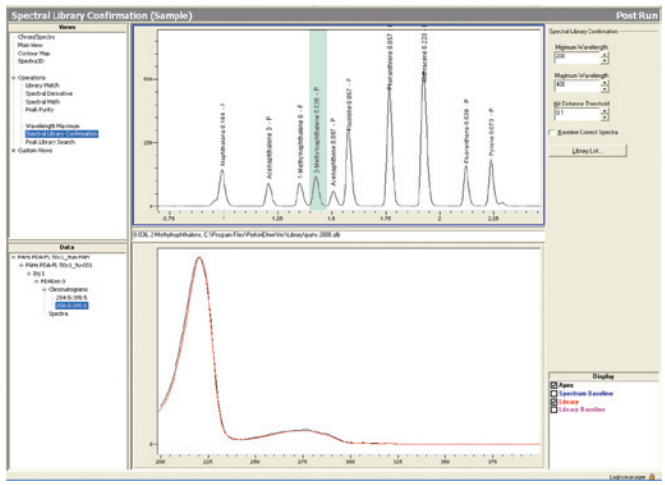
Peak Purity – Quickly evaluate/confirm the peak purity of all components in your chromatogram, both graphically and numerically. All recognized chromatographic peaks are automatically annotated with the corresponding purity index value (PI) and with a "P" (passed) or "F" (failed), relative to the set threshold value. In addition, when selecting a particular peak, the upslope and downslope spectra are graphically displayed for comparison, including a graphical difference plot. Peak-specific PI values can automatically be included in each report.



Wavelength Max – Evaluate the absorbance maxima at a glance, for all detected peaks in a chromatogram, using the apex spectra of each peak. For method development, this operation is especially valuable in establishing the optimal wavelength to use for a particular application. It can also be used to define the wavelength programming steps providing optimal sensitivity for all components in a method. For routine analyses, Wavelength Maximum is also a valuable tool to confirm peak identification. Wavelength Max values can be automatically included in reports after each run.



Spectral Library Confirmation – Automatically (or interactively) report component ID confirmation based on the spectral comparison of all labeled peaks, to one or more spectral libraries, according to a user-settable tolerance.



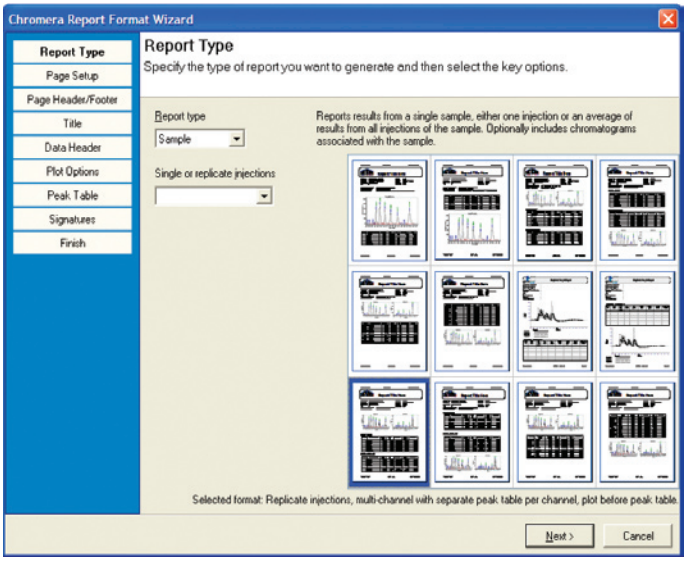
Peak Library Search – Identify unknown peaks using spectral or retention time comparisons, based on one or more spectral libraries

Customizable Views

To further facilitate the user's work experience, the user can customize a preferred primary view. This could include for example, the size/location of any combination of chromatographic, spectral or 3D panes or contour map. In addition, multiple customized views can be saved, depending on the particular focus and/or the needs of individual users.

See and Share Your Results

Chromera makes reporting easy. Include all your chromatographic and spectral information in customized reports using an easy report wizard.



Generate customized reports with the spectral confirmation information you need to assure your chromatography is right on the mark and your samples are running smoothly.

Ret. Time	Component Name	Area	Peak Purity	Wavelength Max	Spectral Library Confirm
1.509	Acenaphthene	103216.97	1.13	225	0.116
1.579	Fluorene	528295.73	5.51	205	0.067
1.767	Phenanthrene	781814.75	1.24	251	0.057
2.121	Fluoranthene	251361.12	1.15	236	0.039
2.238	Pyrene	302869.06	1.22	240	0.073

Build Your Confidence Powerfully Easy

Chromera has been designed from the ground up with a powerfully easy user interface that your staff will learn and run quickly. With a comprehensive suite of 3D spectral analysis tools at your fingertips, you will achieve a deeper understanding of your samples and more confident identification of your chromatographic peaks.

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