



Dear :

ACD/Labs is pleased to present our latest Optical Spectroscopy Newsletter. This edition highlights some of the novel chemometric capabilities imbedded in ACD/Labs software.

To view this newsletter in PDF, visit <http://www.acdlabs.com/newsletters/>

In this Issue:

- A New Way of **Selecting Wavelength Regions**
- **Smart Peak Tracking** Between LC/DAD and LC/MS Runs
- SIMPLISMA Applications in the **Semiconductor Industry**
- What's New in **Version 10** for Optical Spectroscopy
- ACD/Labs at **PITTCON 2007**

Selecting Wavelength Regions—SIMPLISMA-fied

Wavelength selection for calibration and other chemometric analyses has been described as one of the most confusing aspects of spectroscopic analysis.

Simplify it with a new way of judiciously selecting wavelength region that works—even for cases involving ill-defined or unknown component spectroscopy and chemistry.

The purity function in the SIMPLISMA (SIMPLE-to-use Interactive Self-Modeling Mixture Analysis) algorithm can provide a means of narrowing the set wavelength region to be tested to the more significant regions. This algorithm is currently implemented in [ACD/UV-IR Manager](#) and provides an intuitive way of selecting regions that does not require high levels of expertise to use.

If you missed our presentation at EAS 2006, you can see it PITTCON 2007
"A New Deterministic Variable Selection Method for Multivariate Regression Analysis"
 Tuesday, Feb. 27th at 1:30pm
 Room 504A

Smart Peak Tracking—Outrunning the Avalanche

When one chromatographic separation generates three chromatograms, each from different detectors, how do you deal with the avalanche of data? Coordinating LC/DAD, LC/MS, and single wavelength chromatograms offers substantial data management challenges that are made worse by the need to adjoin spectroscopic interpretations for the observed diode array and mass spectrometric features. While you may have considerable expertise in UV-Vis and mass spectrometry, critical evaluation of features one-by-one is rarely fast—especially if the chromatographic separations allowed some co-elutions to take place.

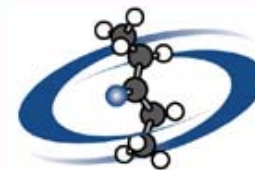
Wouldn't reliable and spectroscopically-aware expert systems that could reduce the interpretation burden prove to be an immense help?

[ACD/Method Development Suite for LC/MS](#)

Designed to give you

- a concise overview of your method development project
- perform spectroscopic interpretation required for peak tracking
- manage all of the associated information

Automatic chromatographic peak tracking across different experiments is based on leveraging spectral similarity with specialized chemometric algorithms for extracting and interpreting components in LC/DAD and LC/MS data sets. The results are presented in a way that is easy for you to critically evaluate and review. This has helped scientists working in the pharmaceutical industry accelerate their method development by up to 80%.



**A d v a n c e d
C h e m i s t r y
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ACD/Labs

More Solutions from ACD/Labs

Advanced Material Science

Impurities and Degradants

Elucidation of Unknowns

Demo Movie
 ACD/UV-IR Manager
 Multivariate Curve
 Resolution
 with SIMPLISMA

View a demonstration of how the software resolves mixtures into pure component spectra and concentrations without prior information about the mixture's composition. Then, view the statistics, number of components, the Intensity Graphs, and Purity Spectra.

view online (Flash 4.48 Mb)
 download movie (exe, 6.67 Mb)

Visit us at
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Attend ACD/Labs' Chromatography Product Manager Michael McBrien's presentation at PITTCON 2007 entitled

"n-Dimensional Map Chromatography—Virtual Resolution of Components Based on Orthogonal Chromatographic Methods"

Sunday, Feb. 25th at 3:15pm
Room 504BC

Impurities in Semiconductors—A Case Study

Infrared spectra of mixtures are very difficult to interpret, so chromatographic or physical separations are often used as a pretreatment. However, there are many cases where isolation of components is either unfeasible or unpractical. The SIMPLISMA curve resolution software offers an alternative way of extracting pure component spectra and concentration profiles from spectral matrices, thus simplifying interpretation of mixtures.

It is difficult to get a true measure of an algorithm without showing it applied to real world examples. At EAS 2006, Michael Boruta presented three interesting case studies on real world data in the semiconductor industry. It was shown that the SIMPLISMA curve resolution algorithm was successful in extracting composition and impurity information from complex mixtures used in the silicon wafer manufacturing process. In the first example, the software was used to help distinguish between good and bad chemical powder lots used in chemical mechanical polishing. In the second example, an aging study of an etching bath solution was used to yield insight into the kinetic behavior of the bath's components over time. Last but not least, SIMPLISMA was used to confirm the presence of trace artifact and impurities in a dilute and polar aqueous photoresist developer.

Download a PowerPoint presentation outlining these particular application examples.

[PDF \(2.11 Mb zip\)](#)

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What's New in Version 10 for Optical Spectroscopy

If you have an older version of our software and haven't seen what's new in [ACD/UV-IR Manager](#) Version 10, download a [PDF copy](#) of the improvements.

ACD/Labs at PITTCON 2007

Visit us at Booth# 1055 to learn more about ACD/Labs software products and services, to discuss scientific advances, or just to say hi.

Oral Presentations by ACD/Labs Staff:

- **IR and Raman Databases for the Analysis of Polymers**
Monday at 1:30pm in the *Spectroscopic Techniques for Polymer Characterization* session (Room 405A)
- **IR and Raman Spectrum: Structure Correlation in the Analysis and Identification of Polymers**
Monday at 1:50pm in the *Spectroscopic Techniques for Polymer Characterization* session (Room 405A)
- **Grouping of High-Throughput XRPD Spectra**
Wednesday at 1:50pm in the *Material Science* session (Room 502A)

Events and News

News

Reel Two and ACD/Labs Collaborate on Better Extraction of Chemical Structures from Patent Data—January 23, 2007 [Read](#)

ACD/Name Ranks Best of the Best According to Recently Published Study—January 11, 2007 [Read](#)

Vertex Pharmaceuticals Purchases ACD/Labs' Nomenclature Software—January 10, 2007 [Read](#)

Upcoming Events

PITTCON 2007
Chicago, IL, USA
February 26–March 1, 2007
Booth #1055

233rd ACS National Conference & Expo
Chicago, IL, USA
March 25–29, 2007
Booth #1065