

Enclosed is the latest newsletter from [Advanced Chemistry Development, Inc. \(ACD/Labs\)](#). This edition contains a summary of recent software advances for chromatographic method development.



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Automatic Molecular Ion Identification for LC/MS

As LC/MS instrumentation has improved, the analysis bottleneck has shifted from sample acquisition to data analysis and interpretation. To ease this burden, ACD/Labs introduces [ACD/IntelliXtract™](#), an innovative new LC/MS software package for automated molecular weight identification and LC/MS data interpretation.

IntelliXtract software mimics the approach an expert mass spectrometrist takes to extract chromatographic components, and interpret the spectrum for each. Adduct ions, multimers, $^{12}\text{C}/^{13}\text{C}$ ratios, isotopes, neutral losses, and fragment ions are considered, providing accurate molecular ion identification in a fraction of the time of manual data review.

Early Findings from an IntelliXtract Tester:

An IntelliXtract software tester presented a talk at PITTCON 2006 titled "Advances in the Extraction of Potential Metabolites and Impurities Using a Self-Optimizing Componentization Algorithm for Peak Extraction and Identification of MS¹ Datasets." It was noted that it took only 3 minutes for the software to find 100% of all the KD5150 impurities, which had been previously identified manually. This suggests that the algorithm can be used with a high degree of confidence in an automated setting. [View the full abstract or download the slides.](#)

Automated Chromatographic Peak Tracking

Accurate tracking of chromatographic peaks from one experiment to the next during method development is a critical step. Peaks may be transposed from run to run, and identifying these misassigned peaks can require a great deal of manual interpretation time. This presentation from PITTCON 2006 describes novel algorithms to take advantage of diode array detection and mass spectrometry in order to automate the chromatographic peak matching process. [Read more on our web site.](#)

Managing Data in LC/MS/DAD Forced Degradation Studies

Today's chromatographers have an unprecedented capacity for generation and collection of data associated with unknown samples. In many cases, the bottleneck in analysis has shifted from data collection to data interpretation. Chromatographic peak tracking and cross-sample component resolution, combined with the necessity of transcribing peak tables into modeling software can require as much or even more time than the data collection itself. [Review a poster, presented at PITTCON 2006, which describes new techniques for management of method development data.](#)

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Update to Free ACD/Column Selector

ACD/Column Selector allows you to scientifically compare and contrast reversed-phase HPLC columns. Don't have a referenced column on hand? Column Selector can help you to find the most equivalent ones. Need a column that is different from yours in a particular way? Column Selector can help with this as well. With this simple tool, you can take the guesswork out of column selection.

This free software was recently updated with 34 new columns. [Download the latest version for Windows.](#)

Meet ACD/Labs at Upcoming Events

Stop by our booth at the following upcoming conferences to say hello, and see the latest advancements in our software.

HPLC 2006

June 18–23, 2006
San Francisco, CA, USA
Booth #608

Join us at HPLC 2006 for our Lunchtime Seminar
Tuesday, June 20, 2006, 12:30–1:30 PM

How to Combine LC-UV-MS Analysis with Advanced Data Interpretation and Organization to Develop More Rigorous Methods, Fast

Learn how software can help you:

- Reliably track chromatographic peaks from run to run, even with significant changes in conditions.
- Organize and manage the large amount of data collected over the course of a project.
- Decrease method development time by up to 80%.

Register here: <http://www.acdlabs.com/um/hplc06/>

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