



Welcome to the latest Chromatography newsletter from ACD/Labs. This edition features recent presentations given by ACD/Labs staff describing how automated peak tracking software can alleviate the crushing pressure of too much data, and the ins and outs of fully automated method development systems. Also get information about ACD/Labs at ASMS and HPLC 2007, and a new freeware offering for the prediction of $\log P$.

In this issue...

- Automated Peak Tracking: More Data Please!
- Fully Automated Method Development: Coming Soon
- New! ACD/Log P Freeware
- ASMS 2007
- HPLC 2007

More Data Please!

Collecting vast amounts of data isn't always worthwhile, because of the burden of data analysis that results. Accurate, automated peak tracking means that it is now possible to evaluate a huge amount of chromatographic data with virtually no manual labor. Two presentations from PITTCON 2007 describe how automated peak tracking facilitates some large-scale chromatography studies.

24-Hour Creation of Chromatographic Prediction Systems



For many years, there have been efforts to create a system to predict the elution of compounds based on their chemical structure. Predictions are based on experimental data, and the accuracy limited by the number and diversity of compounds examined. In the past, retention time and compound information had to be collected manually, which effectively

limited the prediction accuracy. Automated LC/MS peak tracking provides a faster and easier way to build a prediction system.

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HPLC Stationary Phases Classification and Method Development Employing Mass Spectrometry and Modern Software Tools

HPLC stationary phase classification is usually based on a relatively small collection of probe compounds to test analyte-stationary phase retention mechanisms. With this approach, only a few analyte classes are included, and represent a small portion of those possible in HPLC analyses. Automated peak tracking enables a new approach that covers greater



More Solutions from ACD/Labs

[Impurities and Degradants](#)

[High-Throughput](#)

[Failure Analysis](#)

Chromatography Presentations

n-Dimensional MAP Chromatography: Virtual Resolution of Components Based on Orthogonal Chromatographic Methods NDMC

2D chromatography has allowed chromatographers to utilize multiple selectivities independently, resulting in a resolving power unattainable in 1D separations. Recently, chemometric techniques for peak matching across chromatographic runs have enabled the exploitation of complementary retention mechanisms using conventional instrumentation.

The number of "dimensions" that can be applied to the problem is limited only by the number of orthogonal condition sets that can be designed. The benefits of n-Dimensional MAP Chromatography (NDMC), over conventional multidimensional chromatography are clear

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analyte structural diversity and includes more of the important HPLC variables.

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Chromatographic 'Method-O-Matic'

Previous attempts to build fully automated method development systems have fallen short of the goal, primarily because of their inflexibility to established method development protocols (i.e., in older systems, the user had to adapt to the software, not the other way around), and limitations in the accuracy of automated peak tracking. ACD/Labs and our partners, Agilent and Waters, continue to make progress on systems for automated method development. Read about our progress in the following presentations from PITTCON 2007:

Challenges and Considerations for Building an Automated Method Development System

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Automating the Development of Liquid Chromatographic Methods for Impurity and Stability Samples Using High Sensitivity, High Resolution LC/MS

[Download PDF](#) (636 Kb)

ACD/LogP Freeware—Fast & Accurate Predictions at Your Desktop

ACD/Labs is delighted to announce the release of **ACD/LogP Freeware**.

This **add-on** to our drawing package, **ACD/ChemSketch**, will give you easy access to predictions of the octanol/water partition coefficient, also referred to as $\log P$ or K_{ow} .



Continually enhanced since its introduction in 1995, our calculations are based on an experimental data set of over 18,000 reliable $\log P$ measurements, and are used by scientists worldwide through CAS's SciFinder service, and at companies like Pfizer and GSK.

[Read More & Download ACD/LogP Freeware](#)

ACD/Labs at ASMS 2007

Seminar at ASMS

Sunday June 3, 12:30–4:00 pm

LC/MS Data Processing for Small Molecule Analysis

[View the Agenda](#)

[Register Now!](#)

Drop by our **booth (#36)** on the show floor or take a break from the commotion at our **Hospitality Suite** at the Westin Indianapolis, Cabinet Room.

ACD/Labs at HPLC 2007



Identification of Impurities Using Liquid Chromatography Hyphenated with Tandem Mass Spectrometry

"Why is it that as analysts we still invest huge numbers of hours into the extraction of potential impurities from LC/MS and fragment related data by having to perform manual data work-up? Is this not a perfect situation for software to provide a solution?" The potential to perform extraction and determination of molecular weight, and obtain fragment and neutral loss data in a single pass experiment using an increased level of source voltage offers significant opportunities for automation by software.

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Want to see the latest in Method Development and Optimization software in action?

Visit our booth (#59) on show floor.

News and Events

News

Related Fragment Screening: Swift and Easy Elucidation of Drug Metabolites—May 2, 2007 [Read](#)

ACD/Labs and Protasis Shatter the High-Throughput Bottleneck for NMR Analysis—April 16, 2007 [Read](#)

ACD/Labs Software Integrated into ChemSpider Service—April 10, 2007 [Read](#)

Upcoming Events

ASMS 2007

Indianapolis, IN, USA
June 3–7, 2007
Booth #36

HPLC 2007

Ghent, Belgium
June 17–21, 2007
Booth #59

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