

Visionary Software



Advancing Research

Dear :

Advanced Chemistry Development, Inc., (ACD/Labs) is pleased to present our latest Chromatography Newsletter.

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In this Issue:

- Method Development Suite for LC/MS
- Systematic Development of Stability-Indicating Methods
- Efficient Chiral Screening and Purification
- Joint Project with Waters Corporation
- ACD/Labs at PITTCON

## ACD/Method Development Suite for LC/MS

ACD/Method Development Suite for LC/MS is *the only* LC project management and method optimization software that supports full mass spectrometry data (not just the TIC). The software has powerful new features which will help you accelerate your method development:

- Track peaks between runs automatically based on MS or UV spectral similarity
- Get a clear overview of your project by summarizing your data in a peak table, alongside chromatograms, MS, and UV spectra
- The Method Development Assistant can suggest the next experiment(s) to perform

Develop better methods, faster, with new [ACD/Method Development Suite for LC/MS](#).

## Forced Degradation—Stemming the Data Flood



Read the [full article](#).

Maintaining individual degradation samples for a method development project provides better detection limits and fewer components to resolve, but poses a major challenge for data handling and interpretation. In an article for the online journal *The Column*, titled Systematic Development of Stability Indicating Methods, ACD/Labs' Michael McBrien and Margaret Antler discuss some of the challenges and benefits of individual degradation samples for method development.



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**Demo Movie**  
Selecting and Optimizing  
Chromatographic  
Parameters

Review the development of an isocratic separation method for a model mixture of carbohydrates.

[view online](#) (Flash 4.14 Mb)  
[download movie](#) (exe, 8.04 Mb)

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## Chiral Screening—The Problem with Purification

Within the pharmaceutical industry, it has been conservatively estimated that nearly 40% of drugs under development are chiral. Typically, these compounds are purified, rather than using chiral-specific synthesis, putting a significant strain on chiral preparative labs to avoid bottlenecks in the purification process. Application databasing can increase the efficiency of chiral method screening to significantly reduce the number of experiments run, therefore delivering purified samples faster.

### Efficient Chiral Screening and Purification in Support of Medicinal Chemistry

[download PDF](#) (171 Kb)

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## Waters and ACD/Labs Collaborate

In November 2006, ACD/Labs and Waters Corporation announced plans to develop an automated method development solution for LC and LC/MS. The project will integrate ACD/AutoChrom software with Waters® Empower™ 2 software, and AQUITY UPLC® and Alliance® HPLC systems. The automated method development system is expected to reduce method development time for new methods from weeks, to days or less. Preliminary results of this project will be unveiled at PITTCON 2007.

"This level of efficiency and ease of use has never been available to chromatographers before."

Craig Dobbs, Waters Corporation

See a preview of ACD/AutoChrom for Waters and Agilent systems at PITTCON 2007, Booth #1055.

**Contact Us:**  
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## ACD/Labs at PITTCON

Visit us at Booth #1055 to learn more about ACD/Labs software products and services, to discuss scientific advances, or just to say hello. [map](#)

### Oral Presentations by ACD/Labs Staff:

- **n-Dimensional MAP Chromatography: Virtual Resolution of Components Based on Orthogonal Chromatographic Methods**  
Sunday at 3:15PM in the *LC-MS in Environmental, High-Throughput and Other Applications* session (Room 504BC)
- **The Impact of LC/MS Componentization in the Low Level Extraction of Impurities and Related Compounds**  
Tuesday at 9:30AM in the *Identification of Impurities Using Liquid Chromatography Hyphenated with Tandem Mass Spectrometry* session (Room 405A)
- **24-Hour Creation of Chromatographic Prediction Systems**  
Tuesday at 10:45AM in the *Method Development in Chromatography* session (Room 504A)
- **Automating the Development of Liquid Chromatographic Methods for Impurity and Stability Samples Using High Sensitivity, High Resolution LC/MS**  
Wednesday at 8:50AM in the *LC-MS Pharmaceutical/Drug Discovery/Proteomics &*

- **Sample Stability, Composite Samples, and Chromatographic Method Development**  
Wednesday at 10:05AM in the *Application of Liquid Chromatography and Tandem Mass Spectrometry in the Analysis of Active Pharmaceutical Ingredients* session (Room 501BC)

**For more information about  
our software solutions, or to  
request a trial evaluation,  
please e-mail us at:**

**[info@acdlabs.com](mailto:info@acdlabs.com)**

## Events and News

### News

Wockhardt Equips Drug Discovery Researchers with ACD/Labs Software—February 5, 2007 [Read](#)

ACD/Labs Approaches Benchmark in NMR Prediction Accuracy with Release of New Software Version—January 29, 2007 [Read](#)

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

### Upcoming Events

#### **59<sup>th</sup> AAFS Annual Meeting**

San Antonio, TX, USA  
February 19–24, 2007  
Booth #605

#### **PITTCON 2007**

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

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