

Dear :

ACD/Labs is pleased to present our latest MS newsletter. Read about applications for metabolite elucidation and identification, see some of the new products and features available for MS in version 10 of our software, and read about our activities at this year's ASMS in Indianapolis.

In this issue...

- Applications—Dextromethorphan Metabolites and Related Fragment Screening
- What's New—Features and Functionality for MS in Version 10
- ACD/Labs at ASMS 2007

## Making a Molehill Out of a Mountain

Identification and elucidation of drug metabolites is a difficult task. Because of its sensitivity and selectivity, LC/MS is the technique of choice for metabolite studies; however, interpreting the results can be difficult due to the tremendous amount of information generated and expertise needed to sort it all out. The following two application notes outline how software can help alleviate some of these issues.

### *Software-guided Identification of Dextromethorphan Metabolites with ACD/IntelliXtract*



Separating useful information from LC/MS datasets hampered by noise and overlapping components is possible with the right software. Read about how [ACD/IntelliXtract](#) can help by doing some of the routine tasks for you.

[Download PDF](#) (220 Kb)

### *Extraction and Elucidation of Metabolites Using Related Fragment Screening*

Related Fragment Screening takes advantage of similarities in structure of drug metabolites relative to the parent compound. Learn how to organize and interpret this data more easily with the help of specialized software.

[Download PDF](#) (118 Kb)

## What's New in Version 10

Has it been a while since you last looked at [ACD/MS Manager](#)? The latest release has several improvements, making your MS data processing and interpretation faster and easier than ever.

- Neutral loss reactions have been added to the fragment prediction engine. This will **improve assignment of**

## More Solutions from ACD/Labs

[Metabolism Studies](#)

[Impurity and Degradant  
Studies](#)

[Synthetic Chemistry](#)

## Featured Presentations

Advances in the Extraction of Potential Metabolites Using a Self-Optimizing Componentization Algorithm for Peak Extraction and Identification of MS Datasets

[Abstract](#)  
[Download PDF](#)

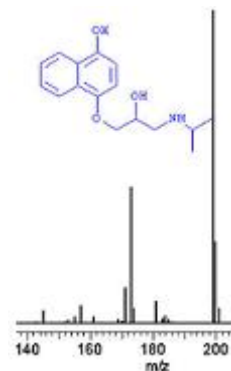
Using ACD/Labs Software to facilitate drug metabolite identification processes

[Abstract](#)  
[Download PDF](#)

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fragments to experimental spectra acquired using low-energy ionization techniques.

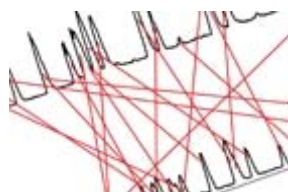
- The Empirical Formulae Generator is now more flexible and easier to use with experimental data. You can now **calculate the charged or neutral formula from the MH<sup>+</sup>, MH<sup>-</sup>, or adduct ions** in the spectrum. And, unlike some other formula generators, MS Manager takes into account the mass of an electron, for the most accurate results.
- Extensive LC/UV processing capabilities have been added, including baseline correction, which **automatically detects the UV spectrum of the solvent background**, and subtracts it, making it easier for you to identify solute peaks.



See [What's New with ACD/MS Manager](#) (PDF, 189Kb)

[ACD/Method Development Suite](#) is improving by leaps and bounds! Here's a taste of the new features our users are most excited about.

- **Automated peak matching based on UV or MS spectral similarity** to accelerate evaluation of screening experiments. Peak matching also aids component detection, even for co-eluting components.
- Not sure which experiment to try next? The **Method Development Assistant** can guide you through the method optimization process, allowing you to optimize your separations more efficiently.
- Advanced project management features which provide a **clear overview of your method development project**. You can even dig down into the raw data when necessary, by providing hyperlinks to LC/UV, LC/MS, and chromatographic data



[Learn more](#)

## ACD/Labs at ASMS 2007

### ACD/Labs 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 show floor or take a break from the commotion at our **Hospitality Suite** at the Westin Indianapolis, Cabinet Room.

## News and Events

### News

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

### Upcoming Events

**ASMS 2007**  
Indianapolis, IN, USA  
June 3–7, 2007

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

Booth #36

Scientists at ACD/Labs Co-Author 'Most Accessed' Paper  
in MRC—April 9, 2007 [Read](#)

**31<sup>st</sup> International Symposium on High  
Performance Liquid Phase Separations  
& Related Techniques (HPLC) 2007**

Ghent, Belgium  
June 17–21, 2007

