

Enclosed is the latest newsletter from [Advanced Chemistry Development, Inc. \(ACD/Labs\)](#). This edition highlights new resources for our mass spectrometry and chromatography software. Read below for more information.

ACD/Labs



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CODA Tool for Identification of Trace Components in LC/MS Data Sets

The [COmponent Detection Algorithm \(CODA\)](#) is a method for fast, automatic identification of mass chromatograms with low noise, low background, and analyte peaks. CODA reduces the size of the data set without losing analytical information, simplifying identification of relevant mass chromatograms. CODA significantly reduces noise in LC/MS data sets, enabling confident detection of trace analyte components.

See examples of CODA with experimental data in the [application notes](#) *Noise Reduction of LC/MS Data Using the Component Detection Algorithm* and *CODA for Noise Reduction in LC/MS Analysis of Urine*.

[ACD/MS Manager](#) contains a unique version of CODA, with advanced features such as baseline correction of mass chromatograms, and peak picking. See how these features improve the quality of data extraction in the poster [Improvements in the Performance of CODA and COMPARELCMS for Generic Data Extraction](#), presented at ASMS 2004.

Current [ACD/MS Processor](#) users can learn how the algorithm works, and how to optimize CODA input parameters with the [technical notes](#) *An Introduction to CODA* and *Optimizing the Parameters Used within CODA*.

Accelerate Chiral Method Development with ChirBase™ for ACD/Labs

The selection of a Chiral Stationary Phase (CSP) with the appropriate mobile phase can be a bottleneck in chiral method development. However, previous separations of similar compounds may provide clues in selecting a CSP. [ChirBase](#), the acclaimed chiral separations database, is now available in [ACD/ChromManager](#) format. Search the database according to chemical structure similarity, substructure similarity, and/or experimental conditions, and find chiral methods for compounds similar to yours. Speed your method development time by taking advantage of over 100,000 previous HPLC chiral separations. [ChirBase/GC™](#) and [ChirBase/CE™](#) are also available, containing 24,000 and 8000 separations respectively.

Structure Based pK_a Prediction with ACD/LC Simulator

Selection of the mobile phase pH is critical when developing LC separation methods, as it allows for control of the analyte ionization and thus its interaction with the stationary phase, and can also improve method robustness. An appropriate mobile phase pH can be selected based on the pK_a values of the compounds to be separated. [ACD/LC Simulator](#) allows you to predict pK_a values based on the structures of your compounds.

Find out more about structure based pK_a prediction in our poster from the HPLC 2004 conference, [Application of Structure-based pK_a Prediction to Reversed-Phase Chromatographic Method Development](#).

Also read the application note, [Application of pK_a Prediction to Chromatographic Method Development](#), for further discussion.

Tools for 2D Chromatographic Data

A technical note describing how to work with 2D chromatographic data, along with example data files is now available—[Viewing and Processing LC/GC and GC/GC Data with ACD/ChromProcessor and ACD/Matrix](#).

Upcoming ACD/Labs Events

Meet our staff and learn more about our software offerings for mass spectrometry and chromatography at the following fall tradeshow:

CPSA (Princeton, NJ, USA)
Oct. 18-21, Booth #5

AAPS (Baltimore, MD, USA)
Nov. 7-11, Booth #2624

Montreux Symposium on LC/MS (Montreux, Switzerland)
Nov. 10-12

EAS (Somerset, NJ, USA)
Nov. 15-19, Booth #442