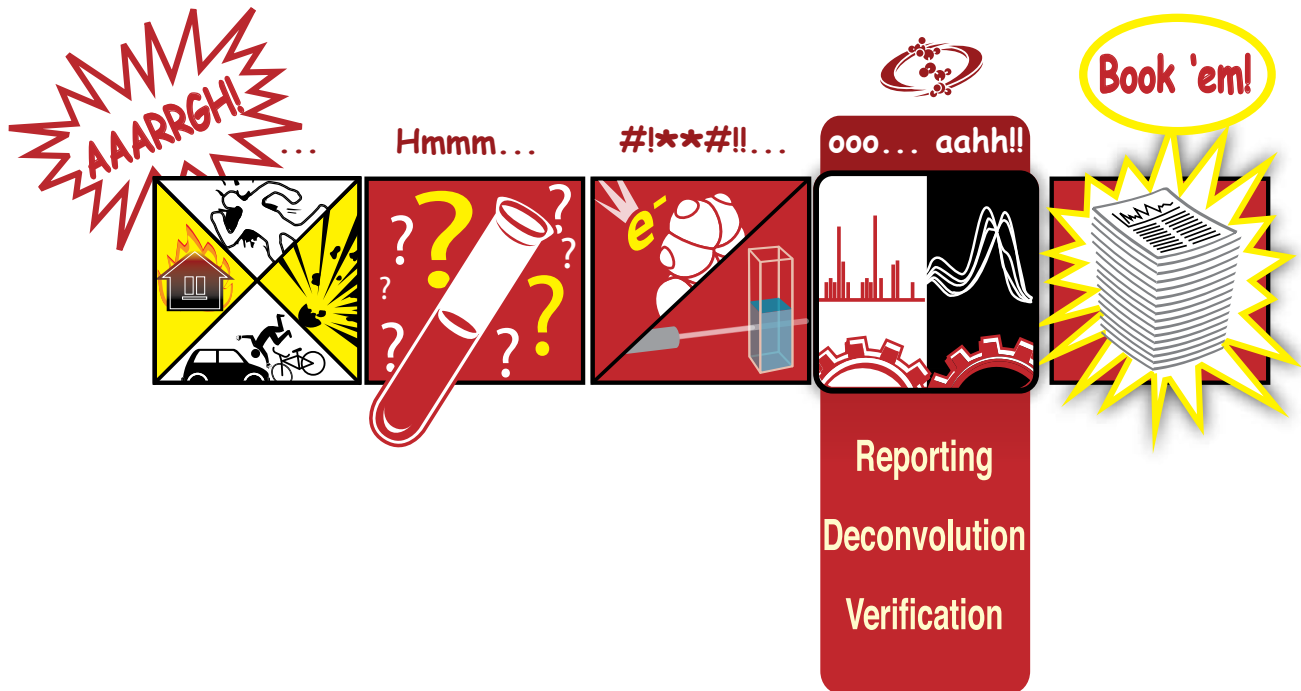# Extract, Identify, and Report Results Faster

With ACD/Labs Analytical Data Management System

The challenge of identifying compounds of interest and reporting results quickly becomes difficult due to the nature of complex forensic samples and the limited abilities of analysis software to produce reports in acceptable formats.
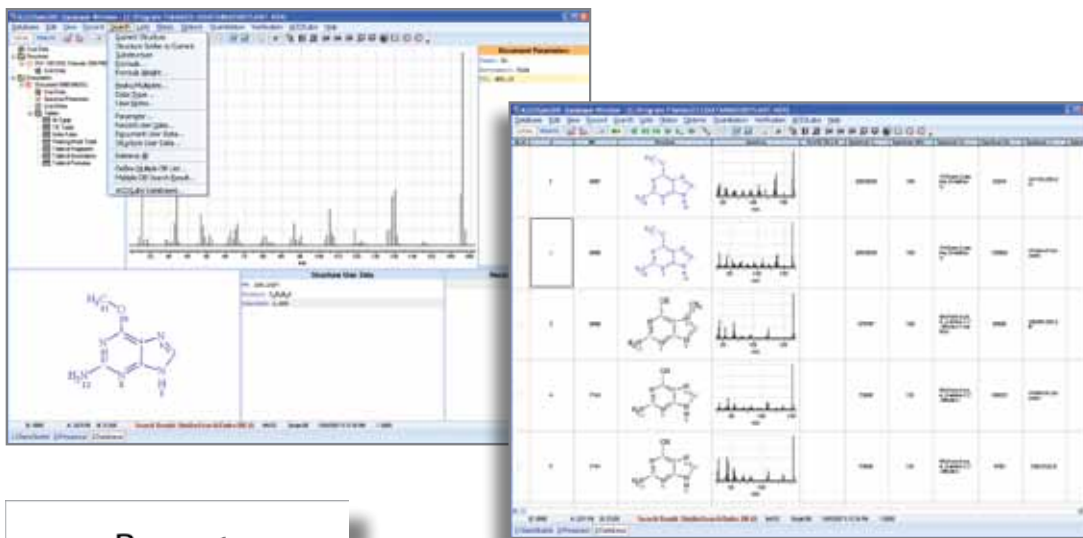
ACD/Labs software offers alternatives to instrument vendor software packages with advanced algorithms for dealing with complex matrices to extract components and identify compounds, as well as flexible knowledge management tools to create customized reports, incorporating all of the information you need, with the click of a button.

Analytical Knowledge Management

Supporting data formats from most major instrument vendors, ACD/Labs can import raw or processed data files from GC/MS, LC/MS, and optical analytical techniques from Thermo, AB SCIEX, Waters, Agilent, Bruker, Varian, Shimadzu, and other instruments.

Apply **advanced processing** to automatically assign [M+H]$^+$ and [M-H]$^-$, and extract components or identify unknown compounds.

Customized Reporting

Generate reports containing all of the information you need, in the format you want, using customized templates for consistency.

Results can also be saved to a spectral database that can be searched by a full or partial spectrum, structure, substructure, and a variety of text-based queries.

Targeted Screening and Identification Tools

Deconvolute and apply advanced filters such as mass defect, isotope pattern analysis, and $^{12}C/^{13}C$ test to complicated matrices and extract all of the components, even those at trace concentrations or when co-eluting with other peaks.

Screen your samples for all of the known compounds you need to find or eliminate, then identify other components that may be present.
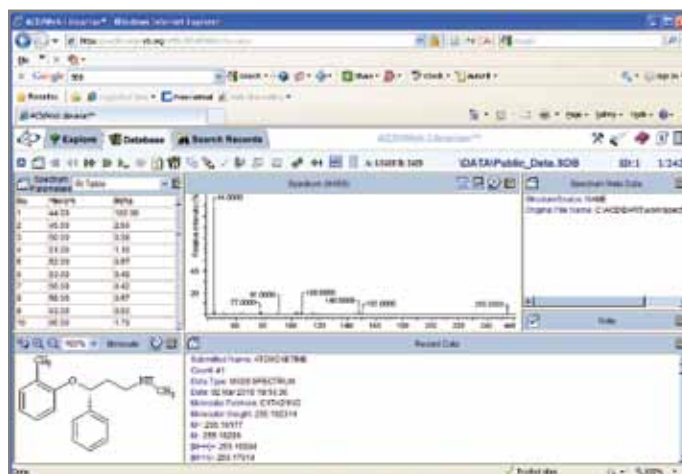
Use spectral matching capabilities in library searches to quickly identify unexpected compounds.

Collaboration and Sharing

Building a database of spectral and chemical data is a convenient way to **share information** across groups or geographic locations. Spectral data from a variety of analytical techniques such as GC/MS, LC/MS, IR, Raman and other optical techniques, and from any variety of instruments can be combined in a single repository that can be searched within an organization or remotely through a **web-based interface**.

Manage access with secure logins and authentication to protect the data from unauthorized use, or allow wider access to other organizations or the public.

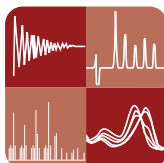## Industry Application: A Forensic Database Administered by RTI International

RTI, with a grant from the National Institute of Justice, and employing ACD/Labs software, created a database of spectral and chemical information on toxins, pharmaceuticals, and illicit substances of relevance to the forensic community. The 'Forensic DB' (www.forensicdb.org), is built from data acquired by users and laboratories around the world and is accessible to the public via a web interface. Users can upload spectra to search for matching examples, perform structure and substructure queries, as well as generate reports.

Forensic DB houses GC/MS and Direct Analysis in Real-Time (DART) MS spectra and associated data; however, the capability also exists for future expansion to include LC/MS, UV, and Raman Data, and even NMR data in the future.
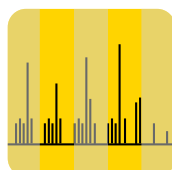
Read more at www.acdlabs.com/forensicdb

ACD/Labs Software Solutions for Forensic Toxicology

Analytical Data Handling

Multi-technique, vendor-independent spectroscopic and chromatographic software for data processing and customized reporting.
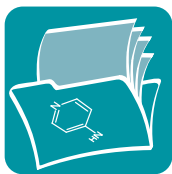
Targeted Screening and Peak Extraction

Advanced deconvolution algorithms help you find targeted compounds as well as other unknowns in complicated samples LC/MS and GC/MS data sets.

Intelligent Compound Recognition

Reduce the time spent on manual interpretation, searching, and validation of GC/MS spectra by searching against the NIST or other commercial libraries.

Databases and Knowledge Management

Create and manage flexible and easily customized databases of chemical structures and analytical data, reactions, reports, and other supporting material as a means of harmonizing and sharing chemical knowledge.

Contact an ACD/Labs representative to learn more about analytical data management with ACD/Labs software.

www.acdlabs.com/finditfaster

ACD/Labs