SHIMADZU
Excellence in Science

For LabSolutions™ LCMS

High Resolution Accurate Mass Library for Forensic Toxicology

LCMS-9030

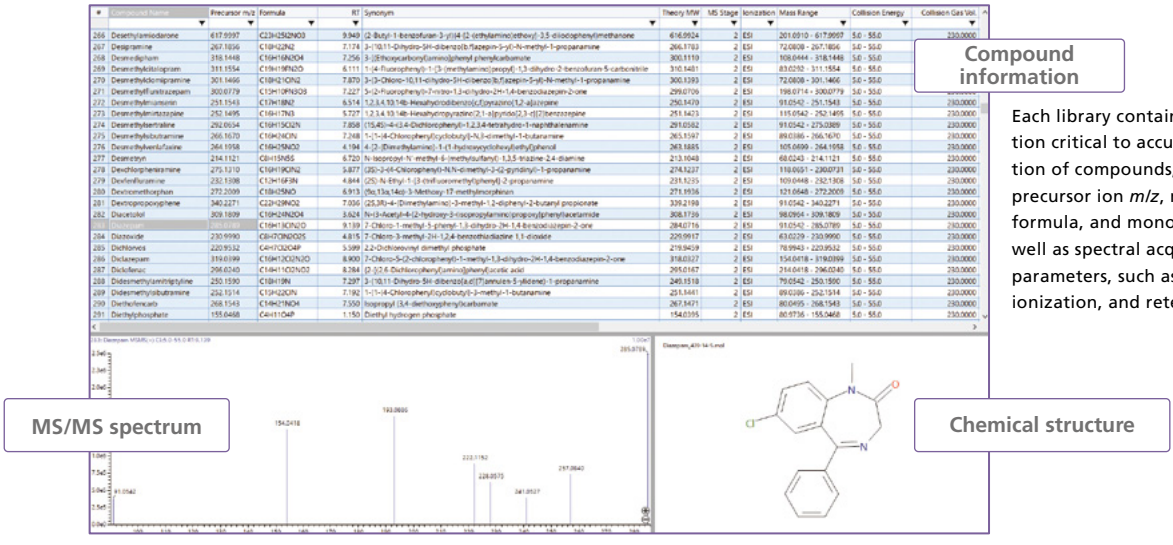
Perform forensic toxicology screening for drugs of abuse, psychotropic drugs, pharmaceuticals, pesticides, and natural toxins using this high-resolution accurate mass database.

MS/MS Spectra for over 900 Toxicological Substances

The High Resolution Accurate Mass (HRAM) Library includes two MS/MS spectral libraries. Each library is built using two different separation conditions and is suitable for targeted or non-targeted screening of drugs of abuse, psychotropic drugs, pharmaceuticals, pesticides, and other compounds of toxicological interest.

Library Contents

Library 1 includes 81 MS/MS spectra and ODS method retention times for various illegal drugs and pharmaceuticals commonly of interest to forensic laboratories. Library 2 includes MS/MS spectra for 901 potentially toxic substances of interest to forensic analysis and clinical research. Retention times and method conditions are based on a Biphenyl column.



Example of Library Entry

Each library contains key information critical to accurate identification of compounds, including precursor ion *m/z*, molecular formula, and monoisotopic mass, as well as spectral acquisition parameters, such as collision energy, ionization, and retention time.

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Simple Data Analysis Using LabSolutions Insight Explore™

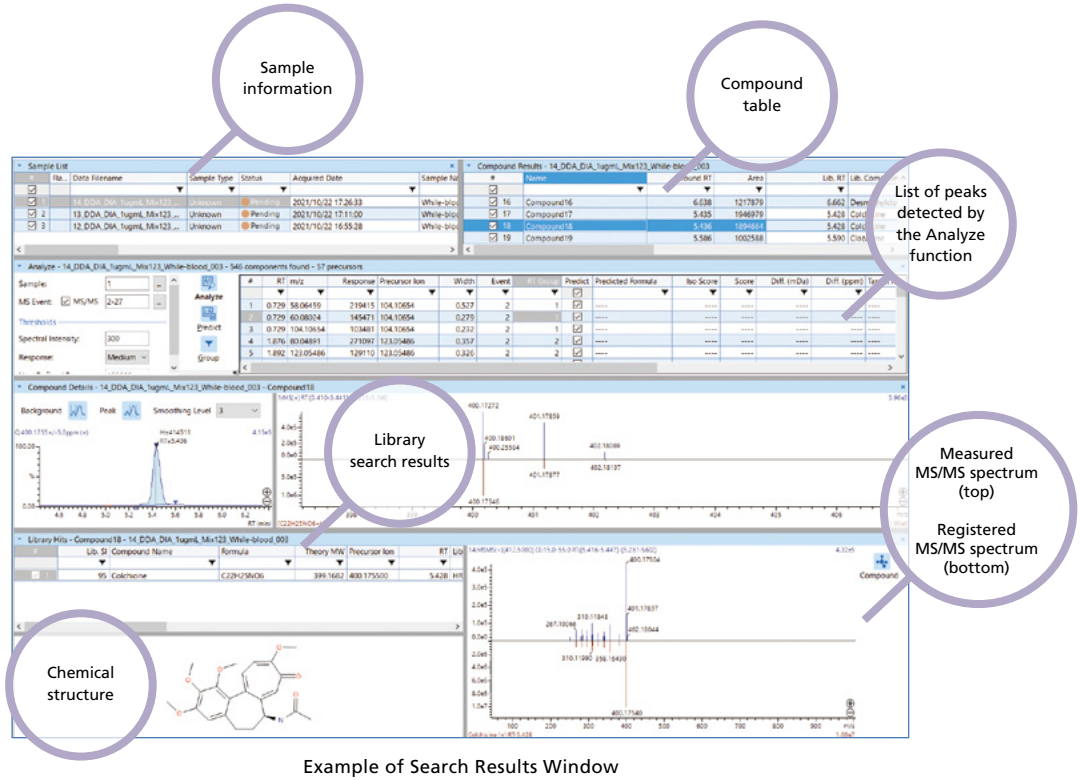
Data acquired with a Shimadzu Q-TOF system can be analyzed easily using LabSolutions Insight Explore software. Library searching and compound identification can be performed in just three steps. Search results are displayed in a format that is visually easy to understand.

Procedure for Compound Identification by Searching the Library

STEP 1 Use Insight's Analyze function to detect peaks in the mass spectrum and register results in the compound table.

STEP 2 Search the MS/MS library for spectra with similarities to detected compounds.

STEP 3 Check library search results along with library similarity score and chemical structure.



Example of Search Results Window

Remarks and Precautions

1. LabSolutions LCMS Ver. 5.113 or later and LabSolutions Insight™ Ver. 3.8SP4 or later are required.
2. This library is intended for research use only. It may not be used for clinical diagnostic applications.

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