C146-E419A

SHIMADZU
Excellence in Science

Screening Software for LC/MS/MS Systems

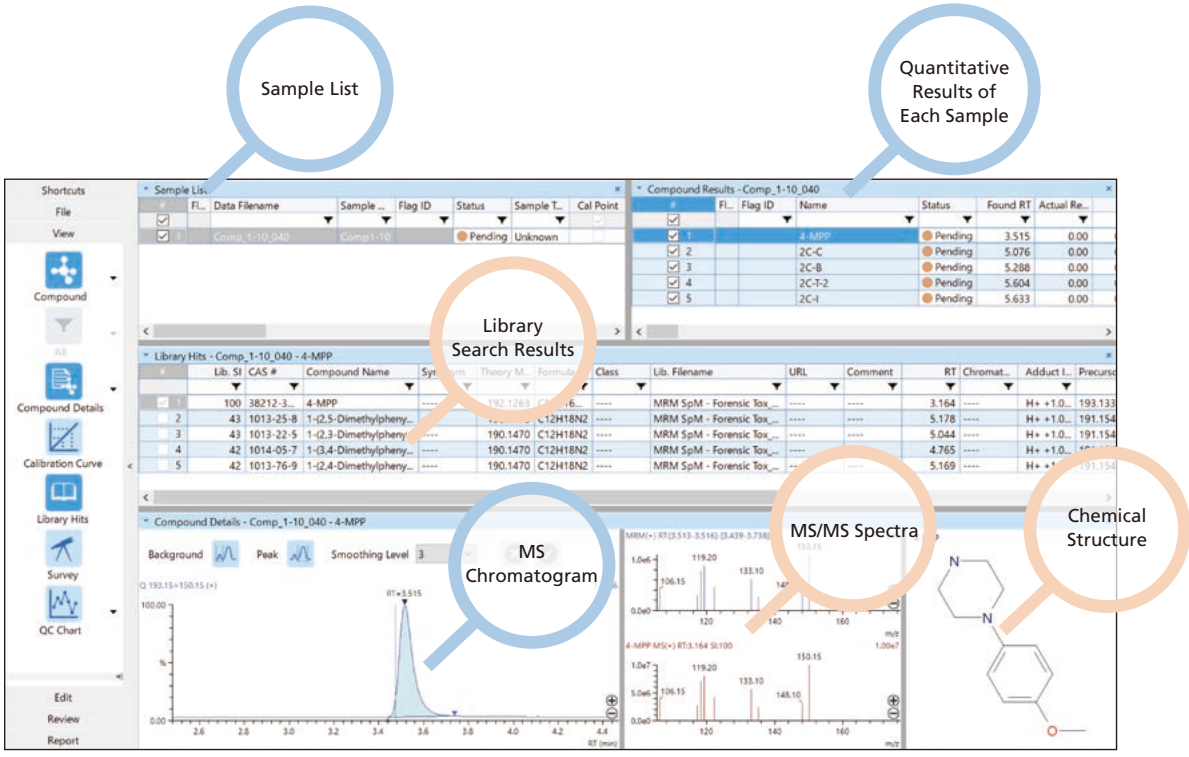
LabSolutions Insight Library Screening

Integrating **Library Search** Into Quantitative Workflows

Technical advances of mass spectrometers have made quantitative multi-target screening in food safety and forensic toxicology easier, faster and more reliable. In turn, this has elevated the need for a sophisticated data review scheme to improve overall turnaround time.

Shimadzu's LabSolutions Insight™ multi-analyte software is designed to streamline complex data analysis workflows. The LabSolutions Insight Library Screening option adds the library search capability to further increase the efficiency of data review and confidence of identifications, both of which will shape the future of routine tests.

View Results at a Glance, Simple and Efficient



In LabSolutions Insight Library Screening, three views is integrated into the data review display of LabSolutions Insight, allowing the reviewer to intuitively judge whether the library search result is adequate.

■Library search results

Displays the candidate matches and their similarity index scores.

■MS/MS spectrum

Displays and allows comparison of an acquired spectrum (upper) against a reference library spectrum (lower) that switches as the user clicks on different candidate hits on the search results. The reference spectrum can be arranged in parallel, as shown above, or reflected upside down for ease of spotting unmatching peaks.

■Chemical structure

Displays the chemical structure of the candidate compound selected in the search result.

As the key benefit of integrating qualitative data analysis into the quantitative platform, the top-ranked candidate name and its similarity index score can be directly displayed in the quantitative results table and be used for flagging. Whereas conventional identification criteria, such as reference ion ratio(s), have necessitated broad data inspection due to frequent occurrence of false-negative and false-positive identifications, similarity index score provides a reliable measure of identification certainty and helps narrow down or pinpoint ambiguous data.

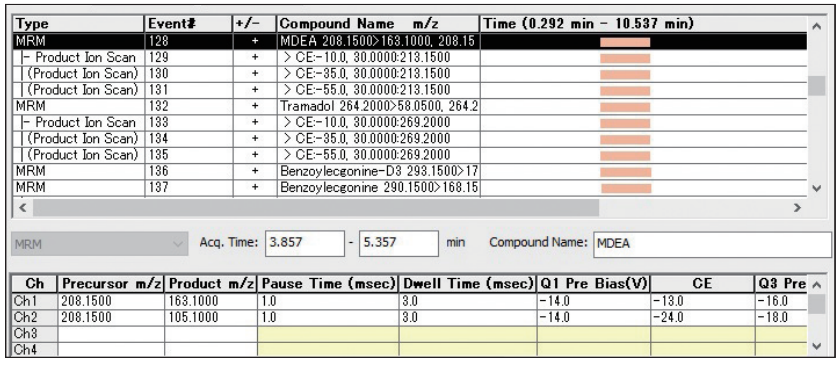
Supports Two Data Acquisition Modes

LabSolutions Insight Library Screening software can screen compounds not only based on mass spectra as usual, but also based on the following characteristic screening methods.

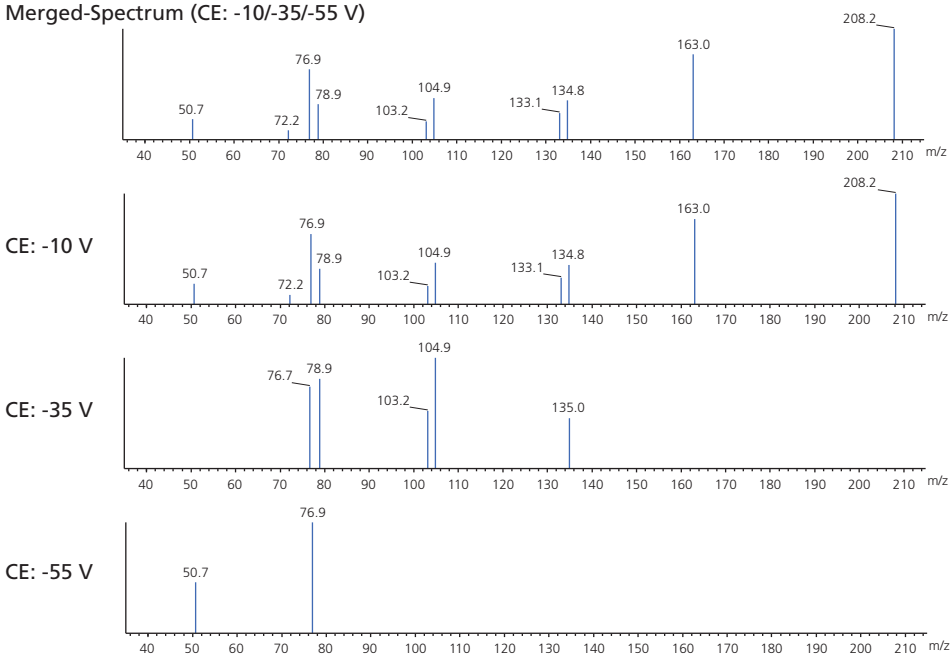
- Screening based on MRM-automatic product ion spectra
- Screening using the MRM Spectrum Mode

Screening Based on MRM-Automatic Product Ion Spectra

Synchronized Survey Scan function is a method for automatically measuring data linked to MRM measurements, one standard technique for acquiring data intended for library searching. In addition to detecting compounds with high sensitivity, MRM also provides three spectra for product ions with different collision energy (CE) levels. LabSolutions Insight Library Screening automatically combines those spectra into a single merged spectrum for library searching. That approach can identify more product ions so that chemical substances with similar structures can be differentiated. The figure below shows an example of a method using the Synchronized Survey Scan function. If the MRM intensity exceeds the threshold value, it automatically starts a product ion scan.



Measurements using the above method result in a merged spectrum that combines product ion spectra for three different collision energy levels. That merged spectrum can be used to search the library.



Enables High-Sensitivity Screening Analysis

MRM Spectrum Mode

Rethink your MRM Limits

Rediscover the capabilities of MRM

The MRM Spectrum Mode is the boundary-breaking technique for simultaneously acquiring quantitative data and MS/MS spectrum for library search. It is a preferred approach for laboratories seeking to improve data processing workflow for the most challenging matrices in food safety and forensic toxicology screening.

Data Acquired in the Same Way as Usual Quantitative Methods

Data for MRM spectra is, in principle, acquired in the same way as for normal measurements. The difference is that MRM measurements are performed comprehensively for all product ions relevant to all target compounds. Another advantage of the MRM Spectrum Mode is the ability to measure all product ions at optimized collision energy levels. Consequently, it can detect the same ions targeted in product ion scans with higher sensitivity. Using this mode for simultaneous multianalyte analysis involves simultaneously measuring several hundred MRM spectra, which is a strength of Shimadzu LC/MS/MS systems, which boast among the highest speeds in the world. Consequently, these Shimadzu systems can perform those measurements without sacrificing sensitivity even at high speeds.

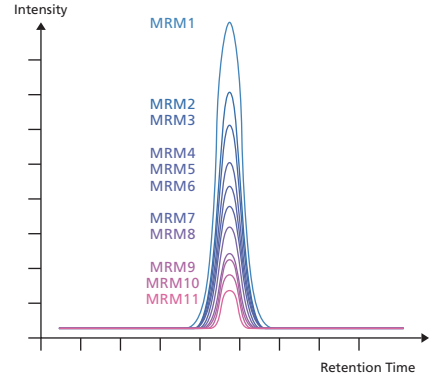
- Reliable data acquisition: Given that the MRM Spectrum Mode continuously monitors all product ions, regardless of their MRM intensity level, the mode can detect even trace quantities of target compounds to ensure none are overlooked.
- Ready-to-use methods and MRM parameters for food safety and forensic applications are provided with LabSolutions Insight Library Screening.

Data Analysis Also Follows the Same Workflow as Normal Quantitative Analysis

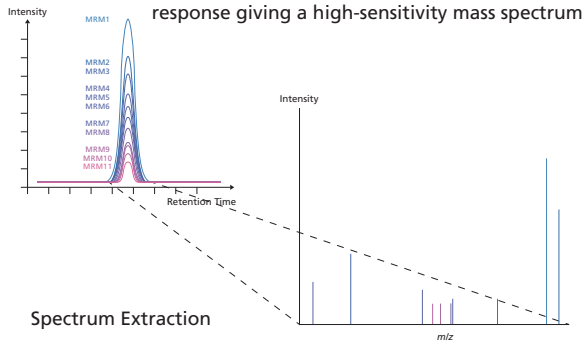
MRM spectrum data can be analyzed in the same window where quantitative results are displayed, using the same workflow as for quantitative analysis. When acquired MRM spectral data is displayed in LabSolutions Insight Library Screening software, all MRM data for each product ion and each compound is automatically merged and converted to a pseudo product ion spectrum, referred to as an MRM spectrum. Then based on the resulting MRM spectrum, added library search functionality is used to identify the compounds by searching a reference library.

- Reliable screening: Because MRM measures multiple product ions necessary for screening, spectral quality is maintained even in low-concentration regions so that compounds can be identified based on high similarity scores.
- Optimized analytical operations: Efficiency of quantitative data acquisition and data analysis are improved by using identification results as an indicator for identifying compounds to be targeted by quantitative analysis.

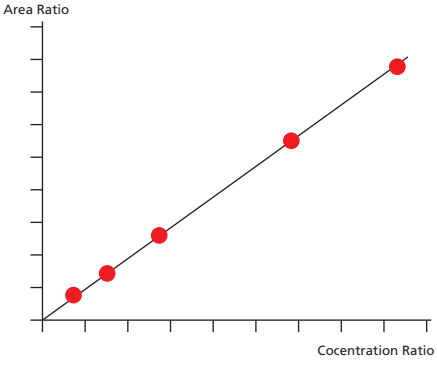
MRM Measurement:
High-Sensitivity and Comprehensive Detection of Product Ions



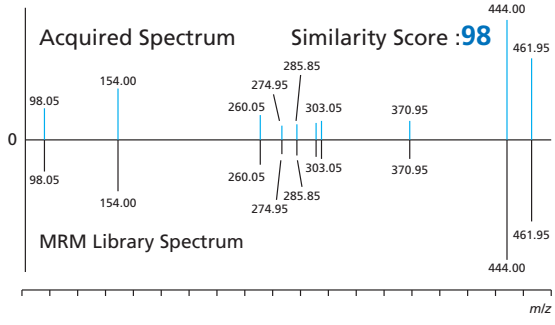
Each product ion is optimized for the highest response giving a high-sensitivity mass spectrum



Quantitation



Library search



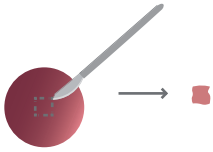
Introducing the workflows

Workload reduction in veterinary drug screening

Thanks to the compliance of manufacturers, the reality of veterinary drug screening is that the vast majority of foodstuff samples being tested do not contain any of the restricted compounds above maximum residual limit if not detected at all. The data review process mainly checks for false-positive detections that occur as a result of matrix interference. This involves subjective judging and manual correction of peak identification. Here introduced is how LabSolutions Insight Library Screening could be used to reduce this process while ensuring that no data is misjudged or overlooked.

Easily and Reliably Detect Rare Positive Results

By specifying somewhat broad automatic identification criteria and performing a library search for target peaks near the predicted retention time, flagging functionality can be used to identify compounds that satisfy the criteria of having taller-than-specified peaks and a high similarity score.



Sample pretreatment by QuEChERS

Data acquisition including MRM spectrum
(MRM transitions are included in Library Screening software)

LabSolutions Insight
Library Screening

- Calibration
- Library search on MRM spectra

If positive

Quantitative analysis
(LC/MS/MS Method Package for Veterinary Drugs)

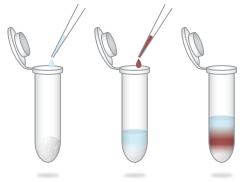
LabSolutions Insight

- Calibration and quantitation
- Reporting

A total solution for toxicology screening

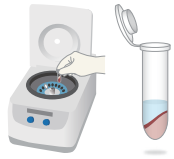
Toxicology screening requires eliminating the possibility of accidentally detecting related compounds with similar structures. Therefore, it requires reliable identification based on library searching. LabSolutions Insight Library Screening provides a convenient platform with both the quantitative and qualitative functionality necessary for toxicology screening. Two types of measurement methods are available, which can be selected depending on the sensitivity desired, the types and number of target compounds being analyzed, or other factors. LC/MS/MS systems can also be configured in combination with pretreatment kits or method packages to provide robust solutions.

① Add the sample



Note: For LC/MS/MS rapid toxicology screening, an internal standard substance is added here.

② Separate with a centrifuge



③ Transfer the supernatant to a vial

Micro Volume QuEChERS Kit

- Change target compounds whenever needed.
- Measure compounds with high sensitivity.

- Target compounds include 231 components commonly analyzed in forensic fields.
- Perform simplified quantitative analysis.

Data acquisition including MRM spectrum
(methods provided with the Library Screening license for panels of 584 or 1208 compounds)

Add/subtract compounds as required

LC/MS/MS Rapid Toxicology Screening System
- Includes one-point calibration curves for quick quantitative analysis

- MRM-triggered product ion scan for all target compounds.

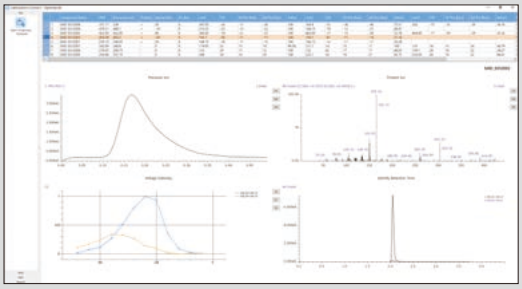
- Calibration and quantitation
- Confirmation by library search
- Reporting

LabSolutions Insight
+ Library Screening

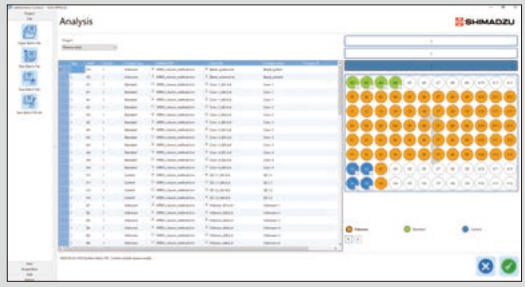
Related Products

LabSolutions Connect™ MRM Software for Linking to Compound Database

The screening methods contain abundance of information that makes it impossible to manually check for missing compounds and inappropriate parameters. LabSolutions Connect MRM is a mandatory software for efficient management of LC/MS/MS methods. With the capability to create a compound database, it can automate most of the processes associated with optimization of MRM acquisition parameters, registering the compounds to database with optimum parameters, and creating methods by extracting relevant information from the database.



1. Reviewing optimization results. Hundreds of compounds can be processed simultaneously.



2. Method file creation and batch analysis.

Method Package

■ LC/MS/MS Method Package for Veterinary Drugs

This software includes two types of high-speed quantitative analysis methods (for either ODS or biphenyl columns) that can be used to detect 129 veterinary drug components in 16.5 minutes. The method for biphenyl columns uses the same analytical condition settings as the MRM spectral data-compatible method template included in LabSolutions Insight Library Screening software.

■ LC/MS/MS Forensic Toxicology Database

This MS/MS database covers a wide range of compounds including drugs-of-abuse, psychotropics, OTC drugs, pesticides, and natural toxins. A ready-to-use screening method for 2,500 compounds is included to allow users to start complex analyses on the day of instrument installation.

■ LC/MS/MS Rapid Toxicology Screening System

The system can be used for screening or simplified simultaneous analysis of 231 components commonly targeted in forensic analysis of banned substances or hypnotic drugs, psychotropic drugs, or other pharmaceuticals. The product includes a QuEChERS-based pretreatment method for a total solution covering all steps from pretreatment to data acquisition and data analysis.

Product Summary

Contents

- LabSolutions Insight Library Screening installation disc for additional features ※1
- MRM spectrum library disc
  - MRM spectrum library including 235 veterinary drugs and 584/1208 toxicological compounds.
  - Template method file for acquisition of MRM spectra
    - Method for veterinary drug screening
    - Method for toxicology screening (584 compounds)※2
    - Method for toxicology screening (1208 compounds)※2
  - Chemical structure (.mol) file of all included compounds
  - SQL-based compound database file containing the optimized MRM parameters※3
  - PDF files indicating compound names and acquisition parameters.
- Instruction manual

Specification

Features for quantitative data analysis, common to LabSolutions Insight product line.

Peak filtering by flagging

Chromatographic peaks can be labelled with conspicuous flags that appear if a peak or data meets user-defined conditions. For example, the concentration flags is setting for data exceeding legal or company limits. A single click can navigate users to flagged peaks to facilitate data review.

Flaggable parameters

Flagging parameters can be set in about 30 different ways, including different alert levels for the same parameter.

Flexible data display for efficient review

All display panes are floatable, dockable and hideable to allow users to design the work field to maximize performance. This is particularly effective with a large monitor or multiple monitors. Sample survey view can display numerous peaks in one view, which can be sorted by flagging or filtering features.

Easy manipulation of quantitative results

Calibration curves can be edited directly on the screen. With one click, you can change the type of calibration curve, the weighting method, whether or not the calibration point passes the origin, and whether or not the calibration point is excluded or added. The parameter change is immediately reflected in quantitative results.

Qualitative features added in the Library Screening option

Displaying Spectra

The spectra obtained by various modes are extracted and drawn according to the peak elution time of the target compound, and are shown side by side with the reference spectrum and chemical structure. The addition of qualitative information increases the reliability of compound identification.

Library search

The acquired MS/MS spectrum data is collectively searched against the library, outputting a list of candidate compounds with high similar scores. Identification information at the top of the list is reflected in the quantified results table, which can be used for efficient data review through flagging and filtering.

※1 Requires prior installation of LabSolutions Insight (version 3.7 SP3 or later).
※2 The methods differ by LC conditions, the 584-compound method uses a C18 column, whereas the 1208-compound method uses a biphenyl column.
※3 Requires LabSolutions Connect (sold separately) for using the compound database.

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