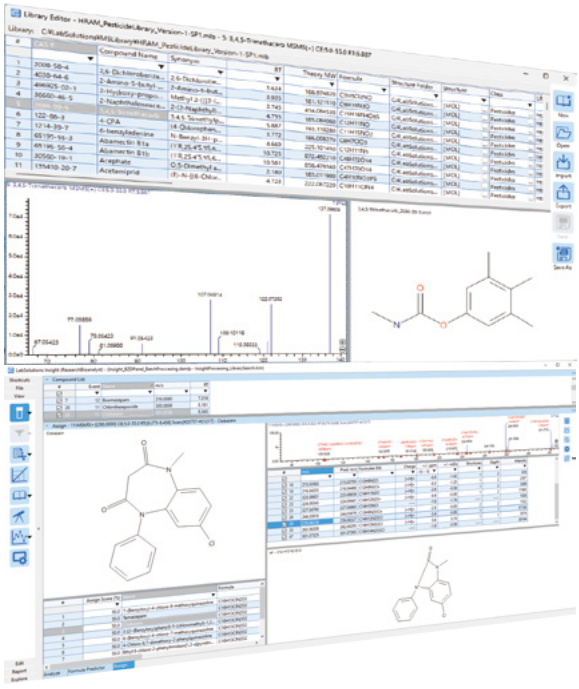
SHIMADZU
Excellence in Science

Multi-analyte Screening Software

LabSolutions Insight Explore



LabSolutions Insight Explore™

Powerful Support for Qualitative Analysis Workflows

LabSolutions Insight Explore software supports a full range of workflows ranging from qualitative to quantitative analysis, providing advanced functionality for precision library searching, structural analysis, and formula prediction based on high-resolution and high-accuracy mass spectrometry data. The software provides comprehensive support for identifying unknown components through compound detection, formula prediction, and library searching. Structures can be queried using accurate mass information or molecular formulae, and fragment assignment for MS/MS spectra is also available. The software also offers batch processing and report generation for qualitative analysis, enabling efficient handling of large datasets in applications such as pesticide screening and illicit drug analysis.
In total, LabSolutions Insight Explore enables efficient qualitative and structural analysis of unknown compounds as well as quantitative analysis.

POINT 01
Pharmaceuticals
Reliable detection of known and unknown impurities from trace samples.

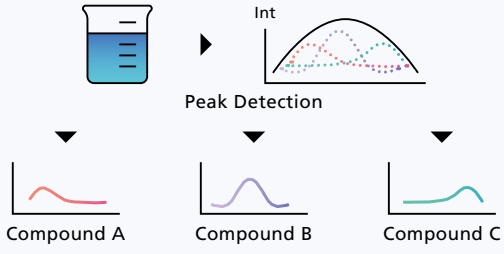
POINT 02
Environment
Reliable detection of contaminants in water and soil.

POINT 03
Forensic Toxicology
Detection of unknown compounds structurally similar to known substances from trace samples.

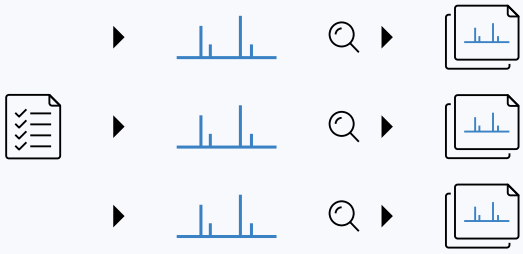
Streamlined Workflow for Unknown Compound Identification

LabSolutions Insight Explore offers streamlined capabilities for essential unknown compound identification workflows.

STEP 01
Candidates Detection
The system detects peaks corresponding to multiple potential compounds hidden within the chromatogram.



STEP 02
Screening
From the detected peaks, it searches for and identifies known compounds.



STEP 03

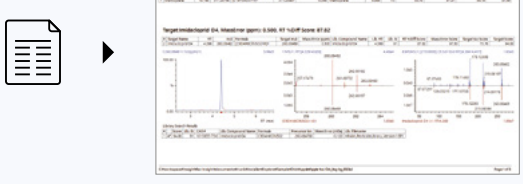
Unknown Compound Identification

For unknown peaks, users can review the chromatograms and spectra, perform library searches, and assign fragment ions to determine compound identities.

STEP 04

Report Generation

Identified compounds are consolidated and output as a comprehensive report.



Efficient Platform for Qualitative Analysis

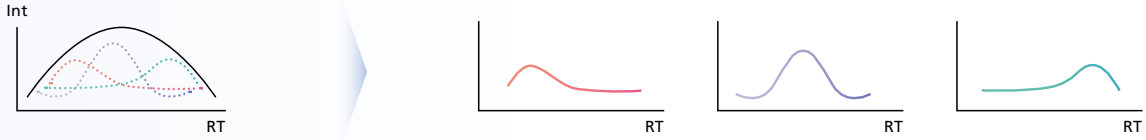
ANALYZE

Core Capabilities that Power the Qualitative Workflow

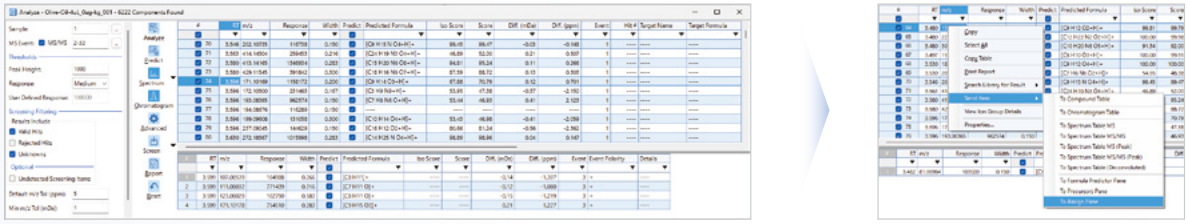
Candidates Detection
Screening
Unknown Compound Identification

High-resolution, high-mass-accuracy mass spectrometers generate enormous volumes of data, making peak identification, qualitative analysis, and quantitation increasingly complex. LabSolutions Insight Explore streamlines these processes with a simple, intuitive workflow that supports everything from qualitative assessment to quantitative analysis.
Analyze serves as the core application of LabSolutions Insight Explore, employing Shimadzu's proprietary Detect algorithm to comprehensively identify peaks corresponding to unknown components within acquired datasets. Starting from Analyze, the software integrates seamlessly with applications such as formula prediction and library searching, enhancing the accuracy of unknown-component characterization and supporting downstream workflows for compound identification and quantitative analysis.

Narrowing Down Unknown Compounds



Searching for Candidate Compounds

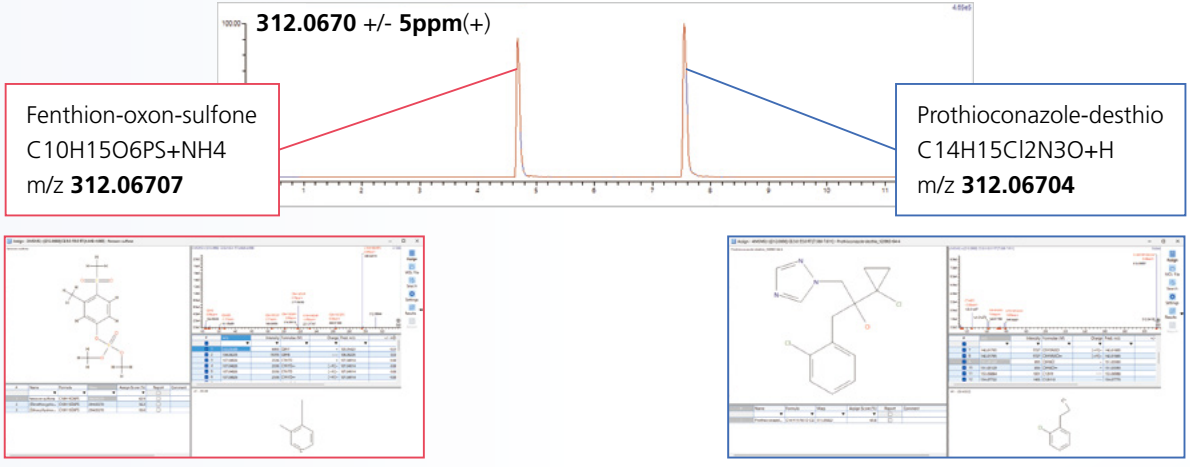


ASSIGN

Rapid Structural Interpretation Using Fragment Information

Unknown Compound Identification

For each acquired high-resolution mass spectrum, the software retrieves candidate molecular structures from online databases and calculates fragment patterns based on those structures. These fragments are then assigned to the corresponding spectral peaks. The compound information obtained from database searches can be output as a candidate list, and the degree of fragment-assignment matching helps support the differentiation of isomers.

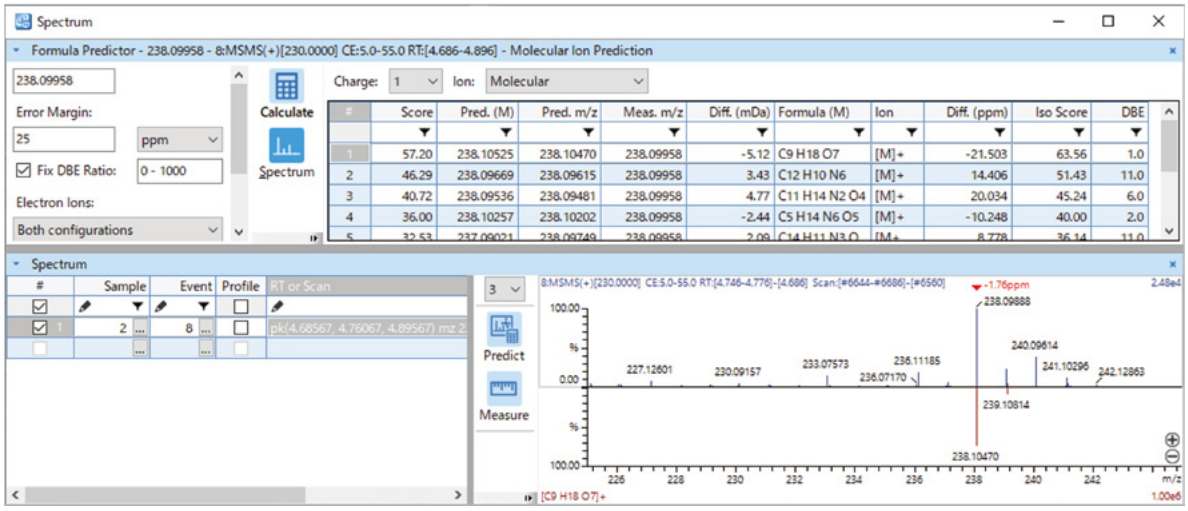


PREDICT

Unknown Compound Identification

Calculating the Composition of Unknown Compounds from Spectral Data

The software calculates elemental compositions based on the measured mass-to-charge ratios (m/z). It then compares the sample's experimental spectrum with the theoretical spectra of candidate compounds, calculating a score that also accounts for isotopic patterns. These combined insights enable users to evaluate the compositional information of the spectrum with greater confidence.

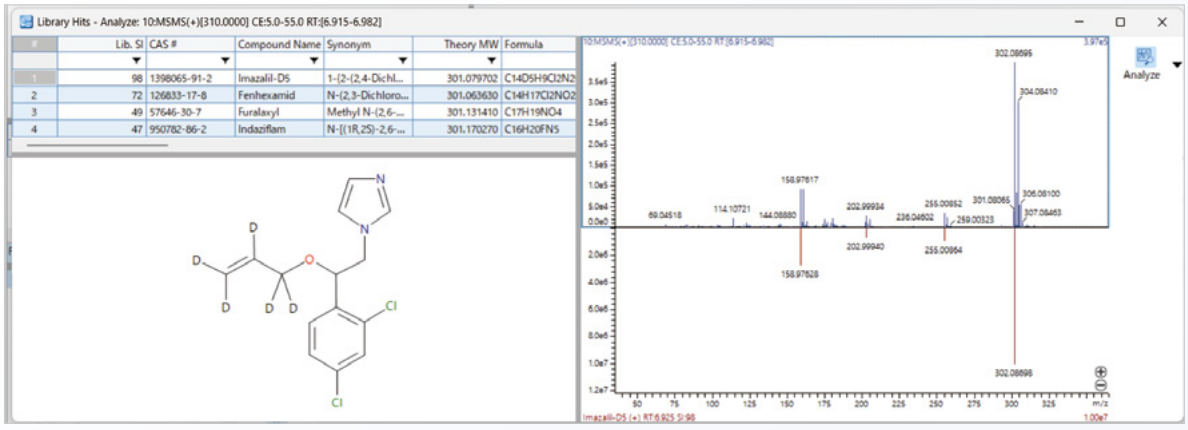


LIBRARY SEARCH

Unknown Compound Identification

High-Speed, High-Performance Library Searching & Editable Results

Library searches can be performed directly using MS/MS spectra. The high-speed, high-performance Insight algorithm rapidly retrieves theoretical spectra and structural information, allowing users to review results simultaneously within a single interface. A table-based library editor is also available, enabling easy modification of library entries.



Supporting a Wide Range of Qualitative Workflows

Qualitative Batch Analysis of Large Sample Sets in Just Four Steps

In applications such as pharmacokinetic studies, illicit drug analysis, and residual pesticide testing, large numbers of samples must be processed under identical conditions. This includes performing qualitative analysis, screening for predefined target compounds, and generating reports summarizing component-detection results. LabSolutions Insight™ Discovery is an application designed to efficiently perform qualitative analysis. It supports this entire workflow—from qualitative analysis of hundreds of samples to final report generation—in just four simple steps.

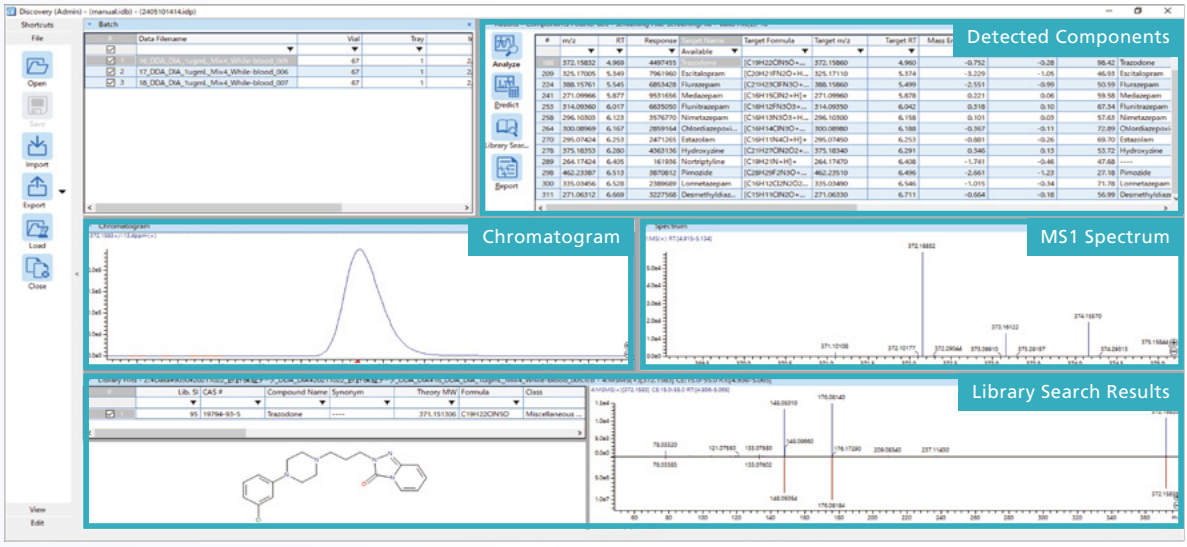
Execute Qualitative Analysis for All Samples in Just Four Steps

STEP 01
Configure
Set up the qualitative batch workflow. In addition to component detection, you can configure screening and library search options.

STEP 02
Load
Import the data files and any associated files required for analysis. Additional data files can be added later as needed.

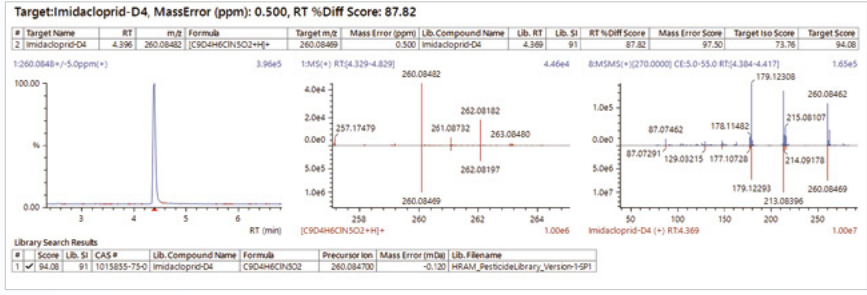
STEP 03
Run
Begin qualitative analysis for all samples with a single click.

STEP 04
Report
Output qualitative analysis results for all samples in MTS format with one click. The report can be used as evidence for component detection results.



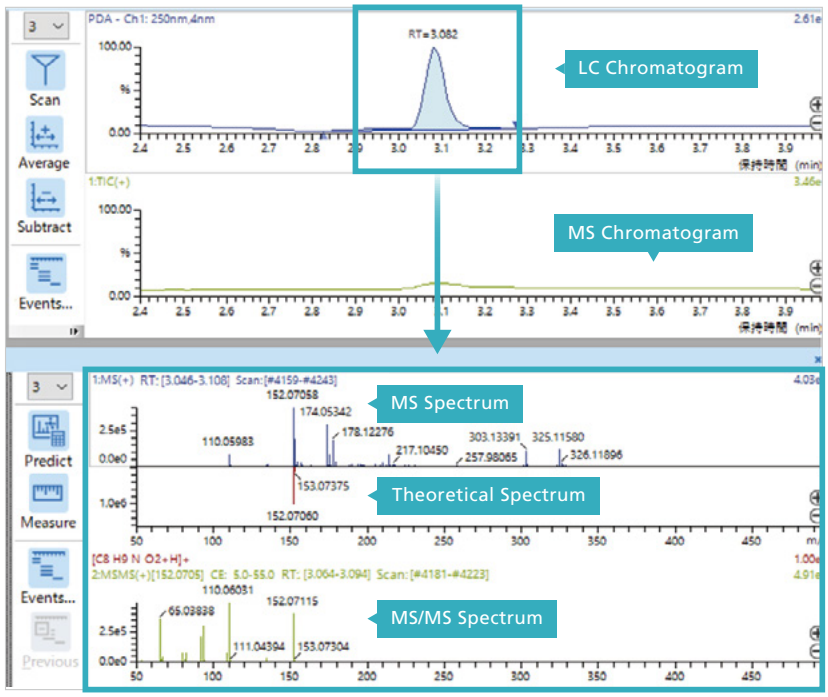
Evidence supporting compound identification can be exported as an MTS-format report.

Note:
LabSolutions Insight Discovery is available only with the file-management version of the software.



Integrated MS Spectra and LC Chromatograms for Impurity Analysis

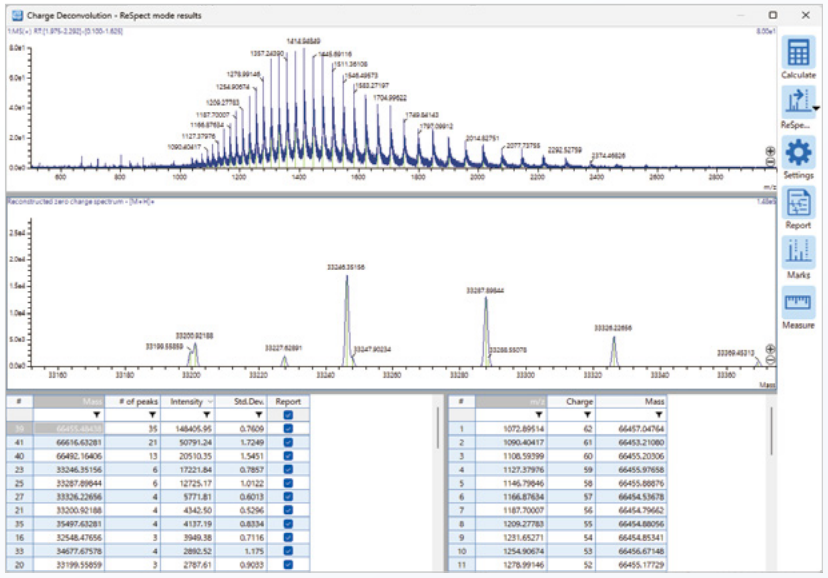
The software allows flexible on-screen arrangement of LC and MS chromatograms and spectra, enabling the display of LC and PDA chromatograms alongside MS data. When used together with LC detectors, this capability supports detailed structural analysis of impurities. For example, in pharmaceutical applications, impurities detected by UV or PDA detectors can be further examined by using MS spectra to determine their structures.



Multi-charged ion analysis algorithm for compounds with high molecular weight

LabSolutions Insight Explore CSD (Charge State Deconvolution) supports multi-charged ion analysis for compounds with high molecular weight. It adopts a multi-charged ion analysis algorithm from Positive Probability Limited that can handle high charge states. This capability is particularly useful for analyzing macromolecular compounds such as peptides.

Note:
LabSolutions Insight Explore CSD is an optional software for LabSolutions Insight Explore.



Software Lineup

LabSolutions Insight Explore	Qualitative analysis software for LCMS.
LabSolutions Insight Explore CSD	Software for qualitative analysis of multiply charged ions in LCMS.

Shimadzu Corporation
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