

Non-Targeted Analysis Software for LC/QTOF Data

LabSolutions Insight™ Profiler



LCMS-9050

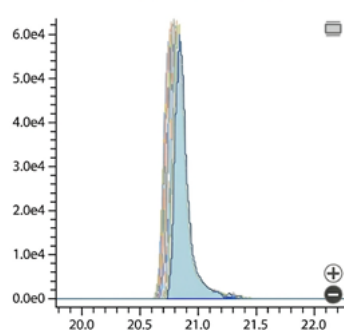
LabSolutions Insight Profiler is a unified, end-to-end workflow for LC/QTOF data processing — with a "single-click" approach. Insight Profiler is purpose-built for non-targeted analysis in suspect screening, unknown identification, and metabolomics across complex sample sets.

Making non-targeted data processing easier and faster

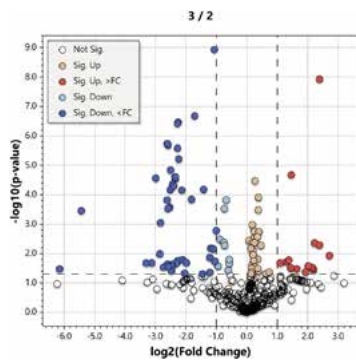
Traditionally, untargeted LC/QTOF workflows demanded sequential processing across multiple platforms. This software consolidates that entire pipeline into a single configurable method.

Load your data, set your parameters once, and a single click drives automated feature detection, alignment, large-scale suspect screening against MS/MS libraries, PCA, loadings plots, and volcano plots — with results comparable to the multi-platform workflow obtained in a fraction of the time. Pre-built method templates accommodate both new and experienced analysts, supporting applications across toxicology, food safety, extractables and leachables, and metabolomics-based biomarker discovery.

1: 150.0531-150.0631(+) - SFC_DDA+_001_Sa... 5.98e4

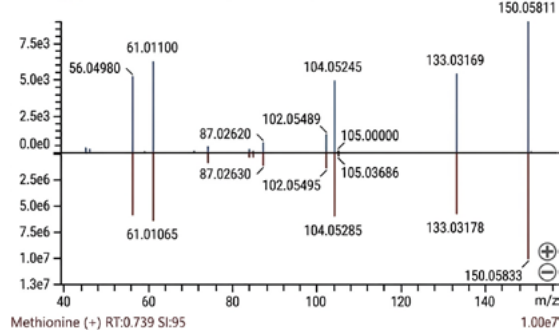


The Analyze non-targeted algorithm extracts compound features from each sample and aligns them across the sample set by accurate mass and retention time.



Integrated statistical tools — t-test, fold-change analysis, PCA scores and loading plots, volcano plots, and box plots — identify components that are shared or significantly different across sample groups.

2:MSMS(+)[150.0582] CE:5.0-55.0 RT:[20.774-21.247]



Suspect screening hits and statistically significant compounds are identifiable against curated Shimadzu and public MS/MS libraries.

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A single click approach to data processing

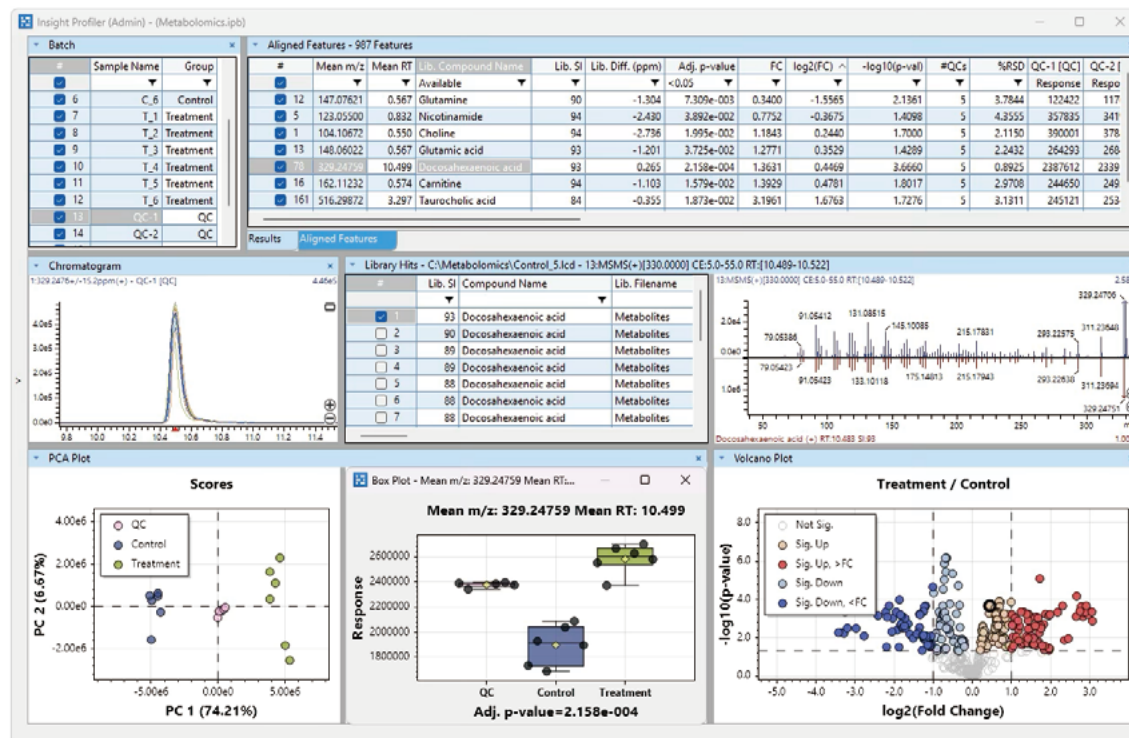
Profiler processing methods can be predefined for specific workflows — whether suspect screening or metabolomics — enabling both new and advanced users to generate results quickly with a single click. Each processing method includes optimized settings for its intended application, creating a streamlined platform for processing complex data sets.

Group variables setup

In a metabolomics example, two groups (control and treatment) were loaded with QCs

Interactive and intuitive data review

Chromatograms, spectra, and library identification results are interactively linked to statistical outputs, including PCA, volcano, and box plots, enabling rapid, context-rich interpretation of complex data sets.



Statistical Processing

The Profiler method was configured to automatically present PCA and volcano plots following analysis on features that met the filtering criteria for this study (based on the pooled QC and group variance tolerances). The box plot is presented on a user-defined component.

Delivering an intelligent workflow for processing complex data sets

From environmental and forensic toxicology screening to extractables and leachables and metabolomics-based biomarker discovery, Insight Profiler's single-click processing methods bring the full power of untargeted LC/QTOF analysis within reach of any laboratory.

Precautions

Requires LabSolutions LCMS Ver. 5.135 SP1 or later.

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