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Application News

LabSolutions Insight Profiler Streamlines Analysis of Untargeted Metabolomics Data from LC/QTOF Analysis

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User Benefits

- Application of LabSolutions Insight™ Profiler, a novel software solution for untargeted analysis, bringing together feature detection and alignment, statistical analysis, filtering and compound identification into a single processing method.
- The workflow has been applied in a study to reveal potential candidate biomarkers of pancreatic cancer.
- LabSolutions Insight Profiler delivers an end-to-end solution for untargeted metabolomics research automating complex data processing from sample analysis through to identification of statistically significant features.

■ Introduction

Advances in untargeted metabolomics increasingly rely on integrated workflows which utilise complex spectral deconvolution, data alignment, and multivariate interpretation. Several applications provide complementary capabilities for data processing and statistical analysis; however, transitioning data across discrete platforms increases workflow fragmentation, especially for large scale metabolomics studies.

In this application, a single software package, LabSolutions Insight Profiler, has been developed to automate feature detection and alignment, statistical analysis and filtering with compound identification, delivering an integrated workflow solution for untargeted analysis applications such as metabolomics.

The data processing application has been applied to a biomarker discovery study with pancreatic cancer serum samples from patients with pancreatic ductal adenocarcinoma (PDAC) and healthy controls analysed by LC/QTOF on the LCMS-9030. The workflow is applicable to any untargeted metabolomics study using the LCMS-9030 or LCMS-9050 QTOF. The research project was approved by the Pancreatic Cancer Research Fund Tissue Bank (PCRFTB) Tissue Access Committee.

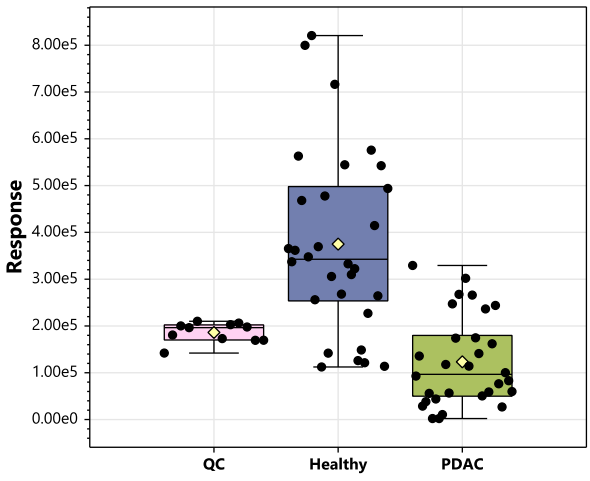


Fig. 1 Boxplot of PC 18:2_18:2 (m/z 782.56936) in positive ion mode; a feature identified as being significantly different between healthy and pancreatic ductal adenocarcinoma (PDAC) profiles.

■ Methods

Serum samples from PDAC patients (n=30) and healthy controls (n=30) were extracted in methanol (1:3 v/v) and diluted 1 in 10 (positive ion mode) or 1 in 2 (negative ion mode) for untargeted metabolomics analysis. The LC/QTOF method (Table 1) was designed for the highest metabolome coverage and has been previously applied to biofluids, tissues, and cell cultures.

In common with established untargeted metabolomics methodologies, quality control (QC) samples were included in the analysis[1]. Pooled QCs were prepared by combining equal aliquots of each sample and were used to equilibrate and stabilise the system at the start of the analysis. Samples were analysed in a random order with a QC injected after every 6 to monitor system performance and filter out any feature that resulted in high variance in signal intensity.

Data were acquired in positive and negative ion mode on the LCMS-9030 operated using LabSolutions™ and processed and analysed using LabSolutions Insight Profiler. The method represents an end-to-end solution for untargeted metabolomics using Shimadzu LC/QTOF.

Table 1. Analytical conditions

[UHPLC conditions] (Nexera X2)	
Column	C18 (2.1x100 mm 1.7 µm)
Oven temp.	50 °C
Flow Rate	0.4 mL/min
Mobile Phase	A: Water + 0.1% formic acid B: Acetonitrile + 0.1% formic acid
Rinse (R0/R1/R2)	IPA/MeOH/MeCN/H_2O (1:1:1:1) + 1% formic acid
Time program (%B)	2% B (0-1 min) → 40% B (2 min) → 90% B (25 min, curve -3) →100% B (27.5-31 min) → 2% B (31.01-35 min)
Injection	0.5 µL, autosampler temperature 4 °C
[MS conditions] (LCMS-9030)	
Interface	ESI:1.5 kV (+) / -3.0 kV (-)
Mode	Data Independent Acquisition (DIA)
Interface temp.	300 °C
Heat block temp.	400 °C
DL temp.	250 °C
Nebulizing gas flow	3 L/min
Heating gas flow	10 L/min
Drying gas flow	15 L/min
CID gas pressure	230 kPa
MS	TOF-MS (*m/z* 60-1000)
MS/MS	*m/z* 40-1000, 27 events , precursor isolation 35 Da collision energy spread 5-55 V
Total cycle time (MS and MS/MS)	~1 second

■ Data Processing using LabSolutions Insight Profiler

Data files from the untargeted metabolomics analysis of PDAC and control serum profiles were first loaded into LabSolutions Insight Profiler. As the initial step, the samples were assigned to one of three groups: 'Healthy', 'PDAC', or 'QC'. Following group assignment, the processing method was applied as a batch to the loaded dataset for automated feature detection, alignment, filtering, and statistical analysis.

The processing method for feature detection used a minimum peak height of 1000 and a low MS response threshold, corresponding to a sum ion signal of at least 10,000 counts across a chromatographic peak. Features were aligned using a mass tolerance of 10 mDa and a retention time tolerance of 0.1 min.

Filtering was performed according to standard criteria for untargeted metabolomics. Features exhibiting high variance in the QC samples (>20% RSD) were excluded, and only features detected in at least 75% of the samples in the PDAC and/or control groups were included for statistical analysis. Missing values were replaced with one-fifth of the minimum value detected for the respective feature in the other samples. The significance threshold for fold change was set at 2, with a p-value threshold of 0.05. For two-group comparisons, p-values were automatically calculated by the software using a t-test.

Compound identification was performed using the automated library-searching functionality of LabSolutions Insight Profiler. The search supports up to five MS/MS libraries and considered several curated and public-domain compound databases, including Shimadzu compound databases (in-house libraries), LipidBlast, HMDB, NIST, MassBank, and MoNA.

Once a processing method has been set-up and saved, it can be applied as a single click by a new user or an advanced expert. The result is a single click operation that can automate complex data processing helping to identify compounds that differ between sample groups (Fig. 2).

Feature Detection and Alignment
Detects and aligns all ion signals that behave as a peak.

Statistics
Applied to identify significant ion signals and remove highly variable ions according to predefined filtering criteria.

Screening and Identification
Using large scale screening lists and multiple libraries to identify ion signals of interest.

Batch
A single, configurable workflow integrates feature detection, alignment, and compound identification, enabling automated batch processing for untargeted analysis.

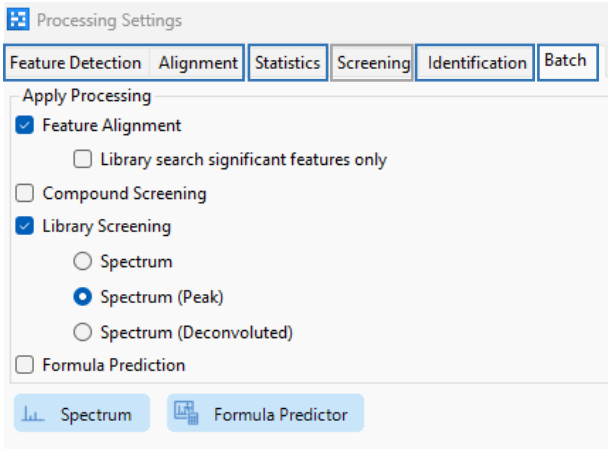


Fig. 2 LabSolutions Insight Profiler Processing Settings editor showing the Batch settings. The Processing Setting editor is used to save a single method for feature detection and alignment, statistical analysis and flexible compound identification, all driven by a batch process to support automated processing. (The method also supports untargeted screening and profiling workflows for LC/QTOF data, though it was not applied in this application).

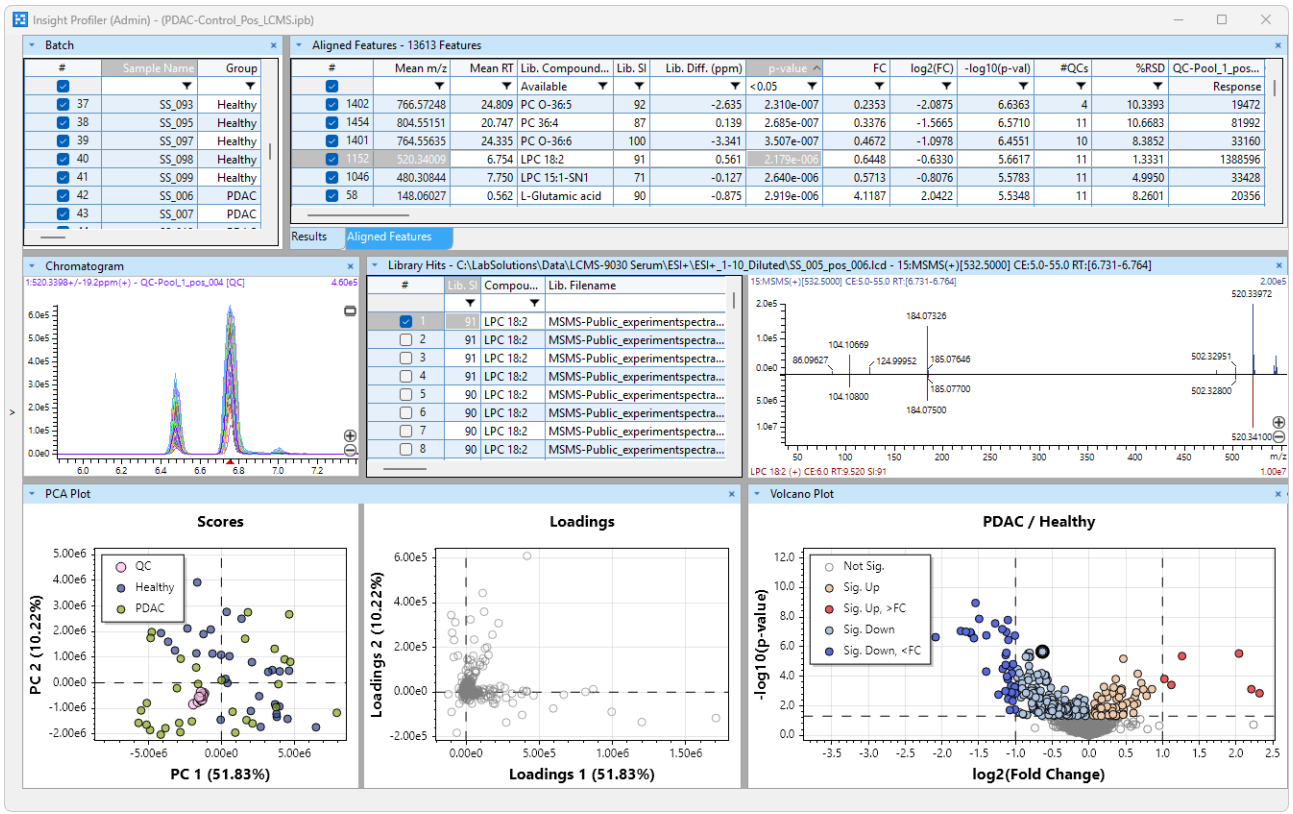


Fig. 3 LabSolutions Insight Profiler applied to the analysis of serum extracts from PDAC patients and healthy controls following untargeted metabolomics analysis (LC/QTOF). Interactive and intuitive data review enables analysis of statistically significant features. Chromatogram, spectrum and library identification are linked with statistical analysis, including PCA/Volcano plots, helping data interpretation to find potential biomarkers.

LabSolutions Insight Profiler enables seamless navigation by linking tables and plots to selected samples and features, supporting fast, intuitive review of statistically significant data (Fig. 3). Selecting a result in the 'Results' or 'Aligned Features' tables highlights it across statistical plots (e.g. PCA loadings, volcano plot).

For any selected feature, 'Chromatogram' displays extracted ion chromatograms across detected samples, while the MS spectrum for the highlighted sample in 'Batch' can be shown in the 'Spectrum' pane.

The PCA scores plot is also linked to the 'Batch' table, highlighting the active sample. PCA and boxplots can be viewed with or without QC samples.

Where available, 'Library hits' lists all matches ranked by similarity index (SI), with highest confidence from authentic standards analysed using equivalent methods.

MSI level 2 identifications can be assigned from third-party library hits; though they do require manual review by the analyst before reporting to prevent misidentification, as highlighted by Theodoridis et al. (2026)[2].

In this study, LabSolutions Insight Profiler analysis of LC/QTOF data revealed clear metabolite differences versus healthy serum controls. Consistent with literature, linoleic acid–containing phospholipids were significantly reduced[3] (e.g. LPC 18:2, PC 18:1_18:2, PC 18:2_18:2, PC 18:2_20:4; Fig. 4). LPE 18:2, LPC 18:1, LPC 18:3, and LPC 20:5 were also decreased. Glutamic acid was significantly elevated in PDAC serum and confirmed to MSI level 1 using an authentic standard.

Lipids were assigned to MSI level 2 via MS/MS matching to LipidBlast. All hits were reviewed manually, and confidence was strengthened by confirming corresponding features in negative ion mode (Fig. 4).

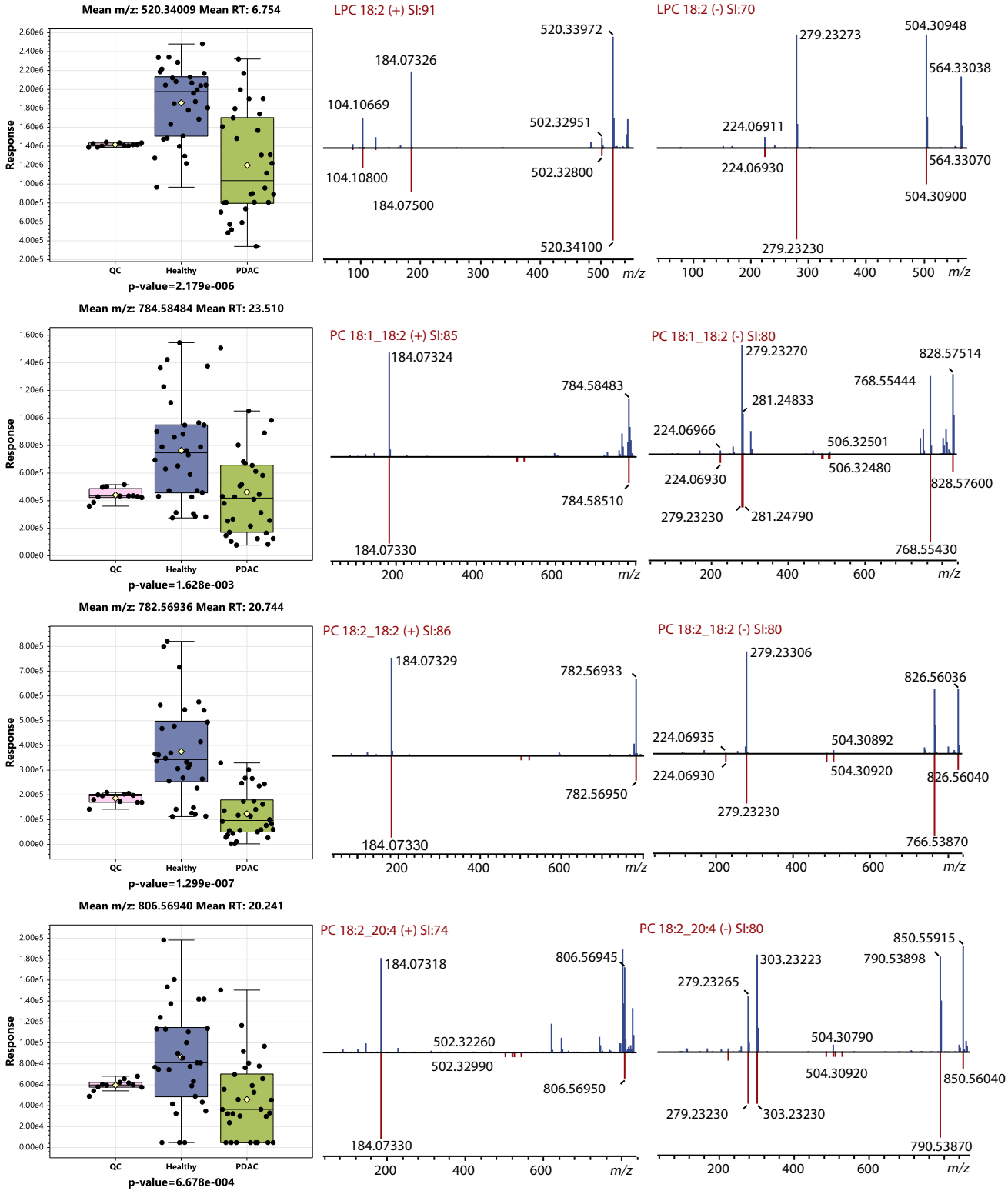


Fig. 4 Boxplots of significantly different features detected by LC/QTOF analysis of PDAC patient serum samples compared to controls. Features were putatively identified in both positive and negative ion mode data to provide higher confidence identifications. The upper spectra show the acquired DIA-MS/MS spectra and the lower spectra are LipidBlast library MS/MS spectra.

■ Conclusion

LabSolutions Insight Profiler is a single software application developed to automate feature detection and alignment, statistical analysis and filtering with spectral annotation. To highlight a workflow for untargeted metabolomics, the software application has been applied to a biomarker discovery study of pancreatic cancer. The analysis of LC/QTOF data with DIA-MS/MS acquired from serum extracts from PDAC patients and healthy controls enabled the detection of statistically significant features distinguishing the two phenotypes that could be identified to metabolomics standards initiative[4] level 1 or 2 within the same processing method. Using a single processing method cascade to automate metabolomics data analysis helps to simplify complex data processing workflows without compromising data quality.

■ References

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