Differential Analysis Function in msFineAnalysis Ver 3 (3): Analysis of Vinyl Acetate Resin by Using Pyrolysis-GC-TOFMS

Related product : Mass Spectrometer(MS)

Introduction

As the performance of mass spectrometers has improved, the demand for differential analysis of trace components in materials has increased. To address this trend, we have added a new differential analysis function to msFineAnalysis, our automated qualitative analysis software specifically designed for GC-HRTOFMS data. In this work we used msFineAnalysis to compare Vinyl Acetate Resins that were measured by using Pyrolysis (Py)-GC-MS.

Analysis detail

Two commercially available Vinyl Acetate Resins (adhesives) (A, B) were used as samples. In order to conduct statistical analysis, GC/EI measurements were performed for n=5. As the condition for differential classification, p-value (an index: the smaller the p-value, the higher the statistical reproducibility) ≦5% and fold change (intensity ratio between samples) ≧1.5 were used to perform differential analysis by using msFineAnalysis. The Table 1 shows the measurements condition details.

Table 1. Measurement and analysis conditions

Py-GC-MS	
Pyrolyzer	EGA/PY-3030D (Frontier Laboratories Ltd)
Mode	Single shot
Furnace	600℃
Gas Chromatograph	7890A GC (Agilent Technologies, Inc.)
Mode	Split mode (100:1)
Column	DB-5msUI (Agilent Technologies, Inc.) 15m x 0.25mm, 0.25μm
Oven Temperature	50°C(1min)-30°C/min -330°C(1.7min)
Carrier flow	He:1.0mL/min

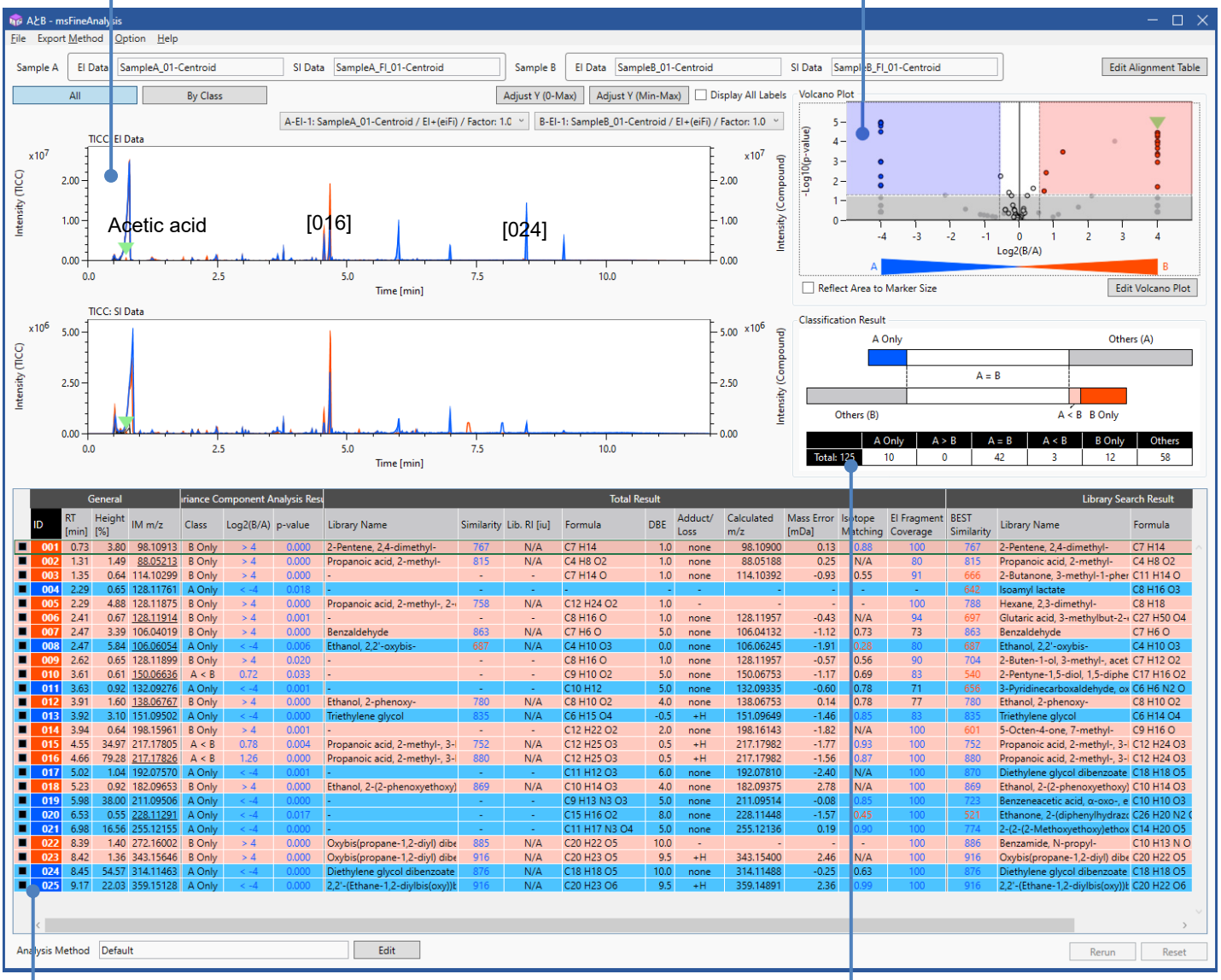
TOFMS	JMS-T200GC (JEOL)
Ionization	EI+:70eV, 300μA FI+:-10kV, 6mA, Carbotec-5μm (CarboTech)
Mass Range	*m/z* 35-600
msFineAnalysis	(JEOL)
Mode	Variance component analysis
Number of data	n=5
p-value	≦5%
Fold change	≧1.5

Results

Figure 1 shows a screenshot of the differential analysis results for the vinyl acetate resins by using msFineAnalysis. In total, 125 peaks were detected. The breakdown of the differential peaks are: 10 peaks that are characteristic of Sample A (peak ID [024] Diethylene Glycol Dibenzoate, etc.), 15 peaks that are characteristic of Sample B ([016] 2,2,4-Trimethyl-1,3-pentadioldiolMonoisobutyrate, etc.), and 42 peaks did not show a difference between sample A and B. Additionally, there were 58 peaks that were judged to have no statistical reproducibility (gray in volcano plot, “other” in classification results).

Chromatogram
Top: GC/EI(TICC/compound peak), Bottom: GI/FI
The color of the compound peak reflects the results of difference judgment
Blue = Strong with Sample A
Red = Strong with Sample B
Yellow = No intensity difference(<2 times)

Volcano plot
X axis: Log2(fold change) Y axis:-Log10(p-value)
Blue = Strong with Sample A
Red = Strong with Sample B
White = No intensity difference(<2 times)
Gray = Low reproducibility



Peak List
The color reflects the results of difference judgement
Blue = Strong with Sample A
Red = Strong with Sample B
Note: Only peak of difference are shown.

Judgement Result
The ones with high reproducibility are classified into A only, A>B, A=B, A<B, B only.
The ones with low reproducibility are classified into others.

Figure 1. Screenshot of msFineAnalysis

Figure 2 shows a screen shot of individual compound analysis result for peak ID [015]. The first library search candidate (similarity 857) indicated 2,2,4-trimethyl-1,3-pentadioldiisobutyrate ($C_{16}H_{30}O_4$: molecular weight 286). However, since *m/z* 217 was detected as the base peak in the FI mass spectrum, it was decided that it is more likely the protonated molecule $[M+H]^+$ for the second candidate (similarity 755) of 2,2,4-trimethyl-1,3-pentadiol Monoisobutyrate ($C_{12}H_{24}O_3$: molecular weight 216). Consequently, the second candidate was selected as the result appropriate choice for the integrated analysis. This example shows that using EI/SI data together, msFineAnalysis makes it possible to obtain highly reliable results.

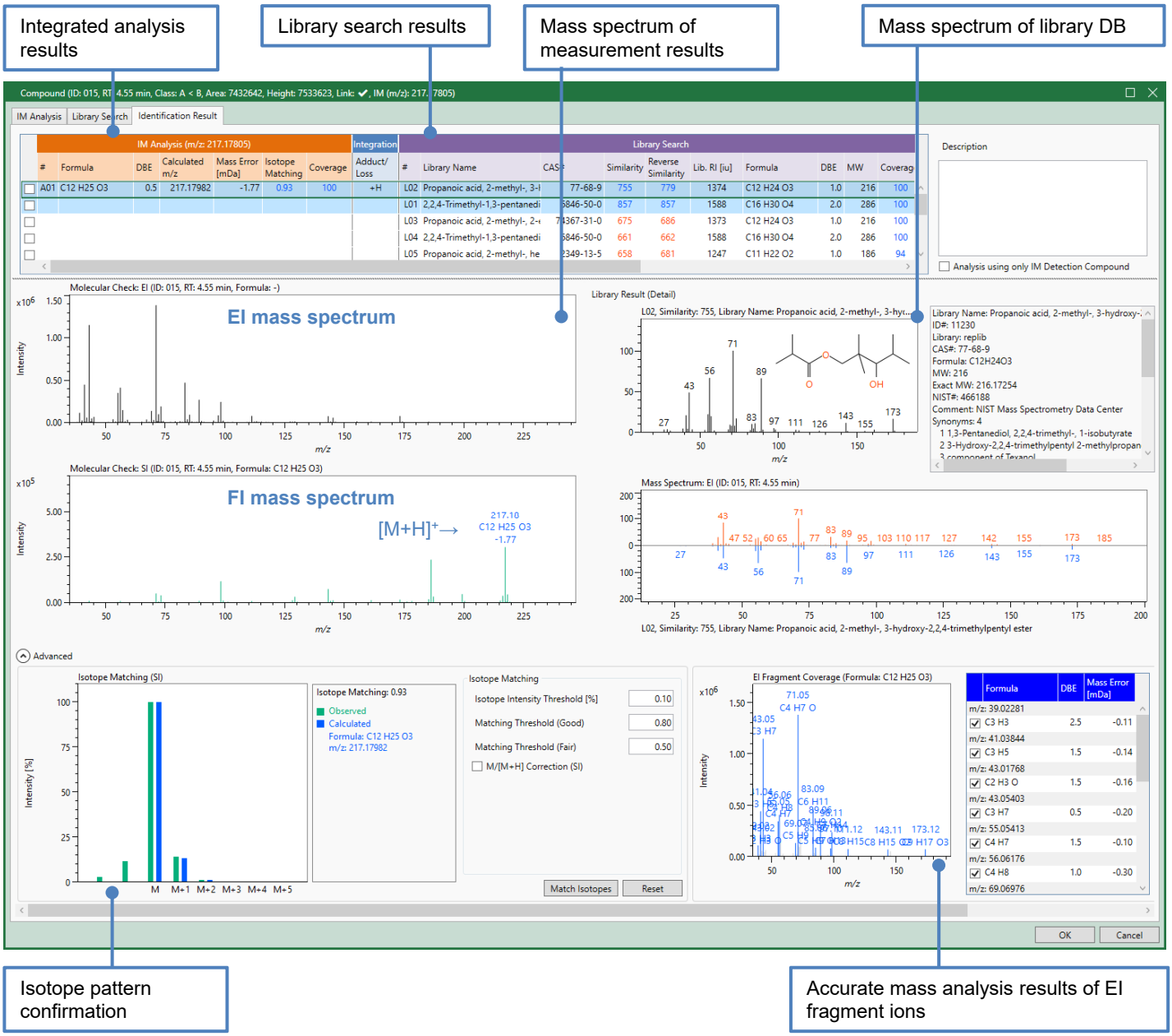


Figure 2. Screenshot of compound window

Summary

The differential analysis function of msFineAnalysis Ver3 enabled us to easily obtain the differential information between two Vinyl Acetate samples. Also, because EI and SI data are analyzed together, msFineAnalysis produces highly reliable qualitative analysis results that can be quickly evaluated by the analyst. And finally, this software in combination with GC-HRTOFMS is especially effective for pyrolysis methods in which many of the compounds produced are not registered in library databases.

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