

Differential Analysis Function in msFineAnalysis Ver 3 (2): Analysis of Coffee Bean Aroma Component using Headspace-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 coffee bean aromas by using headspace (HS)-GC-MS. Additionally, the analysis results were consistent with the characteristics of the production area for the coffee beans.

Analysis detail

Two commercially available coffee beans (A: from Guatemala, B: from Brazil) were used as samples. The measurements were performed with the steps below.

- 1) Put 1g of coffee beans in a 22mL HS vial, pour 15mL of boiling water to 100°C, and seal.
- 2) Cool the sample vial to room temperature, collect 10mL of supernatant liquid, and add 2μL of the internal standard (p-Bromofluorobenzene).
- 3) Separate the above into 2mL each for 5 HS vials and seal.

GC/EI measurements were performed for n=5 in order to conduct statistical analysis of the sample differences. The msFineAnalysis differential analysis conditions involved using p-value (an index: the smaller the p-value, the higher the statistical reproducibility) $\leq 5\%$ and fold change (intensity ratio between samples) ≥ 1.5 . Table 1 shows the measurements condition details.

Table 1. Measurement and analysis conditions

HS-GC-MS		TOFMS	
Headspace sampler	MS62070STRAP (JEOL)	TOFMS	JMS-T200GC (JEOL)
Mode	Trap	Ionization	EI+:70eV, 300μA
Sample heating	60°C, 15min		FI+:-10kV, 8mA,
Gas Chromatograph	7890A GC (Agilent Technologies, Inc.)	Mass Range	Carbotec-5μm (CarboTech) <i>m/z</i> 35-600
Mode	Split mode (30:1)	msFineAnalysis	(JEOL)
Column	ZB-WAX (Phenomenex Inc) 30m x 0.18mm, 0.18μm	Mode	Variance component analysis
Oven Temperature	40°C(3min)-30°C/min -250°C(10min)	Number of data	n=5
Carrier flow	He:1.0mL/min	p-value	$\leq 5\%$
		Fold change	≥ 1.5

Results

Figure 1 shows a screenshot of the differential analysis results for the coffee samples by using msFineAnalysis. In total, 141 peaks were detected. The breakdown of the differential peaks are: Sample A: 6 peaks that are characteristic of Guatemalan coffee aroma (peak ID[006]:furfural, [007]acetic acid, etc.), Sample B: 3 peaks that are characteristic of Brazilian coffee ([001] methylfuran, etc.), and 52 peaks that did not show a difference between Sample A and B. Additionally, there were 88 peaks that were judged to have no statistical reproducibility (gray in volcano plot, "other" in classification results). From Sample A, the Guatemalan coffee, hexanal (aroma of grass), methyl acetate (fruit-like aroma), acetic acid, linalool (citrus/floral aroma) were strongly detected. These results are consistent with the freshness and crispness that are characteristics of the coffee beans from Guatemala. From Sample B, the Brazilian coffee, methylfuran (chocolate-like aroma), dimethyl disulfide (garlic-like aroma) were detected, which is consistent with the richness that is characteristic of coffee beans from Brazil.

Chromatogram

Top: GC/EI(TIC/compound peak), Bottom: GI/FI

The color of the compound peak reflects the results of difference judgment

Blue = Strong with Sample A (Guatemala's)

Red = Strong with Sample B (Brazil's)

Yellow = No intensity difference (<2 times)

Volcano plot

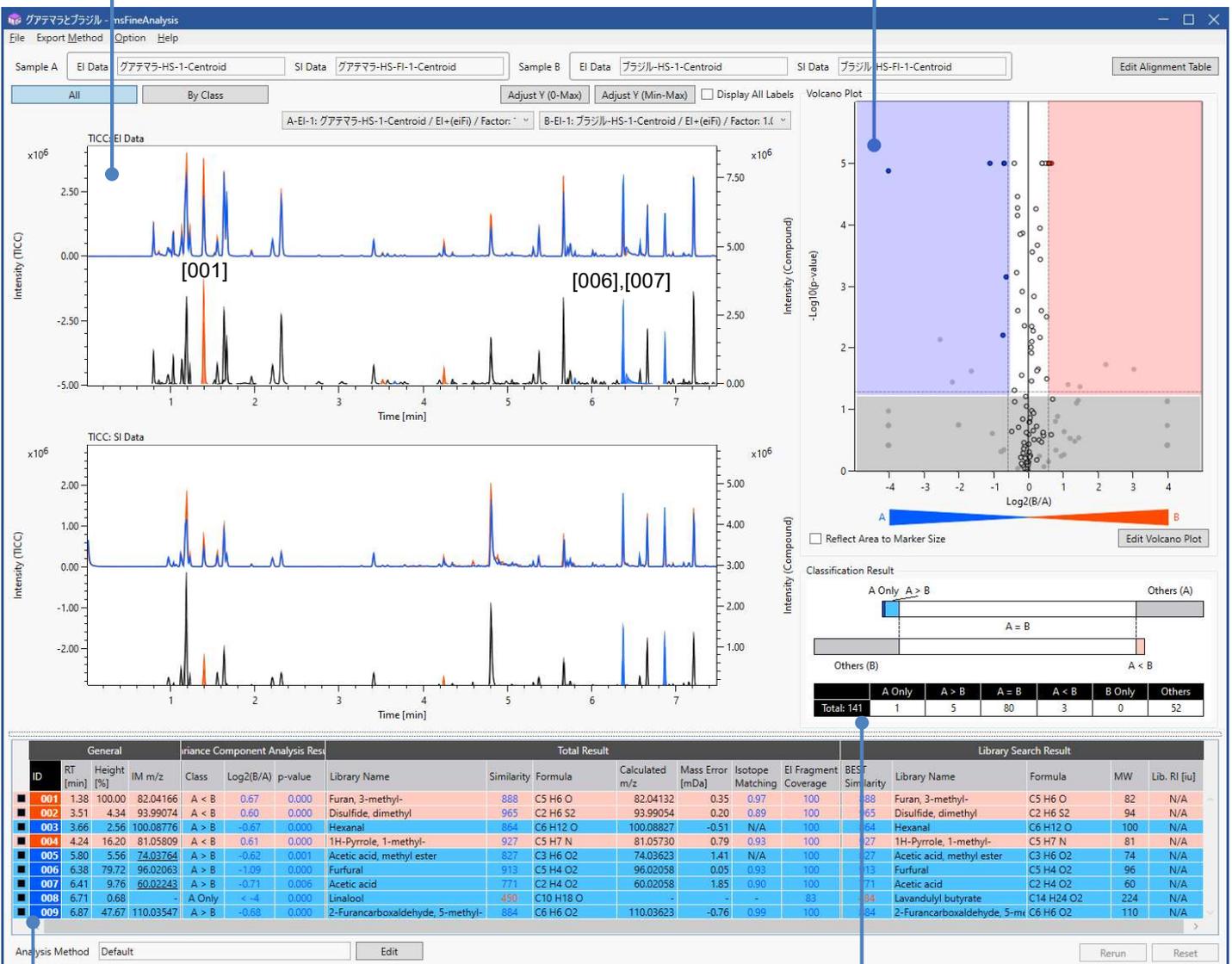
X axis: Log2(fold change) Y axis: -Log10(p-value)

Blue = Strong with Sample A (Guatemala's)

Red = Strong with Sample B (Brazil's)

White = No intensity difference (<2 times)

Gray = Low reproducibility



Peak List

The color reflects the results of difference judgement

Blue = Strong with sample A(Guatemala's)

Red = Strong with sample B(Brazil's)

Note: Only peak of difference are shown.

Classification 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 screenshot of the data alignment (identity determination) of msFineAnalysis. Linalool is represented by a very minor peak with an intensity ratio of 0.68% to the maximum peak, and is likely to be missed by manual analysis. By using peak deconvolution detection, msFineAnalysis allows for the detection of minor peaks that are not obvious in the TICC. Furthermore, the statistical analysis of multiple measurements results in highly reliable qualitative analysis results by removing peaks from the analysis list that are not statistically reproducible.

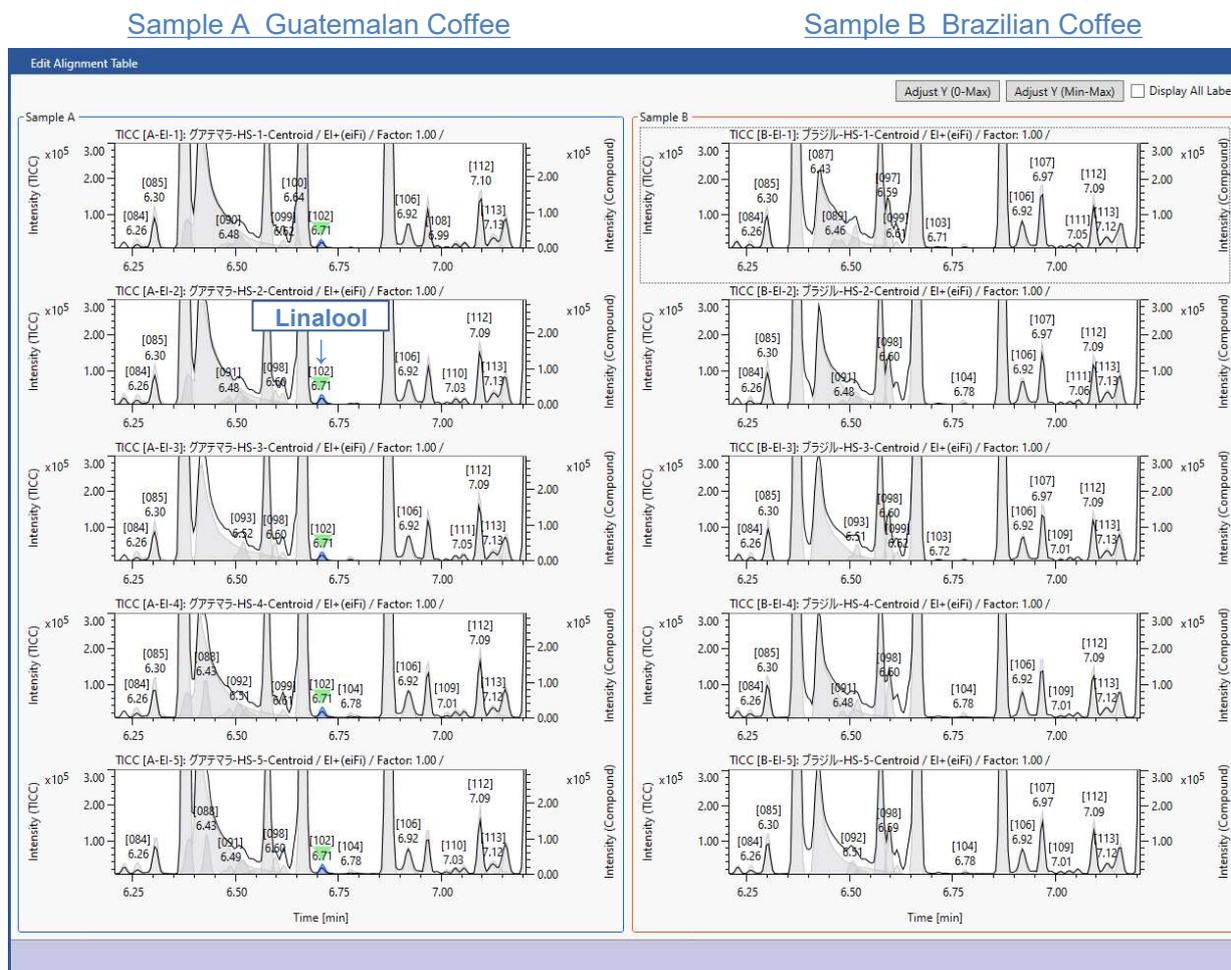


Figure 2. Screenshot of alignment window

Summary

The differential analysis function of msFineAnalysis Ver3 enabled us to easily identify coffee bean aroma components that are consistent with the characteristic of the production region (Guatemalan versus Brazilian). As a result, msFineAnalysis offers sophisticated capabilities such as peak deconvolution and statistical analysis to effectively differentiate samples from each by using trace components such as an aromas for sample differentiation.

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