Analyzing an Off-flavor Component of Adhesive using Group Analysis Function of msFineAnalysis AI

Product used: Mass Spectrometer (MS)

Introduction

Electron ionization (EI) is one of the most popular ionization methods used in gas chromatography-mass spectrometry (GC-MS). Consequently, compounds are typically identified by a mass spectral database search using EI mass spectra. Because molecular ions are often weak or absent in 70 eV EI mass spectra, identification of unknowns can be difficult by EI alone. In these cases, soft ionization (SI) can be very helpful for producing and identifying molecular ions. Recently, JEOL began developing an integrated qualitative analysis workflow that automatically combines and interprets the information from EI and SI data[1]. And then in 2018, we introduced our integrated qualitative analysis software “msFineAnalysis” which uses both EI and SI data to improve compound identification for GC-MS applications. Despite the fact that msFineAnalysis was automatically able to determine the molecular formula and partial structure information from EI fragment ion formulas, the actual structural formulas still required manual analysis using chemical compositions. To address this, we then developed an automated structure analysis software package entitled “msFineAnalysis AI” which uses artificial intelligence (AI) to predict EI mass spectra from chemical structures[2].
The msFineAnalysis AI software has a Group analysis function that enables easy extraction of specific compounds. In MSTips No. 417, we introduced an overview of group analysis function and example of its application for vinyl acetate resin samples. The group analysis function includes a list of characteristic fragment ions and neutral losses as described in MSTips No. 417, as well as an "additive list" containing major additives for polymeric materials and an "off-flavor list" containing off-flavor components. In this MSTips, we will introduce off-flavor compounds analysis results using this group analysis function with “off-flavor list”.

Experimental

A commercially-available adhesive was used as a test sample in this study. We performed Py-GC-HRTOFMS measurements using both EI and field ionization (FI) modes with a combination EI/FI ion source. The qualitative data processing was performed with msFineAnalysis AI (JEOL). Measurement conditions are shown in Table 1.

msFineAnalysis AI

Table 1 Measurement and analysis conditions

Pyrolysis conditions	
Pyrolyzer	EGA/PY-2020D(Frontier Lab)
Pyrolysis Temperature	600°C
GC conditions	
Gas Chromatograph	7890 GC (Agilent Technologies)
Column	DB-5msUI (Agilent) 15m x 0.25mm, 0.25µm
Oven Temperature	50°C(1min)-30°C/min -330°C(1.7min)
Injection Mode	Split mode (100:1)
Carrier flow	He:1.5mL/min

MS conditions	
Spectrometer	JMS-T200GC (JEOL Ltd.)
Ion Source	EI/FI combination ion source
Ionization	EI+:70eV, 300µA
	FI+:-10kV, 6mA/10msec (Carbotec)
Mass Range	*m/z* 35-800
Data processing condition	
Software	msFineAnalysis AI (JEOL Ltd.)
Library database	NIST20, AI Library (JEOL Ltd.)

Results and Discussion

Extraction of off-flavor component by group analysis

Figure 1 shows an example of off-flavor compounds analysis result using group analysis function with “off-flavor list”.
The chromatographic view on the left top shows the GC/EI data with the TICC marked by a solid black line. The bottom left view shows the soft ionization data with the TICC marked by a solid green line. The view on the right shows “Ion List” (applied the off-flavor list) detected in the analysis data. This off-flavor list contains 33 molecular formulas. If a compositional formula registered in this off-flavor list is present in the analysis data, the compound name of the off-flavor component, the type of odor, and the CAS number will be displayed in the Description column. In this study, multiple ions were detected that matched the molecular formula of the off-flavor component. This time, we focused on ion that match acetophenone (Sweet pungent odor, CAS No. 98-86-2) with the molecular formula C_8H_8O.
The blue peaks in each data of Figure1 represent the components containing $C_8H_8O^+$ extracted from the chromatographic deconvolution result. The operator can select an ion such as $C_8H_8O^+$ from the table and click the OK button at the bottom right of the GUI to immediately create a C_8H_8O tab, thus allowing for extraction of the components containing $C_8H_8O^+$ (Figure 2).

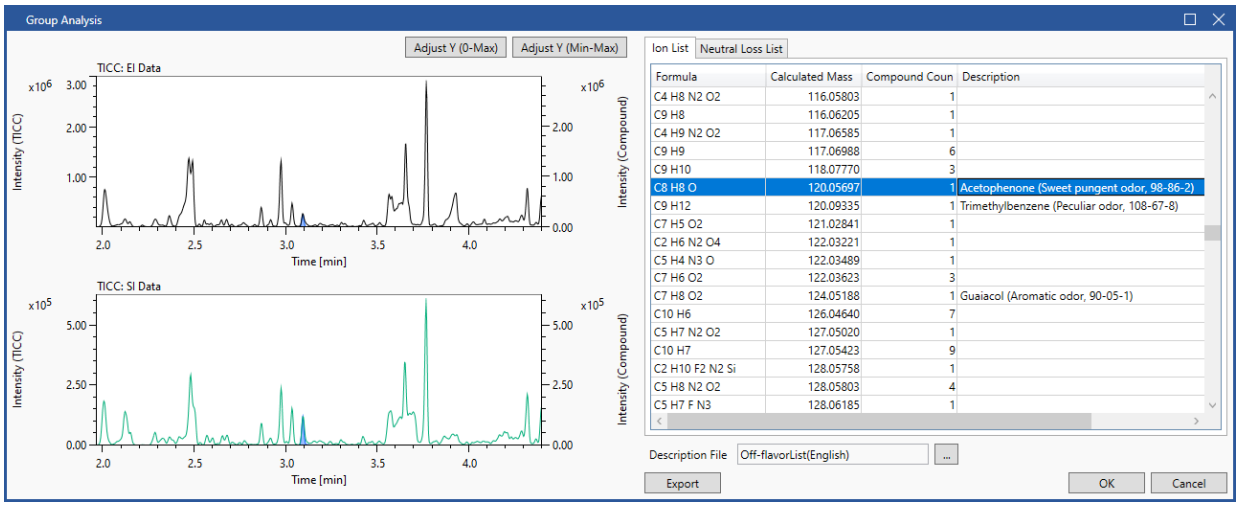

Figure1 Group analysis result using off-flavor list

Figure 2 shows the extracted results for components containing $C_8H_8O^+$ The Group Analysis function displays an “All” tab for the entire analysis results and up to 5 tabs for groups created for ions or neutral losses specified from the exact mass list in Figure 1. The ID and integrated analysis results are then shared between tabs. A total of 60 component peaks were observed in the analysis results, but it was possible to immediately extract only the peak containing $C_8H_8O^+$. Detailed qualitative analysis results for this component are described in the next section.

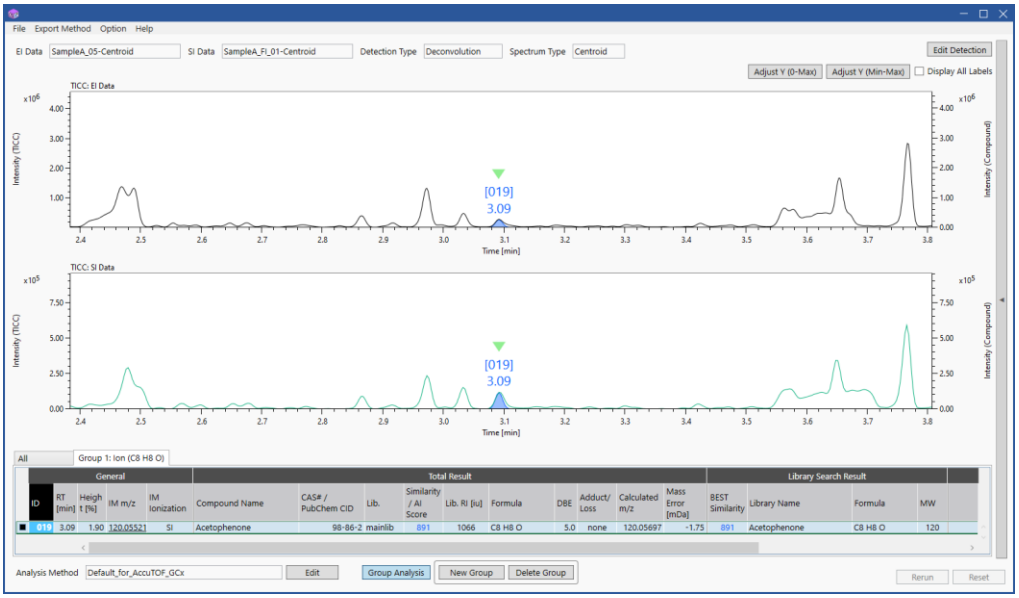

Figure 2 Group analysis result for C_8H_8O ion

Qualitative analysis of off-flavor component

Figure 3 shows the mass spectra of the component extracted by group analysis function. *m/z* 120, which is presumed to be the molecular ion, was detected in both the EI and FI mass spectra, and the FI mass spectrum showed the molecular ion as the base peak. The integrated qualitative analysis result list (top 5 candidates) by msFineAnalysis AI is shown in Table 2 In the NIST Library DB search result, several highly similar compounds were presented. However, based on the estimated elemental composition of the molecular ion, the molecular formula was calculated to be C_8H_8O. Therefore, this component was presumed to be “Acetophenone" (Figure 4). From the above results, it was confirmed that off-flavor component was detected from the commercially available adhesive measured this time.

Even in an analysis such as pyrolysis GC-MS analysis in which many peaks are detected, off-flavor-derived peak could be extracted immediately.

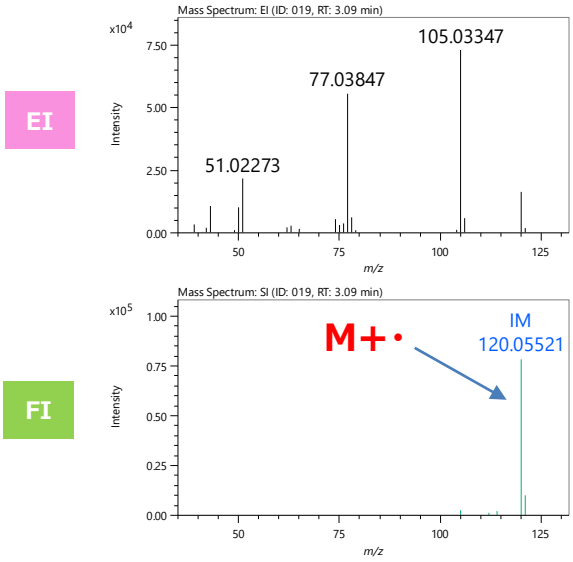

Figure 3 Mass spectra

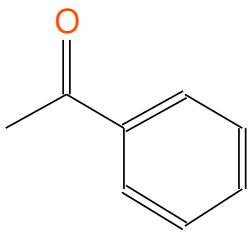

Figure 4 Structual formula of Acetophenone

Table 2 Integrated qualitative analysis result using the msFineAnalysis AI

	Elemental Composition of IM (m/z: 120.05521)							Integration	Library Search									
	#	Formula	DBE	Calculated m/z	Mass Error [mDa]	Isotope Matching	Coverage	Adduct/Loss	#	Library Name	CAS#	Lib.	Similarity	Reverse Similarity	Formula	DBE	MW	Coverage
★	A01	C8 H8 O	5.0	120.05697	-1.75	0.74	86	none	L01	Acetophenone	98-86-2	mainlib	891	903	C8 H8 O	5.0	120	86
									L03	Ethanone, 2,2-dihydroxy-1-phenyl-	1075-06-5	mainlib	832	926	C8 H8 O3	5.0	152	88
									L05	γ-Chlorobutyrophenone	939-52-6	mainlib	817	820	C10 H11 Cl O	5.0	182	100
									L07	N-Methoxy-N-methylbenzamide	6919-61-5	mainlib	808	880	C9 H11 N O2	5.0	165	100
									L08	2-Chloro-1-phenyl-1-propanone	6084-17-9	mainlib	807	873	C9 H9 Cl O	5.0	168	100

Conclusion

In this MSTips, we introduced an example of extracting off-flavor component in non-target analysis using the group analysis function of msFineAnalysis AI. By using the group analysis function, target analysis-like analysis can be performed even in non-target analysis, so detailed analysis in a shorter time can be expected.

Reference

1) M. Ubukata, A. Kubo, K. Nagatomo, T. Hizume, H. Ishioka, A. J. Dane, R. B. Cody, Y. Ueda. Integrated qualitative analysis of polymer sample by pyrolysis–gas chromatography combined with high-resolution mass spectrometry: Using accurate mass measurement results from both electron ionization and soft ionization. Rapid Commun Mass Spectrom. 2020; 34:e8820.

2) A. Kubo , A. Kubota, H. Ishioka, T. Hizume, M. Ubukata, K. Nagatomo, T. Satoh, M. Yoshida, F. Uematsu. Construction of a mass spectrum library containing predicted electron ionization mass spectra prepared using a machine learning model and the development of an efficient search method. Mass Spectrometry. 2023; 12: A0120.

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