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Application News

GC-MS GCMS-QP2050
Headspace Sampler HS-20 NX

Analysis of Aroma Components in Apples Using the Smart Aroma Database™

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User Benefits

- The Smart Aroma Database enables straightforward qualitative analysis of aroma components.
- The HS-20 NX headspace sampler allows for high-sensitivity and convenient analysis of the aroma components in fresh apples.
- Multivariate analysis facilitates an objective evaluation of aroma component differences between samples.

■ Introduction

The aroma components of fruits are one of the key factors that determine their flavor and taste, serving as a significant criterion for consumers when choosing fruits. These aroma components vary based on the type and variety of the fruit, its ripeness, production area, and cultivation environment. The complex interplay of these factors shapes the unique flavors of individual fruits. Therefore, the analysis of aroma components plays an important role in quality control and the development of new fruit varieties.

The compounds that make up the aroma of fruits are diverse, including both volatile and non-volatile components, and their numbers can range from dozens to hundreds. These components, which include alcohols, esters, ketones, and acids, possess various chemical structures and contribute to the aroma of the fruit. Gas chromatography mass spectrometry (GC/MS) offers an effective method for objectively evaluating the relationship between aroma and aroma components.

This article describes an example of analyzing the aroma components in apples using a GCMS-QP2050 gas chromatograph mass spectrometer in combination with an HS-20 NX headspace sampler (Fig. 1).

Fig. 1 GCMS-QP2050 and HS-20 NX
Gas Chromatograph Mass Spectrometer and HS-20 NX Headspace Sampler

■ Sample Preparation and Analysis Conditions

Three types of commercially available apples (one type of Sun Fuji and two types of Jonagold) were prepared as samples.

The apples were peeled, and the edible parts were grated using a grater. Each 1 g sample was placed into a 20 mL crimp-top vial for headspace GCMS, with five samples taken from each type of apple. To prevent changes in the components due to oxidation, the sampling was performed quickly while keeping the apples cool.

The instrument configuration and analysis conditions are indicated in Table 1. The trap model of the HS-20 NX headspace sampler features an electronic cooling trap for concentrating the aroma components to enable high-sensitivity analysis. Consequently, compounds with various boiling points, ranging from low to high, can be concentrated and analyzed.

Table 1 Instrument Configuration and Analysis Conditions

Instrument Configuration	
GC-MS:	GCMS-QP2050
Headspace Sampler:	HS-20 NX
Column:	InertCap Pure-Wax (30 m, 0.25 mm I.D., df = 0.25 µm) Cat No. 1010-68142
Database:	Smart Aroma Database
HS	
Mode:	Trap (Tenax TA)
Oven Temperature:	40 °C
Sample Line Temperature:	100 °C
Transfer Line Temperature:	100 °C
Trap cooling Temperature:	-10 °C
Trap heating Temperature:	280 °C
Trap waiting Temperature:	25 °C
Vial Agitation:	5 times
Multi-Injection:	5 times
Vial Pressure:	80 kPa
Dry Purge Pressure:	60 kPa
Vial Heat-Retention Time:	30 min
Vial Pressurization Time:	1 min
Vial Pressurization Equilibrating Time:	0.1 min
Loading Time:	1 min
Loading Pressurization Time:	0.1 min
Dry Purge Time:	1 min
Injection Time:	3 min
Needle Flush Time:	5 min
Sample Amount:	1 g
GC	
Carrier Gas:	He
Carrier Gas Control:	Pressure
Injection Mode:	Split
Split Ratio:	10
Column Oven Temperature Program:	50 °C (5 min) - (10 °C/min) - 250 °C (10 min)
MS	
Ion Source Temperature:	200 °C
Interface Temperature:	250 °C
Ionization Mode:	EI
Measurement Mode:	Scan (*m/z* 35 to 400)
Event Time:	0.3 sec

■ Results

The results obtained were analyzed using the Smart Aroma Database, with a total of 20 aroma components identified from the three types of apples. The identified aroma components are indicated in Table 2.

Table 2 Identified Apple Aroma Components

Ethyl acetate	Butyl 2-methyl butyrate
Propyl acetate	1-Pentanol
Butyl acetate	Hexyl acetate
Hexanal	1-Hexanol
Isobutanol	*trans*-2-Hexen-1-ol
2-Methylbuthyl acetate	Hexyl butyrate
1-Butanol	Hexyl 2-methylbutanoate
Pentyl acetate	Sulcatol
trans-2-Hexanal	Estragole
Buthyl butyrate	alpha-Farnesene

■ Multivariate Analysis

Three types of apples, with five samples each (for a total of 15 samples), were measured once. The obtained data were analyzed using SIMCA17 multivariate data analysis software (Informatics Co., Ltd.) to perform principal component analysis (PCA) and hierarchical clustering analysis. The PCA score plot (Fig. 2), loading plot (Fig. 3), and the dendrogram from the hierarchical clustering analysis (Fig. 4) are shown.

Based on the PCA score plot, the contribution rate of the first principal component (horizontal axis) is 85.6 %, and the contribution rate of the second principal component (vertical axis) is 10.2 %, totaling 95.8 %. The clear separation of the plots by apple type indicates that there are differences in the aroma of the three varieties. Additionally, the results of the hierarchical clustering analysis show that Jonagold (A) and (B) have relatively similar compositions of aroma components.

Table 3 shows the aroma components that are relatively abundant in Jonagold (A) along with the sensory information for each aroma component registered in the Smart Aroma Database.

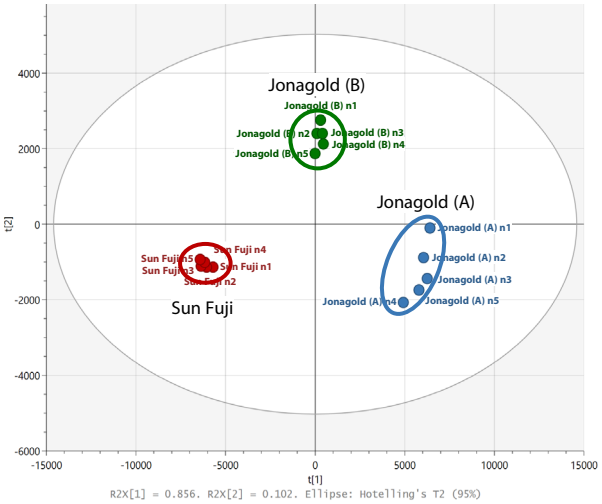

Fig. 2 PCA Score Plot

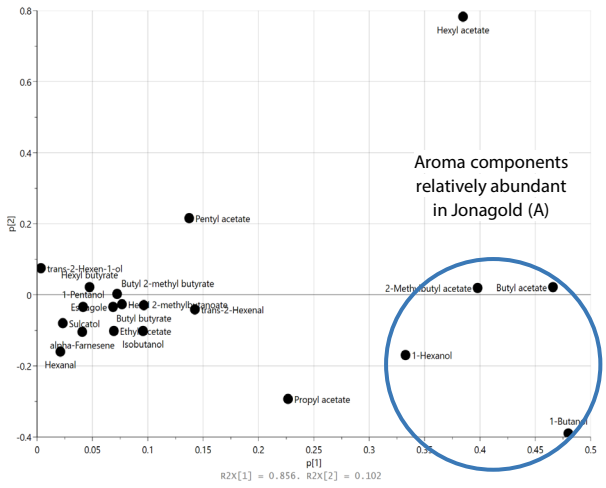

Fig. 3 PCA Loading Plot

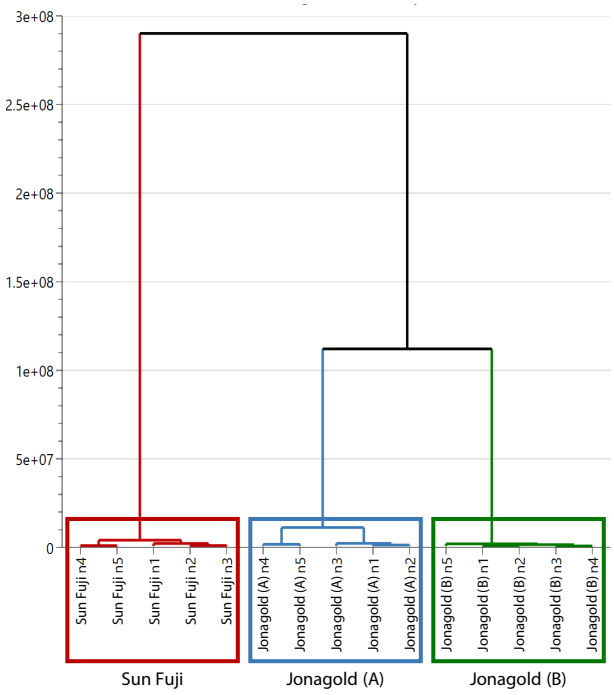

Fig. 4 Dendrogram of Hierarchical Clustering

Table 3 Aroma Components Relatively Abundant in Jonagold (A)

Aroma Component	Sensory Information Registered in the Smart Aroma Database
Butyl acetate	Pear
1-Butanol	Medicine, fruit
1-Hexanol	Resin, flower, green
2-Methylbutyl acetate	Fruit

■ Conclusion

We analyzed the aroma components of three types of commercially available apples using a GCMS-QP2050 gas chromatograph mass spectrometer. By utilizing an HS-20 NX headspace sampler, we were able to analyze the aroma components of fresh apples with high sensitivity, and the Smart Aroma Database made the process convenient.

We consider that scientifically analyzing the differences in aroma components based on factors such as fruit type, variety, ripeness, production area, and cultivation environment is beneficial for quality management and the development of new varieties.

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