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Application News

GC-MS GCMS-QP2020 NX

The Effect of Heating Temperature on Aroma Compounds in E-liquid

Yuto Nakasuji and Toshinari Ishii

User Benefits

- Smart Aroma Database™ strongly supports aroma compounds analysis.
- Users can reduce the time and effort of pretreatment for analysis by using the HS-20 NX.
- The HS-20 NX headspace sampler supports stable analysis over a wide range of temperatures.

Introduction

E-cigarettes have become increasingly popular in recent years. E-cigarettes are used by heating the flavored e-liquid instead of using tobacco leaves, and enjoying the flavor. The vaporization ratio of aroma compounds changes depending on the temperature, since the vapor pressure of each aroma compound is different. Therefore, the flavor of e-liquid is expected to change depending on the temperature. GC/MS analysis is useful for objectively evaluating the correlation between flavors and aroma compounds. In this report, aroma compounds of e-liquid with a simple pretreatment were analyzed under an environment close to the actual use conditions, by using the Smart Aroma Database and the HS-20 NX headspace sampler.

Fig. 1 GCMS-QP2020 NX + HS-20 NX + AOC-30i

System and Analytical Conditions

The HS-20 NX headspace sampler was connected to the GCMS-QP2020 NX gas chromatograph mass spectrometer. For the method, analytical conditions specific to the Smart Aroma Database were used. In this analysis, the progress mode, which is a function of HS-20 NX, was selected. The oven temperature was changed step by step during batch analysis by selecting the progress mode. In this case, analysis was performed at every oven temperature from 150 °C to 270 °C in increments of 20 °C.

In this experiment, a fluit flavored e-liquid was used for the sample, of which 1 mg was directly weighed in a crimp vial for a headspace sampler. Here, a heat resistant crimp cap was used for the vial cap, and a high heat resistance septum for the septum.

Table 1 Analytical Conditions

Analytical Conditions of GC-MS	
Model:	GCMS-QP2020 NX
Column:	SH-I-5Sil MS
Injection Mode:	Split
Split Ratio:	10
Career:	He
Ion Source Temp.:	200 °C
Interface Temp.:	250 °C
Scanning Mode:	Scan
Analytical Conditions of Headspace Sampler	
Mode:	Loop (1 mL)
Insulation Mode:	Progress (Increment : 20 °C)
Oven Temp.:	150 to 270 °C
Transfer Line Temp.:	280 °C
Sample Line Temp.:	280 °C
Vial Compressing Pressure:	100 kPa
Compression Time:	0.5 min
Load Time:	0.5 min
Injection Time:	0.5 min
Balance Time:	0.1 min

Results

As a result, 47 aroma compounds were identified by the Smart Aroma Database. Next, in order to investigate the correlation between the peak area of each aroma compound and temperature, the area value was standardized, and cluster analysis was performed using the statistical analysis software "R." The heat map obtained as the result of cluster analysis is shown in Fig. 2. Here, the vapor pressure of e-liquid increases with increasing temperature. Therefore, the peak area value in Fig. 2 is corrected by the dilution rate with the pressurized gas. The dilution rate by the pressurized gas was calculated based on the measured internal pressure of the vial.

Fig. 2 shows the correlation between the area value of each compound and the oven temperature. From this heat map, the correlation can be confirmed at a glance. Overall, it can be seen that the amount of aroma compounds in the generated gas tends to increase with increasing oven temperature. In particular, there is a significant tendency to increase from 210 °C. On the other hand, the tendency of the area of aroma compounds to change depends on the variety of compounds when viewed in detail.

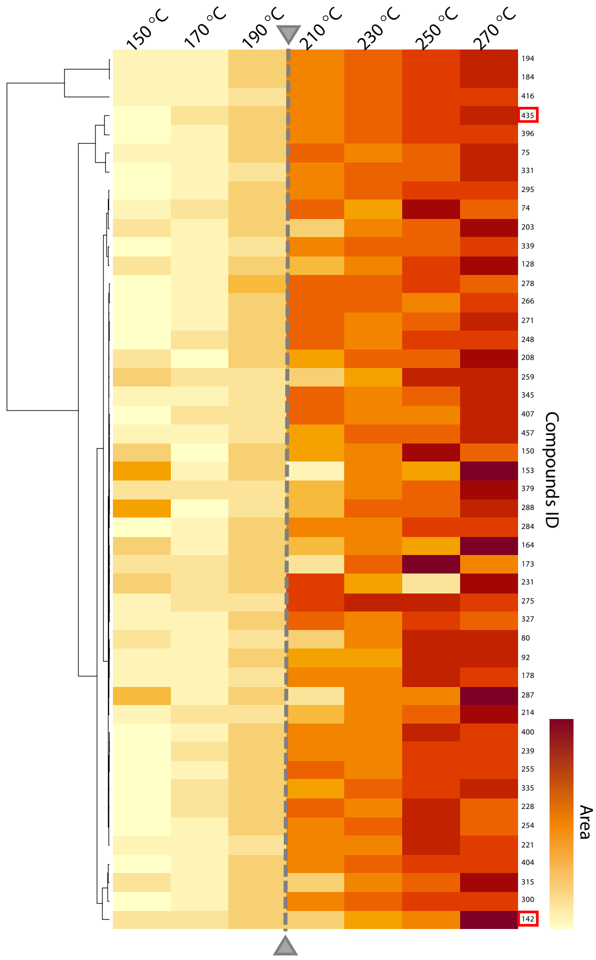

Fig. 2 Correlation between Area Value of Aroma Compounds and Oven Temperature

■ Changes in Aroma Characteristics

Fig. 3 shows the temperature dependence of the quantitative ion peak areas of raspberry ketone and benzonitrile. Here, these two compounds are shown in the red frame in Fig. 2. The area values in Fig. 3 have been corrected taking into consideration the dilution ratio of the pressurized gas, as in the case of Fig. 2. As shown in Fig. 3, the peak area of raspberry ketone increases with temperature, but the tendency decreases from around 210 °C. On the other hand, the peak area of benzonitrile does not change much in the low-temperature range, but the peak area value rapidly increases from 270 °C. These results show that the increasing tendencies of the area values of the two compounds are different.

The Smart Aroma Database also contains sensory information about aroma compounds. According to the sensory information, for example, raspberry ketone smells like raspberry, and benzonitrile smells rancid. From the results of Fig. 2 and Fig. 3, it can be inferred that the raspberry-like scent increases until 210 °C, and the rancid smell increases rapidly from around 270 °C. In this way, by linking changes in aroma compounds with sensory information, it can be applied to strategic scent design and evaluation.

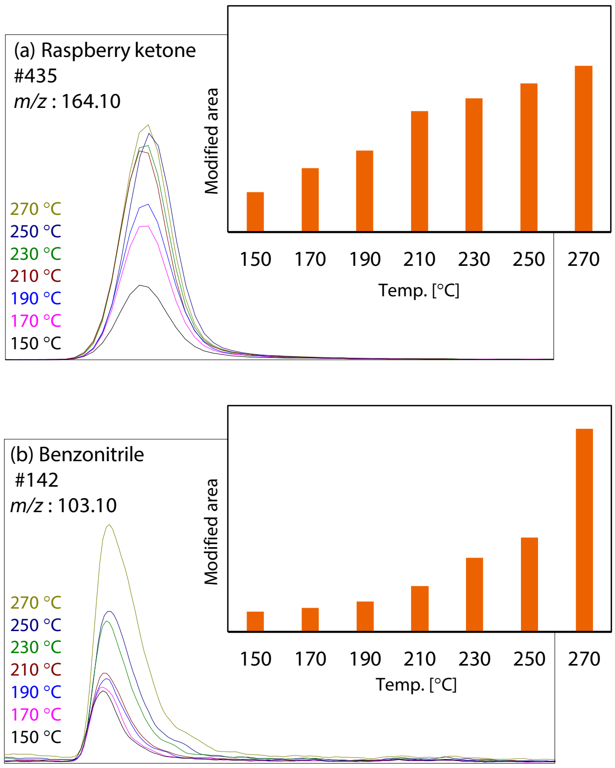

Fig. 3 Correlation between Temperature and Quantitative Ion Peak Area of Raspberry Ketone and Benzonitrile

■ Conclusion

In this application news, the correlation between aroma compounds of e-liquid vapor and heating temperature was evaluated by using a GCMS-QP2020 NX gas chromatograph mass spectrometer and an HS-20 NX headspace sampler.

The Smart Aroma Database strongly supports the analysis of aroma compounds, since the database includes information on characteristic ions, retention indices, and mass spectra for more than 500 aroma compounds. In addition, the database contains sensory information of aroma compounds. Therefore, by linking the analysis results of aroma compounds with sensory information, efficient design and evaluation of fragrance can be expected.

Smart Aroma Database is a trademark of Shimadzu Corporation in Japan and/or other countries.

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