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Application News

GC-MS GCMS-TQ™8040 NX and Smart Aroma Database™

Analysis of Aroma Compounds in Cosmetics Using the Smart Aroma Database

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User Benefits

- More than 500 aroma-related compounds are registered in the Smart Aroma Database to enable efficient analysis of aroma compounds.
- Using the Smart Aroma Database, MRM methods can be easily created to accurately analyze samples with complex matrices such as cosmetics.

■ Introduction

Aromas/fragrances can have a major effect on products, brand image, and other factors, and have an important role particularly in food products and cosmetics. Recently, aromas have been attracting attention as one factor that can affect the impressions people receive. Cosmetics and other personal care products are increasingly being judged not only by skin feel and functional properties but also by their fragrance. However, fragrances are typically evaluated based on sensory testing by humans, but because the sensation of fragrances is influenced by individual preferences and state of health, evaluations are often decided statistically based on a large number of evaluation results. Consequently, due to the high expertise levels and time required for fragrance/aroma evaluations, there has been increasing interest in using instrumental analysis to increase productivity and ensure more consistent quality.

Aroma compounds related to such fragrances can be analyzed by gas chromatography, but even if only the target aroma compounds are analyzed, it can be extremely difficult to analyze the data due to the many contaminants detected together with the targets. Therefore, this article describes an example of analyzing the aroma compounds in cosmetics using the Smart Aroma Database, which is a unique database that contains over 500 aroma compound information.

Fig. 1 AOC-6000 Plus + GCMS-TQ™8040 NX System

■ Analysis Using the Smart Aroma Database

The Smart Aroma Database contains analytical information for about 500 types of important compounds relevant to fragrances. It provides support for the entire process flow from widely-targeted analysis of several hundred important compounds to high-sensitivity target analysis using SIM and MRM mode targeting only the key compounds contained in samples. Using the Smart Aroma Database, creating analytical methods only requires an adjustment of retention times using a standard n-alkane mixture before sample analysis. Then the results can be used to automatically and accurately identify the relevant target aroma compounds based on multiple decision criteria, such as retention times, similarity scores, and ion ratios.

Fig. 2 Analysis Process Flow Using the Smart Aroma Database

■ Samples and Analytical Conditions

Using a system configured with an AOC-6000 Plus autosampler and GCMS-TQ8040 NX gas chromatograph mass spectrometer connected, concentrated volatile compounds were analyzed using the SPME method. A 20 mg sample of a commercial lip gloss product was weighed and sealed in a screw vial for SPME analysis.

First, the compounds contained in the sample were identified by scan-mode analysis using analytical conditions registered in the Smart Aroma Database. Next, SIM and MRM methods were automatically created for the identified compounds and the sample was analyzed by SIM and MRM modes.

Table 1 Analytical Conditions

System	
GCMS Model:	GCMS-TQ8040 NX
Autosampler:	AOC-6000 Plus
Database:	Smart Aroma Database
Column:	SH-I-5Sil MS (30 m × 0.25 mm I.D. 0.25 µm)
AOC-6000 Conditions	
SPME Arrow:	DVB/Carbon WR/PDMS (O.D.: 1.1 m, Film thickness: 120 µm, length: 20 mm)
Conditioning Temp.:	270 °C
Pre Conditioning Time:	10 min
Vial Incubation Time:	15 min
Stirrer Speed:	250 rpm
Sample Extract Time:	30 min
Sample Desorb Time:	1 min
Post Conditioning Time:	5 min
GC Conditions	
Injection Mode:	Split
Split Ratio:	5
Carrier Gas:	He
Carrier Gas Control:	Pressure (83.5 kPa)
Column Temp.:	50 °C (5 min)_10 °C/min_250 °C (10 min)
MS Conditions	
Ion Source Temp.:	200 °C
Interface Temp.:	250 °C
Data Acquisition Mode:	Scan, SIM, MRM
Event Time:	0.3 sec (Scan)
Scan Range:	*m/z* 35 – 400

■ Using the Smart Aroma Database for Scan Mode Analysis

Using the Smart Aroma Database, 31 aroma compounds were detected by scan-mode analysis. The detected compounds and the corresponding library search similarity scores are listed in Table 2.

The Smart Aroma Database includes a library of only registered aroma compounds. That library can narrow down the list of target compounds based on not only retention times and ion ratios but also the similarity scores from searching the library, which can result in more accurate and efficient widely-targeted analysis.

Furthermore, as the sensory information is registered in the Smart Aroma Database, the aroma characteristics of detected compounds can be checked simultaneously when identification results are obtained. Fig. 3 shows a screenshot from the Smart Aroma Database data analysis window displayed in LabSolutions Insight™. Evaluating product aromas requires determining how the respective compounds affect the product fragrance. With the Smart Aroma Database, identification results and sensory information can be checked at the same time, which is useful for basic evaluations used to determine aroma formulations.

Table 2 Summary of Identification Results

Compound	Similarity Score	Compound	Similarity Score
1-Butanol	95	Limonene	96
Methyl Butanoate	96	Benzyl alcohol	94
Ethyl isobutyrate	92	Diethyl malonate	93
Ethyl butanoate	96	(E)-Linalool oxide	84
Ethyl lactate	92	Pentyl butyrate	92
Butyl acetate	97	Linalool	96
Ethyl 2-methylbutyrate	96	Nonanal	94
cis-3-Hexen-1-ol	80	Benzyl acetate	94
Isoamyl acetate	97	(Z)-3-hexenyl butyrate	96
Methyl hexanoate	96	Hexyl butyrate	85
Benzaldehyde	94	Ethyl octanoate	92
Ethyl hexanoate	94	n-Decanal	95
Octanal	88	Benzyl butyrate	81
(3Z)-3-Hexenyl acetate	95	Methyl cinnamate	86
Hexyl acetate	98	gamma-Decalactone	93
		gamma-Undecalactone	93

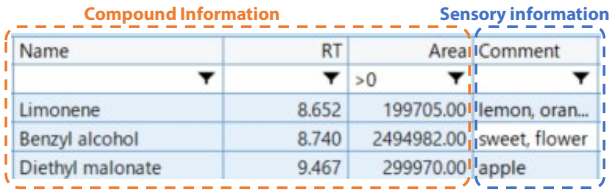

Fig. 3 LabSolutions Insight Data Analysis Window

■ SIM and MRM Mode Analysis

Next, the 31 compounds identified by scan-mode analysis were analyzed using the SIM and MRM methods, which were automatically created by the Smart Aroma Database.

Because fragrance is determined by the balance between respective aroma compounds, it is important that quantitative analysis of aroma compounds is accurate. However, cosmetics and other personal care products often contain fragrances or active ingredients that are natural substances extracted from plants or other sources. Such compounds are typically detected along with multiple interfering peaks, which can make it difficult to accurately quantify target compounds due to overlapping peaks from quantitation ions and contaminants, even for SIM mode analysis of a narrow mass range.

In particular, when comparing multiple analytes, contaminants can vary depending on the sample. When analyzing data from SIM mode analysis, it may be necessary to make appropriate adjustments to quantitation ions or incorrectly identified peaks in accordance with the sample. In such cases, the higher selectivity of MRM-mode analysis can help minimize the effects of contaminants, so that target compounds can be quantitated more accurately and reduce the effort required for data analysis.

Typically, determining MRM-mode analytical conditions is a difficult time-consuming process. However, the Smart Aroma Database can create MRM methods for the selected compounds automatically to ensure advanced MRM-mode analysis can be performed easily without special experience or time-consuming steps. Fig. 4 is a comparison of SIM and MRM-mode analysis results obtained using the Smart Aroma Database. Fig. 4 shows that a large number of contaminant peaks are included near target compounds in SIM mode results, but those targets are detected with greater selectivity in MRM mode results. Thus, for cosmetics and other samples with complex matrices, using the MRM mode can provide an effective way to suppress the effects of contaminants to achieve more accurate quantitation and data analysis with less effort.

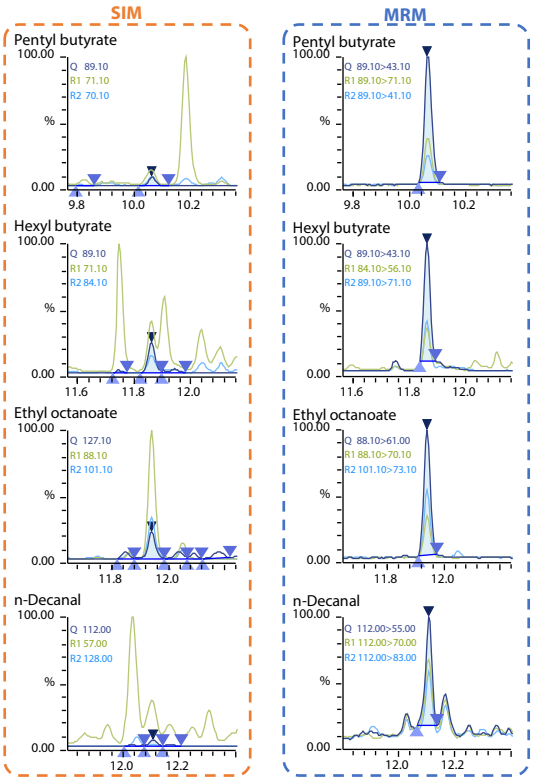

Fig. 4 Comparison of SIM and MRM-Mode Analysis

■ Conclusion

The Smart Aroma Database enabled 31 aroma compounds emitted from lip gloss to be detected. The Smart Aroma Database also helps increase the accuracy and efficiency of aroma compounds qualitative analysis by using mass spectral similarity scores calculated based on the aroma compounds library included with the database to narrow down the list of candidates, rather than using only mass chromatograms and ion comparisons. By analyzing the specified internal standard in advance, it can also provide information about semi-quantitative values useful for development work.

In addition, the Smart Aroma Database can be used to easily create SIM and MRM-mode methods for easily more sophisticated aroma compound analysis, even for cosmetics or other samples with complex matrices.

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