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Off-flavor system of Shimadzu analyzes the odor components in edible oil

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Overview

A simple and fast method of analyzing 150 kinds of odor substances was established for rapid screening of odor components in edible oil with GCMS-TQ8040.

Introduction

Edible oil is an indispensable cooking ingredient and a healthy essential nutrient in people's life. The edible oil will produce different odors during the production or storage process. In the process of oil production, peculiar smells are produced. For example, the oil made from the scorched embryo has a burnt smell, the alkali-smelted oil has a "soap taste", and the leached oil has a solvent taste.

Grease can cause rancid odor due to improper storage conditions, such as unpleasant clams taste, stinky smell, etc. The smell of edible oil directly affects the flavor quality and edible value of the food. So it is essential to establish a rapid and effective method for detecting odor substances in edible oils.

Methods and Materials

Sample preparation

Put the sample of edible oil into a sealed headspace bottle, at a certain temperature, SPME autosampler and GC/MS/MS device were used to pretreat and detect the odor substances from the sample.

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GC/MS/MS analysis

Analytical Conditions

SPME autosampler (AOC-6000, Shimadzu Corporation, Japan)	
SPME fiber	: SPME FIB-C-WR-100/10, PDMS
Aging temperature	: 270°C
Aging time (before extraction)	: 15min
Equilibrium temperature	: 80°C
Equilibrium time	: 5min
Extraction time	: 20min
Desorption time	: 2min
Aging time (after extraction)	: 5min
GC(GC-2010 Plus, Shimadzu Corporation, Japan)	
Analytical column	: InertCap Pure-Wax,30m × 0.25mm× 0.25μm(GL,Japan)
Inlet temp	: 250°C
Col oven temp program	: 50°C (5 min)_10°C/min_250°C(10 min)
Control mode	: constant Linear Velocity (43.3cm/sec)
Split ratio	: 5:1
Carrier gas	: Helium
MS/MS(GCMS-TQ8040, Shimadzu Corporation, Japan)	
Ionization mode	: EI
CID gas	: Argon
Ion source temperature	: 200°C
IF temperature	: 250°C
Detector voltage	: tuning voltage + 0.3kv
Acquisition mode	: SCAN/MRM

Result

The Creation process of odor analysis method

The TQ_MS_Wax_AART method in the odor analysis method package was used to analysis the standard solution of n-alkanes (C9-C33), whose data was used to calculate the retention time of odor substances. The chromatogram of n-alkanes was shown in figure 1.The TQ_MS_Wax_Correct_MRM method was used to analysis three calibration internal standards of 4-bromofluorobenzene, 1, 2-dichlorobenzene-d4 and acenaphthene-d10. The chromatogram of calibration internal standards was shown in figure 2.

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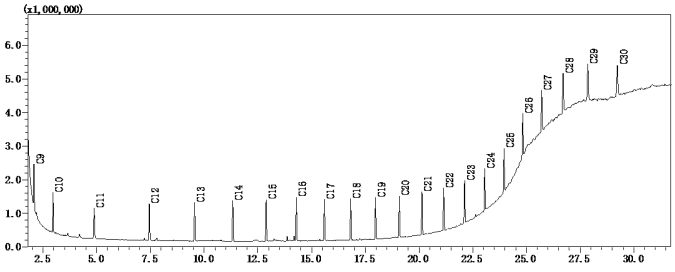

Figure 1　The chromatogram of n-alkanes

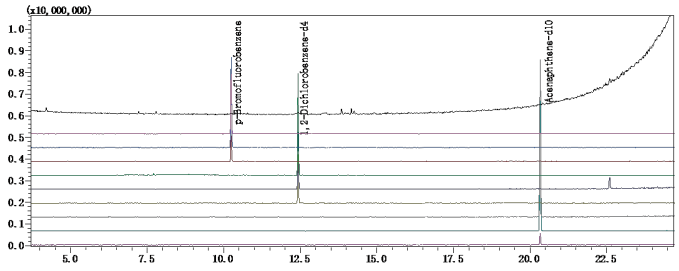

Figure 2　The chromatogram of calibration internal standards

The data of n-alkanes and calibration internal standards and the off-flavor analysis database were used to create a semi-quantitative qualitative method for 150 kinds of odor substances automatetically. The method creation and the method creation completion interfaces of off-flavor analysis database are shown in figure 3 and figure 4.

Figure 3　The method interface of off-flavor analysis database

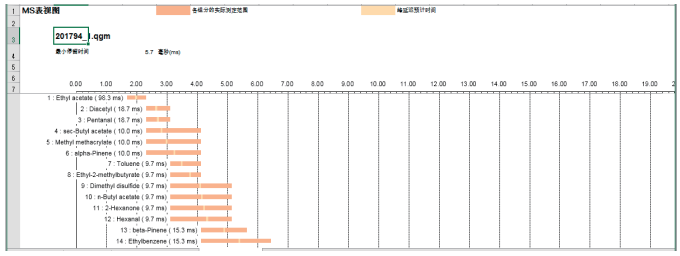

Figure 4　The method completion interface of off-flavor analysis database

The odor screening results of different edible oil

The method created for 150 odor substances was used to detect four edible oil samples, and the test results were shown in table1 to table4.

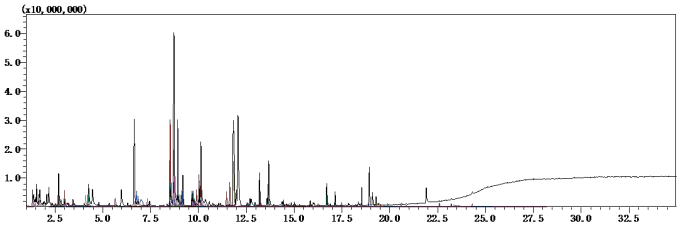

Figure 5　Chromatogram of rapeseed oil

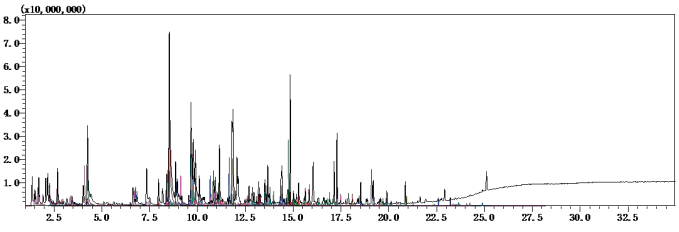

Figure 6　Chromatogram of sesame oil

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Table 1. the odor screening results of rapeseed oil

No.	Compound name	CAS Number	Estimated concentration (pg/mg)	Odor Threshold (pg/mg)	Odor Quality
1	Pentanal	110-62-3	108.0	100	Almond, Pungent, Malt
2	Hexanal	66-25-1	62.9	1	Fat, Tallow, Grass
3	2-Methylpyrazine	109-08-0	14.6	1000	Popcorn
4	2-Octanone	111-13-7	4.0	10	Soap, Gasoline
5	Octanal	124-13-0	8.7	100	Green, Fat, Soap, Lemon
6	trans-2-Heptenal	18829-55-5	39.5	10	Fat, Soap, Almond
7	Dimethyl trisulfide	3658-80-8	0.5	0.1	Cabbage, Fish, Sulfur
8	2-Isobutyl-3-methoxy pyrazine	24683-00-9	0.1	0.01	Earth, Spice,
9	2-Undecanone	112-12-9	27.4	10	Green, Orange, Fresh
10	trans-2-Decenal	3913-81-3	5.5	1	Orange

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Table 2. the odor screening results of sesame oil

No.	Compound name	CAS Number	Estimated concentration (pg/mg)	Odor Threshold (pg/mg)	Odor Quality
1	Toluene	108-88-3	5.6	2000	Paint
2	Dimethyl disulfide	624-92-0	33.3	100	Cabbage, Onion, Putrid
3	Hexanal	66-25-1	175.9	1	Fat, Tallow, Grass
4	2-Heptanone	110-43-0	2.1	10	Soap
5	Styrene	100-42-5	2.0	100	Gasoline, Balsamic
6	2-Octanone	111-13-7	1.8	10	Soap, Gasoline
7	Octanal	124-13-0	26.7	100	Green, Fat, Soap, Lemon
8	trans-2-Heptenal	18829-55-5	75.2	10	Fat, Soap, Almond
9	2-Ethylpyrazine	13925-00-3	43.4	100	Peanut butter, Wood
10	alpha-Methylstyrene	98-83-9	0.1	10	Gasoline, Balsamic
11	Dimethyl trisulfide	3658-80-8	4.0	0.1	Cabbage, Fish, Sulfur
12	Acetic acid	64-19-7	82.7	1000	Sour
13	Benzaldehyde	100-52-7	8.3	1000	Almond, Burnt sugar
14	Propionic acid	79-09-4	19.5	1000	Rancid, Pungent, Soy
15	2-Nonenal	18829-56-6	1.1	1	Paper
16	Isophorone	78-59-1	1.7	100	Saffron, Floral, Hay
17	2-Undecanone	112-12-9	28.4	10	Green, Orange, Fresh
18	trans-2-Decenal	3913-81-3	8.5	1	Orange
19	Salicylaldehyde	90-02-8	6.5	1	Herbal, Stable, Roasted
20	Naphthalene	91-20-3	0.4	10	Tar
21	Caproic acid	142-62-1	0.4	100	Sweat
22	Benzyl alcohol	100-51-6	11.0	100	Sweet, Flower
23	Benzothiazole	95-16-9	2.2	10	Gasoline, Rubber
24	o-Bromophenol	95-56-7	1.9	1	Phenol, Iodine
25	p-Ethylguaiacol	2785-89-9	0.4	0.1	Spice, Clove
26	p-Cresol	106-44-5	0.3	1	Phenol, Medicine, Smoke
27	Eugenol	97-53-0	0.1	1	Honey, Clove
28	Capric acid	334-48-5	0.2	10	Fat, Rancid
29	Isoeugenol	97-54-1	0.3	0.1	Flower
30	Indole	120-72-9	0.7	10	Burnt, Mothball

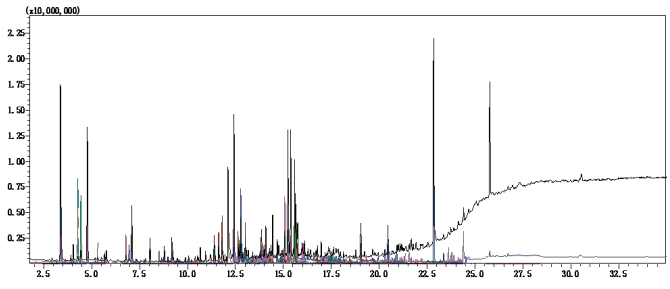

Figure 7　Chromatogram of rancid peanut oil

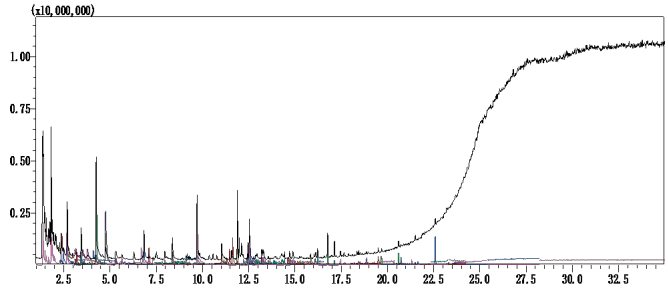

Figure 8　Chromatogram of edible oil used in a restaurant

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Table 3. the odor screening results of rancid peanut oil

No.	Compound name	CAS Number	Estimated concentration (pg/mg)	Odor Threshold (pg/mg)	Odor Quality
1	Ethyl acetate	141-78-6	11.1	1000	Pineapple
2	Pentanal	110-62-3	44.6	100	Almond, Pungent, Malt
3	sec-Butyl acetate	105-46-4	1.9	100	Sweet, Chemical
4	alpha-Pinene	80-56-8	0.2	10	Solvent
5	Toluene	108-88-3	8.3	2000	Paint
6	Hexanal	66-25-1	342.6	1	Fat, Tallow, Grass
7	Ethylbenzene	100-41-4	1.1	100	Gasoline
8	m-Xylene	108-38-3	2.6	2000	Plastic
9	2-Heptanone	110-43-0	1.6	10	Soap
10	Styrene	100-42-5	1.2	100	Gasoline, Balsamic
11	2-Octanone	111-13-7	6.5	10	Soap, Gasoline
12	Octanal	124-13-0	113.6	100	Green, Fat, Soap, Lemon
13	trans-2-Heptenal	18829-55-5	87.4	10	Fat, Soap, Almond
14	Acetic acid	64-19-7	54.7	1000	Sour
15	n-Decanal	112-31-2	2.8	1	Soap, Tallow, Orange peel
16	2-Isobutyl-3-methoxy pyrazine	24683-00-9	0.2	0.01	Earth, Spice, Green pepper
17	Propionic acid	79-09-4	15.0	1000	Rancid, Pungent, Soy
18	2-Nonenal	18829-56-6	6.4	1	Paper
19	1-Octanol	111-87-5	0.2	100	Metal, Burnt, Chemical
20	2-Methylisoborneol	2371-42-8	32.5	0.1	Earth, Musty
21	trans-2-Decenal	3913-81-3	7.8	1	Orange
22	p-Dibromobenzene	106-37-6	32.9	100	Xyene
23	p-Ethylguaiacol	2785-89-9	13.2	0.1	Spice, Clove
24	p-Cresol	106-44-5	0.2	1	Phenol, Medicine, Smoke
25	m-Cresol	108-39-4	0.1	0.1	Plastic, Fecal
26	2,3-Xylenol	526-75-0	0.9	1	Gasoline
27	gamma-Decalactone	706-14-9	0.2	1	Fat, Peach
28	Phenylacetic acid	103-82-2	1.5	10	Flower, Honey
29	Phenylacetic acid	103-82-2	1.5	10	Flower, Honey

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Table 4. the odor screening results of edible oil used in a restaurant

No.	Compound name	CAS Number	Estimated concentration (pg/mg)	Odor Threshold (pg/mg)	Odor Quality
1	Pentanal	110 62-3	15.6	100	Almond, Pungent, Malt
2	Toluene	108-88-3	2.0	2000	Paint
3	Hexanal	66-25-1	40.4	1	Fat, Tallow, Grass
4	Ethylbenzene	100-41-4	0.3	100	Gasoline
5	p-Xylene	106-42-3	0.1	1000	Geranium
6	m-Xylene	108-38-3	0.3	2000	Plastic
7	o-Xylene	95-47-6	0.1	2000	Geranium
8	Octanal	124-13-0	2.5	100	Green, Fat, Soap, Lemon
9	trans-2-Heptenal	18829-55-5	53.5	10	Fat, Soap, Almond
10	Acetic acid	64-19-7	13.4	1000	Sour
11	trans,trans-2,4-Heptadienal	4313-03-5	5.3	2000	Stir-fried oil, Burnt
12	Propionic acid	79-09-4	3.4	1000	Rancid, Pungent, Soy
13	2-Nonenal	18829-56-6	0.3	1	Paper
14	trans-2-Decenal	3913-81-3	1.6	1	Orange
15	alpha-Terpineol	98-55-5	0.5	100	Mint, Anise, Oil
16	Benzyl alcohol	100-51-6	1.0	100	Sweet, Flower
17	o-Bromophenol	95-56-7	1.8	1	Phenol, Iodine
18	p-Cresol	106-44-5	0.1	1	Phenol, Medicine, Smoke
19	m-Cresol	108-39-4	0.1	0.1	Plastic, Fecal
20	Pelargonic acid	112-05-0	0.4	100	Green, Fat
21	Eugenol	97-53-0	0.1	1	Honey, Clove

Conclusions

The GCMS-TQ8040 of shimadzu combined with off-flavor odor analysis database was used to create detection method of 150 kinds of odor substances automatically,using the data of n-alkanes and calibration internal standards. No odor standard was needed for the qualitative and semi-quantitative analysis of odor substances in edible oil. The results show that the method is simple and can be used for the rapid screening of odor substances in edible oil.

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