SHIMADZU

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Analysis of odor components in fish by Shimadzu Off-Flavor system

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1. Overview

In this paper, the Shimadzu GCMS-TQ8050 triple quadrupole GC/MS and AOC-6000 multi-function autosampler were combined with the Off-flavor database to determine the odor components in three kinds of fish meat.

2. Introduction

Fish is rich in nutrients and pleasant flavors and is popular among the public. flavor is one of the main eating qualities of aquatic products, and is an important indicator for customers to evaluate their quality. ordor substances plays an important role in the overall flavor of fish, and are an important sensory evaluation factor for fish. the study of odor substances has important guiding significance for the development of fish falvor and fragrance and improvement of flavor quality of fish meat.

3. Methods and Materials

Accurately weigh 2.0 g of fish sample into a 20 mL headspace bottle and seal with a lid. AOC-6000 solid phase microextraction injection was used, and GCMS-TQ8050 was used for detection

High Speed Mass Spectrometer

Ultra Fast Scan Speed
- Max. 20000 amu/sec

Ultra Fast MRM
- Max. 888 transition /sec

Figure 1 GCMS-TQ8050 triple quadrupole mass spectrometer

4. Result

GC-MS/MS conditions

Injection temp.:250
Injection mode: Split mode
Flow control mode: Linear velocity (40cm/sec)
Column: InertCap Pure-Wax, 30 m × 0.25 mm × 0.25 μm
Column oven temp.: 50℃ (5 min) _10℃/min_250℃ (10 min)
CID gas: Argon
Detector voltage: Tuning result+0.3kV
Interface temp.: 230℃
Ion source temp.: 300℃

The C9~C30 alkane was collected using the TQ_MS_Wax_AART method in the analytical method package to estimate the retention time of the volatile components. The chromatogram of the n-alkane standard is shown in Figure 2. The TQ_MS_Wax_Correct_MRM method was used to determine the calibration internal standard sample containing 4-bromofluorobenzene, 1,2-dichlorobenzene-d4, and acenaphthene-d10. The chromatogram of the internal standard sample was shown in Fig. 3.

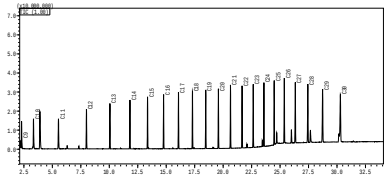

Figure 2 C9~C30 alkane

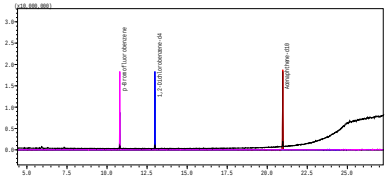

Figure 3 . The chromatogram of the internal standard

The qualitative and semi-quantitative methods for 150 volatile components were automatically created using the internal standard data obtained above and the Off-flavor database.

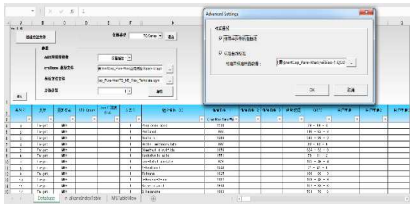

Figure 4.The interface using database to generate screening method

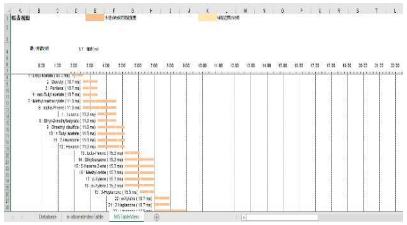

Figure 5.Completion interface of method creation

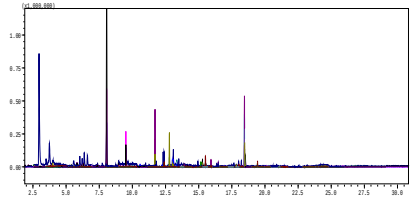

Figure 6.Chromatogram of Jinchang fish

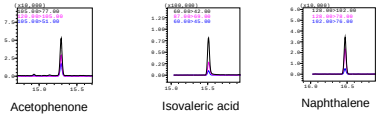

Figure 7.Chromatogram of partial odor component in Jinchang fish sample

Table 1.Screening results of odor components in Jinchang fish samples (concentration unit: pg/mg)

No.	Compound	CAS number	Estimated concentration	Threshold(pg)	Odour characteristics
1	Ethyl acetate	141 - 78 - 6	0.025	1000	Pineapple scent
2	Diacetyl	431 - 03 - 8	0.041	10	Butter scent
3	Ethyl-2-methylbutyrate	7452 - 79 - 1	0.006	1	Apple scent
4	Dimethyl disulfide	624 - 92 - 0	0.005	100	Cabbage, Onion, Putrid
5	Hexanal	66 - 25 - 1	0.011	1	Fat, Tallow, Grass
6	beta-Pinene	127 - 91 - 3	0.009	100	Pine, Resin, Turpentine
7	Mesityl oxide	141 - 79 - 7	0.001	10	Sweet, Chemical
8	p-Xylene	106 - 42 - 3	0.003	1000	Geranium
9	m-Xylene	108 - 38 - 3	0.007	2000	Plastic
10	o-Xylene	95 - 47 - 6	0.003	2000	Geranium
11	2-Heptanone	110 - 43 - 0	0.006	10	Soap
12	Eucalyptol ; Cineol	470 - 82 - 6	0.009	10	Sweet, Mint
13	2-Methylpyrazine	109 - 08 - 0	0.002	1000	Popcorn
14	2-Octanone	111 - 13 - 7	0.005	10	Soap, Gasoline
15	Dimethyl trisulfide	3658 - 80 - 8	0.002	0.1	Cabbage, Fish, Sulfur
16	Butyl cellosolve	111 - 76 - 2	0.415	100	Sweet, Ester
17	trans,trans-2,4-Heptadienal	4313 - 03 - 5	0.002	2000	Stir-fried oil, Burnt
18	Camphor	76 - 22 - 2	0.004	100	Camphor
19	Linalool	78 - 70 - 6	0.006	10	Flower, Lavender
20	Isobutyric acid	79 - 31 - 2	0.300	1000	Rancid, Cheese, Butter
21	Isophorone	78 - 59 - 1	0.002	100	Saffron, Floral, Hay
22	Phenylacetaldehyde	122 - 78 - 1	0.121	10	Sweet, Honey
23	L-Menthol	89 - 78 - 1	0.013	1000	Sweet, Mint
24	Acetophenone	98 - 86 - 2	0.012	1000	Flower, Musty, Almond
25	Isovaleric acid	503 - 74 - 2	0.157	100	Rancid, Sweat, Acid
26	Salicylaldehyde	90 - 02 - 8	0.002	1	Herbal, Stable, Roasted bread
27	alpha-Terpineol	98 - 55 - 5	0.085	100	Mint, Anise, Oil
28	Borneol	507 - 70 - 0	0.005	1	Earth, Musty
29	Naphthalene	91 - 20 - 3	0.010	10	Tar
30	Methyl salicylate	119 - 36 - 8	0.002	1	Peppermint
31	2-Methylnaphthalene	91 - 57 - 6	0.004	1	Sweet, Rancid
32	Benzyl alcohol	100 - 51 - 6	0.009	100	Sweet, Flower
33	1-Methylnaphthalene	90 - 12 - 0	0.003	100	Sweet, Rancid
34	2-Phenylethanol	60 - 12 - 8	0.134	100	Honey, Spice, Rose, Lilac
35	Dibutylhydroxytoluene	128 - 37 - 0	0.025	10	Phenol
36	Benzothiazole	95 - 16 - 9	0.002	10	Gasoline, Rubber
37	Phenol	108 - 95 - 2	0.017	1000	Special and burning smell

5. Conclusions

In this paper, the Shimadzu GCMS-TQ8050 triple quadrupole GC/MS and AOC-6000 multi-function autosampler were combined with the Off-flavor database to determine the odor components in the three fish meats. By collecting N-alkanes and internal standard data, the Off-flavor database was used to automatically create the detecting methods of 150 volatile components for qualitative and semi-quantitative analysis of odor components in fish meat. 37 kinds of odor components were screened in the sample of gold pomfret, 36 kinds of odor components were screened in the sample of ribbonfish , and 21 kinds of odor components were screened in the sample of the saury. The method is simple in operation, fast in analysis, and can be used for rapid screening of odor components in fish meat.