Analysis of blueberry flavor compositions by GC-MS

1 Introduction

Flavor compounds, also known as blended fragrance, are blend of various flavors artificially formulated to have a specific fragrance. Flavors and fragrances can be used to improve, increase and mimic the aroma and taste of foods; they can be used as food additives. The composition of flavor compounds are complex. In the past, analysis of flavor relied mainly on some conventional physical and chemical methods, which were not only slow, but also difficult to understand the composition. However, the emergence of GC-MS solves these problems, which make the flavors and fragrances compositional analysis, from component separation to chemical structure identification, to fulfill the requirement of being convenient, fast and accurate. GC-MS can simultaneously achieve qualitative and quantitative purposes. Thereby, through monitoring the quality of spices and guiding the improvement of flavors and fragrances, it has made significant contribution to the synthesis of new flavors and fragrances.

2 Experiment

2.1 Instruments and reagents

GC-MS3100 (EAST & WEST ANALYTICAL INSTRUMENTS, INC); Equity-5 (30m×0.25mm×0.25um) silica capillary column; 1uL microinjector.

Sample: blueberry flavor

2.2 Analysis conditions

MS conditions： EI source; ion source temperature: 150℃; electron energy: 70eV; scanning mode：full scan; scanning range: 28.5u～400u; scanning period: 0.6s; interface temperature: 260℃; multiplier high voltage: 1200V; solvent delay: 2 min.

GC conditions： Equity-5 (30m×0.25mm×0.25um) silica capillary column; injection port temperature: 260℃; split sampling; sample volume: 0.1 μL; split ratio: 50:1; precolumn pressure: 60 kPa; purge rate: 2ml/min; column temperature program: hold at 35℃ for 2 min, ramp up to 270 °C at 7 °C/min and then hold for 5 min

2.3 Result an discussion

The composition of the blueberry flavor was analyzed by GC-MS3100; Figure 1 is the full scan chromatogram of the essence; through the NIST standard library search combined with manual analysis, a total of 32 components were detected (see Table 1), the main component of which was ethyl Vanillin, vanillin, ethyl butyrate, oleic acid, maltol, palmitic acid, benzyl acetate, octanoic acid,

citronellol, etc.; most of the components have a matching degree of more than 85%. In addition, normalized quantification was performed, and the quantitative results are shown in Table 1.

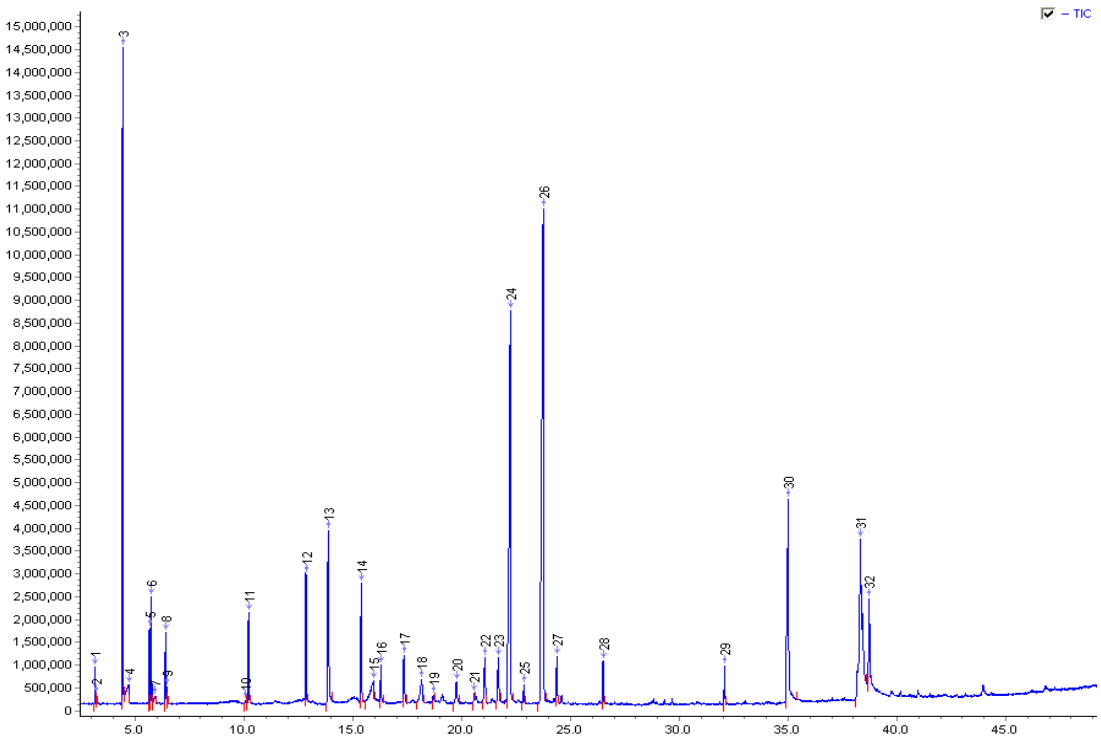

Figure 1 Blueberry flavor full scan chromatogram

Table 1 Analysis results of blueberry flavor composition

No.	Retention timemin /min	Name	CAS	Molecular formula	relative amount %	similarity degree %
1	3.12	1-Butanol, 3-methyl-	123-51-3	$C_5H_{12}O$	0.43	91
2	3.18	1-Butanol, 2-methyl-	137-32-6	$C_5H_{12}O$	0.07	90
3	4.40	Butanoic acid, ethyl ester	105-54-4	$C_6H_{12}O_2$	9.26	91
4	4.68	Butanoic acid	107-92-6	$C_4H_8O_2$	1.18	88
5	5.64	Butanoic acid, 2-methyl-, ethyl ester	7452-79-1	$C_7H_{14}O_2$	1.24	94
6	5.72	Butanoic acid, 3-methyl-, ethyl ester	108-64-5	$C_7H_{14}O_2$	1.56	91
7	5.91	Butanoic acid, 3-methyl-	503-74-2	$C_5H_{10}O_2$	0.26	90
8	6.38	1-Butanol, 3-methyl-,acetate	123-92-2	$C_7H_{14}O_2$	1.13	92
9	6.45	1-Butanol, 2-methyl-,acetate	624-41-9	$C_7H_{14}O_2$	0.22	91
10	10.06	Hexanoic acid	142-62-1	$C_6H_{12}O_2$	0.06	81
11	10.19	Hexanoic acid, ethyl ester	123-66-0	$C_8H_{16}O_2$	1.57	92
12	12.83	Hexanoic acid, 2-propenyl ester	123-68-2	$C_9H_{16}O_2$	2.33	89
13	13.86	Maltol	118-71-8	$C_6H_6O_3$	5.30	90

No.	Retention timemin /min	Name	CAS	Molecular formula	relative amount %	similarity degree %
14	15.37	Acetic acid, phenylmethyl ester	140-11-4	$C_9H_{10}O_2$	2.55	94
15	15.93	Octanoic Acid	124-07-2	$C_8H_{16}O_2$	1.54	87
16	16.27	Methyl Salicylate	119-36-8	$C_8H_8O_3$	0.76	88
17	17.33	6-Octen-1-ol, 3,7-dimethyl-	106-22-9	$C_{10}H_{20}O$	1.01	91
18	18.16	2-Decenal, (Z)-	2497-25-8	$C_{10}H_{18}O$	1.31	90
19	18.70	Nonanoic acid	112-05-0	$C_9H_{18}O_2$	0.17	80
20	19.75	2,4-Decadienal	2363-88-4	$C_{10}H_{16}O$	0.84	89
21	20.57	Benzoic acid, 2-amino- methyl ester	134-20-3	$C_8H_9NO_2$	0.16	88
22	21.05	2-Undecenal	2463-77-6	$C_{11}H_{20}O$	1.35	92
23	21.67	2-Propenoic acid, 3-phenyl-, methyl ester	103-26-4	$C_{10}H_{10}O_2$	1.14	88
24	22.23	Vanillin	121-33-5	$C_8H_8O_3$	15.96	94
25	22.85	3-Buten-2-one,4-(2,6,6-trimethyl-2-cyclohexen-1-yl)-, (E)-	127-41-3	$C_{13}H_{20}O$	0.47	86
26	23.74	Ethyl Vanillin	121-32-4	$C_9H_{10}O_3$	24.11	94
27	24.37	3-Buten-2-one, 4-(2,6,6-trimethyl-1-cyclohexen-1-yl)-, (E)-	79-77-6	$C_{13}H_{20}O$	0.92	91
28	26.49	2(3H)-Furanone, 5-heptyldihydro-	104-67-6	$C_{11}H_{20}O_2$	0.95	92
29	32.07	Isopropyl Myristate	110-27-0	$C_{17}H_{34}O_2$	0.82	90
30	35.00	n-Hexadecanoic acid	57-10-3	$C_{16}H_{32}O_2$	8.64	91
31	38.32	Oleic Acid	112-80-1	$C_{18}H_{34}O_2$	10.30	91
32	38.73	Octadecanoic acid	57-11-4	$C_{18}H_{36}O_2$	2.41	87

3 Conclusion

GC/MS technique is the most effective analytical method for analysis of flavor composition. In this paper, the composition of blueberry flavor was analyzed by domestic instrument GC-MS3100, and 32 substances were identified. Among them, main components were ethyl vanillin, vanillin, ethyl butanoate, oleic acid, maltol, palmitic acid, benzyl acetate, octanoic acid, citronellol, etc. Most of these components have similarity of more than 85%. This method is simple, fast and accurate, and it fully meets the analytical test requirements in this respect.