FLAVOR AND FRAGRANCE ARTICLES

Analysis of pineapple flavor compositions by GC-MS

1 Instruments and reagents

GC-MS3100 Gas Chromatograph/Mass Spectrometer; 1 μL microinjector; pineapple flavor sample

2 Analysis conditions

MS conditions： EI source; ion source temperature: 200℃; electron energy: 70eV; scanning mode: full scan; scanning range: 28.5u～400u; interface temperature: 280℃; multiplier high voltage: 1200V; solvent delay: 1.75min

GC conditions： Equity-5 (30m×0.25mm×0.25um) silica capillary column; carrier gas: high purity helium; injection port temperature: 280℃; split sampling; sample volume: 0.1μL; split ratio: 50:1; precolumn pressure: 60kPa; purge rate: 2ml/min; column temperature program: 35℃ for 1 min, ramp up to 270 ° C at 7 °C/min and then hold for 5 min.

3 Analysis results

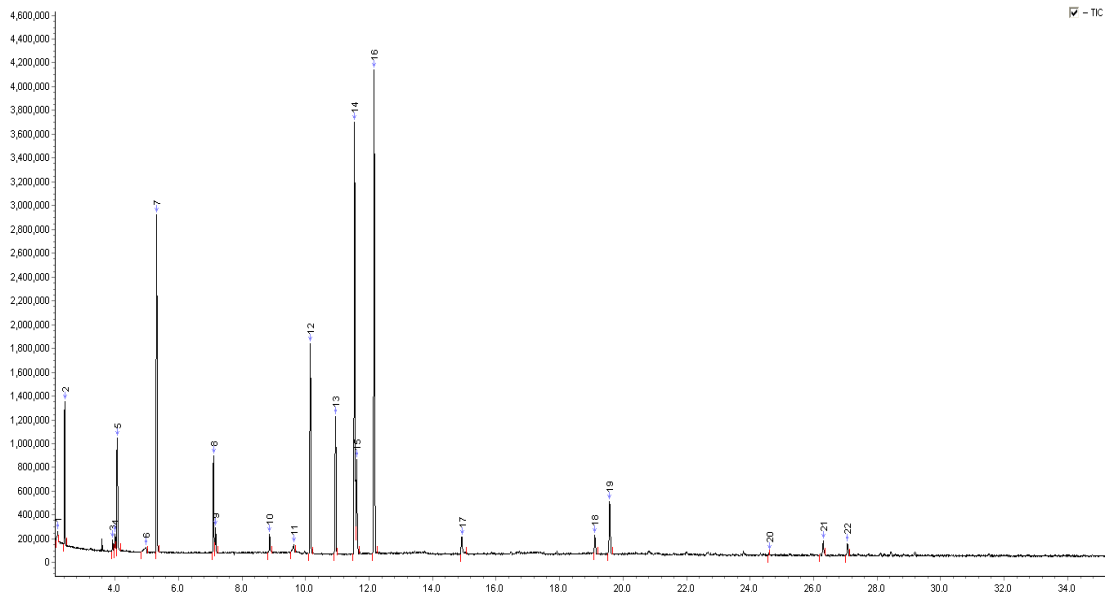

Figure 1 Pineapple flavor's TIC chromatogram

Table 1 Analysis results of pineapple flavor composition

Peak No.	Retention time, min	Name	CAS No.	Molecular formula	relative amount, %	similarity degree, %
1	2.20	Acetic acid	64-19-7	$C_2H_4O_2$	0.49	80
2	2.41	Ethyl Acetate	141-78-6	$C_4H_8O_2$	4.42	90
3	3.93	Ethane, 1,1-diethoxy-	105-57-7	$C_6H_{14}O_2$	0.37	88
4	3.99	1-Butanol, 3-methyl-	123-51-3	$C_5H_{12}O$	0.59	91
5	4.06	(S)-(+)-1,2-Propanediol	4254-15-3	$C_3H_8O_2$	5.39	90
6	4.98	Butanoic acid	107-92-6	$C_4H_8O_2$	0.63	79
7	5.31	Butanoic acid, ethyl ester	105-54-4	$C_6H_{12}O_2$	12.73	94
8	7.10	1-Butanol, 3-methyl-, acetate	123-92-2	$C_7H_{14}O_2$	3.98	91
9	7.17	1-Butanol, 2-methyl-, acetate	624-41-9	$C_7H_{14}O_2$	1.11	90
10	8.86	Butanoic acid, 3-oxo-, ethyl ester	141-97-9	$C_6H_{10}O_3$	0.92	85
11	9.63	Hexanoic acid	142-62-1	$C_6H_{12}O_2$	0.59	85
12	10.15	Hexanoic acid, ethyl ester	123-66-0	$C_8H_{16}O_2$	8.80	94
13	10.95	D-Limonene	5989-27-5	$C_{10}H_{16}$	6.30	92
14	11.54	Propanoic acid, 2-methyl-, 3-methylbutyl ester	2050-01-3	$C_9H_{18}O_2$	20.49	90
15	11.61	Butanoic acid, 2-methylbutyl ester	51115-64-1	$C_9H_{18}O_2$	4.64	89
16	12.16	Hexanoic acid, 2-propenyl ester	123-68-2	$C_9H_{16}O_2$	21.36	92
17	14.92	4H-Pyran-4-one, 2-ethyl-3-hydroxy-	4940-11-8	$C_7H_8O_3$	1.12	93
18	19.11	Vanillin	121-33-5	$C_8H_8O_3$	0.96	90
19	19.58	Cyclohexanepropanoic acid, 2-propenyl ester	2705-87-5	$C_{12}H_{20}O_2$	2.76	88
20	24.60	Undecanal	112-44-7	$C_{11}H_{22}O$	0.15	80
21	26.30	Isopropyl Myristate	110-27-0	$C_{17}H_{34}O_2$	0.79	84

4 Conclusion

The composition of pineapple flavor was analyzed by GC-MS3100, and the separation effect was good. The qualitative analysis was performed through NIST standard library search combined with manual analysis, and 21 compounds have been determined; most of them have similarity of more than 85%. This method is simple, rapid and accurate. The results show that GC-MS 3100 is a very effective instrument for flavor composition analysis.