

ANALYSIS OF FRAGRANCE COMPOUNDS

USING THE QP-5000 GC/MS

Foods contain many fragrance components. These compounds include alcohols, esters, aldehydes, ketones and terpenes. The ratios of these compounds present in the food determine each distinctive aroma. In addition, many aromas can be simulated by mixing the above compounds.

Due to the large numbers of these aroma-producing compounds, it is necessary to perform separation as part of the analysis so GC (gas chromatography)

is used. Identification of the components is made from mass spectra generated by a mass spectrometer.

Here, approximately 100 fragrance compounds, including alcohols, esters, aldehydes, ketones and terpenes, were placed in a mixture and analyzed using GC/MS. Figure 1 shows the TIC (total ion chromatogram). Table 2 lists the components.

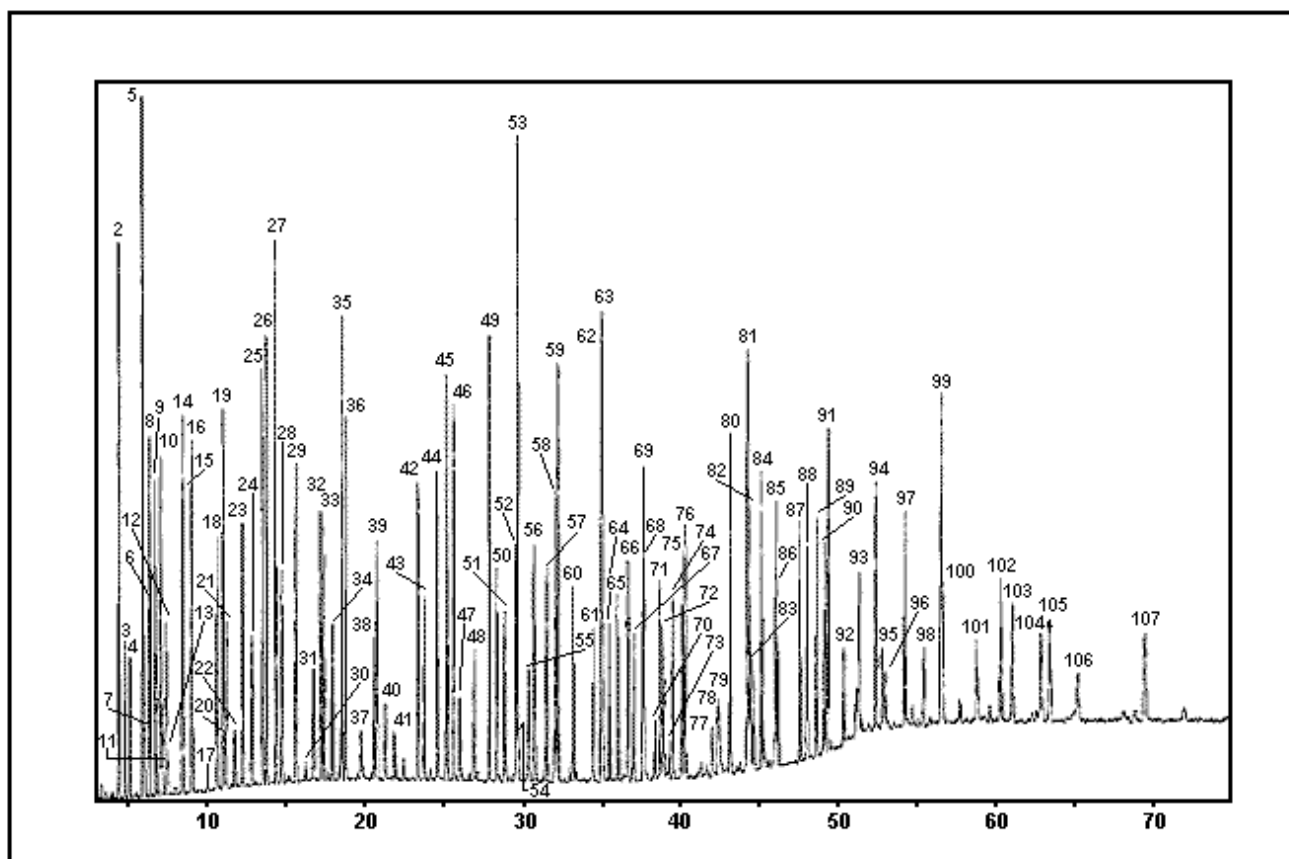


Figure 1 – TIC of Flavour

	Compound Name	Alcohol	Ester	Aldehyde	Ketone	Terpene	Other
1	Ethyl acetate		○				
2	Diethyl acetal						○
3	Ethyl alcohol	○					
4	Ethyl propionate		○				
5	n-Butyl acetate		○				○
6	Chloroform						
7							
8	Ethyl n-butyrate		○				
9	Ethyl 2-methyl butyrate		○				
10	Ethyl i-valerate		○				
11	n-Butyl acetate		○				
12	n-Hexanal			○			
13	n-Butyl alcohol	○					
14	n-Amyl acetate		○				
15	n-Butyl alcohol	○					
16	Methyl amyl ketone				○		
17							
18	n-Amyl propionate		○				
19	Limonene						○
20	2-Methyl butyl alcohol	○					
21	n-Amyl furmate		○				
22	2-Hexanal			○			
23	Ethyl caproate		○				
24	n-Amyl alcohol	○					
25	1-Amyl n-butyrate		○				
26	n-Hexyl acetate		○				
27	Methyl n-hexyl ketone				○		
28	1-Amyl 1-valerate		○				
29							
30							
31	Ethyl lactate		○				
32	n-Hexanol	○					
33	Ethyl n-hexyl ketone				○		
34	Allyl caproate		○				
35							
36	Methyl n-heptyl ketone				○		
37	t-3-Hexanol	○					
38							
39	Ethyl caprylate		○				
40	Acetic acid						
41	Furfural			○			
42	Methyl n-octyl ketone				○		
43	Tetrahydro furfuryl alcohol	○					
44	Benzaldehyde			○			
45	Ethyl nonanoate		○				
46	Linalcol					○	
47							
48	Diethyl malonate		○				
49	Methyl n-nonyl ketone				○		
50	Ethyl levulinate		○				
51	Methyl benzoate		○				
52	Ethyl caprate		○				
53	1-Menthol						○
54							

Table 2 – List of Compounds

	Compound Name	Alcohol	Ester	Aldehyde	Ketone	Terpene	Other
55	Furfuryl alcohol	○					
56	Ethyl benzoate		○				
57	Phenyl diethyl acetate		○				
58							
59	Methyl n-decyl ketone				○		
60	Benzyl acetate		○				
61	Methyl phenyl acetate		○				
62	Dimethyl benzyl carbinyl acetate		○				
63	Allyl caprate		○				
64	Ethyl phenyl acetate		○				
65	allyl β-cyclohexyl propionate		○				
66	Phenethyl acetate		○				
67	Anethol					○	
68	Caproic acid						○
69	Ethyl laurate		○				
70	1-2-Decenal			○			
71	Benzyl n-butyrate		○				
72	Benzyl alcohol	○					
73	Phenetyl propionate		○				
74	1-Butyl phenyl acetate		○				
75	Dimethyl benzyl carbinylbutyrate		○				
76	Phenyl ethyl alcohol	○					
77							
78							
79	Phenyl ethyl propionate		○				
80	Phenethyl 1-valerate		○				
81	Methyl n-tridecyl ketone				○		
82	Anisaldehyde			○			
83	γ-Nonalactone						○
84	Ethyl myristate		○				
85	Triacetine						○
86	Methyl cinnamate		○				
87	Benzylidene acetone				○		
88	Ethyl cinnamate		○				
89	γ-Decalactone						○
90	Eugenol					○	
91	Phenethyl caproate		○				
92	δ-Decalactone						○
93	Heliotropine						○
94	γ-Undecylactone						○
95	Anisalcohol		○				
96	Cinnamy alcohol		○				
97	Diethyl sebacle			○			
98							
99	γ-Deodecylactone						
100	Phenethyl octanoate			○			
101	δ-Dodecylactone						○
102	TEC						○
103	Benzophenone				○		
104	Ethyl vanillin						○
105							
106	Vanillin						○
107	Benzyl benzoate		○				

Table 2 – Continued

Apparatus	: Shimadzu GCMS QP5000		
Column	: DB-WAX 60m 0.25mmi.d. df=0.25µm		
Column Temp.	: 70°C (5min) – 3°C/min → 210°C (30min)		
Inj. Temp.	: 250°C	Int. Temp.	: 230°C
Carrier gas	: He 180kPa	Split Ratio	: 100 : 1

Table 1 – Analytical Conditions

Figure 2 shows a full scan mass chromatogram of peaks 10 to 18. As seen from this data, peaks 15 and 16 represent two overlapping components. Figures 3 and 4 show the library search results based on the background subtracted mass spectrum. The results indicate that peak

15 is butyl alcohol and peak 16 is isoamyl methyl ketone. In this type of complex chromatogram, using a mass spectrometer enables the investigator to determine if a chromatographic peak is homogeneous.

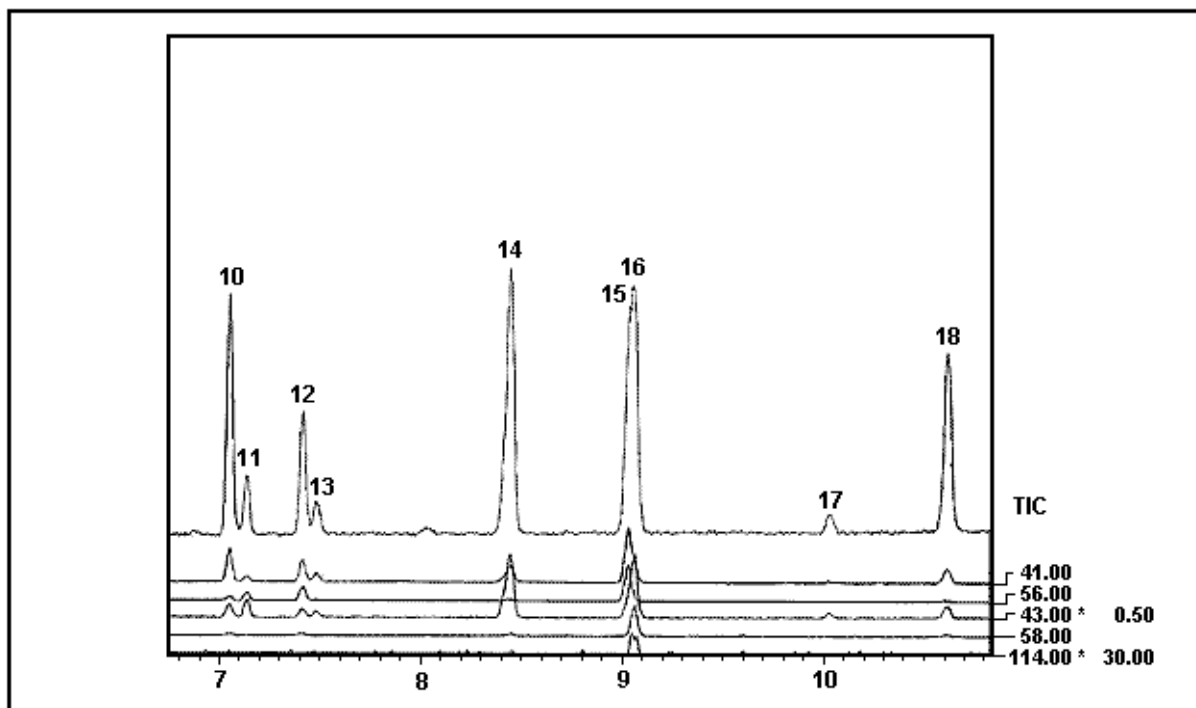


Figure 2 – Mass Chromatogram

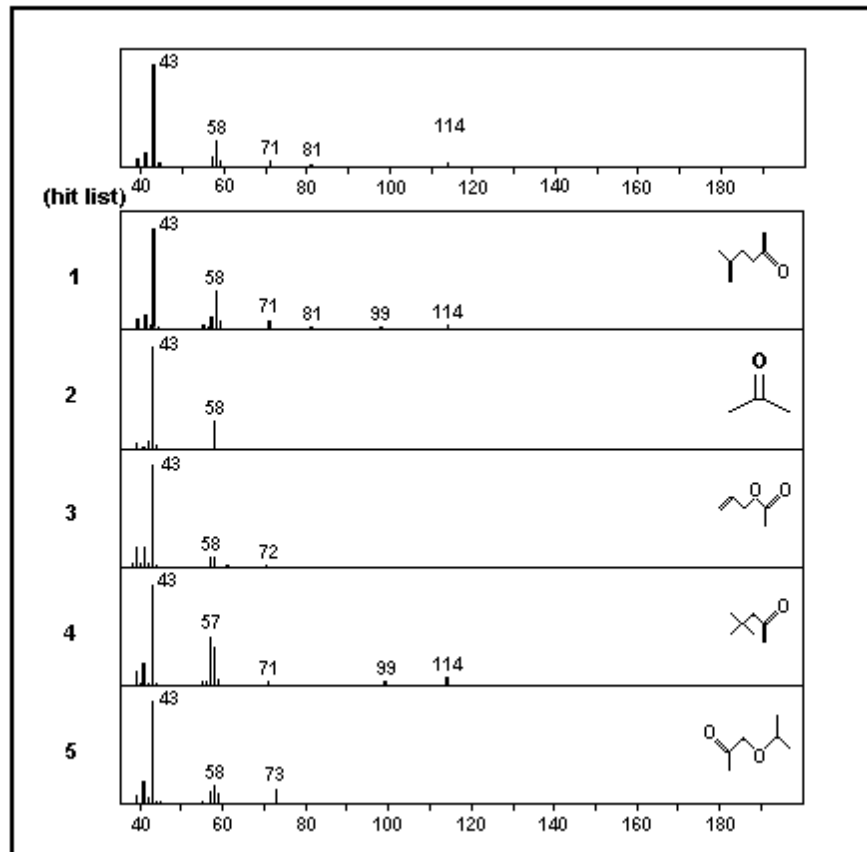


Figure 3 – Library Search of Peak 15

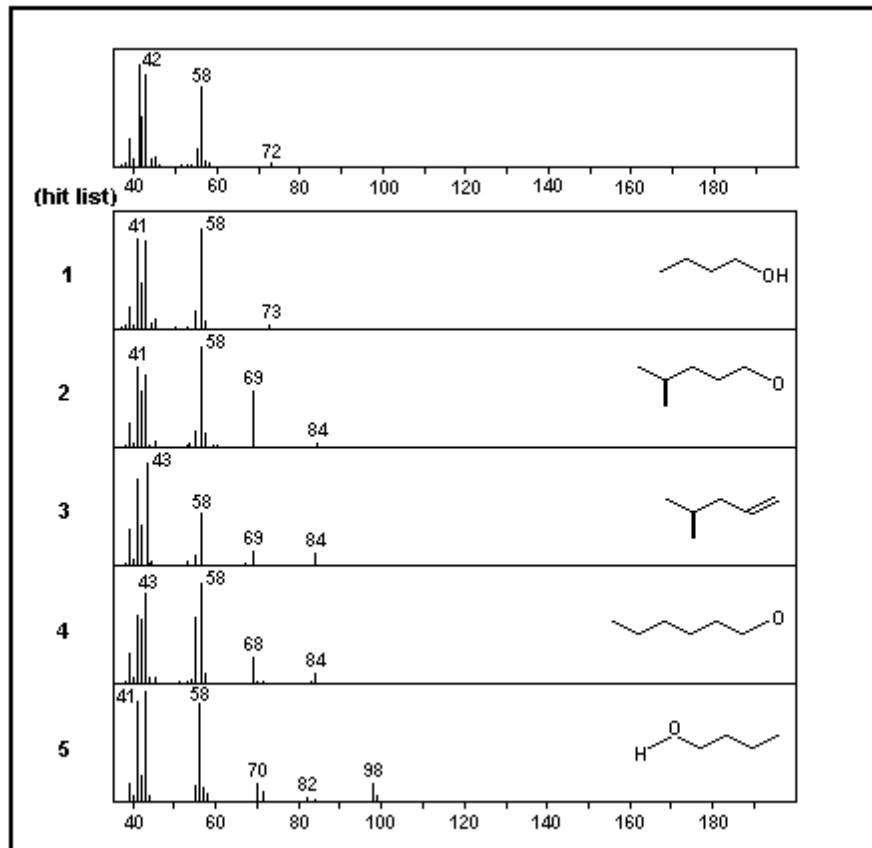


Figure 4 – Library Search of Peak 16