# 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.

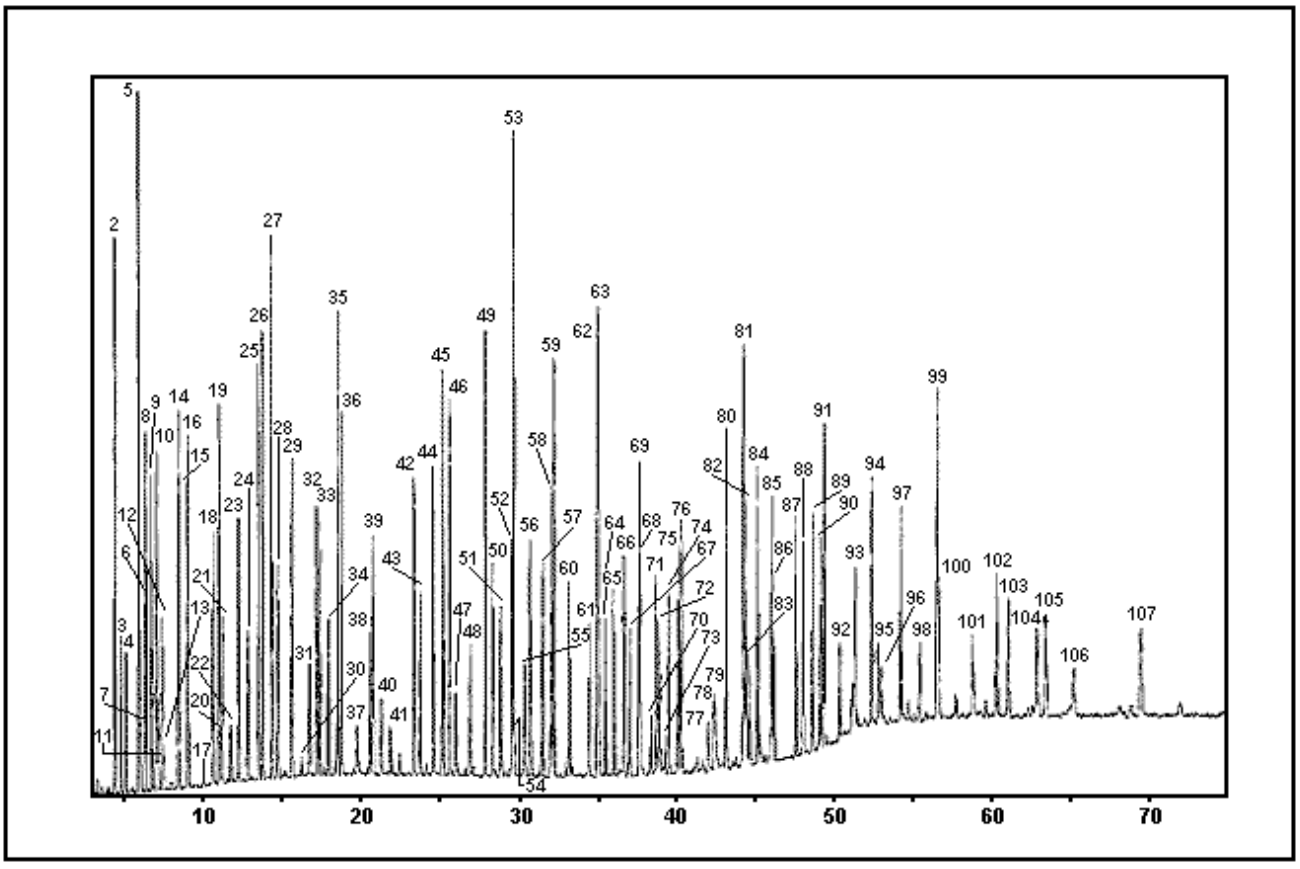


**Figure 1 – TIC of Flavour**

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

**Table 2 – List of Compounds**

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

**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.

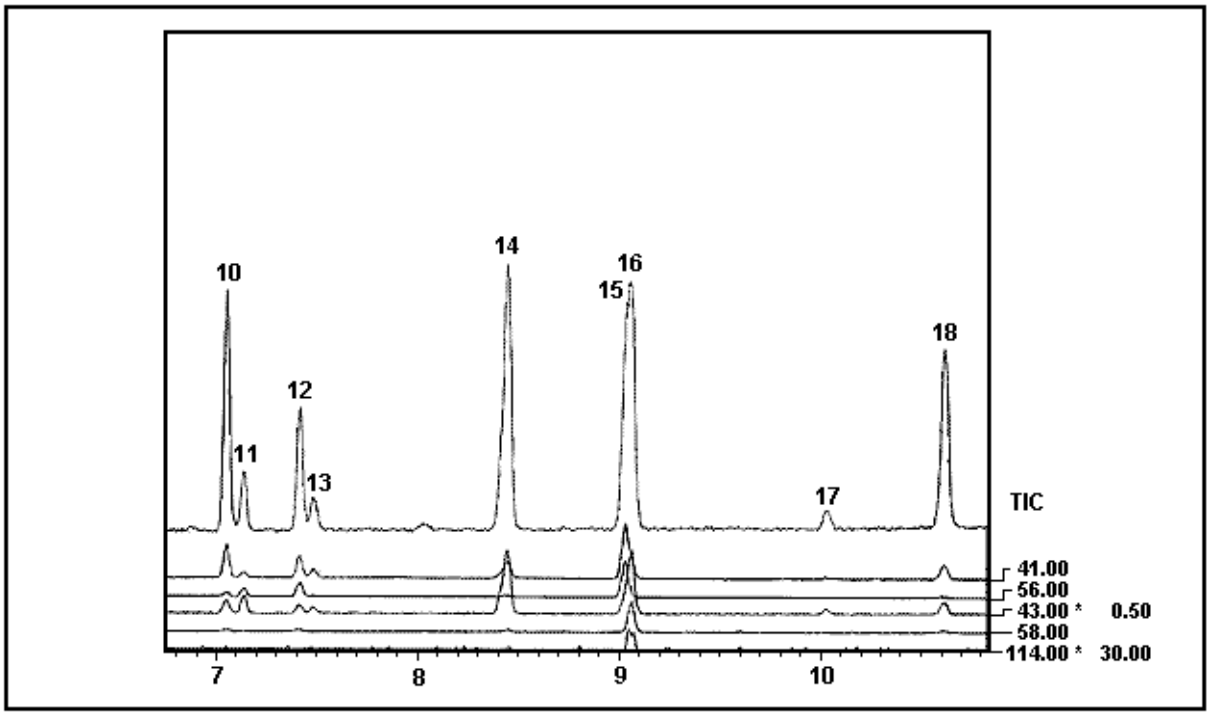


**Figure 2 – Mass Chromatogram**

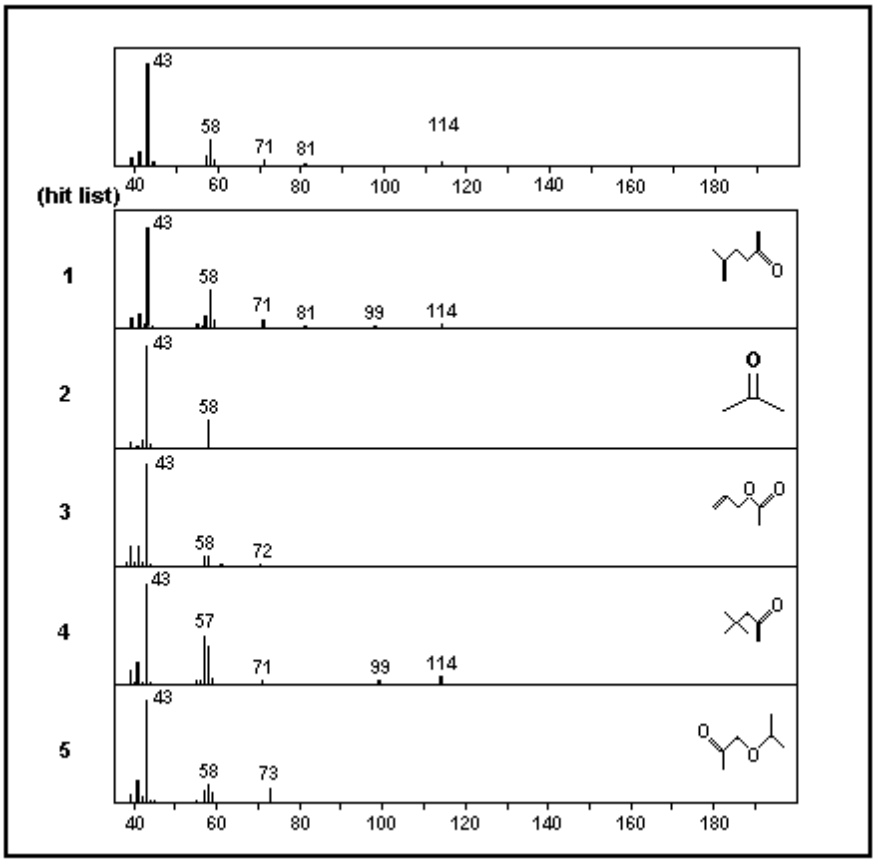


**Figure 3 – Library Search of Peak 15**

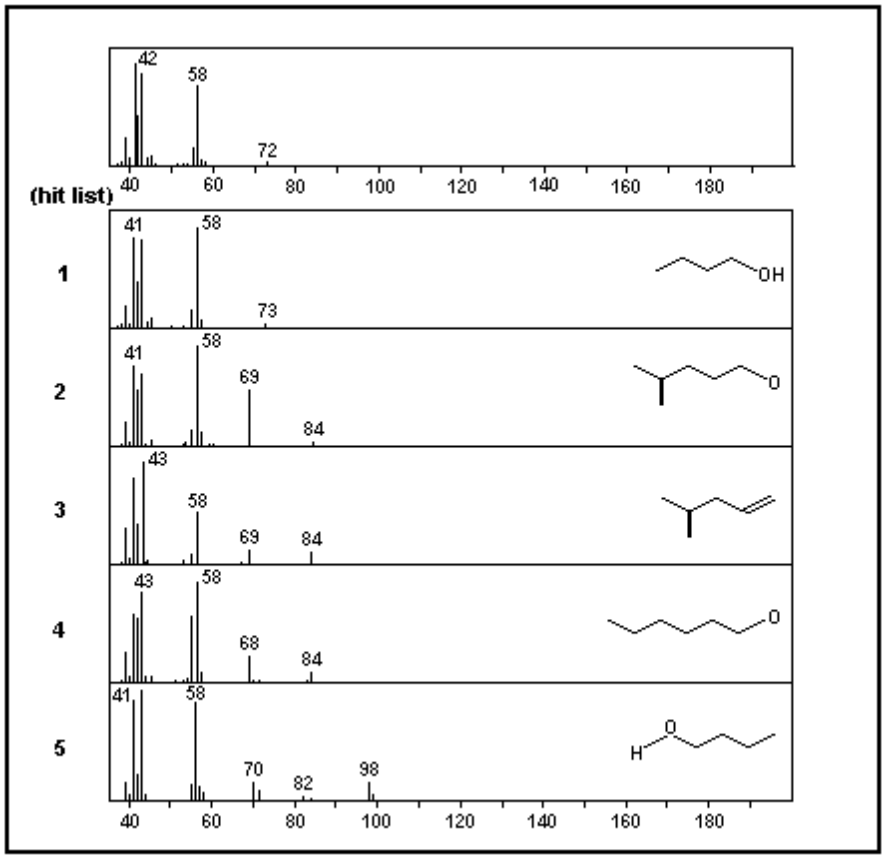


**Figure 4 – Library Search of Peak 16**