1.1 Analysis of Fatty Acids (1) - GCMS

•Explanation

Fatty Acids exist in a great many food products. And derivatization process is used to measures them. The aims of derivatization process are as follows.

1) Weaken the polarity of compounds.
2) Lower the boiling point.
3) Increase molecular ion peak and ion intensity in high mass region.

In the case of fatty acids, derivatization process is used to achieve item 1). The methyl esterization or trimethylsilylation can be used but generally methyl esterization employing diazomethane is used for the derivatization.

Normally, the molecular ion peak that displays the molecular weight is detected for the Ei mass spectrum's saturated fatty acid methyl ester and, as determination of molecular weight is easy, a carbon count is possible.

However, the molecular ion peak often does not appear when the level of unsaturation increases, which means that not only molecular weight but also the carbon count and unsaturated level cannot be determined. In such cases, the Ci mass spectrum is measured. With the Ci mass spectrum, the ion denoting the molecular weight appears as an ion (M+1) with added proton in the molecular weight for detection of molecular weight + 1 ion. Measuring the Ei and Ci mass spectra enables qualitative analysis of compounds in fatty acid methyl ester measuring. Also, the columns used in this measuring include the slightly polar column DB-1 and polar column DB-WAX. The polarity column produces peaks in the saturated and unsaturated order while the slightly polar column produces peaks in the reverse order.

•Analytical Conditions

Instrument	: GCMS-QP5000
Column	: DB-WAX 0.25mm×30m df=0.25μm
Col.Temp.	: 60℃-250℃ (10℃/min)
Inj. Temp.	: 250℃
I/F Temp.	: 250℃
Carrier Gas	: He(100kPa)
Reagent Gas	: Isobutane

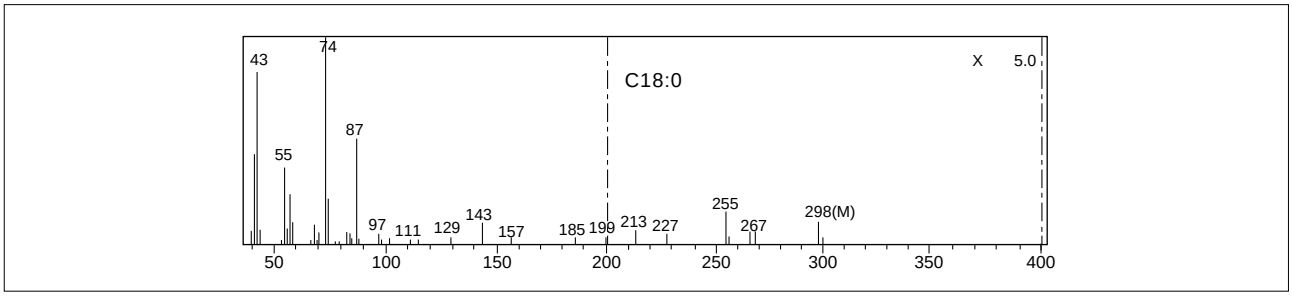

Fig. 1.1.1 Ei mass spectrum of C18:0

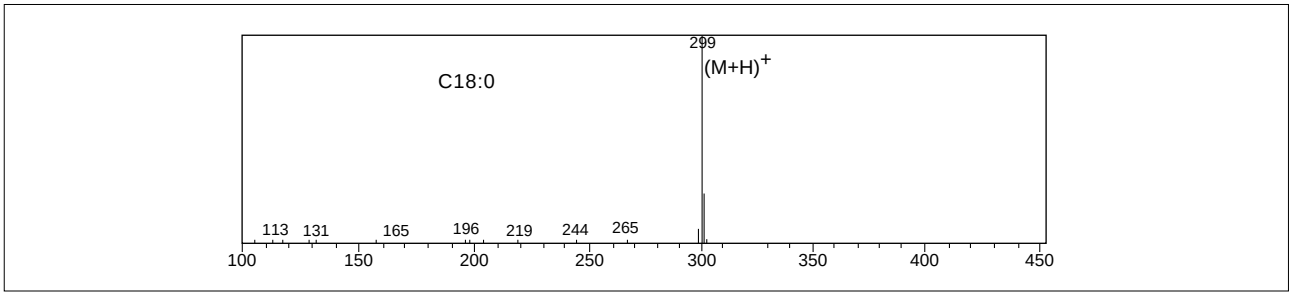

Fig. 1.1.2 Ci mass spectrum of C18:0

1.1 Analysis of Fatty Acids (2) - GCMS

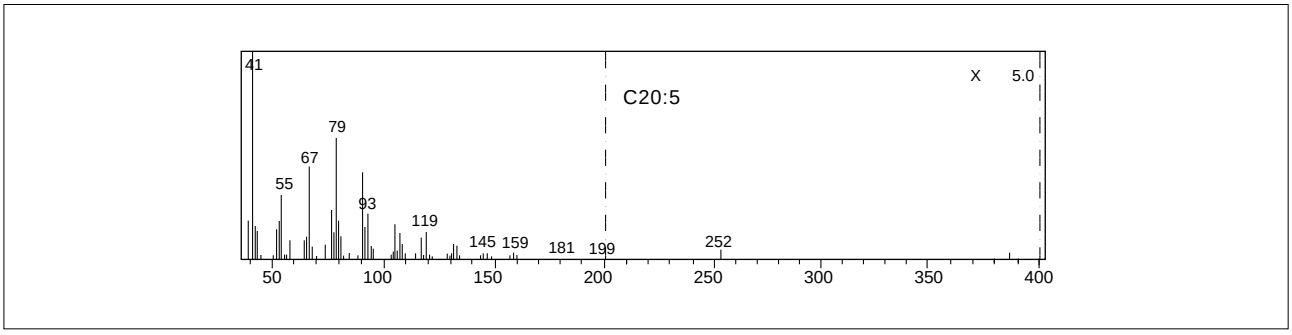

Fig. 1.1.3 Ei mass spectrum of C20:5

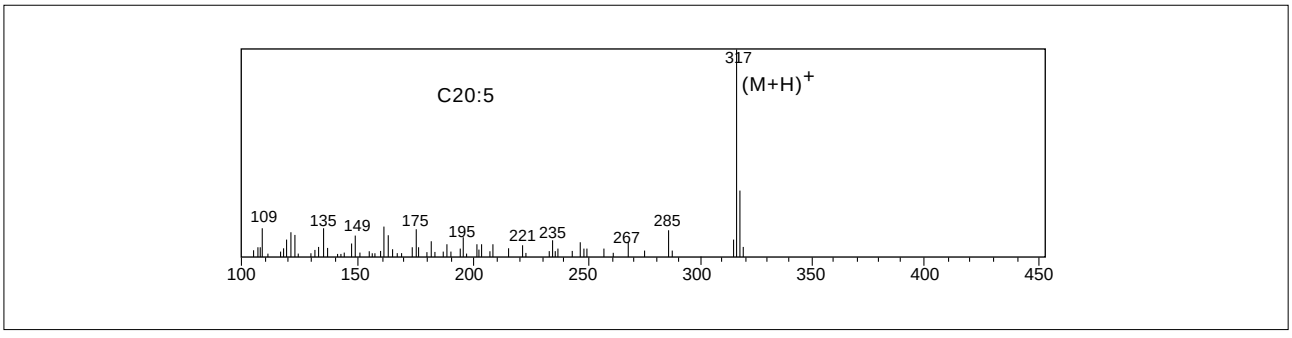

Fig. 1.1.4 Ci mass spectrum of C20:5

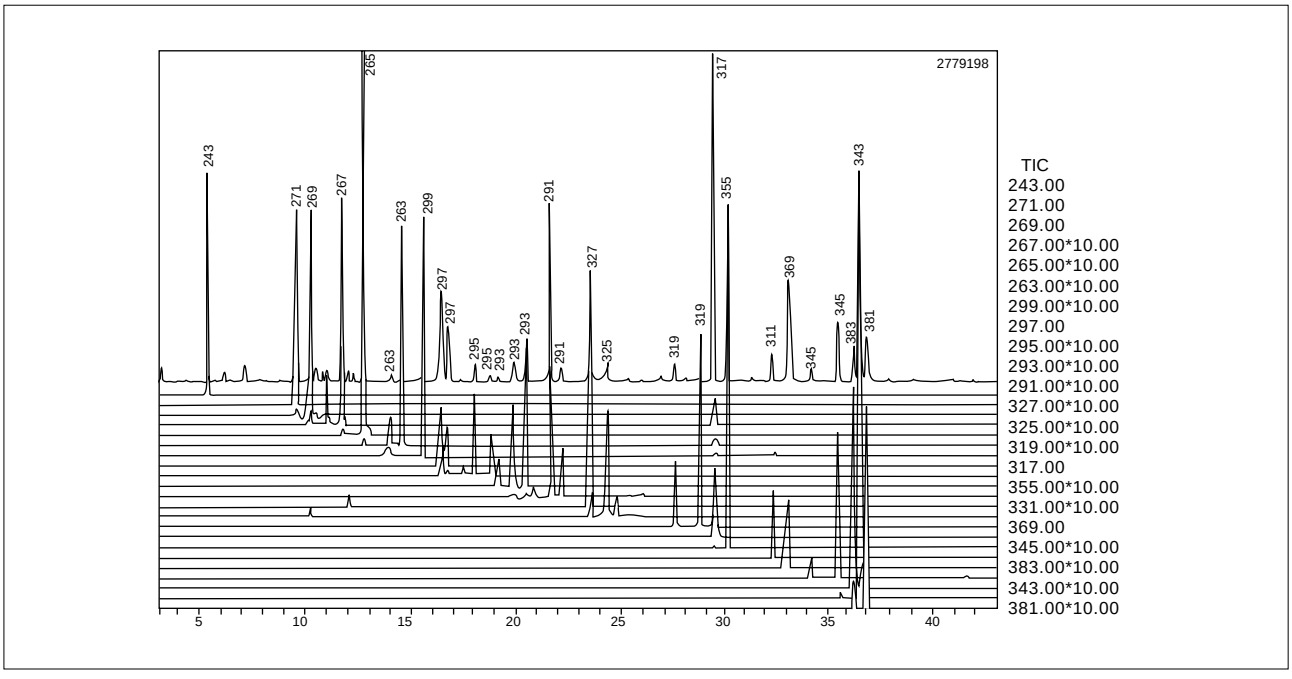

Fig. 1.1.5 Mass chromatogram of protonized molecules for fatty acid methyl ester