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Identification of an Edible Oil by GC/MS

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Edible oils are lipids that are liquid at room temperature and are normally found in human diet. Lipids are fatty acids and their derivatives, such as triglycerides.[1] An edible oil can be characterised based on its fatty acids content or composition.

A gas chromatograph-mass spectrometer (GC/MS) offers a convenient way to determine the fatty acid composition of an edible oil, because by using a GC/MS, one can physically separate the fatty acids and identify them in a single analysis.

In the analysis of fatty acids, normally the fatty acids are derivatised.[1] One commonly used method of fatty acid derivatisation is conversion of the fatty acids into their methyl esters, which is carried out to: (1) reduce the polarity of the analytes; (2) lower the boiling point of the target analytes. The target analytes in this case are the corresponding fatty acid methyl esters (FAMEs). Methyl esterification can be done by using diazomethane or BF_3-Methanol solution.

Here we describe the application of GC/MS for identifying an edible oil based on the fatty acid composition of the oil. In the present case, we derivatised the fatty acids into the FAMEs by using BF_3-Methanol (10% v/v) solution prior to the GC/MS analysis. The analytical conditions are shown in Table 1, and the chromatograms are shown in Figure 1 and Figure 2.

The FAMEs were identified by matching their mass spectra to the mass spectra in the NIST mass spectral database. The mass spectral matching were performed using the GCMSsolution software's *Similarity Search* function, which allows an analyst to compare an unknown mass spectrum with more than one hundred thousand reference mass spectra in less than one minute. The results of the mass spectral matching can be shown graphically, as shown in Figures 3a and 3b.

The fatty acid composition of the oil was obtained from the area% of the FAMEs peaks in the chromatogram (see Table 2 for the area% values). The fatty acid composition indicates that the oil was palm oil.[2]

REFERENCE:

1. Lipid Library, Lipid Analysis Unit, Scottish Crop Research Institute, Scotland http://www.lipid.co.uk

2. "Palm Oil", http://www.britanniafood.com/german/invite_02.htm

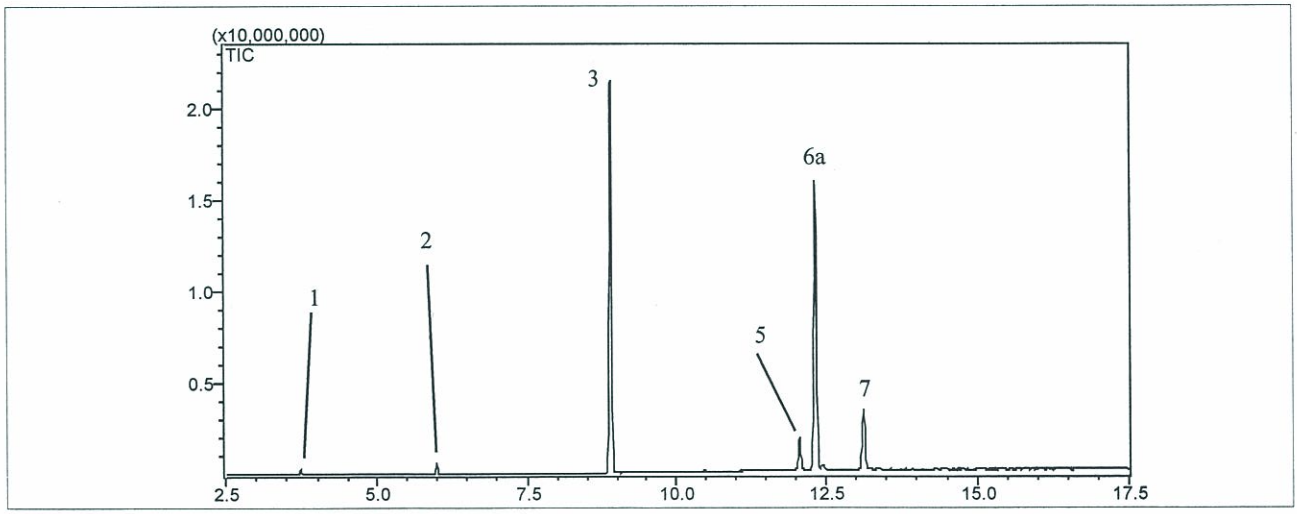

Figure 1. Full chromatogram of the FAMEs mixture obtained from the derivatisation of the edible oil. The chromatogram was obtained using the GC/MS analytical conditions shown in Table 1. Major components, as well as some of the minor components, of the fatty acids are shown : 1) 12:0; 2)14:0; 3)16:0; 5)18:0; 6a)18:1; 7)18:2.

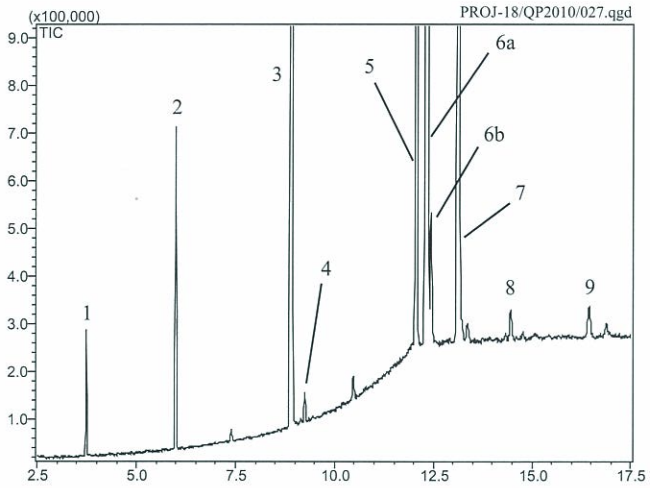

Table 1. Analytical Conditions

Instrument	:	GCMS-QP2010 with GCMSsolution Software
Column	:	Polyethylene glycol (DB-WAX), 30 m x 0.25 mm x 0.25 µm
Injection method	:	Split (Split ratio 100:1)
Injection temp.	:	250°C
Column temp.	:	120°C (0 min)→ 180°C (10 min) @ 5°C/min → 200°C (4 min) @ 5°C/min
Carrier gas	:	Helium, 99.9995% purity
Linear velocity	:	37.5 cm/sec (Constant Linear Velocity mode)
Interface temp.	:	250°C
Ionisation mode	:	Electron Impact
Ion source temp.	:	200°C
Acquisition mode	:	SCAN

Figure 2. Enlarged chromatogram of the FAMEs mixture, showing all of the fatty acid components. The peak numbers refer to those shown in Table 2.

Table 2. Fatty acid composition (% as methyl esters) in the oil.

Peak No.	*Ret. Time (min)*	*Fatty acid*	*Area %*	*Peak No.*	*Ret. Time (min)*	*Fatty acid*	*Area %*
1	3.73	12:0	0.3	6a	12.33	18:1 (*cis*)	39.3
2	5.99	14:0	1.2	6b	12.44	18:1 (*trans*)	
3	8.91	16:0	45.8	7	13.13	18:2	8.7
4	9.25	16:1	0.1	8	14.47	18:3	0.2
5	12.10	18:0	4.1	9	16.44	20:0	0.3

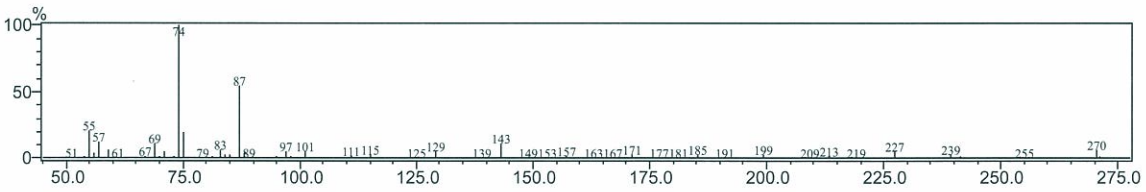

Figure 3a.

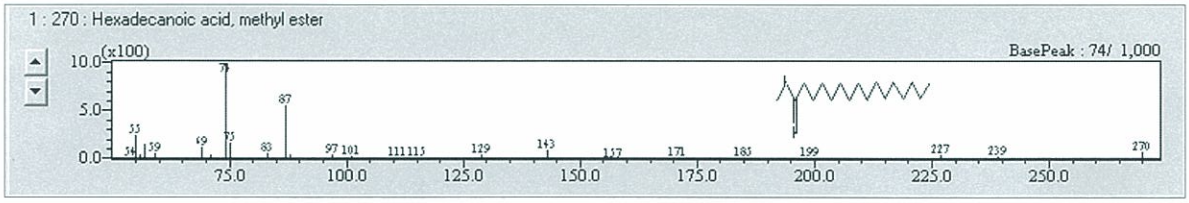

Figure 3b.

Figure 3. a) Mass spectrum (EI) of 16:0 fatty acid methyl ester obtained from the sample analysis; b) Mass spectrum (EI) of 16:0 fatty acid methyl ester in NIST library.

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