The analysis of edible oils using ATR FTIR

Spectroscopy is ideal for analysing the content of oil.

Introduction

EDIBLE OILS ARE A SERIES OF related natural compounds differing in their degree of unsaturation and chain length. Chemically, these compounds are esters of various fatty acids with a single trifunctional alcohol (glycerol), and are hence called triglycerides.

The degree of unsaturation of an edible oil is an important factor in its suitability as a food product. Saturated fats in dietary products have been implicated as a contributing cause of heart disease.

Consequently, there is now greater emphasis on the production of healthier brands of cooking fats, margarine and butter which contain percentages of linoleic acid (polyunsaturates).

Figure 1: Gateway ATR

However, polyunsaturates suffer from auto-oxidation leading to rancidity, which in the food industry has traditionally been monitored by time-consuming titrimetric methods.

Alternatively, fats and oils have been analysed by gas chromatography, where samples require prior chemical derivatisation.

Infrared spectroscopy can be complementary to these techniques for analysing edible oils. It is comparatively easy to identify absorbance bands that can be assigned to C-H vibrations in both saturated and unsaturated compounds. Peak height or area measurements allow the degree of unsaturation to be measured.

Experiment

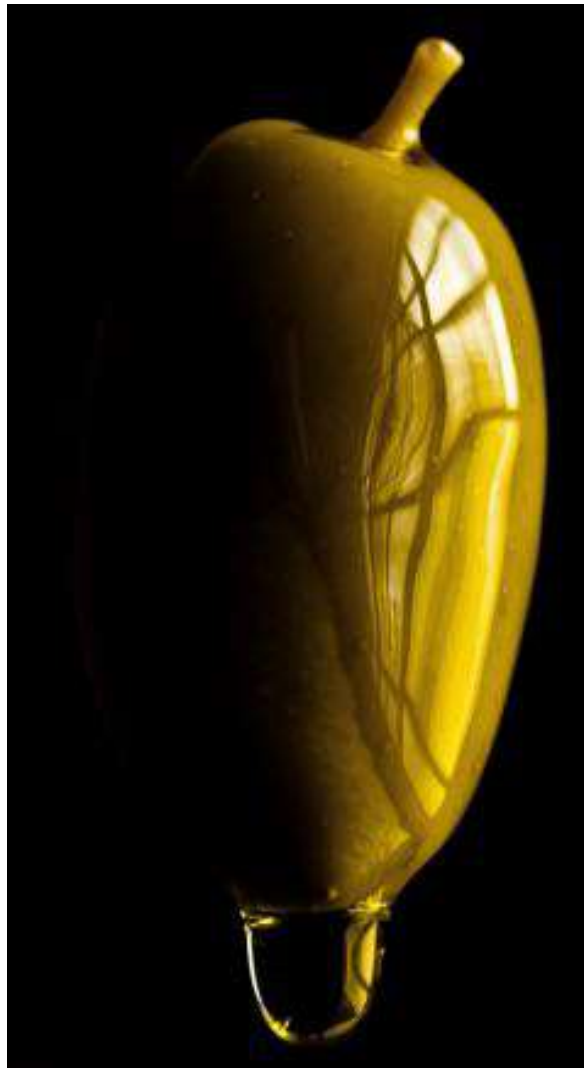
The use of the Gateway ATR (fig.1) allows convenient and rapid analysis of viscous liquid or semi-solid samples. No sample preparation is required as liquid samples can be poured onto the recessed trough or pastes spread onto the crystal surface.

The sample trough is fabricated in a chemically inert ATR crystal (typically Zinc Selenide) innovatively held in a corrosion resistant metal plate without the use of bonding adhesive.

The sample trough is easily removed for cleaning, by washing with a suitable solvent and wiping with a soft tissue without damages.

The non-bonded design of the crystal to the metal plate allows the metal plate to be retained; the top plate can be changed more economically by changing only the ZnSe crystal. The accessory requires minimal alignment and is available to fit all types of FT-IR spectrometer.

Six different types of natural oil were spread in turn on the ZnSe crystal and spectra was recorded on a modern FT-IR spectrometer, fitted with a DTGS detector. Data collection conditions were set for 64 scans at 4cm^{-1} resolution, with the sample chamber un-purged. The spectrum of the bare ZnSe crystal was used as a background.



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> A valuable guide for the onset of rancidity.

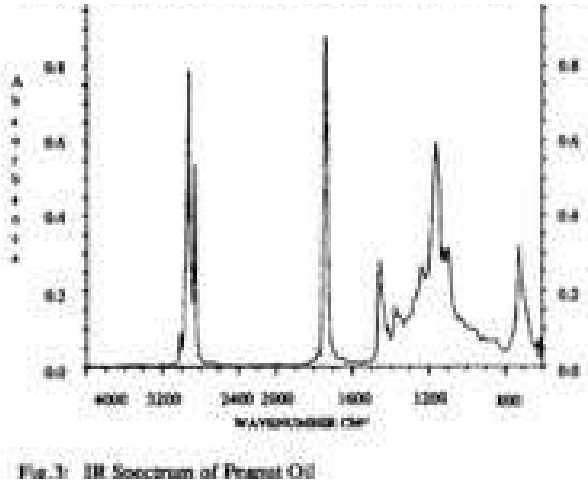

Fig. 3: IR Spectrum of Peanut Oil

Figure 2: IR spectrum of peanut oil

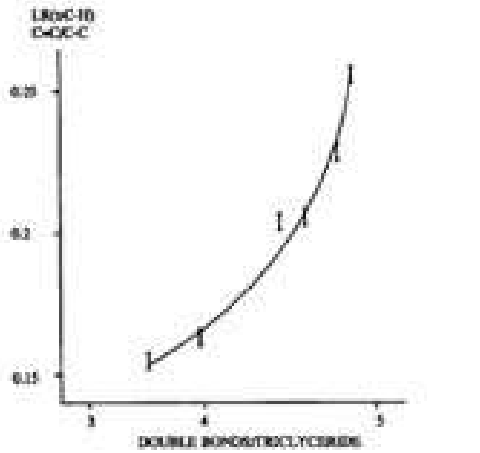

Fig.4: Double bond correlation between infrared and titrimetric analysis.

Figure3: double bond correlation between infrared and titrimetric analysis

Results and discussion

The spectrum shown (fig.2) was obtained from peanut oil without sample preparation using the Gateway ATR.

By selecting two C-H absorption peaks (3009cm-1 and 2854cm-1) that are indicative of unsaturated and saturated environments respectively, it is possible to measure the unsaturated and saturated ratio (by height and/or area) of the oil being tested.

This was done for a series of natural oils including sesame, peanut, sunflower, saffron, soya bean and corn oils. In order, the most unsaturated oil as deduced from ATR measurements was saffron oil, followed by sunflower, soya bean, corn, sesame, and peanut oil.

A plot of the infrared unsaturated-saturated ratio against the corresponding number of double bond in a triglyceride measured by titrimetry is shown in graph (fig. 3). It is evident that the infrared analysis correlates well with the traditional procedure.

Conclusion

As well as offering a fast and accurate sampling method, infrared analysis also yields ready information on the water content of the fat and on the presence of contaminants, a valuable guide of the onset of rancidity.

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