Fatty acid composition analysis for glycerides in edible oils using thermal desorption/pyrolysis DART®-QTOFMS

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Introduction

Increasing attention is being given to the varying health effects of different edible oils. Edible oils are predominantly acylglycerols (fatty acids esterified with glycerol, also known as glycerides), with different fatty acid substituents associated with positive and negative health effects. Analytical methods that can quickly and easily determine the fatty acid composition of edible oils are thus of increasing importance. In this report, we introduce fatty acid composition analysis results of glycerides in edible oil and food items using ionRocket coupled with Direct Analysis in Real Time Quadrupole Time of Flight Mass Spectrometry (TDP/DART®-QTOFMS).

Easy analysis method for fatty acids acid substituents of glycerides

Materials and Methods

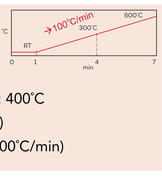
◆ **Materials:**

Medium chain Triglyceride (MCT)
Heavy cream (35.0% milk fat)
Vegetable based cream (40.0% vegetable fat)
Ice cream (15.0% milk fat)
Ice cream (13.0% vegetable fat)

◆ **Analytical methods:**

Thermal desorption/pyrolysis(TDP) / DART®-QTOFMS (Fig. 1)
3 µL of sample were put into the POT.
Mass spectra were measured as the samples were heated.
The fatty acid substituents were identified by MS/MS spectral analysis.

Mass Spec.: compact (Bruker)
Ion Source: DART®-SVP (IonSense)
Ionization gas: Helium
Helium gas temperature: 400°C
TDP device: ionRocket (BioChromato)
Temperature program : RT → 600°C(100°C/min)



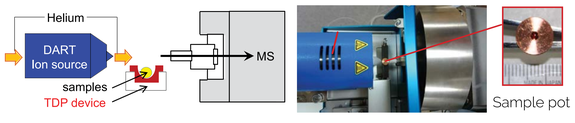


Fig. 1 TDP/DART®-QTOFMS System

Results and Discussions

An example of analysis using TDP/DART® MS

--- Sample: Medium chain Triglyceride (MCT) ---

It was confirmed that glycerides were detected at around 200-300°C (Fig. 2).

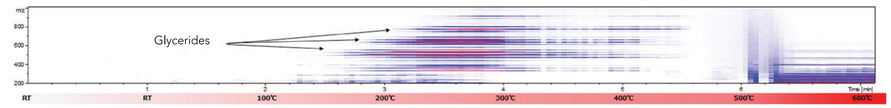


Fig. 2 Heat map of MCT

Results of the analysis of several peaks were observed around *m/z* 500, *m/z* 630, and *m/z* 760 at around 200-300°C (Fig. 2). As most of the detected mass peaks contained six oxygen atoms, they were assumed to be triglycerides (Fig. 3, upper mass spectrum). From their MS/MS spectral analysis, fragments suspected to be derived from the elimination of fatty acids constituting glycerides were obtained. Results for the MS/MS spectrum of triglycerides *m/z* 654.57 ($[C_{39}H_7 2O_6+NH_4]^+$) in MCT supported the elimination of three fatty acids caprylic acid (C8), capric acid (C10), and oleic acid (C18) (Fig. 3, lower MS/MS spectrum). Thus, it was summarized that the fatty acids constituting glycerides of MCT was C8, C10 and C18.

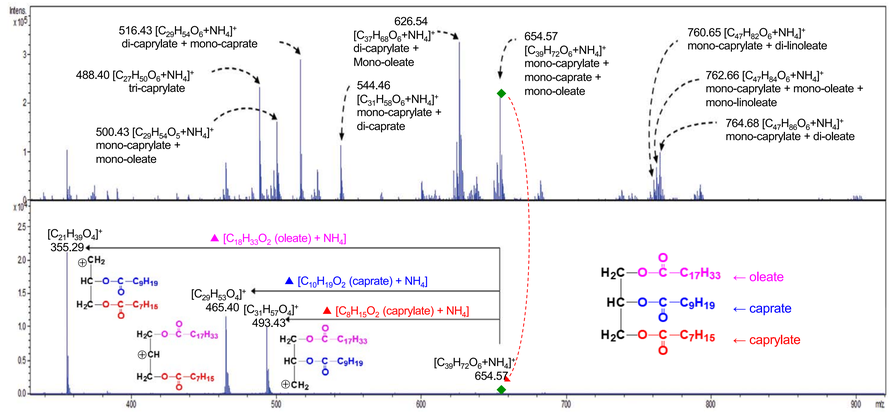


Fig. 3 Mass spectra collected from 200 to 300°C and MS/MS spectra of *m/z* 654.57; MCT

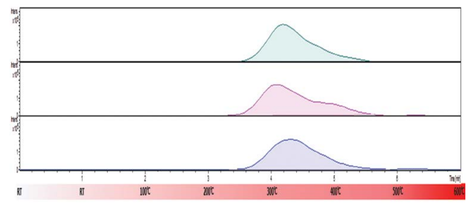


Fig. 4 Fig. 4 Reproducibility of EIC of *m/z* 654.57

The shape and the peak area value of extracted ion chromatograms show good reproducibility (Fig. 4, CV= 1.51% 、n=3).Thus, this analysis method is useful for quantitative analysis.

Discrimination between animal fats and vegetable fats

--- Sample: Heavy cream (35.0% milk fat) & Vegetable based cream (40.0% vegetable fat) ---

Both samples showed similar mass spectra, but the MS/MS spectra of same *m/z* showed different spectral pattern, the fatty acids constituting glycerides of milk fat were C4 ~ C18 and that of vegetable fat were C8 ~ C12. Thus, this method enables discrimination between animal fats and vegetable fats by using MS/MS spectral pattern as a marker (Fig. 5)

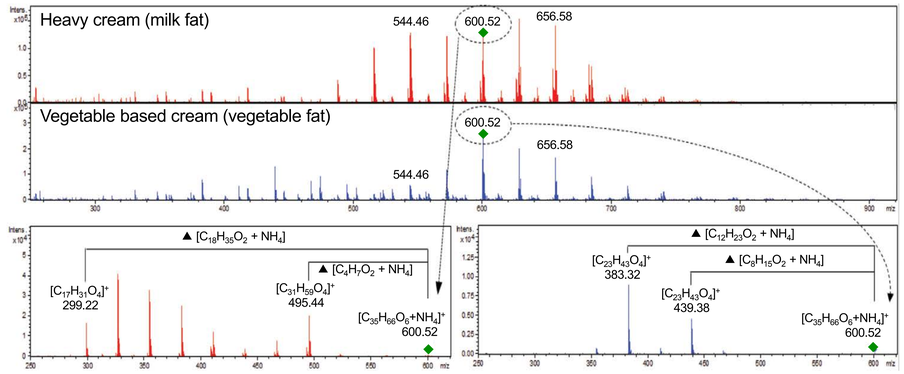


Fig. 5 Mass spectra taken at 200-300°C and MS/MS spectra of *m/z* 600.52; Heavy cream and Vegetable based cream

Application: Do these ice creams contain vegetable fats or animal fats?

--- Sample: Ice cream (15.0% milk fat) and Ice cream (13.0% vegetable fat) ---

As a result of analyzing ice cream, samples which comprise a mixture of fats and other raw materials, it was confirmed that the blend of fats in the sample can be revealed by the MS/MS spectral pattern. This method is also confirmation that these analyses can be performed without any pre-treatment such as dehydration or extraction.

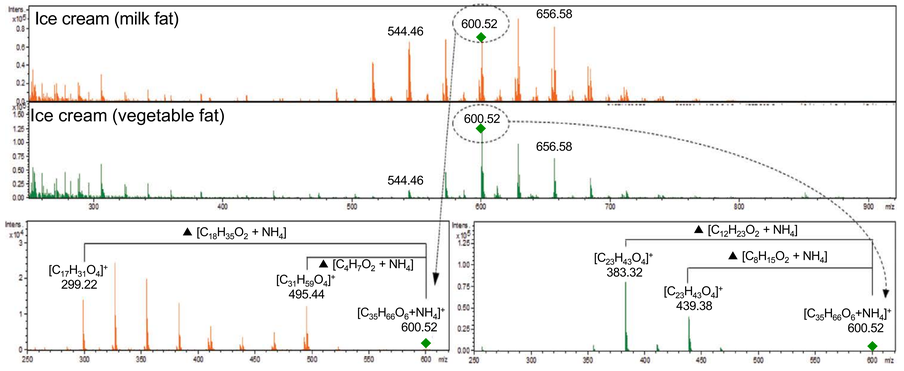


Fig. 6 Mass spectra taken at 200-300°C and MS/MS spectra of *m/z* 600.52; Ice cream (milk fat and vegetable fat)

Conclusion

It was confirmed that TDP/DART®-QTOFMS enables easy identification of fatty acid substituents of glycerides contained in food items, without any pre treatment. Thus, this method could be a useful method for R&D and quality control.