SHIMADZU
Excellence in Science

High Performance Liquid Chromatograph Mass Spectrometer LCMS™-2050

Application News

Simple Method for Screening Analysis of Vegetable Oils Using a Single Quadrupole Mass Spectrometer

Takanari Hattori and Yasuko Shibayama

User Benefits

- Simple analysis of fatty acids and other components of vegetable oils can be done with just one quadrupole LC-MS system.
- Samples can be introduced directly by flow injection for high-throughput analysis that takes only 1 minute.
- eMSTAT Solution™ performs multivariate analysis on mass spectra for easy identification of characteristic components.

■ Introduction

Edible fats and oils mainly consist of triacylglycerols (TAGs), which are composed of three fatty acid molecules and a glycerol, and different fats and oils contain different types and amounts of fatty acids. Recent trends in health consciousness have led to growing interest in edible fats and oils that contain omega-3 fatty acids, such as DHA, EPA, and α-linolenic acid. Free fatty acids also indicate the degree of refinement and oxidative degradation of edible fats and oils, which is why analyzing free fatty acids in edible fats and oils is increasingly of interest.

This Application News describes a simple method for screening fatty acids and other components in vegetable oils that uses flow injection and a single quadrupole LC-MS system. Introducing samples by flow injection enables high throughputs of one sample per minute, which is a useful feature for the rapid analysis of multiple samples.

■ Samples and Sample Preparation

Eight commercially available vegetable oils (soybean, rapeseed, sunflower seed, olive, grapeseed, coconut, linseed, and perilla) were analyzed. Each vegetable oil was diluted 100 times with 2-propanol. DHA was added during dilution for a final concentration of 10 ppm to serve as an internal standard.

■ Equipment and Analytical Conditions

Analysis was performed using the system shown in Fig. 1, which combines a Nexera™ series system and the LCMS-2050. The LCMS-2050 is a single quadrupole mass spectrometer that offers excellent ease of use and performance in a compact form. Typically, flow injections contaminate mass spectrometers because samples are directly injected into them without sending them through a column. However, the robustness and ease of maintenance of the LCMS-2050 when it is contaminated makes it suitable for use with flow injections. The analytical conditions used are shown in Table 1.

Fig. 1 Nexera™ and LCMS™-2050 System

Table 1 Analytical Conditions

[Flow Injection Conditions] (Nexera XR)	
Flowrate:	0.1 mL/min (0 min)→0.05 mL/min (0.1 min) →0.1 mL/min (0.65 min) →1 mL/min (1 min)
Mobile Phase:	Methanol
Injection Volume:	3 µL
[MS Conditions] (LCMS-2050)	
Ionization:	ESI/APCI (DUIS™), Positive and Negative mode
Mode:	Scan (*m/z* 50-2000)
Interface Voltage:	+3.0 kV / -3.0 kV
Nebulizing Gas Flow:	2.0 L/min
Drying Gas Flow:	5.0 L/min
Heating Gas Flow:	7.0 L/min
Desolvation Temp.:	500 °C
DL Temp.:	250 °C

■ Data Analysis

The mass spectral data was converted to JCAMP file format by LabSolutions™ LCMS and then underwent multivariate analysis using eMSTAT Solution. eMSTAT Solution comes with statistical analysis and discriminant analysis modes, and even users unfamiliar with statistical analysis can use it to tailor the data analysis to their application (Fig. 2). Each sample was analyzed four times to create a data set for multivariate analysis.

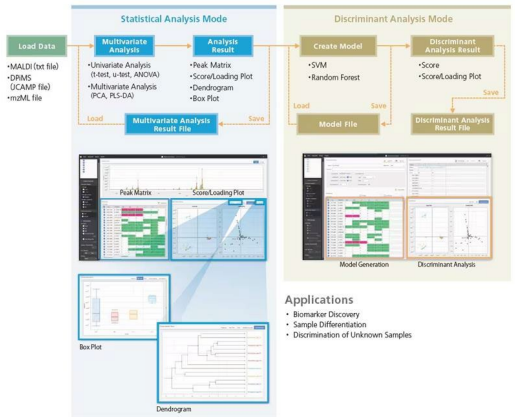

Fig. 2 eMSTAT Solution™ Workflow

■ Simple Screening Analysis

Analyzing the eight vegetable oil samples in negative mode resulted in the detection of 118 peaks. The data was corrected based on the DHA internal standard and then subjected to principal component analysis. The resulting score and loading plots are shown in Fig. 3. The data obtained was clustered into the following four groups: oils high in α-linolenic acid (an omega-3 fatty acid), oils high in linoleic acid (an omega-6 fatty acid), oils high in oleic acid (an omega-9 fatty acid), and coconut oils high in medium-chain fatty acids, such as lauric acid. So each group reflected the fatty acid composition of the vegetable oil samples within them.

The relative peak intensity of each fatty acid was calculated relative to the internal standard, and this was used to determine the percentage composition of fatty acids in each vegetable oil. As shown in Fig. 4, this analysis found that the fatty acid compositions of each vegetable oil were quite close to the reference values in parentheses.[1)]

■ Conclusion

This Application News describes a simple method for screening vegetable oils using a single quadrupole LC-MS system. By analyzing a range of vegetable oil samples in negative mode and then performing statistical analysis on the resulting mass spectral data, the vegetable oils could be grouped based on their compositional fatty acids. The percentage compositions of fatty acids in each vegetable oil calculated by this method were close to the reference values, suggesting that this method could be used in quality control or to identify fake products. Because this method uses flow injection, it has a high throughput, with an analysis time of just 1 minute, making it suitable for the rapid analysis of large numbers of samples. The adoption of this screening method promises to advance technological and product development in the food sector.

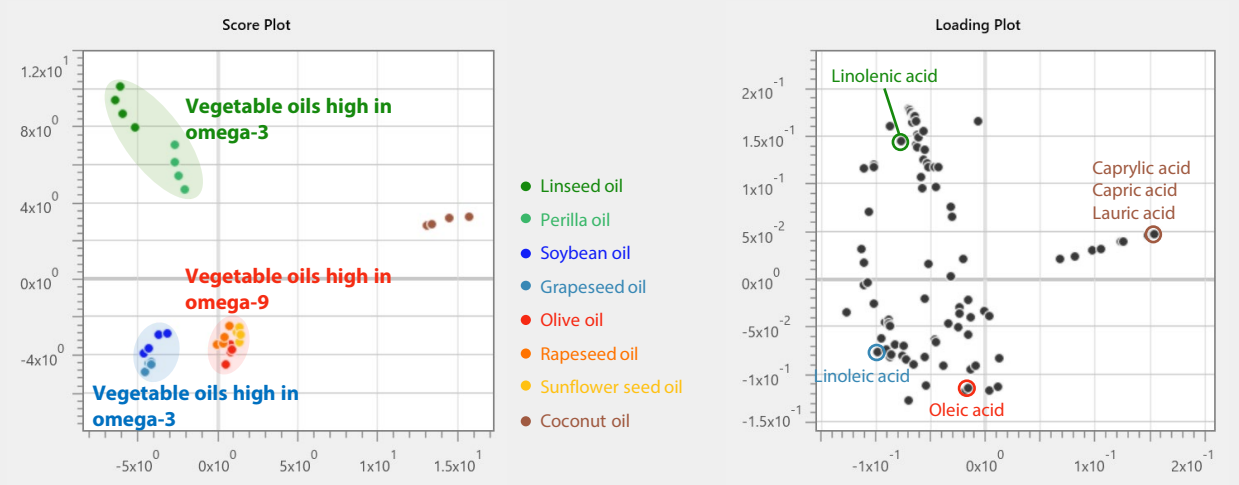

Fig. 3 Results of Principal Component Analysis (Negative Mode)

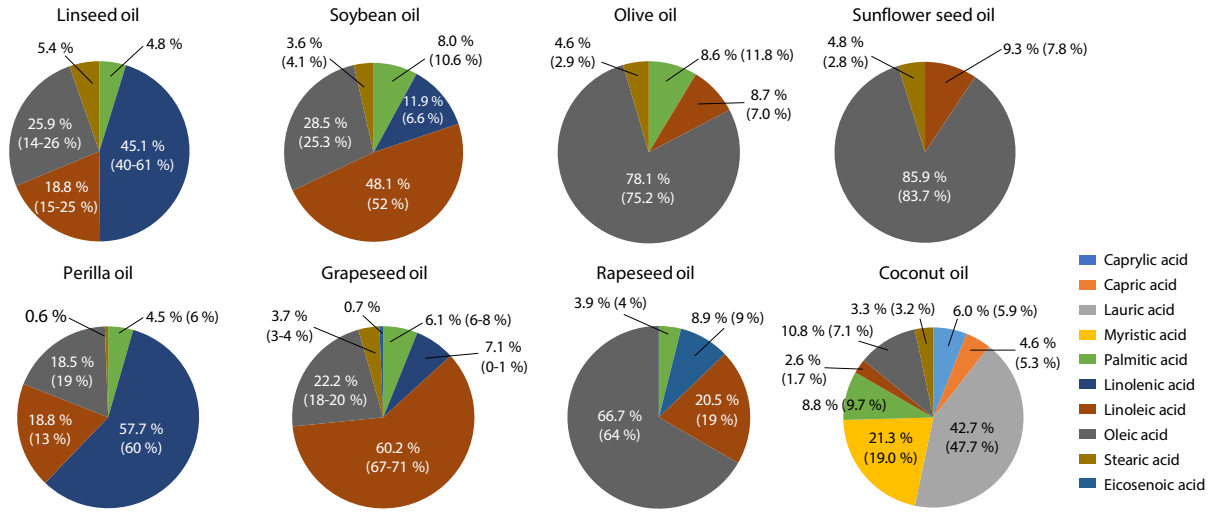

Fig. 4 Fatty Acid Compositions (%)

<References>

1) Kaneda Co., Ltd. "List of Vegetable Oils and Fats," (Accessed November 14, 2023)

<Related Application News Articles>

1. Simple and Rapid Identification of Vegetable Oils Using a Benchtop MALDI-TOF Mass Spectrometer and eMSTAT Solution™ Statistical Analysis Software Application News No. B84

01-00674-EN First Edition: Mar. 2024

SHIMADZU
Shimadzu Corporation
www.shimadzu.com/an/