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Application News

No.C109

Liquid Chromatography Mass Spectrometry

# Application of Direct Analysis in Real Time (Part 2) Rapid Analysis of Triglycerides and Fatty Acids in Food Oil Using LCMS-2020

DART (Direct Analysis in Real Time), when used with a mass spectrometer, permits quick analysis of analyte compounds without the need for sample pretreatment. Application News C108 introduced an analysis of free fatty acids and amino acids in food products using the LCMS-2020 equipped with DART as the ion source.
Fatty acids present in foods are often bound to triglycerides, and when people ingest these triglycerides, not only do they serve as a source of energy, people acquire the physiological functions of the various fatty acids. Therefore, there is interest in research associated with triglyceride molecular species. Generally, LC and GC are used for triglyceride analysis, but these methods are known to have such drawbacks as complicated sample preparation, long analysis time and carryover.
Here, using the same system as that used for the previous Application News, No. C108, we introduce an example of analysis of lipids in food containing triglycerides, without conducting any sample preparation.

## DART-MS Analytical Conditions

The analytical system used consisted of the DART SVP ion source (IonSense, Inc., MA, USA), and the LCMS-2020 single quadrupole mass spectrometer. The LCMS-2020, with its maximum 15,000 u/sec high-speed scanning and 15 msec ultra-high-speed polarity switching, permits one-second multiple scanning over the range of *m/z* 50 to 1500 using dual, positive – negative polarity. These features made it possible to simultaneously detect a spectrum of triglycerides (positive ion detection) and fatty acids (negative ion detection). And, since analysis can be conducted by simply exposing the sample to the gas discharged from the DART ion source, measurement time was kept to about ten seconds per sample, thereby achieving high-throughput analysis.

**Table 1 Analytical Conditions**

| | |
|---|---|
| DART Heater Temperature | : 400 ˚C |
| Scan Type | : *m/z* 50-1500 (Positive / Negative) |
| Neburizing Gas Flow | : 1.5 L/min. |
| Drying Gas Flow | : 5.0 L/min. |
| DL Temperature | : 250 ˚C |
| Block Heater Temperature | : 400 ˚C |

## Analysis of Triglycerides and Fatty Acids in Various Food Oils

The mass spectra of food product oils and fats (shortening and lard) with known fatty acid composition are shown in Fig. 1 and Fig. 2, respectively. The monoglycerides, diglycerides and triglycerides were detected in the positive ion mass spectra of both samples. As for the negative ions, linoleic acid and oleic acid were primarily detected in the shortening, while oleic acid was primarily detected in the lard.

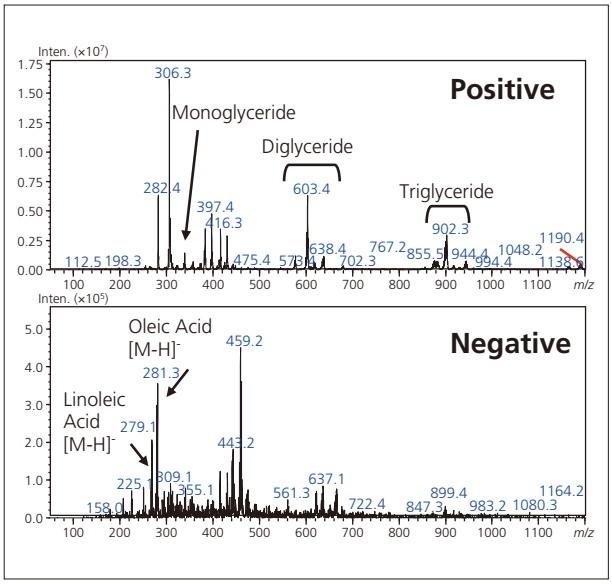


**Fig. 1 Mass Spectra for Shortening**

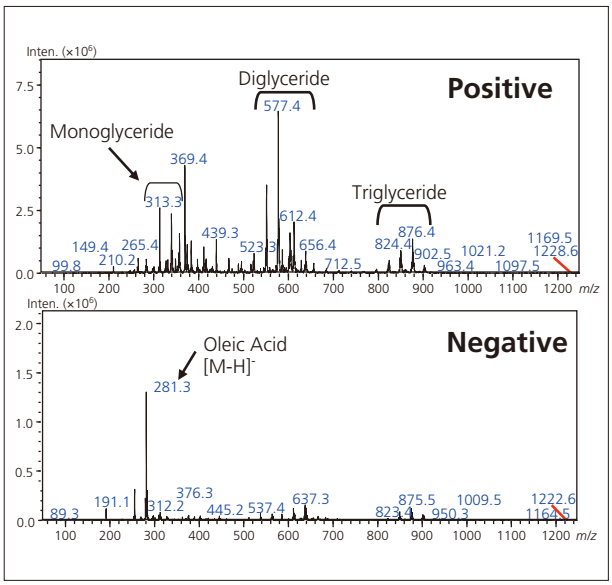


**Fig. 2 Mass Spectra for Lard**

Shown below are expanded views of the MS spectra of the negative ions in shortening and lard, respectively, over the range of *m/z* 200 to 320 (Fig. 3, Fig. 4). The intensity of the peak originating from palmitic acid is weak in the shortening, while oleic acid and linoleic acid are detected with strong intensity. On the other hand, the peaks of oleic acid and palmitic acid in the lard indicate they were detected with strong intensity.

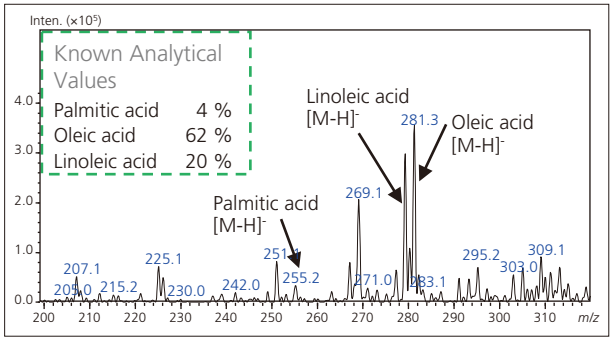


**Fig. 3 Negative Mass Spectrum for Shortening (*m/z* 200-320)**

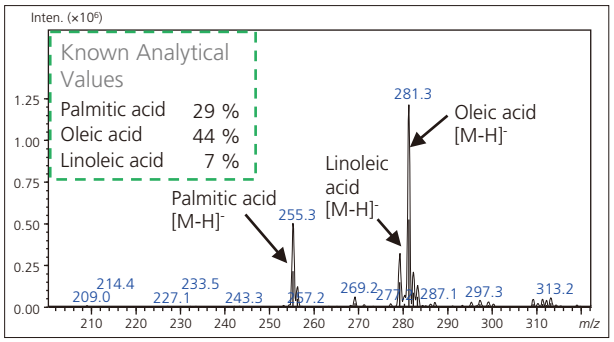


**Fig. 4 Negative Mass Spectrum for Lard (*m/z* 200-320)**

An expanded view of the mass spectrum of positive ions in the range of *m/z* 800 to 920 is shown below. (The triglyceride fatty acids in the figure are displayed only in the combined state.) In the case of shortening, peaks derived from the triglycerides comprising oleic acid or linoleic acid are clearly detected, such as triolein (OOO), in which all three fatty acids consist of oleic acid, indicating that the result is related to the free fatty acid composition. From the mass spectra for lard, on the other hand, peaks derived from the triglycerides comprising oleic acid and palmitic acid are detected.

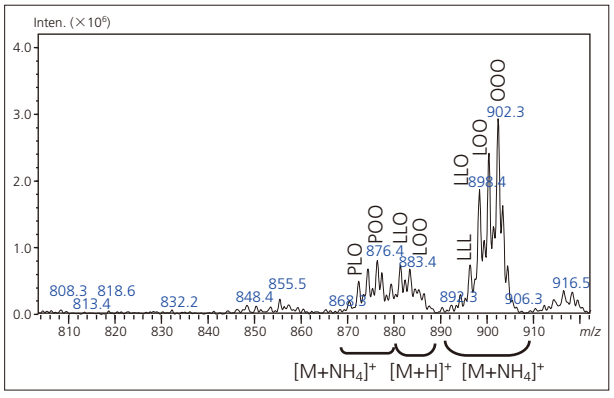


**Fig. 5 Positive Mass Spectrum for Shortening (*m/z* 800-920)**

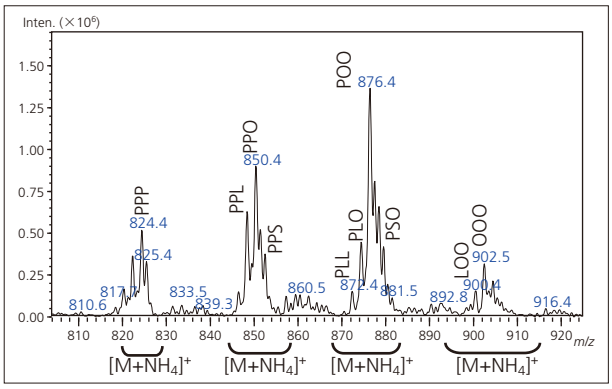


**Fig. 6 Positive Mass Spectrum for Lard (*m/z* 800-920)**

The same trend is seen with the monoglycerides and diglycerides peaks. The positive MS spectra for lard from *m/z* 300 to 380 and *m/z* 540 to 620 are shown in enlarged views (Fig. 7, Fig. 8). The peaks derived from the monoglyceride and diglyceride oleic and palmitic acids are seen.

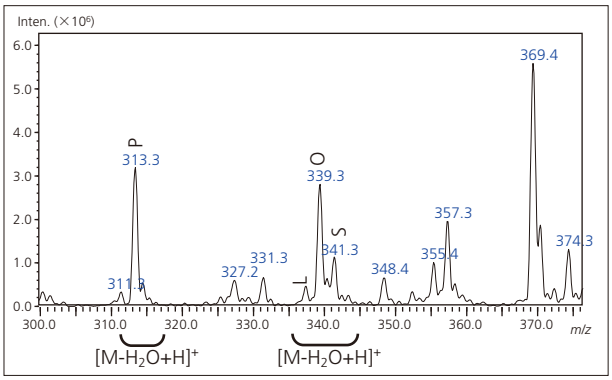


**Fig. 7 Positive Mass Spectrum for Lard (*m/z* 300-380)**

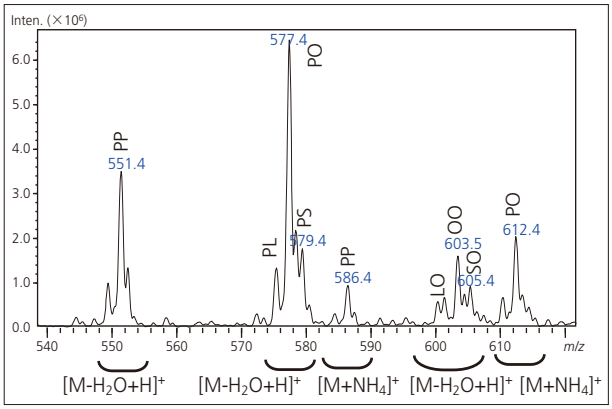


**Fig. 8 Positive Mass Spectrum for Lard (*m/z* 540-620)**

[Acknowledgment]
We wish to express our sincere gratitude to Shun Wada (professor emeritus at Tokyo University of Marine Science and Technology) and the Japan Inspection Institute of Fats & Oils for the food and oil samples, in addition to their kind cooperation in the analysis of the data.

*DART is a product of IonSense Inc. (http://www.ionsense.com/).

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LCMS-2020

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