SpiralTOF-TOF

Structural Analysis of Tristearin

Introduction:

The JMS-S3000 SpiralTOF™ is a MALDI-TOF MS that uses an innovative spiral ion optical system to achieve the highest resolution currently available for a MALDI instrument. Additionally, this system can be equipped with a TOF-TOF option that can acquire high-energy collision-induced dissociation (HE-CID) product ion spectra for monoisotopically selected precursor ions. The resulting HE-CID product ion spectra provide detailed structural information about compounds like triglycerides by means of charge-remote fragmentation (CRF).[1]

Tristearin is a triglyceride found in fats that consists of three stearic acid moieties (Fig. 1). In this work, we report the structural analysis of tristearin by using the HE-CID capabilities of the SpiralTOF-TOF.

Results and Discussion:

The sample was dissolved with NaI in methanol to promote Na^+ adduct formation. PEG 1000 was used as an external calibration standard. Initially, the sample was measured in Spiral mode and showed a signal at *m/z* 913.8231 (Fig. 2). This ion was consistent with the expected $[M+Na]^+$ calculated mass of 913.8194. Next, the product ion spectrum of this monoisotopically selected *m/z* was obtained using the TOF-TOF mode (Fig. 3). The resulting mass spectrum showed a fragmentation pattern consistent with the occurrence of CRF. Fig. 4 shows the enlarged *m/z* 600-920 mass range in which the labeled peaks are clearly reflected in the structure shown in Fig. 5. It should be noted that these fragment ions were detected when CRF occurred to one of the three stearin branches present in the molecule.

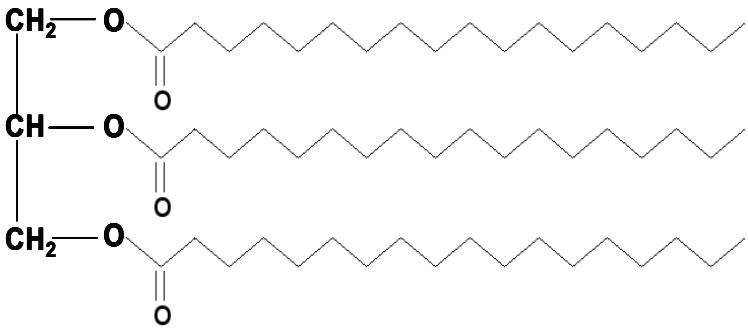

Figure 1. Structure of tristearin.

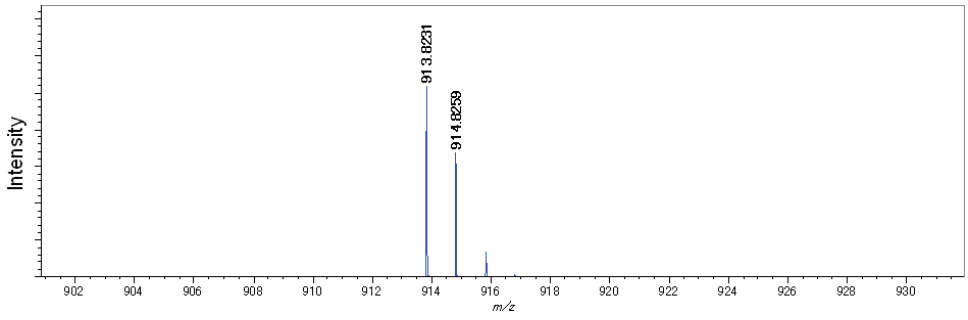

Figure 2. Mass spectrum of tristearin.

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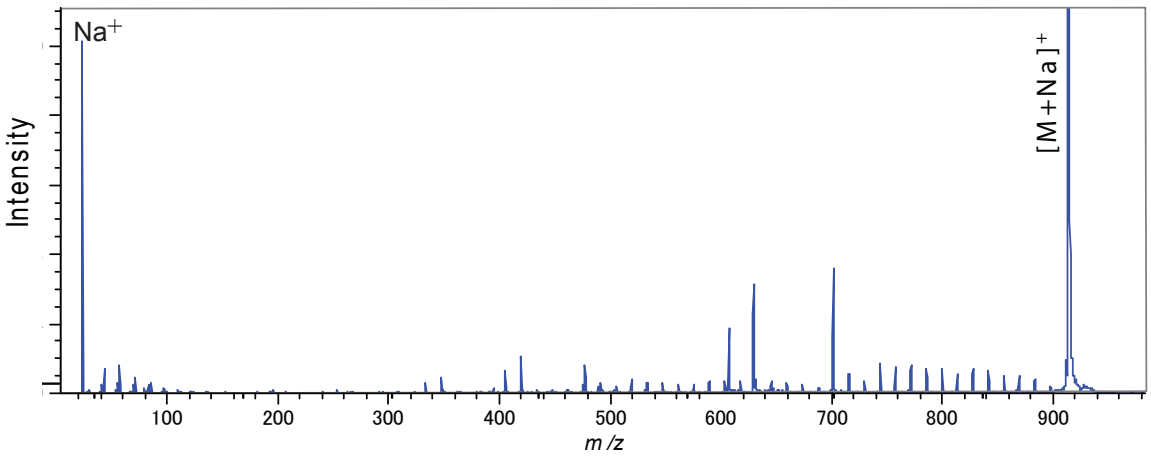

Figure 3. Product ion spectrum for the sodium adduct of tristearin.

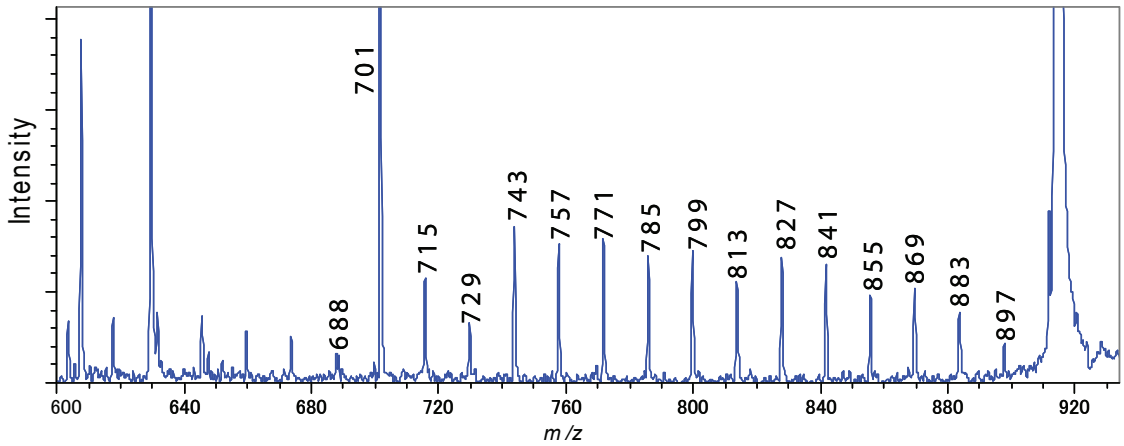

Figure 4. Product ion spectrum for the sodium adduct of tristearin (enlarged between *m/z* 600-920).

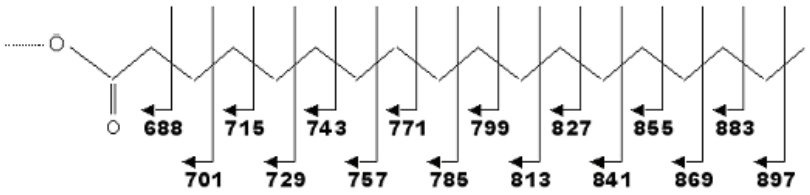

Figure 5. Peak assignments for the product ion spectrum.

Conclusions:

Using the TOF-TOF method, the JMS-S3000 "Spiral-TOF" can acquire HE-CID product ion spectra that show clear CRF mass spectral patterns. Therefore, the structural analyses of compounds like tristearin are easily performed using this technique.

References:

1) Kubo, A., et al., JASMS, 2012. in press.