SpiralTOF-TOF

Structural Analysis of Triolein

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] In this work, we report the structural analysis of triolein, a triglyceride that contains 3 oleic acid moieties (Fig. 1), by using HE-CID capabilities of the SpiralTOF-TOF.

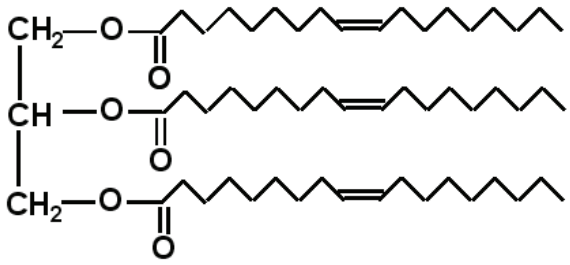

Figure 1. Structure of triolein.

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* 907.7782 (Fig. 2). This ion was consistent with the expected $[M+Na]^+$ calculated mass of 907.7725. Next, the product ion spectrum for this peak was acquired 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 reflected in the structure shown in Fig. 5. Each of the major peaks between *m/z* 684-753 and between *m/z* 807-821 (except *m/z* 808) shows a difference of 14Da which is consistent with successive losses of CH_2 along the oleic acid backbone. However, the *m/z* 808, which is 1Da from *m/z* 807, is a peak that specifically appears when unsaturated bonds are present in the structure.[2] Additionally, the low intensity peaks between *m/z* 753-807 also confirm the presence of the unsaturated bonds at this position. As noted previously, all of these product ion peaks are consistent with CRF occurring along an oleic acid branch within triolein.

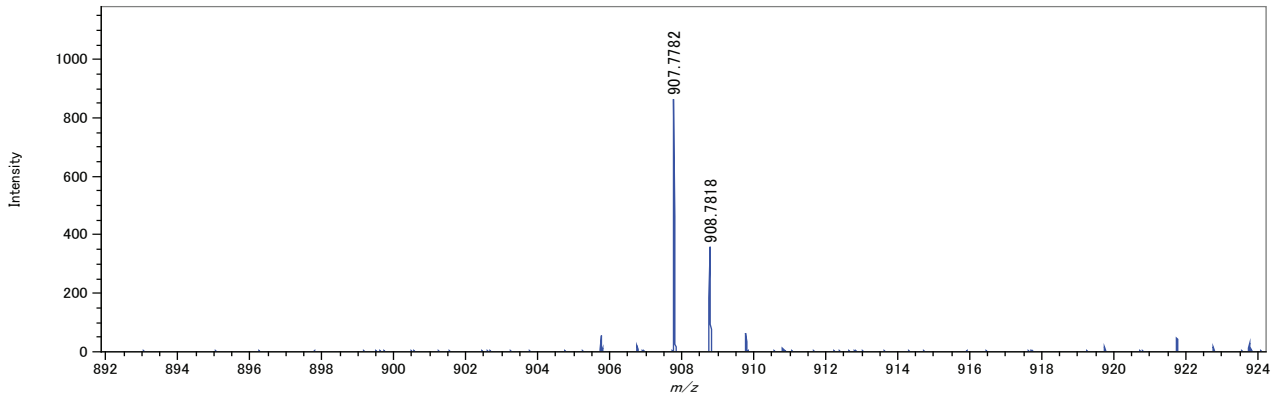

Figure 2. Mass spectrum for the sodium adduct of triolein.

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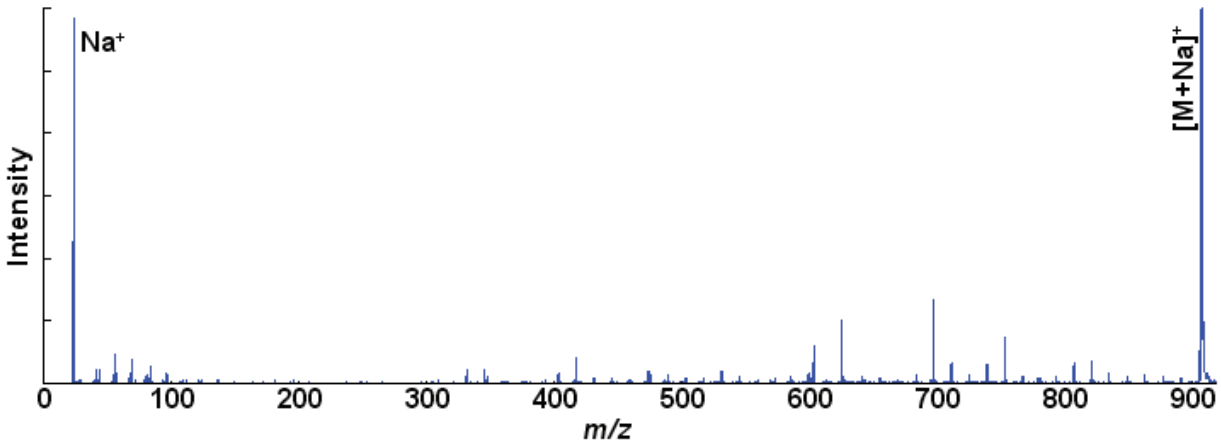

Figure 3. Product ion spectrum for the sodium adduct of triolein.

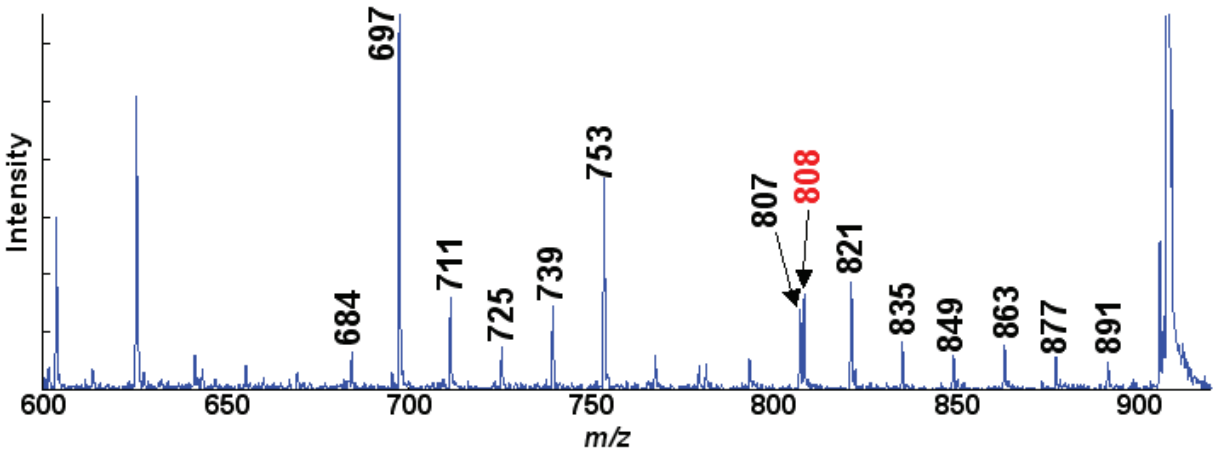

Figure 4. Product ion spectrum for the sodium adduct of triolein (enlarged between *m/z* 600-920).

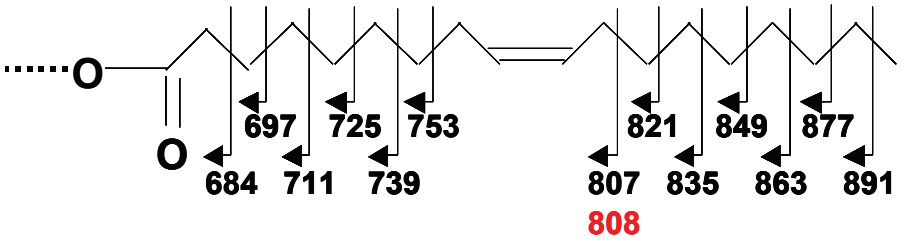

Figure 5. Peak assignments for the product ion spectrum.

Conclusions:

The data for triolein demonstrates that the JMS-S3000 "SpiralTOF" can acquire HE-CID product ion spectra with clear CRF mass spectral patterns. Additionally, this method allows for easy determination of unsaturated bond locations in the carbon chains.

References:

1) Kubo, A., et al., JASMS, 2012. in press.
2) N. Akimoto, *Journal of the Mass Spectrometry Society of Japan* 46 (1998) 228.