

# **SpiralTOF-TOF**

## High-Energy CID MS/MS Analysis of Small Organic Molecules

### Introduction

The JMS-S3000 SpiralTOF<sup>TM</sup> is a MALDI-TOF MS that uses an innovative spiral ion optics system to achieve the highest resolution currently available for a MALDI instrument. As a result, small organic molecules can be analyzed on this system with minimal interferences from the matrix peaks. Additionally, the JMS-S3000 is available with a TOF-TOF option that can acquire highenergy collision-induced dissociation (CID) product ion spectra for monoisotopically selected precursor ions. In this work, we analyzed several small organic molecules by using the JMS-S3000 with the TOF-TOF option.

#### **Results and Discussion**

The proline sample was measured using positive ion mode which produced an  $[M+H]^+$  ion at m/z 116. This ion was monoisotopically selected as the precursor ion for TOF-TOF analysis. The resulting high-energy CID

product ion spectrum is shown in Fig. 2a. The overall MS/MS spectrum was very simple for this sample with the low mass ions m/z 43 and m/z 70 attributed to the fragments shown in Fig. 3.

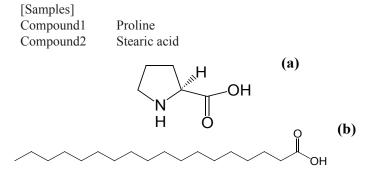


Figure 1. Structural formula of (a) Proline and (b) Stearic acid.

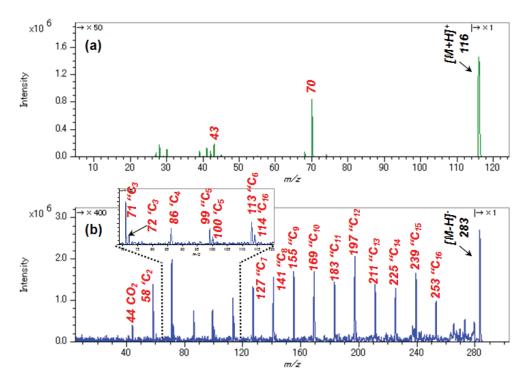


Figure 2. Product ion spectra of (a) Proline  $(m/z \ 116 \ [M+H]^+)$  and (b) Stearic acid  $(m/z \ 283 \ [M-H]^-)$ .

The stearic acid sample was then measured using negative ion mode which produced an [M-H] ion at m/z 283. This ion was monoisotopically selected as the precursor ion for TOF-TOF analysis. The resulting high-energy CID product ion spectrum is shown in Fig. 2b. This spectrum showed a mass spectral pattern that was attributed to charge remote fragmentation (CRF) by high-energy CID. CRF occurs during CID when the charge is localized to a particular location on the molecule (in this case on the –COO) and the bonds that are cleaved are located at positions away from this charge. 1.2 This technique is very useful for structural analysis. Fig. 4 shows the identity of each peak based on the overall structure of stearic acid.

#### **Conclusions**

The JMS-S3000 "SpiralTOF" with TOF-TOF option can be used to measure both the [M+H]<sup>+</sup> and [M-H]<sup>-</sup> precursor ions even for small organic molecules. Furthermore, this technique can be used to acquire high-energy CID product ion spectra that show CRF which involves the systematic cleavage of C-C bonds within the molecular structure.

#### Reference

- 1) W. J. Griffiths, Y. Yang, J. A. Lindgren, and J. Sjövall, Rapid Commun. Mass Spectrom., 10, 21-28, (1996).
- 2) M. Gross, Int. J. of Mass Spectrom., 200(1–3), 611–624, (2000).

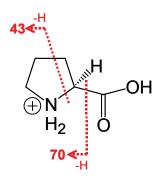


Figure 3. Fragment ions of Proline (m/z 116 [M+H]+).

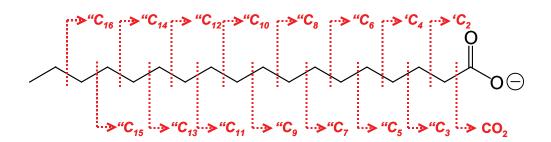


Figure 4. MASCOT MS/MS Ion search result of tBSA by TOF-TOF mode.