SpiralTOF-TOF

Analysis of the Natural Organic Compound YTX by Using TOF-TOF Option

Introduction

Yessotoxin (YTX) is one of the substances that cause food poisoning when humans consume toxic shellfish. The structure of this compound has been previously analyzed by high-energy collision induced dissociation (CID) using a traditional four sector tandem double focusing mass spectrometer.[1]

In this work, we analyzed YTX by using a JMS-S3000 SpiralTOF™ equipped with the optional TOF-TOF analyzer to generate a high energy CID product ion spectrum.

Results and Discussion

Fig. 1 shows the YTX mass spectrum acquired using polyalanine as an external calibrant. The spectrum shows a peak at *m/z* 1061.513, which is suspected to be the monoisotopic ion $[M-2Na-SO3+H]^-$ (calculated value 1061.609). There was also a $[M-Na]^-$ peak observed for YTX at *m/z* 1164.450 (calculated value 1163.548). Among these peaks, the product ion spectrum was acquired from $[M-2Na-SO_3+H]^-$, which had been previously analyzed using a traditional four sector tandem double focusing mass spectrometer.1 Fig. 2 shows the high-energy CID results generated by the SpiralTOF-TOF. The negative charge was fixed to the sulfate ester end of the molecule, causing charge remote fragmentation (CRF) to occur. As a result, the spectrum showed peaks that systematically reflected the structure of YTX, as shown in Fig. 3. This data closely resembles the results obtained using a traditional four sector MS/MS system.[1]

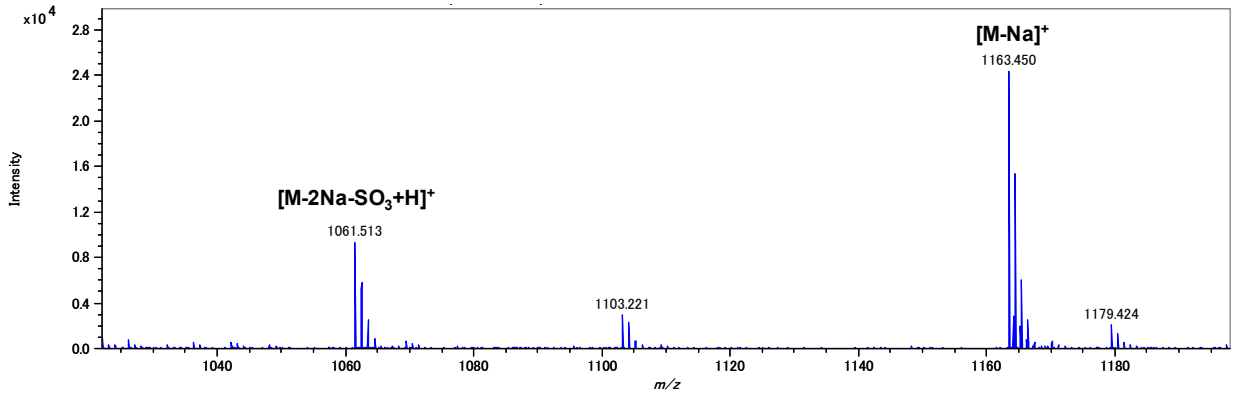

Figure 1. Mass spectrum of YTX.

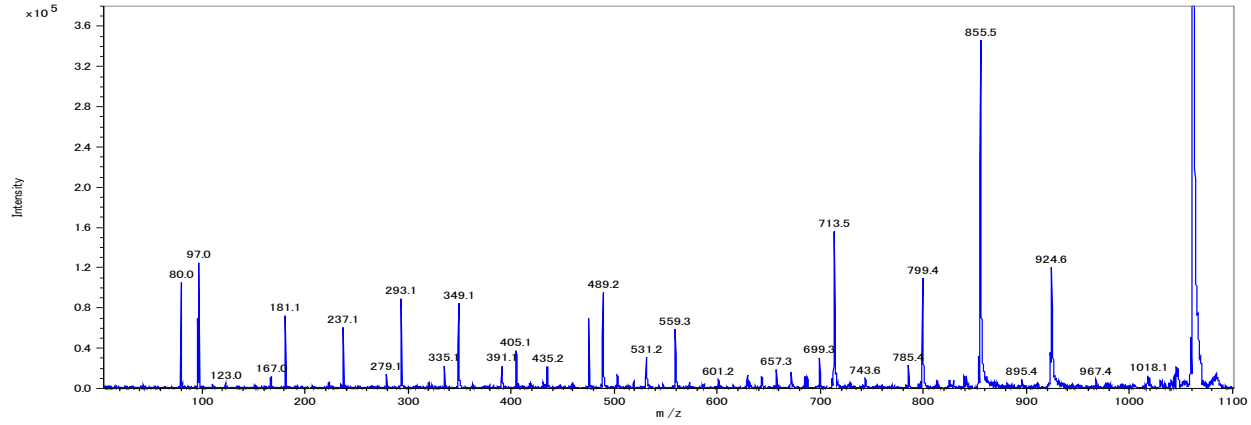

Figure 2. Product ion spectrum of $[M-2Na-SO_3+H]^-$

MS-050813A

Conclusions

As this data demonstrates, high energy CID analysis using SpiralTOF-TOF clearly detected the peaks resulting from CRF, Which enabled analysis of samples that are complex in structure such, as natural organic compounds.

Acknowledgement

We wish to express our thanks to Prof. Michio Murata of the Department of Biomolecular Sciences, Department of Physics, Graduate School of Science, Osaka University, for providing the YTX samples.

Reference

[1] H. Naoki, M. Murata, T. Yasumoto, Rapid Communication of Mass Spectrometry 7 (1993) 179

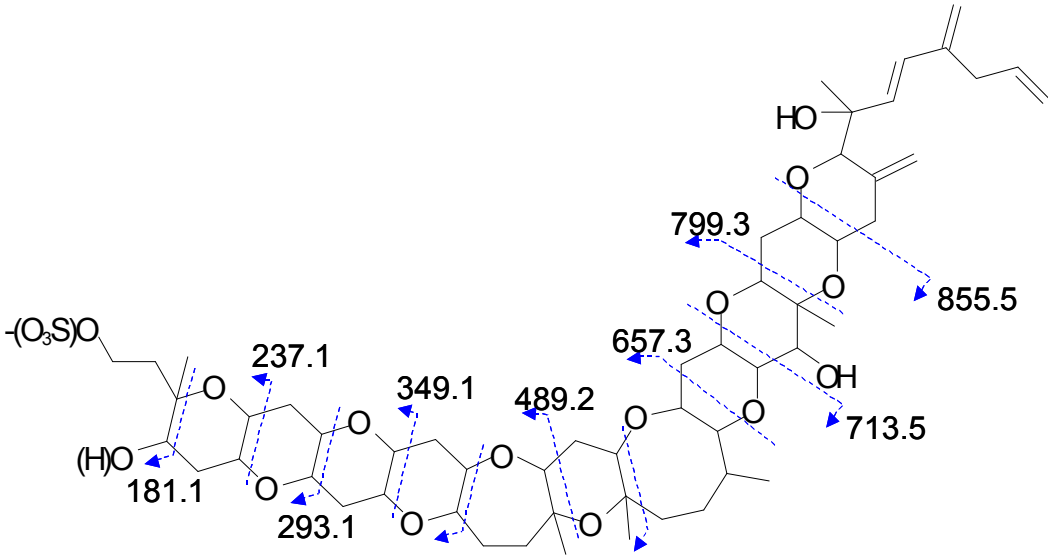

Figure 3. Structure of YTX and fragmentation pattern.