

SpiralTOF-TOF

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

Introduction

Sperm activating and attracting factor (SAAF) is a naturally occurring substance produced by ascidians (sea squirts) to promote the fertilization process. Previously, the structure of this compound was characterized by high-energy collision induced dissociation (CID) using a traditional four sector tandem double focusing mass spectrometer.¹

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

Results and Discussion

Fig. 1 shows the SAAF mass spectrum acquired using

PEG sulfate 600 as an external calibrant. The spectrum shows a peak at m/z 515.301, which is suspected to be the monoisotopic ion $[M-2Na-SO_3+H]^-$ (calculated value 515.305). In addition, peaks from SAAF are observed at two other masses: $[M-2Na+H]^-$ at m/z 595.255 (calculated value 595.261) and $[M-Na]^-$ at m/z 617.237 (calculated value 617.242). Among these peaks, the product ion spectrum was acquired for the $[M-2Na-SO_3+H]^-$ ion, 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 SAAF, as

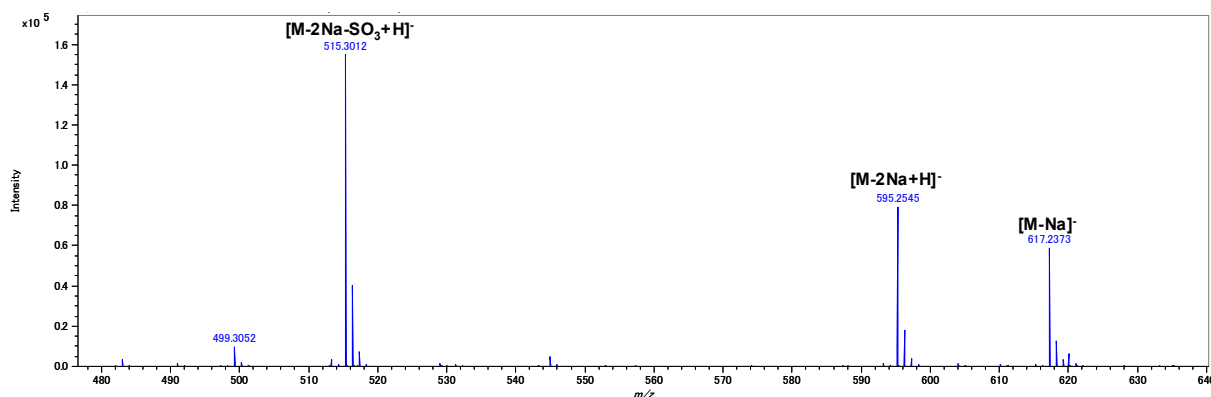


Figure 1. Mass spectrum of SAAF.

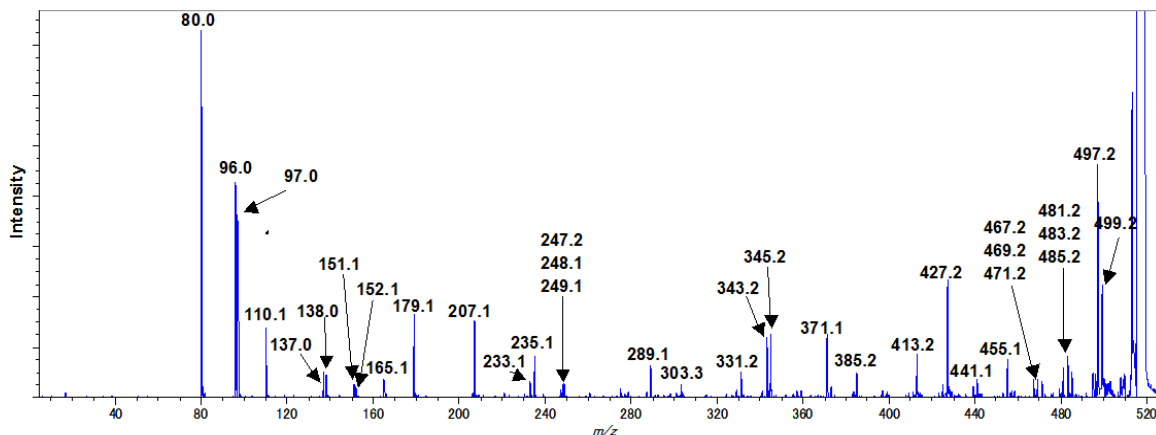


Figure 2. Product ion spectrum of $[M-2Na-SO_3+H]^-$.

shown in Fig. 3. This data closely resembles the results obtained using a traditional four sector MS/MS system.¹

Conclusions

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

Acknowledgment

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Reference

[1] M. Yoshida, M. Murata, K. Inaba, and M. Morisawa, Proceeding of the National Academy of Sciences of the United States of America 99 (2002) 14831-14836.

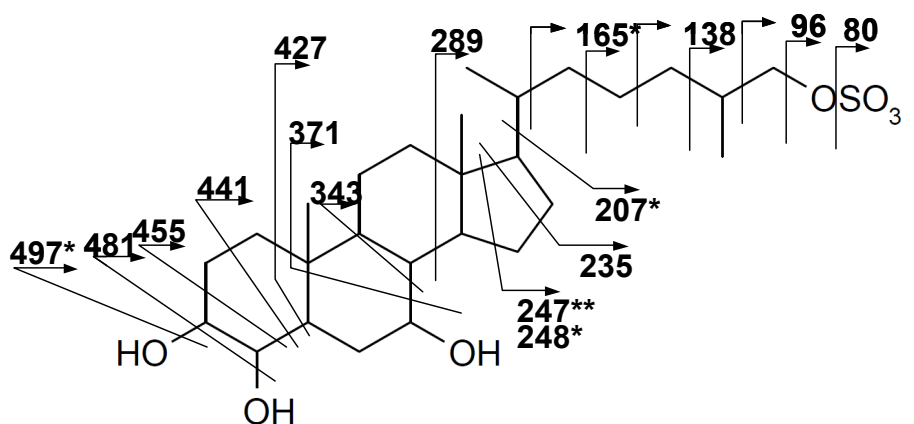


Figure 3. Structure of of SAAF and fragmentation pattern. (Asterisks show dehydrated ions.)