

SpiralTOF-TOF

Structural Analysis of a High Molecular Weight Peptide

Introduction:

The JMS-S3000 SpiralTOF™ is a MALDI-TOF MS that uses an innovative spiral ion optics system to achieve the highest resolution currently available for a MALDI instrument. Additionally, the JMS-S3000 is available with a TOF-TOF option that acquires high-energy collision-induced dissociation (CID) product-ion spectra for monoisotopically selected precursor ions. In this work, we analyzed a high molecular weight peptide by using the JMS-S3000 SpiralTOF with the TOF-TOF option.

Experimental:

Sample: ACTH18-39
(Arg-Pro-Val-Lys-Val-Tyr-Pro-Asn-Gly-Ala-Glu-Asp-Glu-Ser-Ala-Glu-Ala-Phe-Pro-Leu-Glu-Phe)
Matrix: α-Cyano-4-hydroxycinnamic acid (CHCA)

Results and Discussion:

The high-energy CID product-ion spectrum for protonated ACTH18-39 $[M+H]^+$ (m/z 2456.2) is shown in Fig. 1. Each product ion was labeled using the Biemann convention (Fig. 2) in which the a-, b-, and d-ion series are fragments generated from the N terminus of the ACTH18-39 molecule. The SpiralTOF MS/MS data in Fig. 1 show that the sequence information is clearly represented by the a-ion series from a2 to a21. The immonium ions (Fig. 3) and the d-ion series (produced by fragmentation of the a-ion series) were also observed in the mass spectrum.

Conclusions:

The JMS-S3000 SpiralTOF with the TOF-TOF mode produced high energy CID product ion spectra that clearly identified the sequence for the high molecular weight peptide ACTH18-39.

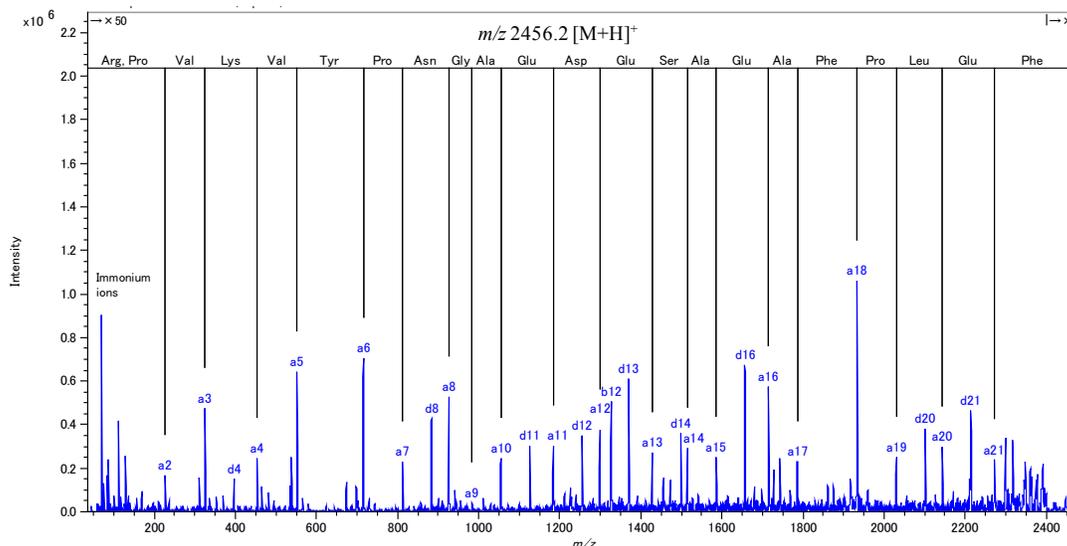


Figure 1. Product ion spectrum of ACTH18-39 (m/z 2456.2, $[M+H]^+$).

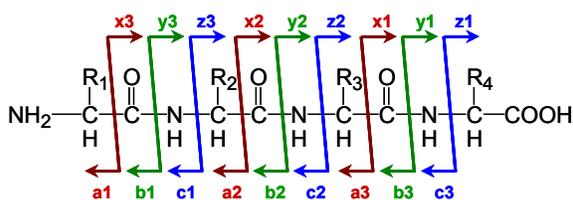


Figure 2. Fragment ion series.

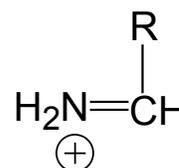


Figure 3. Immonium ion.