

# Peptide Analysis using Field Desorption (FD) of JMS-T2000GC AccuTOF<sup>™</sup> GC-Alpha

Product used: Mass Spectrometer (MS)

### Introduction

Field Desorption (FD) is an ionization method that utilizes the tunneling effect in a high electric field generated between an emitter coated with a sample and an electrode to which a high voltage is applied. It is known as a soft ionization method that provides only molecular weight information because the internal energy given to the sample during ionization is low and fragmentation is unlikely to occur. In FD measurements, the sample-coated emitter is introduced directly to the ion source using a dedicated probe. Therefore, it is possible to measure difficult-to-volatile compounds, polar compounds, thermally unstable compounds, etc., which are difficult to measure with GC-MS. The combination of FD and time-of-flight mass spectrometer (TOFMS) enables calculation of the molecular formula of the measured compound. An overview of FD and sampling technique in the gas chromatograph time-of-flight mass spectrometer JMS-T2000GC AccuTOF™ GC-Alpha are described in <u>MSTips No. 355</u> and <u>MSTips No. 403</u>.

In this MSTips, we report the results of the analysis of the peptide angiotensin I using FD of the JMS-T2000GC as an example of analysis of a highly polar compound.

# **Experimental**

Commercially available angiotensin I human acetate salt hydrate was used as the sample (Figure 1). Angiotensin I was prepared to 10 mg/mL using a 0.1% TCA:methanol mixture (1:1). Then, 1 μL each of this sample and 1 mg/mL copper(II) phthalocyanine (α-type) methanol solution (used as a mass drift corrector) were applied to the emitter for measurement. A gas chromatograph time-of-flight mass spectrometer JMS-T2000GC AccuTOF<sup>™</sup> GC-Alpha was used for the measurements. An EI/FI/FD combination ion source was used, and FD was used as ionization method. Other detailed measurement conditions are shown in Table 1.

**MS** conditions

Spectrometer

Ion Source

Mass Range

**Table 1 Measurement conditions** 

EI/FI/FD combination ion source

 $\rightarrow$  51.2 mA/min  $\rightarrow$  50 mA)

m/z 50 - 1,600

JMS-T2000GC AccuTOF<sup>™</sup> GC-Alpha (JEOL Ltd.)

FD+ (Cathode Voltage: -10kV, Emitter Current: 0 mA



Formula:  $C_{62}H_{89}N_{17}O_{14}$ 

Figure 1 Structural formula of angiotensin I

#### Results

Figure 2 shows the TICC for this measurement. Two peaks were detected; the left peak was derived from angiotensin I, and the right peak was derived from copper phthalocyanine.



# Figure 2 Total ion current chromatogram

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JEOL JEOL Ltd.

3-1-2 Musashino Akishima Tokyo 196-8558 Japan Sales Division Tel. +81-3-6262-3560 Fax. +81-3-6262-3577 www.jeol.com ISO 9001 • ISO 14001 Certified

Figure 3 shows the mass spectrum created from the peak of angiotensin I. The [M+H]<sup>+</sup>, [M+2H]<sup>2+</sup>, [M+3H]<sup>3+</sup> of angiotensin I were detected (Figure 3). Table 2 shows the elemental composition estimated result of these peaks. The mass error was calculated to be within -1.5 mDa, which is a good value. Furthermore, the isotope pattern of [M+H]<sup>+</sup> was roughly the same as the simulation result (Figure 4), indicating that good measurement results were obtained. Essentially, peptides cannot be measured using a GC-MS due to its high polarity. But FD which is a direct MS method can be used for peptides analysis, then molecular formula of the peptide can be easily calculated using a FD-TOFMS system.



Figure 3 Mass spectrum of angiotensin I

Ion Type	Measured <i>m/z</i>	Formula	Calculated m/z	Mass Error [mDa]
$[M+H]^+$	1296.68462	C62 H90 N17 O14	1296.68477	-0.15
[M+2H] <sup>2+</sup>	648.84471	C62 H91 N17 O14	648.84602	-1.31
[M+3H] <sup>3+</sup>	432.89845	C62 H92 N17 O14	432.89977	-1.32







# Conclusions

In this MSTips, we introduced the analysis results of angiotensin I as an analysis example of highly polar compound using FD. As a result of the analysis, it was confirmed that protonated molecule related to molecular weight could be observed, and furthermore, accurate mass could be obtained with good accuracy. These results indicate that FD can be used to analyze highly polar compounds that are difficult to measure by GC-MS.

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