SHIMADZU
Excellence in Science

Application News

No. B68

MALDI-TOF Mass Spectrometry

Rapid Measurement of Low-molecular Compounds Using a Benchtop MALDI-TOF Mass Spectrometer - Direct Detection of Antiseptic Components in Oral Care Products -

MALDI-TOF mass spectrometry is generally considered as an effective analysis method for molecules having a high molecular weight such as proteins and peptides. However, this method can also be used for low-molecular compounds as a rapid, simple analysis method. In particular, since the analysis is hardly affected by salts that may be contained in samples, target components in the product can be analyzed directly without any pretreatment such as purification. For example, commercially available oral care products contain bactericidal components (povidone-iodine, chlorhexidine gluconate, etc.), and such low-molecular antiseptic components can be directly detected from the products.

This article introduces examples of detecting antiseptic components from commercially available oral care products using a benchtop MALDI-TOF mass spectrometer.

S. Nakaya

MALDI-TOF Mass Spectrometer

For the analysis, a benchtop MALDI-TOF mass spectrometer "MALDI-8020" (Fig. 1) was used. This is a positive ion mode-only instrument which is downsized while maintaining the performance of AXIMA Assurance. This newly designed MALDI-TOF mass spectrometer is equipped with a 200 Hz solid laser for the ionization laser, a full automated ion source cleaning device and an oil-free diaphragm pump.

Fig. 1 Appearance of Benchtop MALDI-TOF MS "MALDI-8020"

Direct Detection of Povidone-iodine in a Product

Povidone-iodine is a low-molecular polymer having a bactericidal effect and surface-active action and also is a medical product which is contained in oral care products such as gargle medicines or mouthwashes. A small quantity of mouthwash (A) available over-the-counter was spotted on the MALDI target plate, and added 0.5 µL of matrix solution, and then dried and analyzed.

The mass spectrum obtained by analysis is shown in Fig. 2.

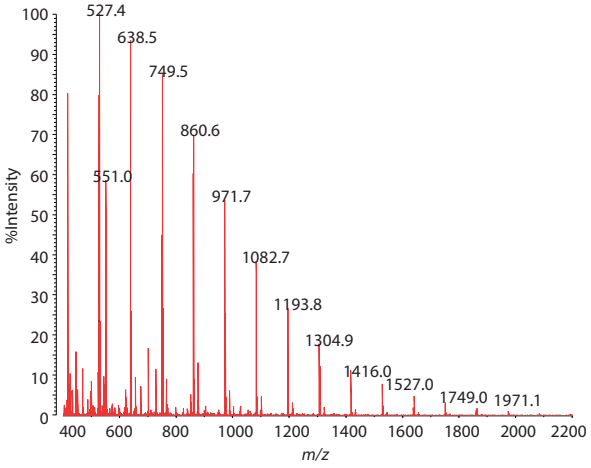

Fig. 2 Mass Spectrum of Mouthwash (A)
Measurement mode: Positive Linear

By enlarging the obtained mass spectrum, signals having a difference in mass originating from polyvinylpyrrolidone, which is a component of povidone-iodine, were observed as shown in Fig. 3.

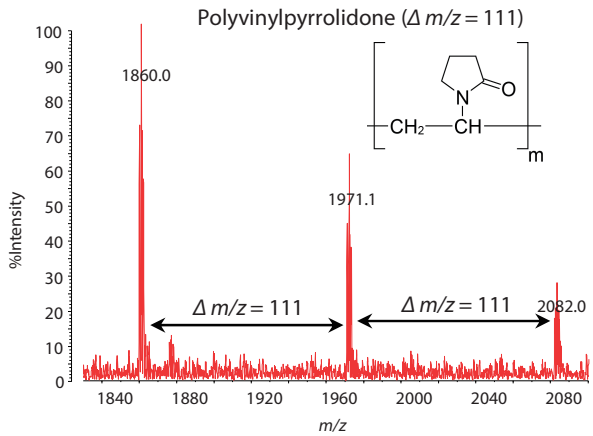

Fig. 3 Enlarged View of Mass Spectrum of Mouthwash (A)
Measurement mode: Positive Linear

Direct Detection of Chlorhexidine in a Product

Chlorhexidine is contained in products in the form of gluconate. In the same way as with povidone-iodine, a small quantity of mouthwash (B) available over-the-counter was spotted on the MALDI target plate, and added 0.5 µL of matrix solution, and then dried and analyzed. The mass spectrum obtained by analysis is shown in Fig. 4. Signals originating from chlorhexidine were observed in the spectrum.

Since chlorhexidine has two chlorine atoms, a characteristic isotope distribution is obtained. When the measured spectrum is compared with the theoretical isotope distribution, we can see that they are identical.

As demonstrated above, use of the benchtop, positive linear mode-only MALDI-TOF mass spectrometer "MALDI-8020" enables rapid and easy determination of low-molecular compounds contained in products without the need of pretreatment.

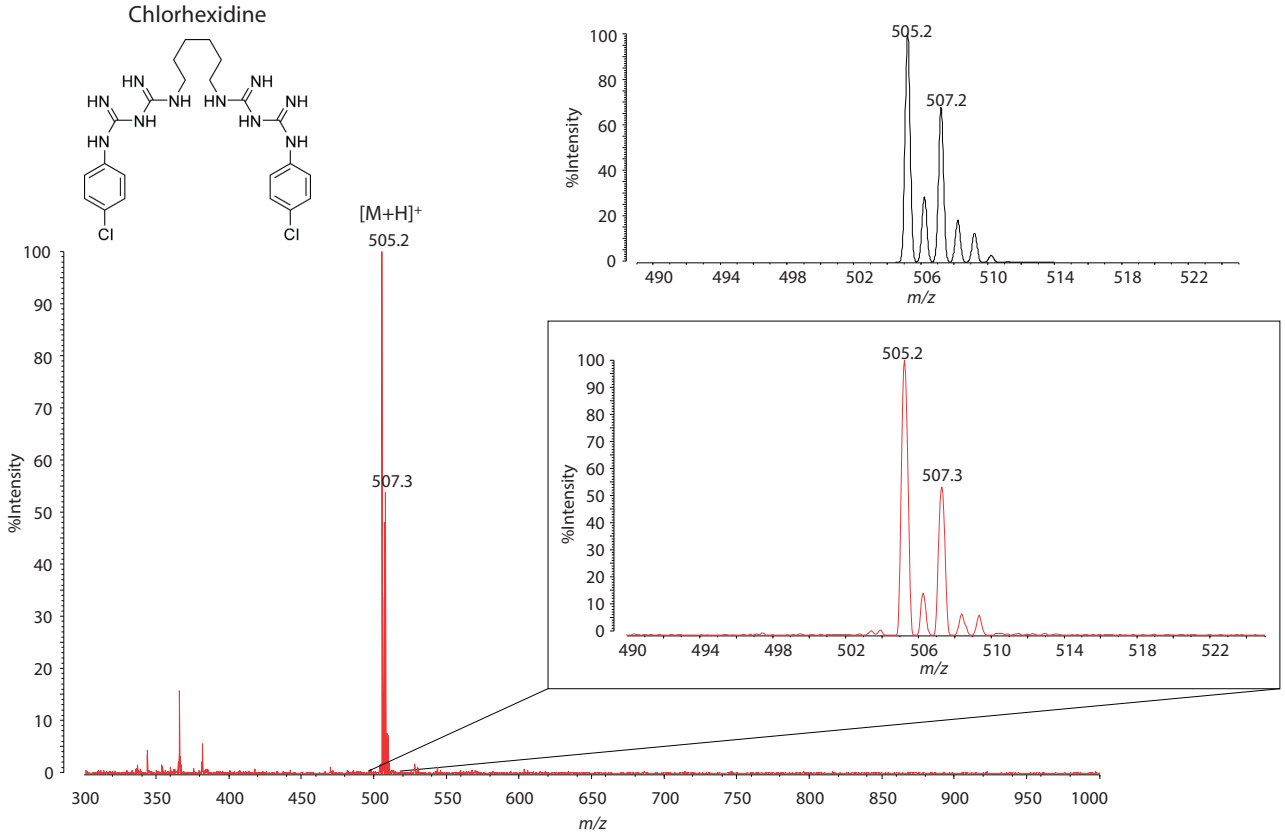

Fig. 4 Mass Spectrum of Mouthwash (B) and Theoretical Isotope Distribution of Chlorhexidine
Red: Measured Spectrum, Black: Theoretical Isotope Distribution
Measurement mode: Positive Linear

First Edition: Oct. 2017

Shimadzu Corporation
www.shimadzu.com/an/