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Application News

No. C158

Direct Probe Ionization Mass Spectrometer

15 Second Screening Analysis of Cyanide in Blood Serum Without Pretreatment

Recent years have witnessed an increasing trend in incidents of crime and poisoning involving various legal drugs and toxic substances. The diversity in the types of used substances has lead to such incidents becoming a social problem. In the fields of forensic medicine, forensic toxicology, and critical care, finding and identifying causative agents is a problem that requires establishment of an analysis method that is both quick and highly sensitive. There is also growing demand in these workplaces to further simplify the complex pretreatment processes and instrument operations as well as to increase analysis speed. While various analysis instruments have been utilized until now for analyzing specific components in blood, most instruments require complex pretreatment, such as extracting the target component from blood. What is needed is a screening method that best reduces the time and labor required to perform analysis.

Probe electrospray ionization (PESI) is a direct ionization technique that ionizes sampled target components by sampling samples using an ultrafine and minimally invasive probe and applying high voltage to the probe tip. This technique enables sample analysis without the need for a chromatograph (Fig. 1).

The DPiMS-2020, which combines PESI with a mass spectrometer, is suitable for simple screening analysis because it enables quick analysis of target components in samples without pretreatment regardless of whether samples are in liquid or solid form.

This article introduces a rapid screening method for detecting cyanide in blood serum that does not require pretreatment by utilizing the DPiMS-2020 and In-Source CID.

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Analysis Sequence Without Pretreatment

Potassium cyanide was added to blood serum to obtain a final concentration of 10 µg/mL and then taurine and naphthalene dialdehyde were added to perform derivatization.[*1] The obtained cyanide derivative (Fig. 2) was added to blood serum and used as the sample.

While complex pretreatment, such as that shown in Fig. 3, is required in conventional blood serum analysis, analysis that utilizes PESI can be performed using blood serum that contains cyanide derivatives either as-is or diluted with water by injecting it onto a small (10 µL) sample plate and setting the sample plate in the instrument.

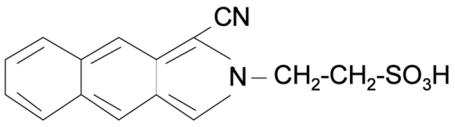

Fig. 2 Cyanide Derivative (MW 300)

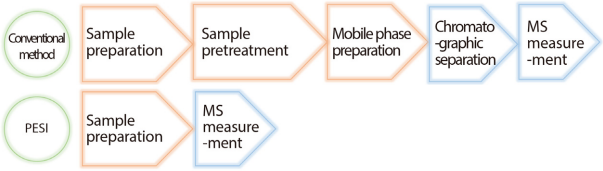

Fig. 3 Analysis Sequence Without Pretreatment

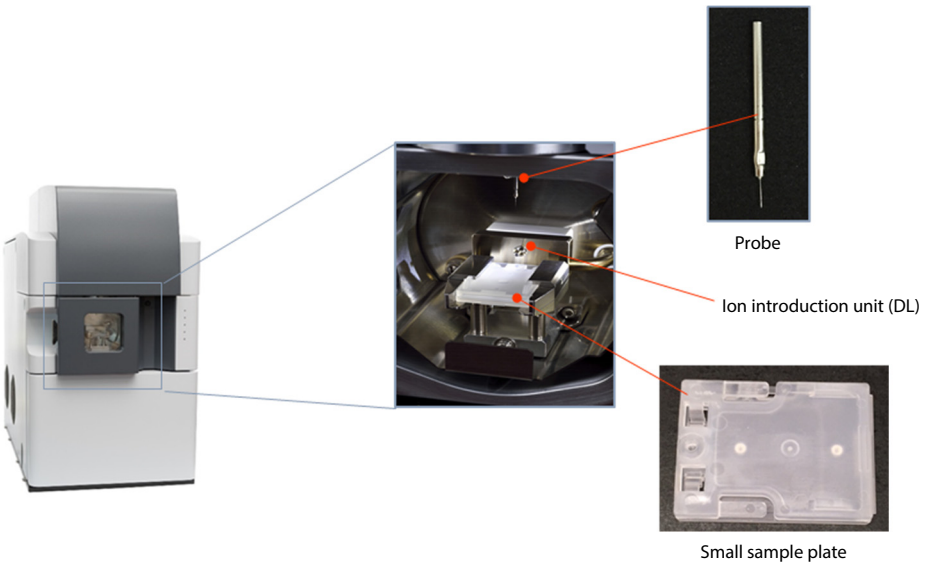

Fig. 1 DPiMS-2020

Structural Analysis Using In-Source CID Analysis

While a triple quadrupole mass spectrometer is usually used for structural analysis, a single quadrupole mass spectrometer can also obtain molecular structure information as well as molecular weight information by setting the lens system to a high voltage.
Analysis that utilizes PESI results in a unique mass chromatogram (Fig. 4) because the probe is driven at a constant frequency to repeat a process of sampling followed by ionization by applying a high voltage.
Fig. 5 shows the mass chromatogram obtained in our example. Applying a voltage of –80 V to DL bias and Q-array bias allows molecular structure information to be obtained and enables quick and simple screening analysis for cyanide in blood serum.
For reference, Fig. 6 shows the product ion (MS/MS) mass spectrum of the cyanide derivative obtained using the LCMS-8040 triple quadrupole mass spectrometer.

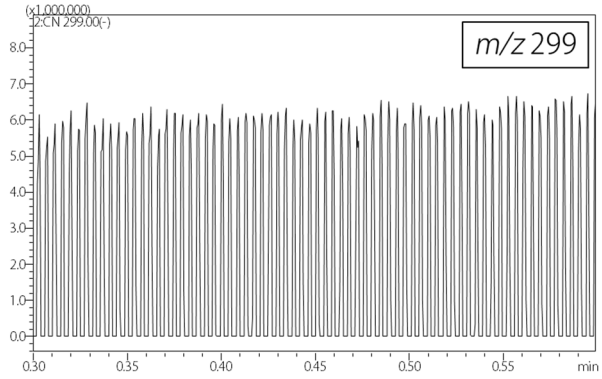

Fig. 4 Mass Chromatogram from DPiMS-2020

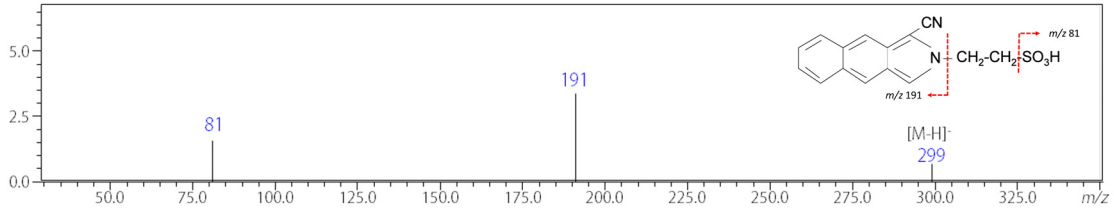

Fig. 5 Mass Spectrum from DPiMS-2020

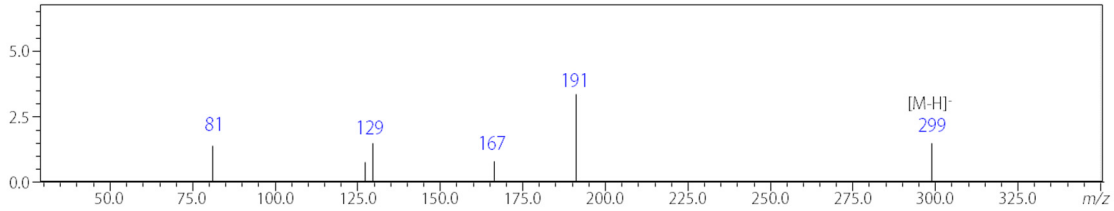

Fig. 6 Product Ion Mass Spectrum from LCMS-8040 (Reference)

DPiMS-2020 Analysis Conditions

When performing analysis using the DPiMS-2020, the drive conditions of the PESI probe and the analysis conditions of the mass spectrometer must be set.

Table 1 and 2 list the drive and analysis conditions respectively.

Table 1 PESI Drive Conditions

Ionization position	: –37 mm
Ionization stop time	: 100 msec
Sampling position	: –46 mm
Sampling stop time	: 50 msec
Probe speed	: 250 mm/s
Probe acceleration	: 0.63 G

Table 2 Mass Spectrometer Analysis Conditions

DL temperature	: 250 °C
Heater block temperature	: 35 °C
Interface voltage	: –2.45 kV (ESI – Negative mode)
DL bias voltage	: –80 V (*m/z* 299)
Q-array bias voltage	: –80 V (*m/z* 299)

References
*1 S. Chinaka, N. Takayama, Y. Michigami, and K. Ueda. *J. Chromatogr. B.* 713: 353–359 (1998)

Acknowledgments
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The product described in this document has not been approved or certified as a medical device under the Pharmaceutical and Medical Device Act of Japan. It cannot be used for the purpose of medical examination and treatment or related procedures.

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