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Application News

No. B90

Probe Electrospray Ionization Mass Spectrometer

Rapid Analysis of Drugs in Forensic Specimens Using the DPiMS™-8060

The analysis of drugs and toxic substances in forensics generally uses body fluid samples such as blood and urine due to their ease of handling and consideration for data collection. However, there are cases where the sampling of body fluid is difficult, such as from decomposed or charred bodies or hemorrhagic deaths. In such situations, organs may be used as samples instead. Since the instrumental analysis of organs requires complex pretreatment due to the complexity of the components within the organs, it takes time until the analysis results can be obtained.

Researches until now have focused on speeding up and simplifying the pretreatment of organs using the QuEChERS method. In order to further shorten the time needed for organ analysis, this article introduces a direct analysis method of drug content in organs with minimal pretreatment and analysis time using the newly developed DPiMS-8060 mass spectrometer (Fig. 1) which combines probe electrospray ionization (PESI), a novel ionization method, with tandem mass spectrometry.

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Fig. 1 **DPiMS™-8060**

Qualitative Analysis

Analysis using the DPiMS-8060 involves repeatedly piercing the sample organ with a probe. At the same time, a voltage is applied to the probe tip to ionize the sample that adheres to the probe surface and introduce it directly into the mass spectrometer.

On June 26, 2016, 1-cyclohexyl-4-(1,2-diphenylethyl)-piperazine (hereinafter, MT-45) was designated as a narcotic in Japan. We used forensic samples of organs (liver, brain, kidney, heart, lung) with MT-45 intake and performed qualitative analysis of the MT-45 in those organs by product ion scanning. The results are shown in Fig. 2. We also analyzed the expected metabolites of MT-45 by product ion scanning, of which the results are shown in Fig. 3.

Preparation of samples is simple with no complex pretreatment. The analysis samples for this research were prepared by cutting a 3 mm square section from each organ and setting each section in a sample plate. Then 35 µL of a 1:1 solution of 10 mmol/L ammonium formate aqueous solution and ethanol was dripped onto each sample. With this step the samples are ready for analysis.

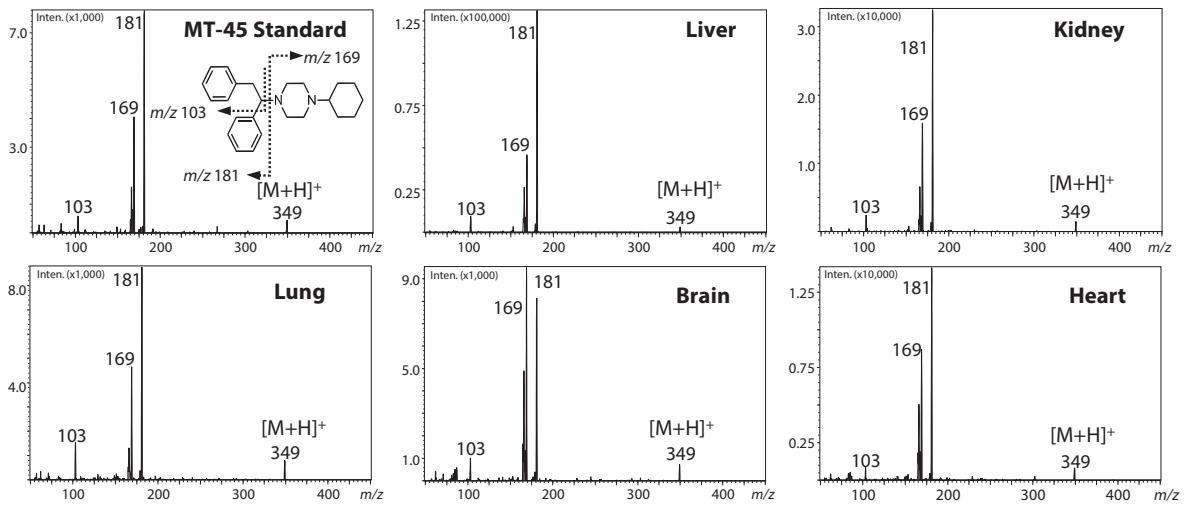

Fig. 2 **Structural Formula of MT-45 and Product Ion Scan Results of MT-45 in Each Organ**

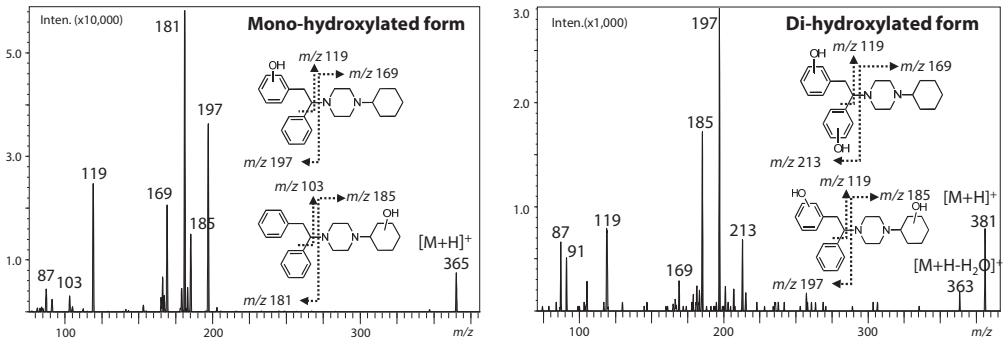

Fig. 3 **Structural Formulae of MT-45 Metabolites and Product Ion Scan Results of Expected MT-45 Metabolites in Liver**

Quantitative Analysis

Organ samples were prepared by the QuEChERS method. Using the obtained sample solution and the standard addition method, quantitation was performed using the DPiMS-8060 and an LC-MS/MS to compare quantitation values.

A calibration curve (n=6) was created by analyses using the conditions listed in Table 1. The linearity (r) of the calibration curve was higher than 0.996 and the accuracy (%RE) was within -5.0 to 9.4, demonstrating favorable analysis precision. Fig. 4 shows the calibration curve.

The drug concentration in each organ was quantitated using this calibration curve and the results are shown in Table 2.

The results show that the values obtained using the DPiMS-8060 and those with an LC-MS/MS are overall of the same level. Furthermore, since the DPiMS-8060 does not require the time for elution that an LC does, the time required for a single analysis is only 0.5 min. This means that by using the DPiMS-8060, the measurement time can be reduced by 97.5 %.

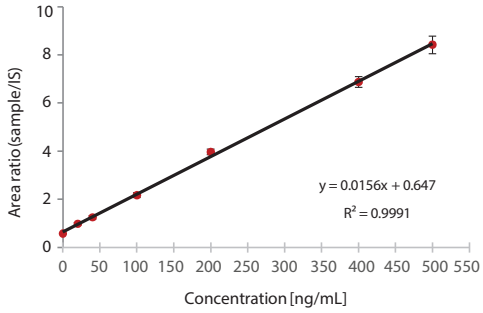

Fig. 4 **MT-45 Calibration Curve by Standard Addition**

Table 1 **Analytical Conditions Using DPiMS-8060**

Collision Energy	25 V
Mass Range	*m/z* 50-450
Scan Speed	405 u/sec
Event Time	1 sec
Desolvation Line	250 °C
Heat Block	50 °C
Polarity	Positive
Acquisition time	0.5 min/event

Table 2 **Comparison of DPiMS-8060 and LC-MS/MS Quantitation Results**

Section	DPiMS-8060 (µg/mL)	LC-MS/MS (µg/mL)
Liver	4.1	3.9
Brain	1.6	1.5
Heart	1.8	2.0
Lung	8.7	10.9
Kidney	1.7	1.5
Measurement time	**0.5 min**	20 min

Conclusion

The DPiMS-8060 enabled rapid detection of a narcotic in organs without any pretreatment.

In addition, application of the DPiMS-8060 to quantitative analysis is also possible with minimal pretreatment.

These results suggest that the use of the DPiMS-8060 is viable as a simple and rapid method for analyzing the drug and toxic substance content in organs in the field of forensics.

Acknowledgments
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References
Usui, K.; Murata, T., et al. *Drug Test Anal.* **2018, 10**, 1033–1038.

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