Illegal Drugs Analysis by Thermal Desorption and Pyrolysis Combined with Direct Analysis in Real Time- Mass Spectrometry (TDP/DART-MS)

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Introduction

Drugs present in biological and autopsy specimens cannot be detected without first selecting the pretreatment and the appropriate analytical conditions for the drugs. Thus, it is extremely important to investigate the analytical method suitable for specific compounds and samples. However, in recent years the situation in which new substances appear one after another, including New Psychoactive Substance (NPS) that threaten society, it is very difficult to examine individually the analytical conditions that are appropriate for each new substance. Thus, the comprehensive analysis system for drugs that require minimal investigation of pretreatment and analytical conditions are greatly desired.
So, we are investigating an analytical method for directly analyzing drugs in blood and urine that does not require any pretreatment.

Methods and Samples

The samples were standard drugs mixture (Table 1), and drugs mixture loaded blood and urine (i.e., blank blood and blank urine samples with drugs mixture added).
Mass spectra were obtained by using a TripleTOF5600+ (SCIEX) Q-Tof mass spectrometer combined with a DART ion source (IonSense LLC) and an ionRocket Thermal Desorption and Pyrolysis (TDP) device (BioChromato, Inc.). The ionRocket was mounted between the DART ion source and the mass spectrometer. We conducted our study by assessing whether drugs could be detected by using this analytical system (Figure 1).

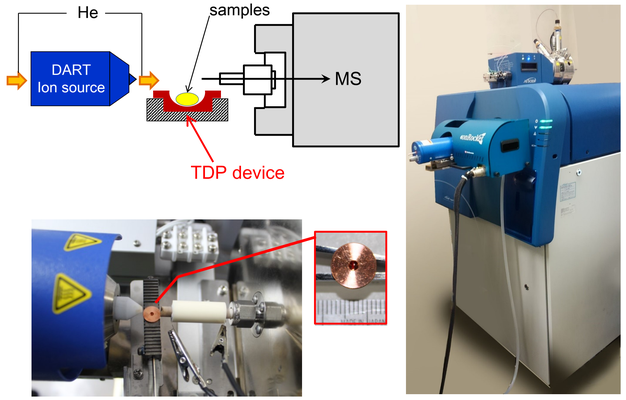

Figure1 TDP/DART-MS system

Table1 samples

Sample name	Elemental composition	M_{mi}
5F-AEB	$C_{20}H_{28}FN_3O_3$	377.21092
5F-CUMYL-PICA	$C_{23}H_{27}FN_2O$	366.21019
Br-DRAGON FLY	$C_{13}H_{12}BrNO_2$	293.00459
4 acetoxy DMT	$C_{14}H_{18}N_2O_2$	246.13628
4 acetoxy DiPT	$C_{18}H_{26}N_2O_2$	302.19888

Results

◆ Analysis by DART-MS

At first, in order to determine the analysis condition, drugs standard were analyzed by DART-MS. All samples were detected as the protonated ion.

Analytical condition

Ionization:
- DART positive
- Set temperature: 400 degree Celsius
- Ionization gas: Helium

MS measuring method:
- Information Dependent Acquisition method (IDA)
- Mass range: *m/z* 100 - 1000

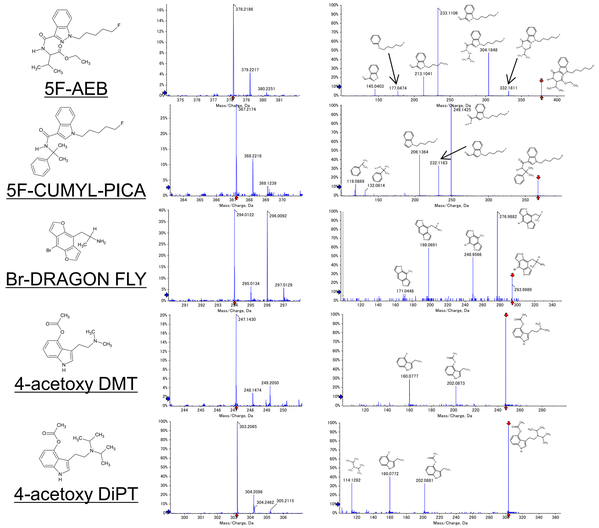

Figure2 MS spectra and MS/MS spectra of drugs standard

◆ Analysis by TPD/DART-MS

5μL of sample solutions were put into the POT (Figure2) and samples were gradient heated by TDP device.

Analytical condition

Temperature program:
- Ambient temperature to 420 degree Celsius at a rate of 70 degree Celsius / min(Figure3).

Ionization:
- DART positive
- Set temperature: 400 degree Celsius
- Ionization gas: Helium

MS measuring method:
- Information Dependent Acquisition method (IDA)
- Mass range: *m/z* 100 - 1000

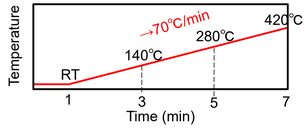

Figure3 Temperature program of TDP device

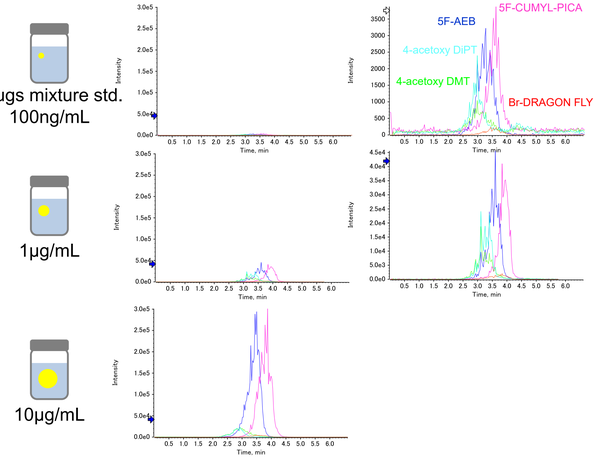

Figure4 Extracted ion currentgram of 100ng/mL, 1μg/mL and 10μg/mL drugs mixture std. in MeOH

As a results of drugs mixture standards, each drugs were separated and detected through thermal gradient heating for all samples, and thermal desorption profiles were highly reproducible for individual drugs. Moreover, this analysis system was seemed to have the potential of quantitative analysis for drugs, as the drug's ion intensity were increased with increasing drugs concentrations in the samples (Figure4).

As for drugs mixture in blood, when we analyzed the blood samples that was pretreated by using dispersive solid-phase extraction for removing phospholipid, whereupon the intensity were dramatically improved (Figure5).

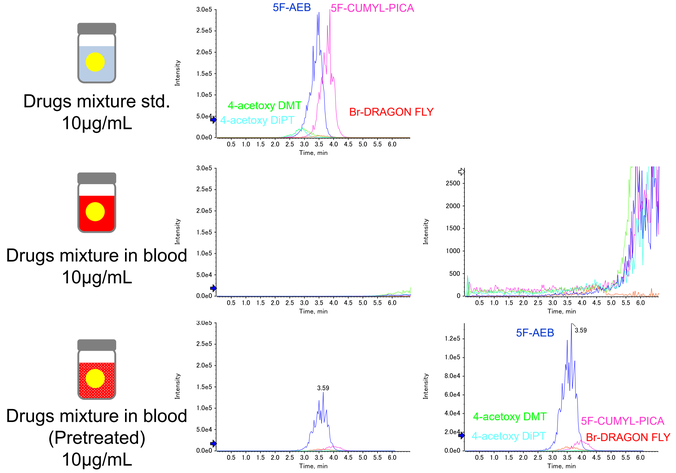

Figure4 Extracted ion currentgram of 10μg/mL drugs mixture std. in MeOH, blood and pretreated by using dispersive SPE for removing phospholipid

Conclusion

- ◆ TPD/DART-MS, DART-MS combined with the thermal desorption and pyrolysis device enabled to acquire a mass spectrum through thermal gradient heating.
- ◆ Each drugs were separated and detected by using TDP/DART-MS.
- ◆ This analysis system was seemed to have the potential of quantitative analysis for drugs.

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