K1 An Improvement for High Sensitivity of Drug Screening by Thermal Desorption and Pyrolysis Combined With Direct Analysis in Real Time-Mass Spectrometry (TDP/DART®-MS)

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Learning Overview: After attending this presentation, attendees will understand the value of TDP/DART®-MS for the rapid identification and screening of forensic drugs in biological and autopsy specimens (e.g., urine and blood).

Impact on the Forensic Science Community: This presentation will impact the forensic science community by explaining how TDP/DART®-MS can be effectively applied as an identification and screening technique for the forensic drugs present in biological and autopsy specimens.

Introduction: Drugs present in biological and autopsy specimens cannot be detected without first selecting the pretreatment and analytical conditions appropriate for the drugs. However, in recent years, the situation in which new substances appear one after another, including New Psychoactive Substance (NPS) that threaten society, makes it very difficult to optimize the analytical conditions for each new substance. Thus, there is a need for a comprehensive analysis system that requires minimal investigation of pretreatment and analytical conditions. So, an analytical method for directly analyzing drugs in blood that does not require any pretreatment is being investigated. In a previous study, TDP/DART®-MS was used to separate and detect drugs in urine.[1] The detected ions were correctly identified according to their measured accurate mass and product ion spectra. Moreover, for the quantitative analysis, urine calibrator curves were prepared at concentrations ranging 0.01μg/ml–1μg/ml and the curves were linear in that range. However, the detection sensitivity was not satisfactory, so the current investigation aims to improve the detection intensity of drugs.

Materials and Method: The samples were standard drug mixture solutions and drug mixture-fortified blood and urine. The standard drug mixture solution consisted of 38 kinds of illegal drugs (e.g., cationics, cannabinoids, and phenethylamines). Mass spectra were obtained by using a quadrupole Time-Of-Flight (qTOF) mass spectrometry equipped with a DART® ion source and a TDP unit. The TDP unit was mounted between the DART® ion source and the mass spectrometry. Mass spectra were measured in positive-ion mode after the samples were heated from room temperature to 300°C. Additionally, to improve the detection intensity, the following two methods were considered: the solvent extraction for deproteinization treatment, and modifications to the analysis systems. In the former case, ethanol (EtOH), methanol (MeOH), and acetonitrile (ACN) were used and in the latter case, the glass tee-tube (the HOOD) was attached between an ion source and the qTOF This glass tee-tube can work for preventing the diffusion of volatilized drugs from the blood samples.

Results and Discussion: Each drug was separated and detected through thermal gradient heating for all samples, and thermal desorption profiles were highly reproducible for individual drugs. The detected ions were correctly identified according to their measured accurate mass and product ion spectra. ACN was the best for deproteinization treat for this investigation, since ACN was attained the highest sensitivity. In addition, when using the HOOD, the peak area of the extracted ion current gram of each drugs was more intense, and it was thought that the volatilized drugs had been ionized more efficiently by attaching the HOOD. Moreover, the calibration curve was linear regardless of the presence or absence of HOOD. Finally, it was confirmed that the heating rate of the TDP device was also effective for improving the detection intensity of drugs, as increasing the heating rate has improved the separation of the peaks and improves the peak intensity.

Reference(s):

1. Hiroko A. et al. Illegal Drugs Analysis by Thermal Desorption and Pyrolysis Combined With Direct Analysis in Real Time-Mass Spectrometry (TDP/DART®-MS). *Proceedings of the American Academy of Forensic Sciences*, 69th Annual Scientific Meeting, New Orleans, LA. 2017.

Drug Screening, TDP/DART®-MS, Urine and Blood