

# Application Data Sheet

## No.101

### GC-MS

Gas Chromatograph Mass Spectrometer

## Analysis of Toxicological Substances in Whole Blood Using the Smart Forensic Database (2)

Smart Forensic Database is an MRM database containing retention indices, MRM transitions, collision energies, and quantitation/confirmation ion ratios for 201 toxicological substances often involved in poisonings. Smart MRM, which is provided with the GCMS-TQ8040, can create analysis methods for Scan/MRM and MRM automatically from the database.

This article introduces an example of using a simultaneous Scan/MRM measurement method created from the Smart Forensic Database to measure a whole-blood sample, and then applying the GC/MS Forensic Toxicology Database to the scan data obtained.

### GC/MS Forensic Toxicological Database

The GC/MS Forensic Toxicological Database is intended for Scan analysis, and is registered with 726 toxicological compounds (1476 types). The database contains toxicological substance names, quantitation and confirmation ions, retention indices, and standard mass spectra. The retention times for the registered toxicological substances are accurately estimated simultaneously from low-boiling point components to high-boiling point components, using measurement data from a standard n-alkane mixture via the GCMSsolution AART function. It is easy to determine whether samples contain toxicological substances by using the mass chromatograms for the quantitation and confirmation ions contained in the database.

### Experimental

Liquid-liquid extraction via EXtrelut® NT3 was used to pretreat the whole-blood sample. The collected whole-blood sample was measured into 1 mL portions for acidic fractionation and basic fractionation, and each portion was diluted with 1 mL of Milli-Q water. The acidic fraction was adjusted to a pH 5 using 10 % hydrochloric acid, and the basic fraction was adjusted to a pH 9 using 10 % ammonia water. The respective solutions were added to the EXtrelut® NT3 columns and left to stand for 30 minutes, after which each was eluted with a 10 mL chloroform:isopropanol (3:1) mixture. The extracted solutions of acidic fraction and basic fraction were then mixed, and after dessication with silica gel and drying in a nitrogen airflow, the sample solution was re-dissolved in a 200 µL chloroform:isopropanol (3:1) mixture.

### Analytical Conditions

The conditions registered in Smart Forensic Database were used as the GC-MS/MS analysis conditions. For the compounds subject to MRM measurement, a simultaneous Scan/MRM analysis method was created, in which the 201 components registered in the database were set.

Table 1: Analytical Conditions

GC-MS:	GCMS-TQ8040		
Column:	Rx <sup>i</sup> -5SiMS (Length 30 m, 0.25 mm I.D., df=0.25 µm)		
Glass liner:	Splitless insert with wool (PN: 221-48876-03)		
[GC]		[MS]	
Injection temp.:	260 °C	Interface temp.:	280 °C
Column oven temp.:	60 °C (2 min) → (10 °C /min) → 320 °C (15 min)	Ion source temp.:	200 °C
Injection mode:	Splitless	Acquisition mode:	Scan/MRM
Flow control mode:	Linear velocity (45.6 cm/sec)	Scan event time:	0.1 sec
Injection volume:	1 µL	Scan mass range:	m/z 43 – 600
		Scan speed:	10,000 u/sec
		MRM event time:	0.3 sec
		Total loop time:	0.4 sec

## Results

The extracted whole-blood samples were measured in the simultaneous Scan/MRM analysis mode. By analyzing the scan data using the GC/MS Forensic Toxicological Database, pentedrone, a type of cathinone, was identified (Fig. 1). If a simultaneous Scan/MRM analysis is done, the obtained MRM data can be analyzed via Smart Forensic Database to identify toxicological substances often involved in poisonings, while the scan data can be analyzed to confirm identifications using the mass spectra, or to screen for approximately 1400 toxicological substances using the GC/MS Forensic Toxicological Database.

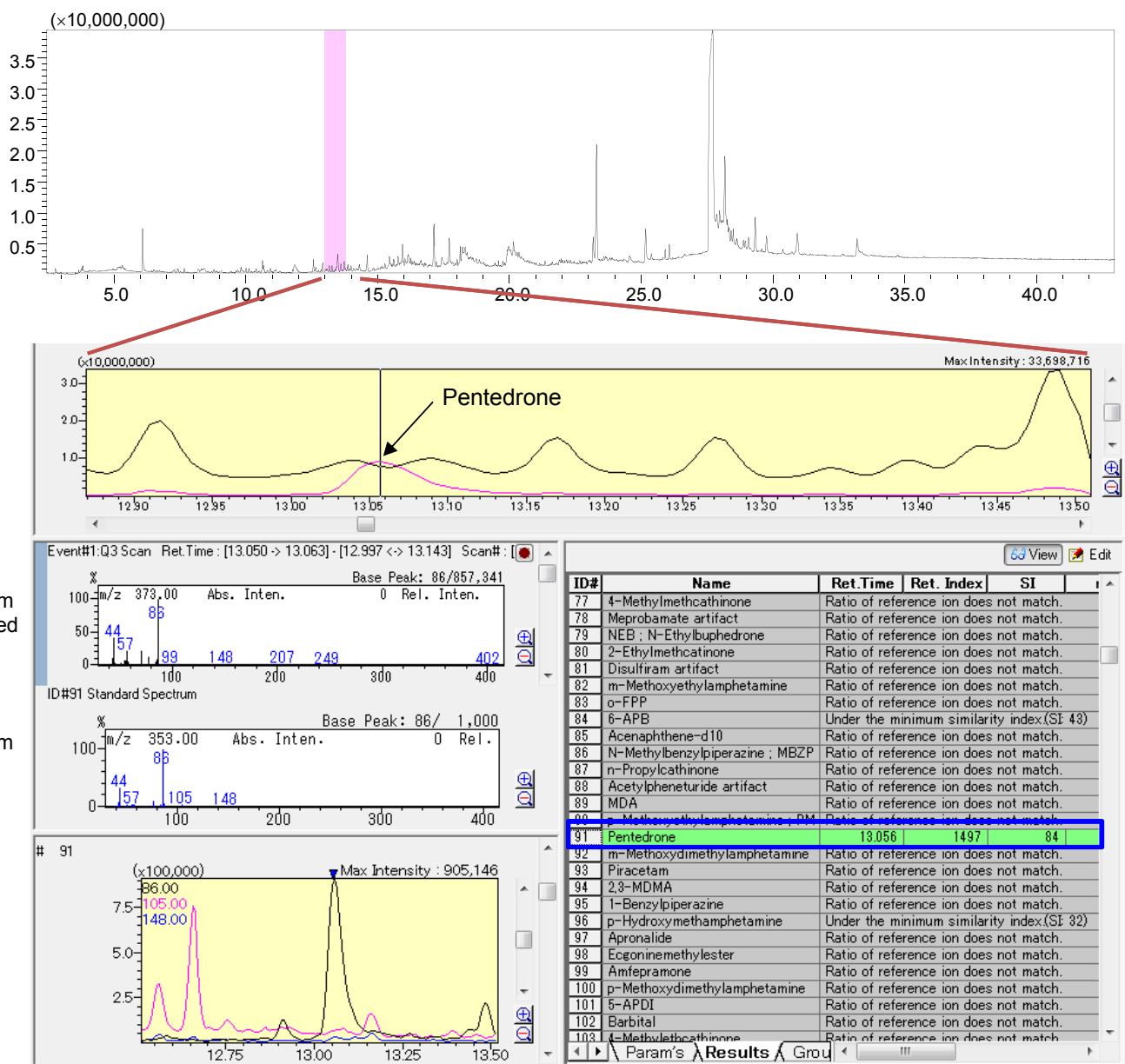


Fig. 1: Results from an Analysis of the Scan Data from a Whole-Blood Sample Using the GC/MS Forensic Toxicological Database

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