Shimadzu's Smart Forensic Database Enables Fast, Accurate Analysis of

TOXICOLOGICAL SUBSTANCES

in Whole Blood

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Excellence in Science

For many forensic laboratories, *there is a need for a simpler, faster and more effective way to conduct analysis.* These labs face the challenge of delivering accurate results for an increasing number of samples. To improve productivity and confidence in results, they need more advanced instrumentation and software solutions designed specifically for forensic analysis.

Shimadzu's Smart Forensic Database helps you easily and automatically create multiple reaction monitoring (MRM) methods for GC-MS/MS toxicological analysis.

Registered Compounds

COMPOUND CLASSIFICATION	NUMBER OF REGISTERED COMPOUNDS
Drugs of Abuse	51
Psychotropic Drugs	200
General Drugs	87
Pesticides	125
Others	5
ISTDs	18
TOTAL	486

The Smart Forensic Database

includes 486 forensic toxicological substances, such as:

- **Abused drugs**
- **Psychotropic drugs**
- **Pharmaceuticals**
- **Pesticides**

With this sophisticated database, you no longer need to configure complicated analysis conditions. It contains information on over **1,200 MRM transitions,** collision energies and confirmation ion ratios for all of the registered compounds. In addition, retention indices are registered for all of the components, so that users can easily update retention times using the **Automatic Adjustment of Retention Time (AART) function.**

POWER

READY

FAILURE

SHIMADZ

GCMS-TQ8050
GAS CHROMATOGRAPH MASS SPECTROMETER

| Serial#	Type	Acq. Mode	Method No.	Compound Name (E)	Ret. Index 1	Ret. Time	Cas#	Comment	Ion1				Ion2		
									Type	m/z	CE	Rati	Type	m/z	CE	Rati
1	Target	MRM	1	Valproic acid	1108		99 - 66 - 1	Psychotropic Drugs	T	102.0>73.0	6	100.00	Ref.1	102.0>55.0	21	32.79
2	Target	MRM	1	Valproic acid-TMS	1156		0 - 00 - 0	Psychotropic Drugs	T	201.1>75.0	12	100.00	Ref.1	174.1>145.0	6	92.43
3	Target	MRM	1	Phentermine	1171		122 - 09 - 8	Drug of Abuse	T	134.0>117.0	9	100.00	Ref.1	134.0>115.0	15	86.53
4	Target	MRM	1	Bromisovalum artifact	1181		0 - 00 - 0	Psychotropic Drugs	T	139.0>122.0	15	100.00	Ref.1	137.0>120.0	18	98.09
5	Target	MRM	1	Methamidophos	1237		10265 - 92 - 6	Pesticides	T	141.0>95.0	8	100.00	Ref.1	95.0>64.0	12	46.66
6	Target	MRM	1	Dichlorvos	1244		62 - 73 - 7	Pesticides	T	185.0>93.0	14	100.00	Ref.1	145.0>109.0	12	37.35
7	Target	MRM	1	Ethosuximide	1249		77 - 67 - 8	Psychotropic Drugs	T	113.0>69.0	15	100.00	Ref.1	113.0>41.0	27	48.63
8	Target	MRM	1	Amphetamine-TFA	1304		0 - 00 - 0	Drug of Abuse	T	140.1>69.0	24	100.00	Ref.1	140.1>113.1	6	19.62
9	Target	MRM	1	Propofol	1359		2078 - 54 - 8	General Drugs	T	178.1>163.1	12	100.00	Ref.1	163.1>117.1	15	97.08
10	Target	MRM	1	Propofol-TMS	1391		0 - 00 - 0	General Drugs	T	250.1>235.1	9	100.00	Ref.1	235.1>233.1	6	107.38
11	Target	MRM	1	Ephedrine-2TFA	1391		50 - 98 - 6	Drug of Abuse	T	154.1>110.1	12	100.00	Ref.1	154.1>69.0	24	61.50
12	Target	MRM	1	Methamphetamine-TFA	1413		0 - 00 - 0	Drug of Abuse	T	154.1>110.1	12	100.00	Ref.1	118.1>91.0	24	19.64
13	Target	MRM	1	Acephate	1450		30560 - 19 - 1	Pesticides	T	136.0>94.0	14	100.00	Ref.1	142.0>96.0	9	25.28
14	Target	MRM	1	Metolcarb	1462		1129 - 41 - 5	Pesticides	T	108.0>77.0	24	100.00	Ref.1	108.0>90.0	12	40.39
15	Target	MRM	1	Ecgoninemethylester	1503		106293 - 60 - 1	Drug of Abuse	T	96.0>81.0	18	100.00	Ref.1	82.0>55.0	15	51.48
16	Target	MRM	1	Apronalide	1503		528 - 92 - 7	Psychotropic Drugs	T	141.0>81.0	6	100.00	Ref.1	142.0>82.0	6	95.08

Chlorpromazine in Whole Blood

Concentration in whole blood: 50 ng/mL
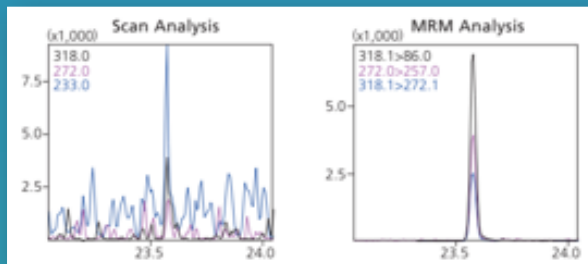
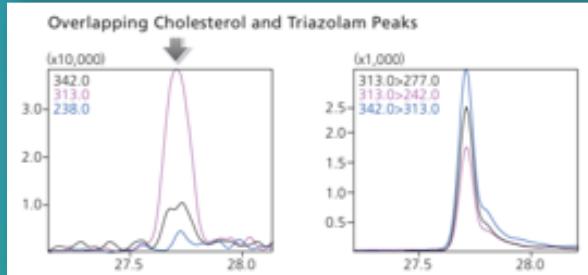Clearer peak detection via high-sensitivity analysis

Blank Whole Blood Sample
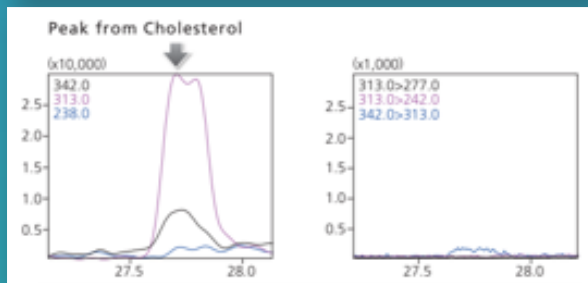
Clearer peak detection via high-separation analysis

Triazolam-Spiked Whole Blood Sample

Concentration in whole blood: 50 ng/mL

MRM Provides Improved Selectivity and Sensitivity

The GC-MS/MS MRM mode detects forensic toxicological substances with improved sensitivity. That's because mass separation is performed in two stages to separate background interference from biological samples from the target compounds. This makes it easy to determine whether biological samples contain forensic toxicological substances and *significantly reduces data analysis times.*

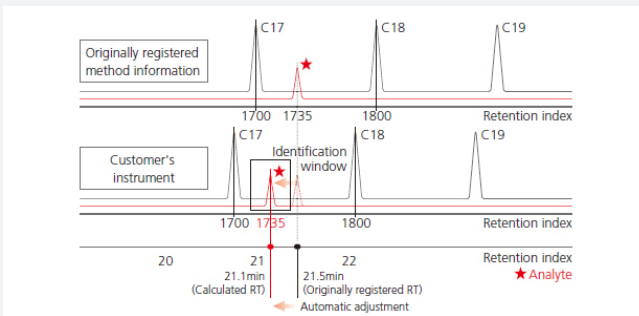# Automatically Create Optimal MRM Methods

In multicomponent simultaneous analysis, it can be difficult to configure the dwell, event and loop time-measurement settings in the MRM program. To address this challenge, Shimadzu offers the Smart MRM program. This program automatically determines the **optimal time-measurement settings** and creates a **high-sensitivity method**. Using the AART function, it creates the MRM method based on the retention time information for target compounds.
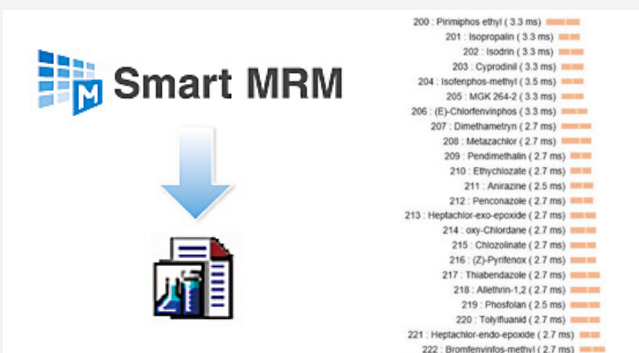
5

1 Perform an n-alkane analysis.

2 Update the retention times using AART.

Originally registered method information

C17   C18   C19

1700 1735 1800   Retention index

Customer's instrument

Identification window

C17   C18   C19

1700 1735   1800   Retention index

20   21   22   Retention index
       21.1min   21.5min   ★ Analyte
    (Calculated RT) (Originally registered RT)
        ← Automatic adjustment →

3 Use Smart MRM to create the MRM method automatically.

Smart MRM

200 : Pirimiphos ethyl (3.3 ms)
201 : Isopropalin (3.3 ms)
202 : Isodrin (3.3 ms)
203 : Cyprodinil (3.3 ms)
204 : Isofenphos-methyl (3.5 ms)
205 : MGK 264-2 (3.3 ms)
206 : (E)-Chlorfenvinphos (3.3 ms)
207 : Dimethametryn (2.7 ms)
208 : Metazachlor (2.7 ms)
209 : Pendimethalin (2.7 ms)
210 : Ethychlozate (2.7 ms)
211 : Anirazine (2.5 ms)
212 : Penconazole (2.7 ms)
213 : Heptachlor-exo-epoxide (2.7 ms)
214 : oxy-Chlordane (2.7 ms)
215 : Chlozolinate (2.7 ms)
216 : (Z)-Pyrifenox (2.7 ms)
217 : Thiabendazole (2.7 ms)
218 : Allethrin-1,2 (2.7 ms)
219 : Phosfolan (2.5 ms)
220 : Tolylfluanid (2.7 ms)
221 : Heptachlor-endo-epoxide (2.7 ms)
222 : Bromfenvinfos-methyl (2.7 ms)

Easy as 1-2-3: Creating the MRM Method Using the Smart Forensic Database

MRM method development can be time-consuming and labor-intensive — if you don't have the right software solution. With Shimadzu's Smart Forensic Database, method development is **quick** and **easy**. In just three simple steps, you can develop a new MRM method.

GCMS Forensic Toxicological Database Containing 1400+ Compounds

In addition to the Smart Forensic Database, Shimadzu also offers the Forensic Toxicological Database for GCMS. This database **contains over 1400 compounds**, enabling rapid screening for compound identification and confirmation. When you use Shimadzu's Forensic Toxicological Database, you can analyze data from simultaneous scan/MRM measurements.

This allows for semi-quantitation of trace levels of these compounds and comprehensive screening of a larger panel of compounds. And, when you combine this database with the Smart Forensic Database, you can collect **precise quantitation data for over 480 compounds.**

Smart Forensic Database in Action

Using the Smart Forensic Database, we ran a simultaneous scan/MRM measurement method to measure a whole blood sample. We then used the Forensic Toxicological Database to analyze the scan data.

Preparation

First, we pretreated the whole blood sample using liquid-liquid extraction via EXtrelut®. The collected whole blood sample was measured into 1 mL portions for acidic fractionation and basic fractionation. Each portion was subsequently diluted with 1 mL of Milli-Q® water. The acidic fraction was adjusted to a pH of 5 using 10% hydrochloric acid, and the basic fraction was adjusted to a pH of 9 using 10% ammonia water.

The respective solutions were then added to the EXtrelut NT3 columns. After thirty minutes, each solution was eluted with a 10 mL chloroform:isopropanol (3:1) mixture. The extracted solutions of acidic fraction and basic fraction were mixed, desiccated with silica gel and dried in a nitrogen airflow. Lastly, the sample solution was re-dissolved in a 200 μL chloroform:isopropanol (3:1) mixture.

Analytical Conditions

The conditions registered in the Smart Forensic Database were used as the GC-MS/MS analysis conditions. For the compounds subjected to MRM measurement, a simultaneous scan/MRM analysis method was created, in which the **486 components registered** in the database were set.

Analytical Conditions

GCMS	GCMS-TQ8040
Column	Rxi®-5Sil MS (Length 30 m, 0.25 mm I.D., df=0.25 μm)
Glass Liner	Splitless insert with wool (PN: 221-48876-03)

[GC]	
Injection temp	260 °C
Column oven temp	60 °C (2 min) -> (10 °C/min) -> 320 °C (15 min)
Injection mode	Splitless
Flow control mode	Linear velocity (45.6 cm/sec)
Injection volume	1 μL

| [MS]	
Injection temp	280 °C
Ion source temp	200 °C
Aquisition mode	Scan/MRM
Scan event time	0.1 sec
Scan mass range	m/z 43 – 600
Scan speed	10,000 μ/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. Using the Forensic Toxicological Database, we were able to analyze the scan data and identify pentedrone, a type of cathinone.

With the scan data you obtain, you can detect trace quantities of toxicological substances typically found in poisonings. Additionally, the scan data can be analyzed to confirm identifications using the mass spectra. You can also screen for approximately **1400 toxicological substances** using the Forensic Toxicological Database.

Mass Spectrum for the Identified Peak

Mass Spectrum Registered in the Database
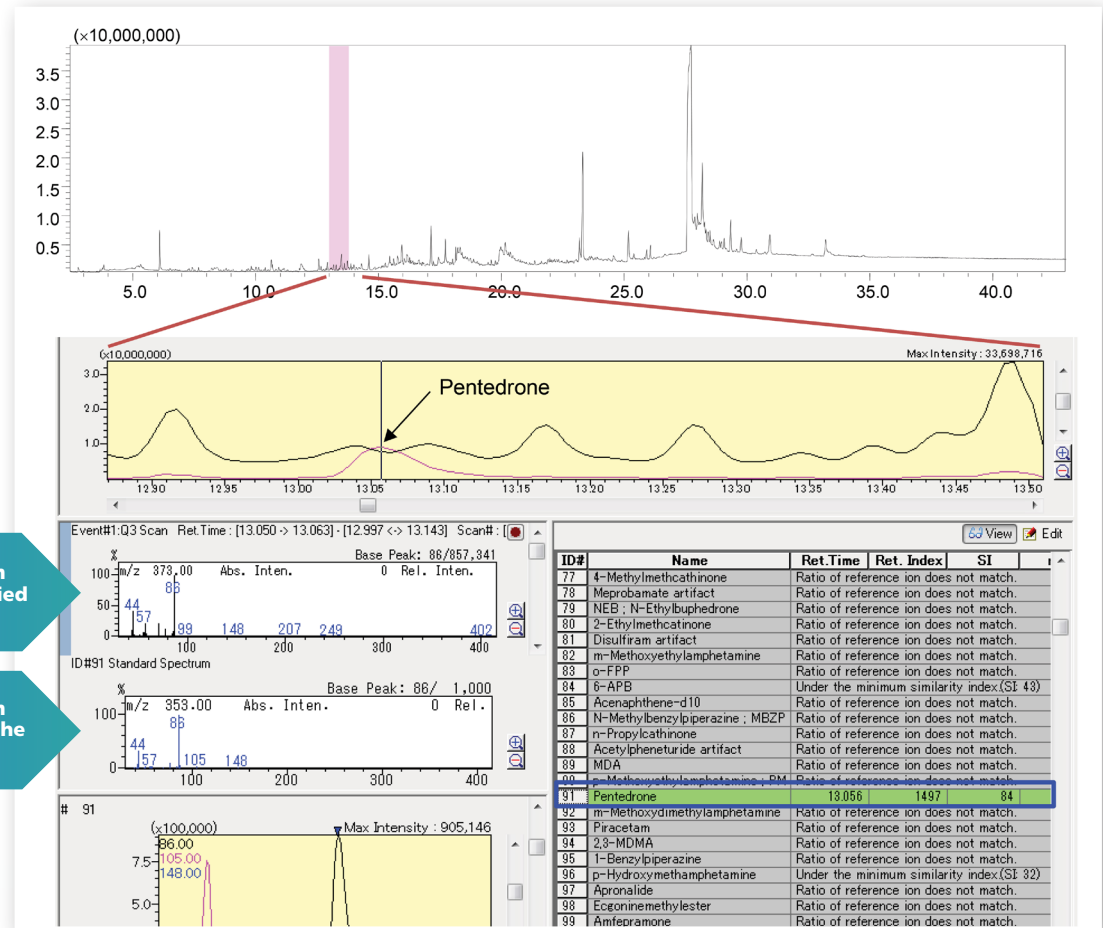
Results from an analysis of the scan data from a whole blood sample using the GCMS Forensic Toxicological Database.

Final Thoughts

Ensuring fast, reliable analysis is critical to the ongoing success of your forensics lab or research facility. That's why Shimadzu offers the **Smart Forensic Database** to ensure rapid, reliable MRM method development for GC-MS/MS toxicological analysis. With 486 forensic toxicological substances, 1,476 toxicological compound types and information on 1,200 MRM transitions, the Smart Forensic Database helps you keep up with everyday demands.

To learn more about how Shimadzu can help you optimize your forensic analysis, visit www.InvestigateYourLab.com.

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