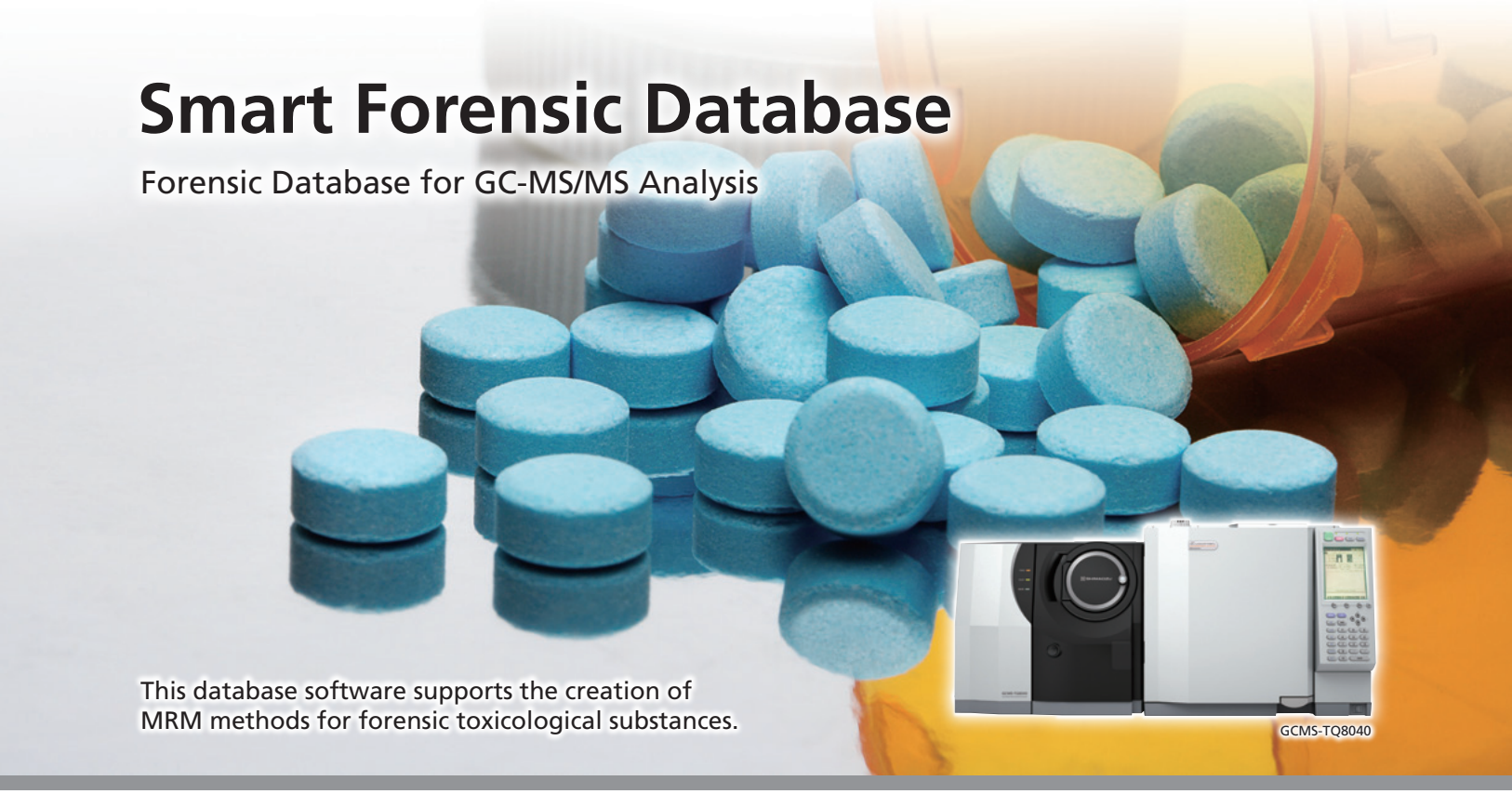
SHIMADZU
Excellence in Science

Smart Forensic Database

Forensic Database for GC-MS/MS Analysis



This database software supports the creation of MRM methods for forensic toxicological substances.

1. Supports Creation of MRM Methods for Forensic Toxicological Analysis Using GC-MS/MS

The database is registered with a total of 201 forensic toxicological substances often involved in poisonings, such as drugs of abuse, psychotropic drugs, pharmaceuticals and pesticides, and includes 1200 MRM transitions. For all registered compounds, it contains information on MRM transitions, collision energies, and confirmation ion ratios, so there is no need to configure complicated analysis conditions. Furthermore, retention indices are registered for all of the components, enabling easy updating of retention times via the AART (Automatic Adjustment of Retention Time) function.

Categories of Toxicological Substances Registered in Smart Forensic Database

	Number of Registered Compounds
Drugs of abuse	20
Psychotropic drugs	120
General drugs	20
Pesticides	40
Rodenticides	1

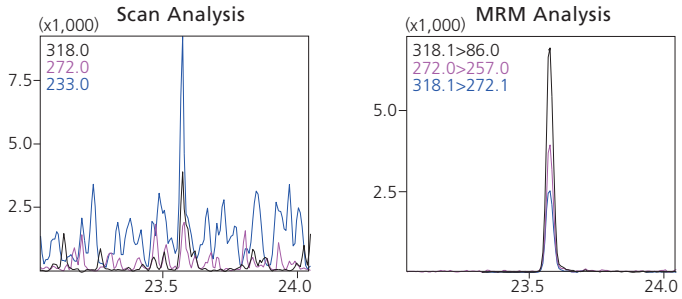
Serial#	Type	Acq. Mode	Method No.	Compound Name (E)	Ret. Index 1	Ret. Time	Cas#	Comment	Ion1			
									Type	m/z	CE	Rati
1	Target	MRM	1	Valproic acid	1108		99 - 66 - 1	Psychotropic Drugs	T	102.0>73.0	6	100.00
2	Target	MRM	1	Valproic acid-TMS	1156		0 - 00 - 0	Psychotropic Drugs	T	201.1>75.0	12	100.00
3	Target	MRM	1	Phentermine	1171		122 - 09 - 8	Drugs of Abuse	T	134.0>117.0	9	100.00
4	Target	MRM	1	Bromisovalum artifact	1181		0 - 00 - 0	Psychotropic Drugs	T	139.0>122.0	15	100.00
5	Target	MRM	1	Methamidophos	1237		10265 - 92 - 6	Pesticides	T	141.0>95.0	8	100.00
6	Target	MRM	1	Dichlorvos	1244		62 - 73 - 7	Pesticides	T	185.0>93.0	14	100.00
7	Target	MRM	1	Ethosuximide	1249		77 - 67 - 8	Psychotropic Drugs	T	113.0>69.0	15	100.00
8	Target	MRM	1	Amphetamine-TFA	1304		0 - 00 - 0	Drugs of Abuse	T	140.1>69.0	24	100.00
9	Target	MRM	1	Propofol	1359		2078 - 54 - 8	General Drugs	T	178.1>163.1	12	100.00
10	Target	MRM	1	Propofol-TMS	1391		0 - 00 - 0	General Drugs	T	250.1>235.1	9	100.00
11	Target	MRM	1	Ephedrine-2TFA	1391		60 - 98 - 6	Drugs of Abuse	T	154.1>110.1	12	100.00
12	Target	MRM	1	Methamphetamine-TFA	1413		0 - 00 - 0	Drugs of Abuse	T	154.1>110.1	12	100.00
13	Target	MRM	1	Acephate	1450		30560 - 19 - 1	Pesticides	T	136.0>94.0	14	100.00
14	Target	MRM	1	Metolcarb	1462		1129 - 41 - 5	Pesticides	T	108.0>77.0	24	100.00
15	Target	MRM	1	Ecgoninemethylester	1503		106293 - 60 - 1	Drugs of Abuse	T	96.0>81.0	18	100.00
16	Target	MRM	1	Apronalide	1503		528 - 92 - 7	Psychotropic Drugs	T	141.0>81.0	6	100.00

Smart Forensic Database

2. Provides Improved Selectivity and Sensitivity via MRM

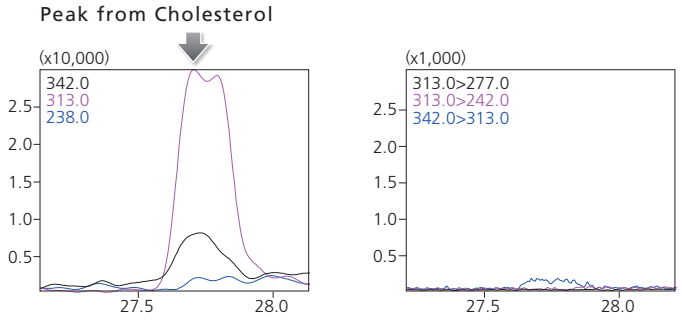
With GC-MS/MS MRM mode, mass separation is performed in 2 stages, so background interferences from biological samples are easily separated from the target compounds, and the forensic toxicological substances are detected with improved sensitivity. Thus, it is easy to determine whether biological samples contain forensic toxicological substances, and data analysis times are substantially reduced.

Chlorpromazine in Whole Blood
(Concentration in whole blood: 50 ng/mL)



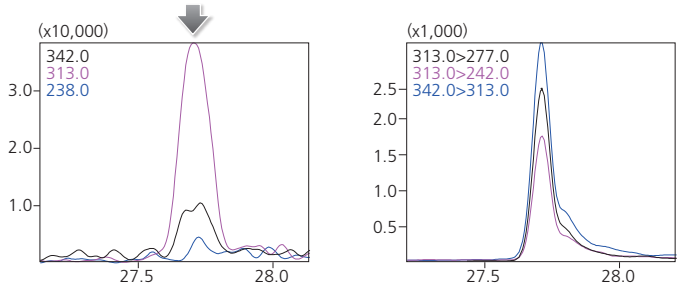
Clearer peak detection via high-sensitivity analysis

Blank Whole-Blood Sample



Clearer peak detection via high-separation analysis

Triazolam-Spiked
Whole-Blood Sample
(Concentration in whole blood: 50 ng/mL)



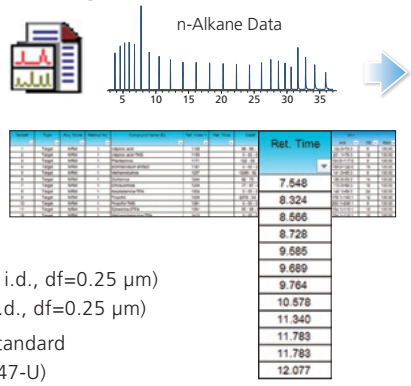
3. Creates Optimal MRM Methods Automatically

The Smart MRM program creates MRM methods automatically. In multicomponent simultaneous analysis, it is difficult to configure the dwell, event, and loop time-measurement settings in the MRM program. Smart MRM, however, automatically determines the optimal time-measurement settings, and creates a high-sensitivity method. The MRM method is created based on the retention time information for target compounds, using the AART function.

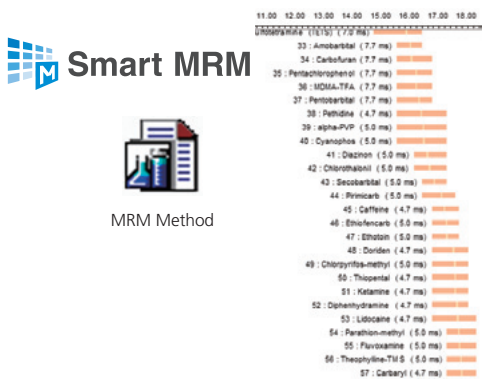
MRM Method Creation Steps Using Smart Forensic Database

1. Perform an n-alkane analysis.

2. Update the retention times using AART



3. Use Smart MRM to create the MRM method automatically.



Items Provided by the User

Analysis columns: Rxi®-5Sil MS (30 m, 0.25 mm i.d., df=0.25 µm)
Or DB-5ms (30 m, 0.25 mm i.d., df=0.25 µm)

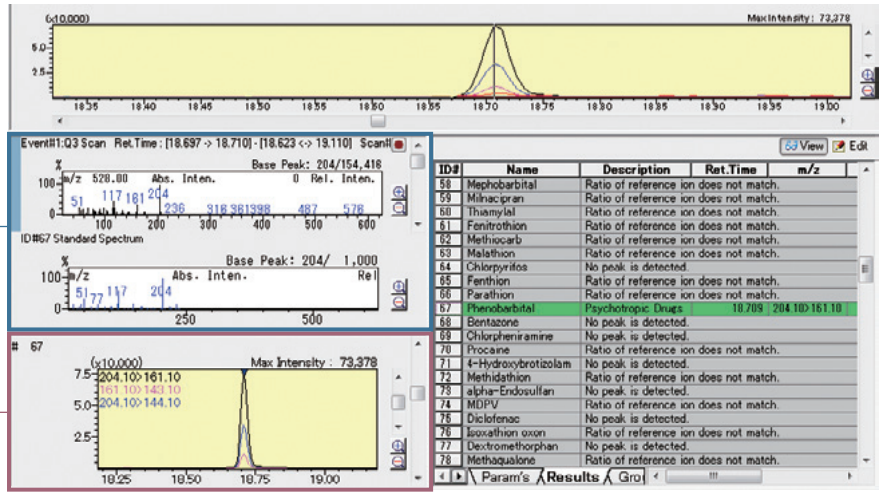
n-Alkane: C8-C40 Alkane Calibration Standard
(SIGMA-ALDRICH, Cat#: 40147-U)

4. Combination with the GC/MS Forensic Toxicological Database in Simultaneous Scan/MRM Measurement

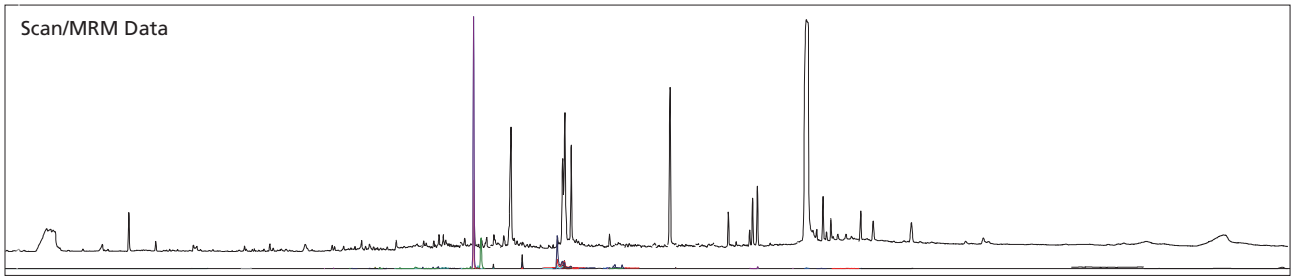
Scan data obtained with simultaneous Scan/MRM measurements can be analyzed using the GC/MS Forensic Toxicological Database, which is used to screen for forensic toxicological substances. MRM data can be used for trace quantity analyses of toxicological substances often involved in poisonings, which are registered in the Smart Forensic Database, while the scan data can be used to screen for drugs of abuse using the GC/MS Forensic Toxicological Database, which includes many designer drugs.

Improved Identification Reliability via Confirmation Using Scan Mass Spectrum

High-Sensitivity, High-Separation Detection via MRM Mass Chromatograms

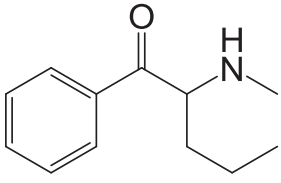


MRM Data + Smart Forensic Database

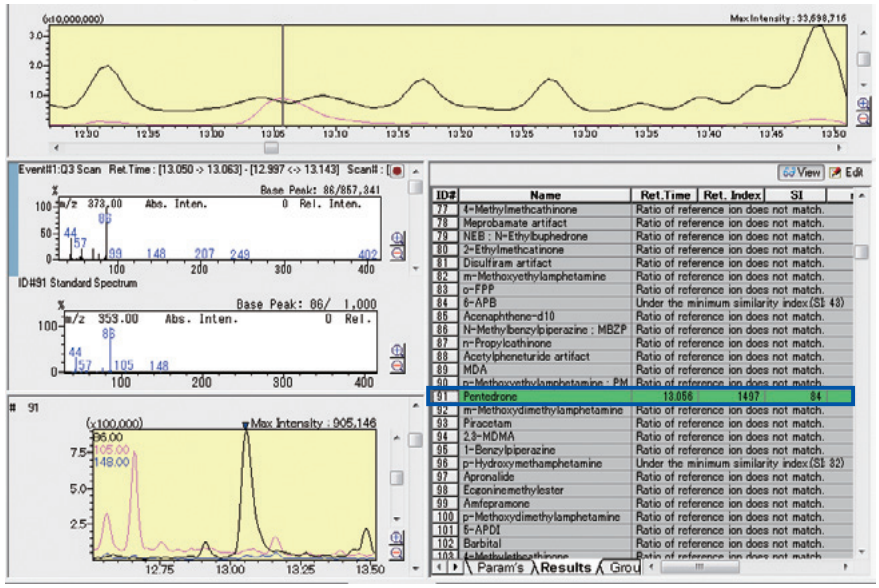


Scan Data + GC/MS Forensic Toxicological Database

Detection of Pentedrone



Pentedrone



Applicable Systems

GCMS-TQ8040, GCMS-TQ8030

Operating Environment

OS: Microsoft® Windows® 7 Professional

Excel: Microsoft® Excel® 2010 (32-bit version), Excel® 2013 (32-bit version)

Workstation software: GCMSsolution ver. 4.20 or later

Smart Forensic Database

Forensic Database for GC-MS/MS Analysis

Compounds Registered in Smart Forensic Database

Compound Name	Compound Name	Compound Name	Compound Name
Valproic acid	Diphenhydramine	Oxazolam-TFA	Heroin
Valproic acid-TMS	Lidocaine	Sertraline	Prazepam
Phentermine	Parathion-methyl	Haloxazolam-TFA	7-Acetamidoclonazepam-2TMS
Bromisovalum artifact	Fluvoxamine	Dosulepin	Permethrin-2
Methamidophos	Theophylline-TMS	Desmethylclotiazepam-TMS	Lormetazepam-TMS
Dichlorvos	Carbaryl	Fludiazepam	7-Aminoflunitrazepam-TMS
Ethosuximide	Mephobarbital	Cloxazolam-TFA	Nimetazepam
Amphetamine-TFA	Milnacipran	Carbosulfan	Lormetazepam
Propofol	Thiamylal	Clomipramine	7-Aminonimetazepam
Propofol-TMS	Fenitrothion	Lorazepam	Fentanyl
Ephedrine-2TFA	Methiocarb	RAZ-609-2TMS (Haloxazolam metabolite)	alpha-Hydroxymidazolam-TMS
Methamphetamine-TFA	Malathion	EPN	Olanzapine
Acephate	Chlorpyrifos	Bromazepam-TMS	7-Aminonitrazepam
Metolcarb	Fenthion	Ethylmorphine	3-Hydroxyprazepam
Ecgoninemethylester	Parathion	Diazepam	Flurazepam
Apronalide	Phenobarbital	Lorazepam-2TMS	Nitrazepam
Barbital	Bentazone	Quazepam	Zolpidem
Oxamyl	Chlorpheniramine	Flutazolam artifact	7-Aminoclonazepam
Isoprocarb	Procaine	Desalkylflurazepam	Clonazepam
XMC	4-Hydroxybrotizolam	Mofezolac	Hydroxyzine
Phenacetin-TMS	Methidathion	Morphine	JWH-203
Xylylcarb	alpha-Endosulfan	Furathiocarb	Estazolam
Ethenzamide	MDPV	THC	Alprazolam
Fenobucarb	Diclofenac	Ethyl loflazepate-TMS	Haloperidol
Propoxur	Isoxathion oxon	Chlorpromazine	Ethyl loflazepate
Acetaminophen-2TMS	Dextromethorphan	7-Aminonitrazepam-2TMS	Prochlorperazine
Allobarbital	Methaqualone	Clorazepic acid artifact	alpha-Hydroxyalprazolam-TMS
MDA-TFA	Isoxathion	Clotiazepam	Tofisopam
Bendiocarb	Amitriptyline	Nitrazepam-TMS	Etizolam
Acetaminophen	Trimipramine	Desmethyldiazepam	Triazolam
Phenacetin	Mianserin	Methotrimeprazine	Brotizolam
Tetramethylenedisulfotetramine (TETS)	Nortriptyline	Chlordiazepoxide artifact	alpha-Hydroxytriazolam-TMS
Amobarbital	Cocaine	6-Acetylmorphine	M-VI-TMS (Etizolam metabolite)
Carbofuran	Imipramine	7-Aminoflunitrazepam-TFA	Thioridazine
Pentachlorophenol	beta-Endosulfan	Clobazam	M-III-TMS (Etizolam metabolite)
MDMA-TFA	Primidone	Benfuracarb	Noscapine
Pentobarbital	Desipramine	Oxazolam	7-Acetamidoclonazepam
Pethidine	Medazepam	Paroxetine	LSD
alpha-PVP	Desalkylflurazepam-TMS	Zotepine	JWH-018
Cyanophos	5-MeO-DIPT	Mexazolam	alpha-Hydroxybrotizolam-TMS
Diazinon	M-4 (Quazepam metabolite)	Mexazolam-TMS	Yohimbine
Chlorothalonil	Desmethyldiazepam-TMS	Midazolam	Quetiapine
Secobarbital	Pentazocine	Delorazepam	M-II-TMS (Estazolam metabolite)
Pirimicarb	Promethazine	Flunitrazepam	Pericyazine
Caffeine	Biperiden	Flutoprazepam	M-II (Estazolam metabolite)
Ethiofencarb	Setiptiline	Clonazepam-TMS	Trazodone
Ethotoin	Endosulfan sulfate	Bromazepam	Spiperone
Doriden	Carbamazepine	Permethrin-1	Tadalafil
Chlorpyrifos-methyl	Maprotiline	7-Aminoflunitrazepam	Sildenafil
Thiopental	Oxazepam	Amoxapine	Vardenafil
Ketamine			

Remarks and Precautions

1. Shimadzu makes no warranty regarding the accuracy of information included in the database or the usefulness of information obtained from using the database.
2. Be sure to perform tests using standards to confirm qualitative and quantitative information obtained with the given system.
3. To reliably identify registered substances using this database, measure samples using the instrument parameters specified in the method template files included in the product.
4. This database is for research purposes. It cannot be used for clinical diagnostic applications.

Shimadzu Corporation
www.shimadzu.com/an/