

Forensic Database for GC-MS/MS Analysis

Smart Forensic Database Ver. 2

Serial	Type	Acq. Inst.	Method No.	Compound Name (E)	Ret. Index	Ret. Time	Case#	Comment	Type	m/z	CE	Ratio
1	Target	MRU	1	Valproic acid	1108		99-66-1	Psychotropic Drugs	T	102.0>73.0	6	100.00
2	Target	MRU	1	Valproic acid-TMS	1156		0-00-0	Psychotropic Drugs	T	201.1>75.0	12	100.00
3	Target	MRU	1	Phenamine	1171		122-09-8	Drugs of Abuse	T	134.0>117.0	9	100.00
4	Target	MRU	1	Bromodiphenyl ether	1181		0-00-0	Psychotropic Drugs	T	139.0>122.0	15	100.00
5	Target	MRU	1	Methamidophos	1237		10265-92-6	Pesticides	T	141.0>95.0	8	100.00
6	Target	MRU	1	Dichlorvos	1244		62-73-7	Pesticides	T	185.0>93.0	14	100.00
7	Target	MRU	1	Ethosuximide	1249		77-67-6	Psychotropic Drugs	T	113.0>69.0	15	100.00
8	Target	MRU	1	Amphetamine-TFA	1304		0-00-0	Drugs of Abuse	T	140.1>69.0	24	100.00
9	Target	MRU	1	Propoxy	1359		2078-64-8	General Drugs	T	178.1>163.1	12	100.00
10	Target	MRU	1	Propoxy-TMS	1391		0-00-0	General Drugs	T	260.1>235.1	9	100.00
11	Target	MRU	1	Ephedrine-2TFA	1391		50-98-6	Drugs of Abuse	T	164.1>110.1	12	100.00
12	Target	MRU	1	Methamphetamine-TFA	1413		0-00-0	Drugs of Abuse	T	154.1>110.1	12	100.00
13	Target	MRU	1	Acetamin	1450		30560-19-1	Pesticides	T	136.0>94.0	14	100.00
14	Target	MRU	1	Metolach	1462		1129-41-5	Pesticides	T	108.0>77.0	24	100.00
15	Target	MRU	1	Epoconazole	1500		106293-60-1	Drugs of Abuse	T	96.0>81.0	18	100.00
16	Target	MRU	1	Apronala	1503		528-92-7	Psychotropic Drugs	T	141.0>81.0	6	100.00

Supports Simultaneous Analysis of Forensic Toxicological Substances in Biological Samples Using GC-MS/MS

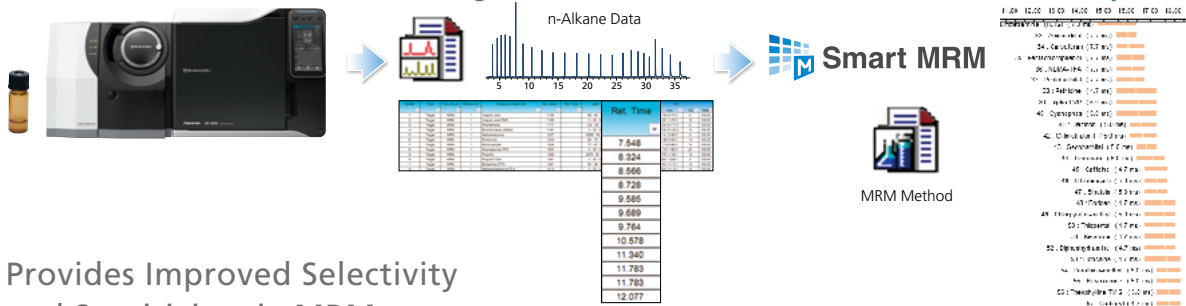
Smart Forensic Database™ is registered with information for MRM analysis of forensic toxicological substances often involved in poisonings, such as drugs of abuse, psychotropic drugs, pharmaceuticals and pesticides. The Smart Forensic Database enables simultaneous high-sensitivity analysis of approximately 480 compounds by adding information about 285 forensic toxicological substances. The database contains information on retention indices, MRM transitions, collision energies, and confirmation ion ratios, eliminating the 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.

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.

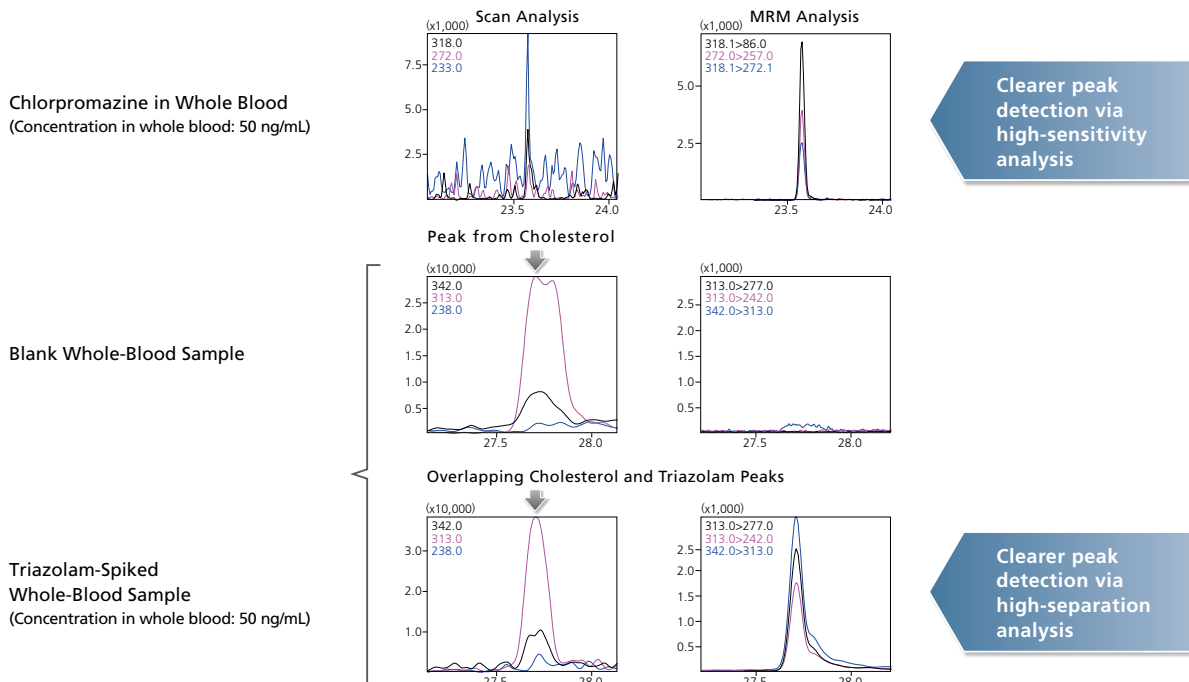
MRM Method Creation Steps Using Smart Forensic Database

1. Perform an n-alkane analysis.
2. Update the retention times using AART.
3. Use Smart MRM™ to create the MRM method automatically.



Provides Improved Selectivity and Sensitivity via MRM

With GC-MS/MS MRM mode, mass separation is performed in two stages. As a result, 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.

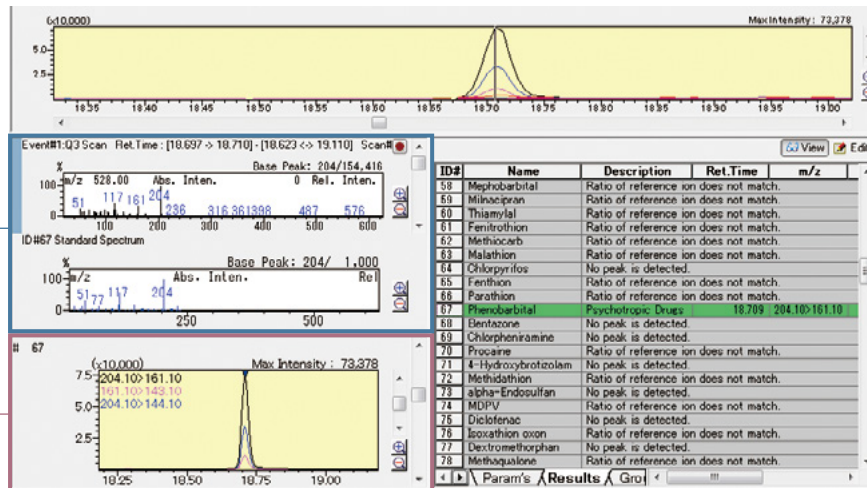


Combination with the GC/MS Forensic Toxicological Database in Simultaneous Scan/MRM Measurement

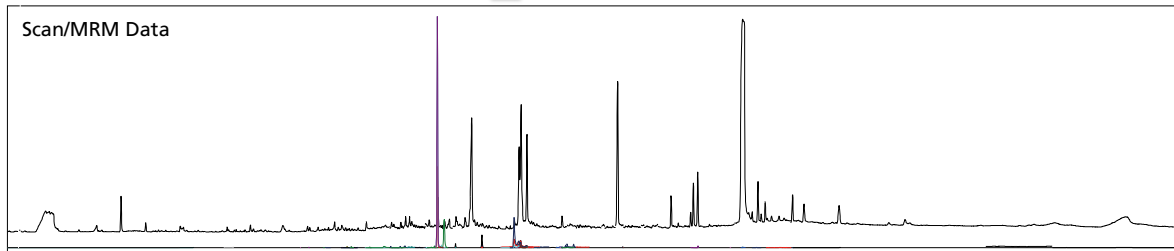
Scan data obtained with simultaneous Scan/MRM measurements can be analyzed using the GC/MS Forensic Toxicological Database, which is used to screen for forensic toxicological substances. MRM data can be used for trace quantity analyses of toxicological substances often involved in poisonings, which are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

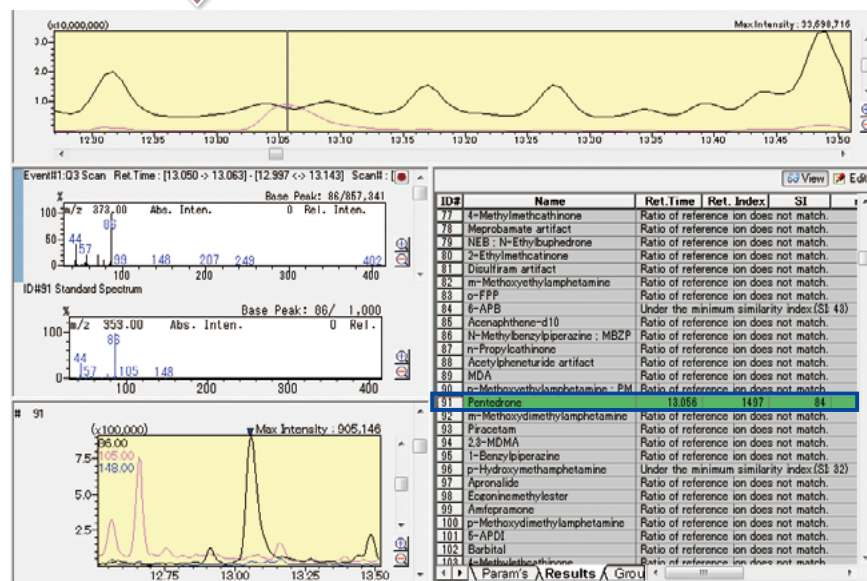
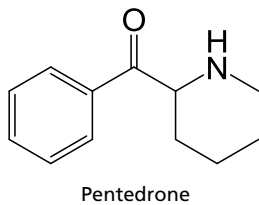


MRM Data + Smart Forensic Database



Scan Data + GC/MS Forensic Toxicological Database

Detection of Pentedrone



Specification

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

Derivatization classification	Number of registered compounds
Underivatized	418
TMS derivatized	59
TFA derivatized	9
Total	486

Configuration

Database file and method file

Applicable Systems

GC-MS: GCMS-TQ™ series

Operation environment

Workstation software: GCMSsolution™, LabSolutions™ DB GCMS, LabSolutions CS

Excel®: Microsoft® Excel® 2021, 2019 (32-bit, 64-bit editions)

Microsoft® Excel® 2016 (32-bit edition)

Recommended consumables

n-alkane: C8-C40 Alkanes Calibration Standard (Sigma-Aldrich)

Analysis columns: SH-I-5Sil MS (30 m, 0.25 mm i.d., df=0.25 μm, P/N 221-75954-30)

or DB-5ms (30 m, 0.25 mm i.d., df=0.25 μm)

Remarks and Precautions

1. The accuracy of the information contained in the database and the usefulness of information obtained as a result of the use of this information is not guaranteed.
2. Be sure to test the qualitative and quantitative information obtained with this system using a standard sample for confirmation.
3. To reliably identify substances registered with this database, perform measurement using the system requirements of the method template file included with the product.
4. GC/MS Forensic Toxicological Database is only available with GCMSsolution.

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