C146-E319B

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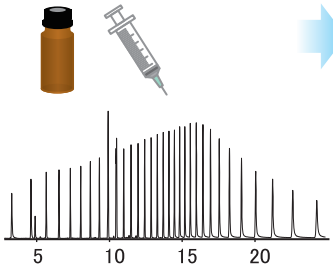
GC/MS/MS Forensic Toxicology Database

Quick-DB Forensic

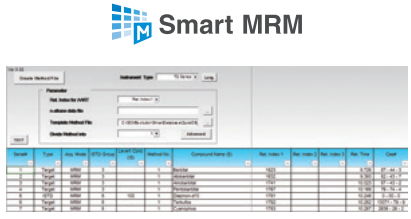
Provides a Total Solution for All Processes of Toxicological Analysis

Quick-DB™ Forensic is a GC/MS/MS database for forensic toxicological analysis that includes information for the sample preparation, analysis and data processing of 68 toxicological drug components common in toxicology cases. In combination with the GCMS-TQ™ series Gas Chromatograph-Mass Spectrometer, it provides a total solution for all analytical processes.
Due to the simple QuEChERS method used for the sample preparation, even first-time users can pretreat samples easily. In addition to analytical conditions, such as for optimized MRM transitions, the database also includes retention indices, calibration curve information, and other data processing conditions. The database also includes an automatic method creation function (Smart MRM™) for creating analytical methods easily. Due to the preexisting calibration curve information, semi-quantitative values can be calculated easily without using standards. Furthermore, it features a performance management function that automatically determines the system status. By using this function, users can quickly identify areas with low performance to ensure optimized performance throughout the analysis.

1 Analyze n-alkanes.



2 Automatically create an analytical method using Smart MRM.



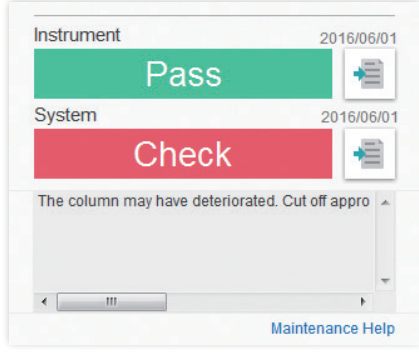
Smart MRM

3 Use the created analytical method for measurement.

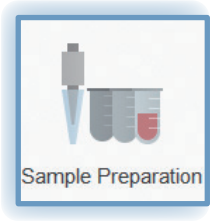
Simple-to-Operate Dedicated Software

The dedicated launcher displayed on-screen helps navigate the necessary operations. Therefore, even first-time users can analyze samples easily by simply following the instructions on the launcher.
During autotuning or when measuring performance check (negative control) samples, the software automatically uses a performance check function to check the status of the MS, consumable use times, and columns in order to evaluate the overall status of the system.

If specific control parameter criteria are not satisfied, the optimal steps for restoring the system status are displayed in a message box.

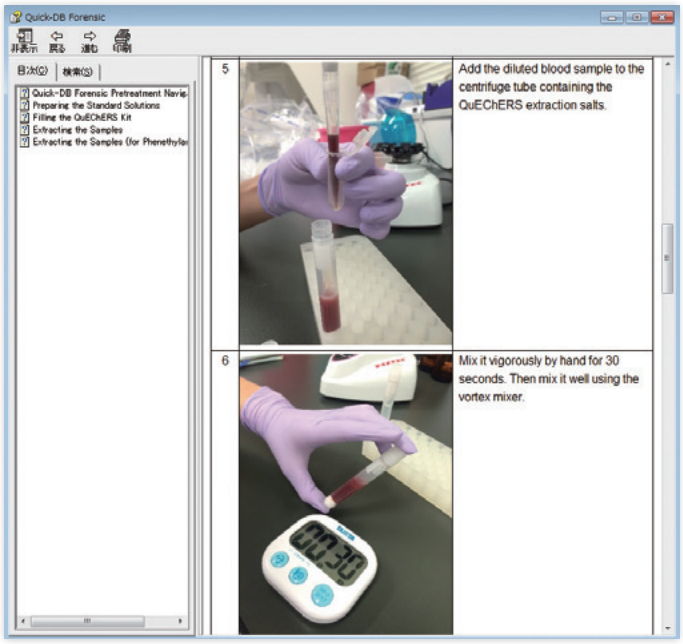


Quick-DB Forensic Launcher Screen



Navigates Appropriate Pretreatment Steps

For toxicological analysis of whole blood samples, the extraction and purification processes have been optimized using the QuEChERS method.
Preparing samples is simplified by using the Sample Preparation navigator to display photographs with instructions for each step of the QuEChERS cleanup process.



Sample Preparation Navigator

Collect a whole blood sample.

↓

Add the internal standards.

↓

Extract the sample using the QuEChERS method.

↓

Clean up the sample by dispersive solid phase extraction (dSPE).

↓

Concentrate and dry the sample.

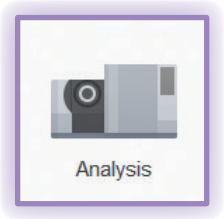
↓

Analyze the sample by GC/MS/MS.

Q-sep® QuEChERS extraction salts packet (Restek Corporation)

Q-sep QuEChERS cleanup kits (Restek Corporation)

Overview of QuEChERS Protocol

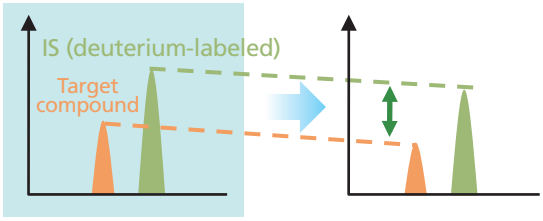


Achieve Analysis without Standards

To improve the accuracy of semi-quantitation without a standard, the internal standard that is selected and the recovery rate of sample preparation need to be considered. For internal standards, the Quick-DB Forensic database uses six types of deuterium-labeled toxicological substances that exhibit the same behavior as registered compounds. By using the calibration curve information from a whole blood sample spiked with a standard and pretreated, the quantitative error due to matrix interference, recovery rates of sample preparation, and other factors, which can have a significant effect on quantitative accuracy, can be reduced and accurate semi-quantitation values can be obtained without using a standard.

Using a Deuterium-Labeled Internal Standard to Correct for Sensitivity Variations

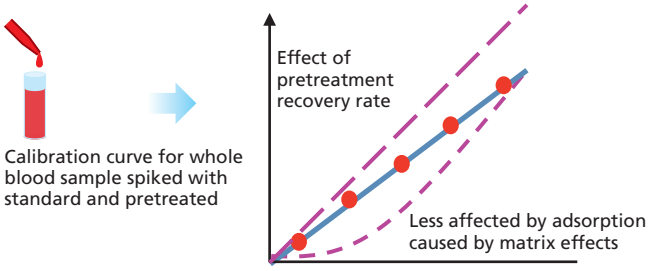
Deuterium-labeled internal standards can also be used to correct for GC-MS/MS sensitivity variations, even if the variations cause the response to target compounds in calibration curves to be different than in a customer's instrument.



Database Calibration Curve Customer's GC-MS

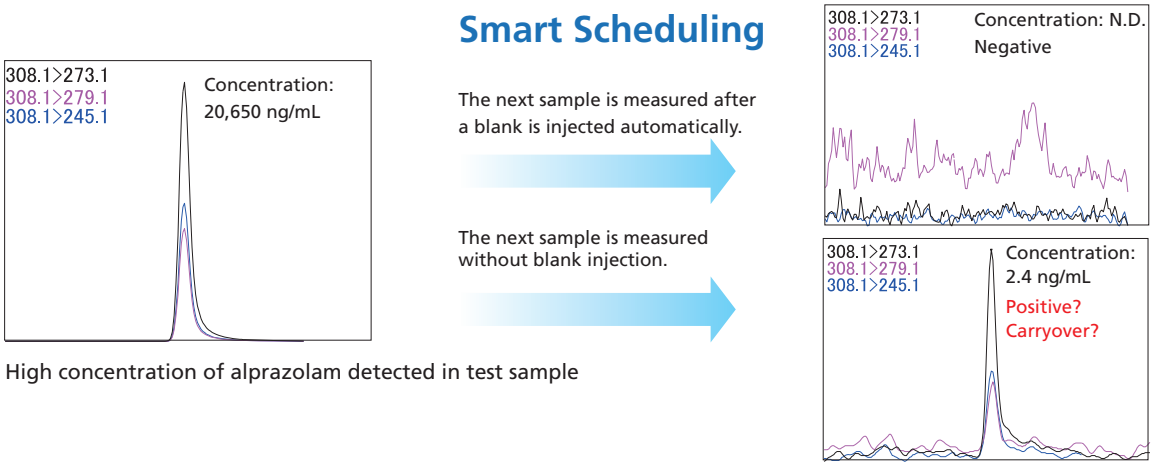
Using a Calibration Curve for a Pretreated Sample to Correct for Recovery Rates

By using the calibration curve information from a pretreated sample, accurate quantitative values can be obtained. The calibration curve information is used to correct differences in recovery rates for each target compound or correct for effects caused by adsorption, which occurs when creating calibration curves using standards.



Smart Scheduling Injects Blanks Automatically

If a high concentration of a target compound is detected in a test sample, carryover within the system may cause doubt about a false positive in the next test sample. If that occurs, the test sample is normally measured again to confirm the results. This may be an impossible task if only a small quantity of sample is available and pretreatment must be done.
Therefore, the Quick-DB Forensic database includes a Smart Scheduling function. This function automatically measures a solvent blank if the concentration of a target compound measured in a test sample is higher than a specified value. Smart Scheduling can prevent the risk of carryover causing a false positive.



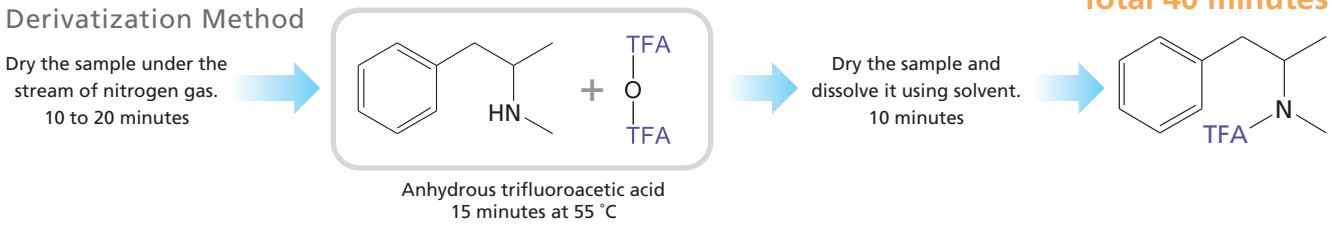
High concentration of alprazolam detected in test sample

Automates Time-Consuming Derivatization Processes*

Due to the limited amount of mass spectral information available for phenethylamine drugs, such as methamphetamine, MDA, and MDMA, as well as their tendency for adsorption, they are normally derivatized for measurement. The manual derivatization process requires significant time and can be difficult and lengthy. In contrast, the Quick-DB Forensic database enables on-column TFA derivatization using MBTFA (N-Methylbis-trifluoroacetamide). The test samples can be automatically TFA-derivatized and measured by simply placing the test samples and derivatizing agent in the auto-injector.

Manual TFA Derivatization Method

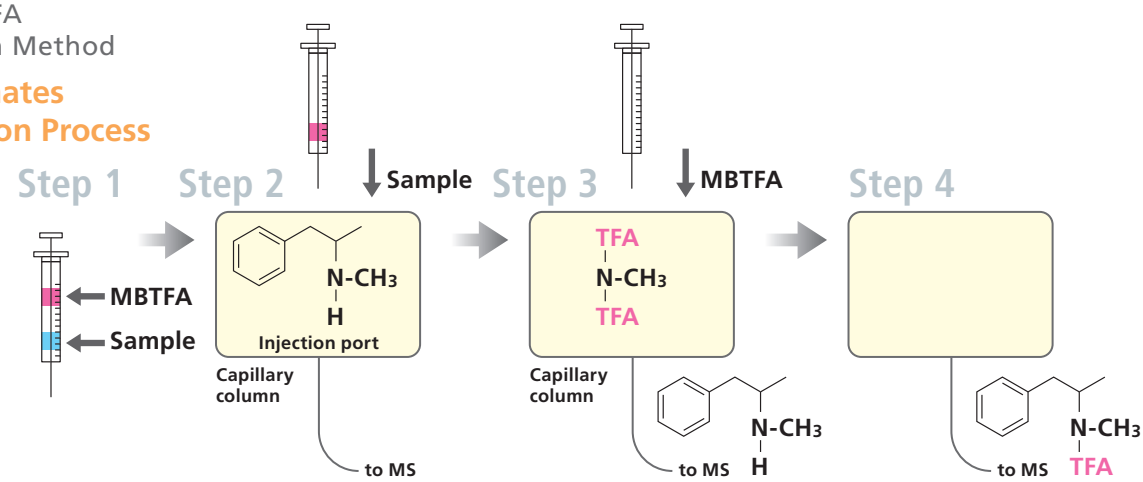
Total 40 minutes



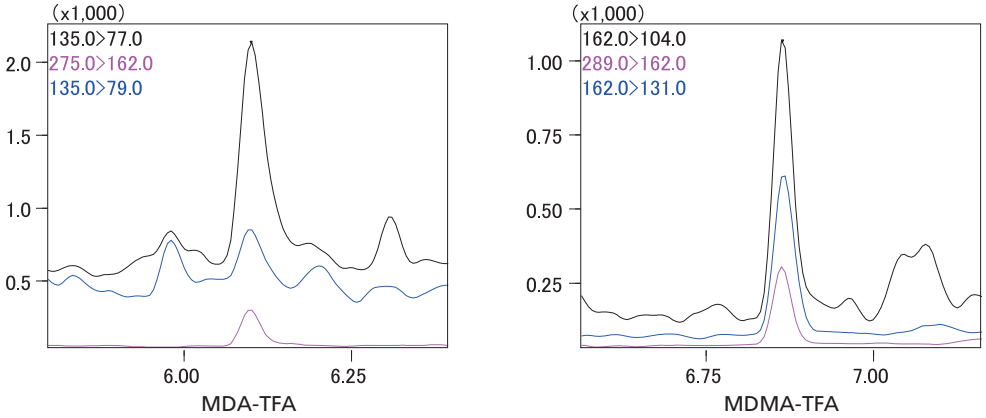
Anhydrous trifluoroacetic acid
15 minutes at 55 ˚C

On-Column TFA Derivatization Method

Fully Automates Derivatization Process

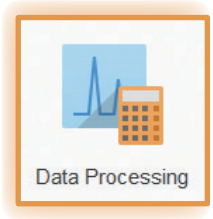


Step 1 An MBTFA derivatizing agent and test sample are successively aspirated into a syringe.
Step 2 The mixture is injected into the sample injection port. The sample is vaporized in the injection port and delivered to the capillary column.
Step 3 After waiting a few seconds for the target components to enter the capillary column, the MBTFA derivatizing agent is injected.
Step 4 The target components are derivatized inside the capillary column and then analyzed by GC-MS.



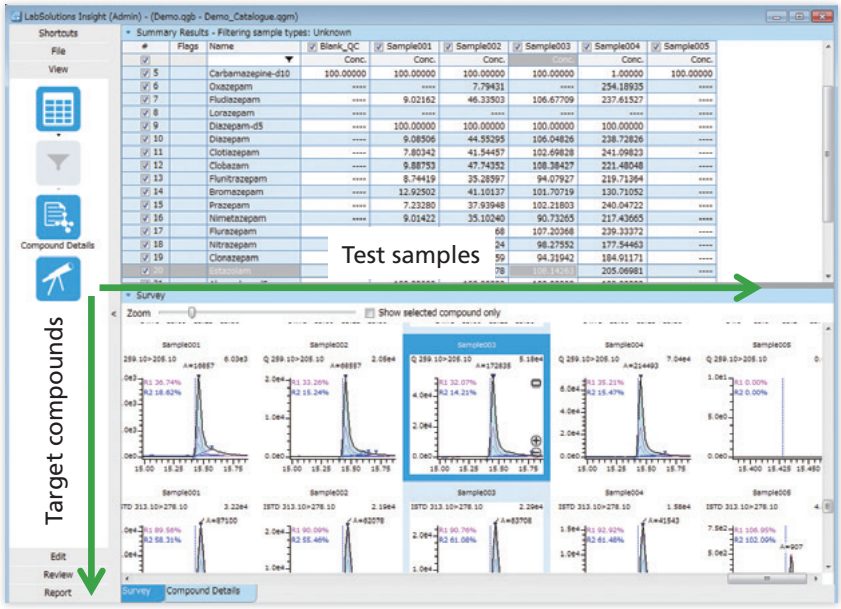
Mass chromatogram of phenethylamine drug (concentration: 10 ng/mL) added to whole blood sample

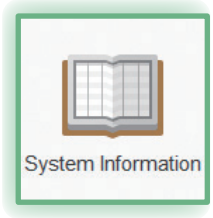
*AOC-20i and AOC-20s are required for this automation.



More Efficient Multianalyte Data Processing

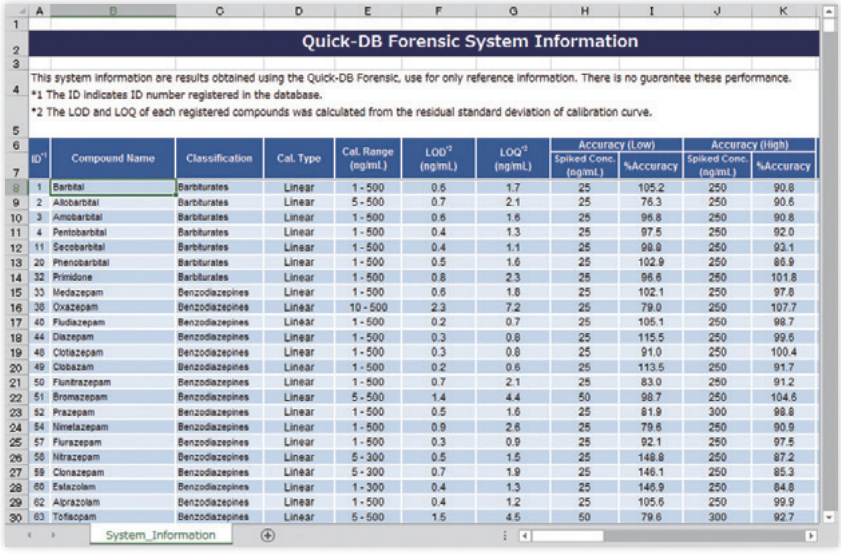
Quantitation results for a series of data sets can be displayed at the same time for data processing using LabSolution Insight. In addition, chromatograms for each test sample data can be displayed side-by-side for each target compound, making it easy to confirm semi-quantitation results.





Performance Information Obtained Using this System Can Be Confirmed

System performance results, such as the limit of detection (LOD), limit of quantitation (LOQ) and recovery of sample preparation, using this system are registered. The quantitation limit, pretreatment recovery rate, and other values for detected compounds can be confirmed as reference information.
If customer wants to increase the number of registered compounds, the information can also be registered.



Quick-DB Forensic System Information

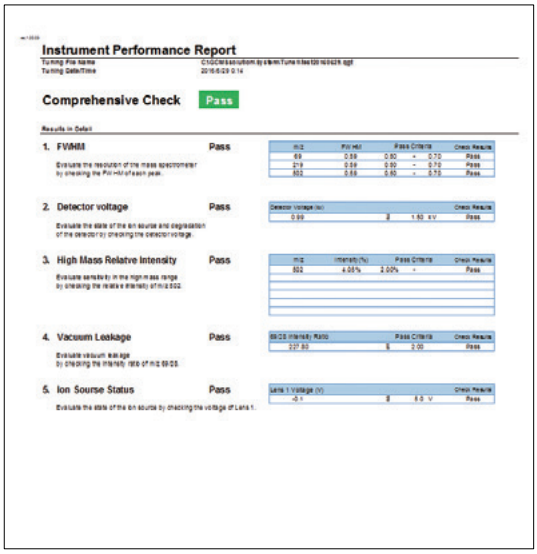
This system information are results obtained using the Quick-DB Forensic, use for only reference information. There is no guarantee these performance.
*1 The ID indicates ID number registered in the database.
*2 The LOD and LOQ of each registered compounds was calculated from the residual standard deviation of calibration curve.

ID*1	Compound Name	Classification	Cal. Type	Cal. Range (ng/mL)	LOD*2 (ng/mL)	LOQ*2 (ng/mL)	Accuracy (Low) Spiked Conc. (ng/mL)	Accuracy (Low) %Accuracy	Accuracy (High) Spiked Conc. (ng/mL)	Accuracy (High) %Accuracy
1	Barbital	Barbiturates	Linear	1 - 500	0.6	1.7	25	105.2	250	90.8
2	Allobarbital	Barbiturates	Linear	5 - 500	0.7	2.1	25	76.3	250	90.6
3	Amobarbital	Barbiturates	Linear	1 - 500	0.6	1.6	25	96.8	250	90.8
4	Pentobarbital	Barbiturates	Linear	1 - 500	0.4	1.3	25	97.5	250	92.0
11	Secobarbital	Barbiturates	Linear	1 - 500	0.4	1.1	25	98.8	250	93.1
20	Phenobarbital	Barbiturates	Linear	1 - 500	0.5	1.6	25	102.9	250	86.9
32	Primidone	Barbiturates	Linear	1 - 500	0.8	2.3	25	96.6	250	101.8
33	Medazepam	Benzodiazepines	Linear	1 - 500	0.6	1.8	25	102.1	250	97.8
38	Oxazepam	Benzodiazepines	Linear	10 - 500	2.3	7.2	25	79.0	250	107.7
40	Fludiazepam	Benzodiazepines	Linear	1 - 500	0.2	0.7	25	105.1	250	98.7
44	Diazepam	Benzodiazepines	Linear	1 - 500	0.3	0.8	25	115.5	250	99.6
48	Clotiazepam	Benzodiazepines	Linear	1 - 500	0.3	0.8	25	91.0	250	100.4
49	Clobazam	Benzodiazepines	Linear	1 - 500	0.2	0.6	25	113.5	250	91.7
50	Flunitrazepam	Benzodiazepines	Linear	1 - 500	0.7	2.1	25	83.0	250	91.2
51	Bromazepam	Benzodiazepines	Linear	5 - 500	1.4	4.4	50	98.7	250	104.6
52	Prazepam	Benzodiazepines	Linear	1 - 500	0.5	1.6	25	81.9	300	98.8
54	Nimetazepam	Benzodiazepines	Linear	1 - 500	0.9	2.6	25	79.6	250	90.9
57	Flurazepam	Benzodiazepines	Linear	1 - 500	0.3	0.9	25	92.1	250	97.5
58	Nitrazepam	Benzodiazepines	Linear	5 - 300	0.5	1.5	25	148.8	250	87.2
59	Clonazepam	Benzodiazepines	Linear	5 - 300	0.7	1.9	25	146.1	250	85.3
60	Estazolam	Benzodiazepines	Linear	1 - 300	0.4	1.3	25	146.9	250	84.8
62	Alprazolam	Benzodiazepines	Linear	1 - 500	0.4	1.2	25	105.6	250	99.9
63	Tofisopam	Benzodiazepines	Linear	5 - 500	1.5	4.5	50	79.6	300	92.7

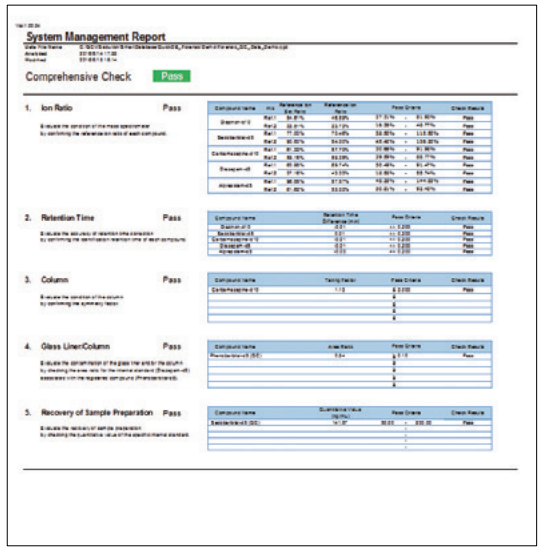
System_Information

Performance Report for Quickly Confirming System Status

System performance details displayed on the launcher in real time can also be output in specialized evaluation reports. Two performance management methods are used: one to evaluate instrument performance via MS tuning and the other to evaluate system performance by measuring the performance check sample. These two methods ensure any problems can be confirmed in an easy-to-understand manner.



Instrument Performance Report



System Performance Report

Specifications

■Product Contents

Quick-DB Forensic launcher program, database files, method files, batch files, report format files, and 2-step AOC control software

■Applicable Instruments

GC/MS	: GCMS-TQ series
Auto-injector	: AOC™-20i+s
Workstation	: GCMSsolution™ (Ver. 4.44 or later) + LabSolutions Insight™ (Ver. 2.0 SP1 or later)

■Required Parts and Reagents

Column	: SH-Rxi™-5Sil MS 30 m × 0.25 mm I.D., df = 0.25 µm (P/N 221-75954-30)
Pretreatment	: Q-sep QuEChERS extraction salts packet (AOAC 2007.01) (Restek Corporation P/N: 26238)
	: Q-sep QuEChERS cleanup kit (Restek Corporation P/N: 26424)
Internal standard substance	: Alprazolam-D5 (SIGMA-ALDRICH, Cat: A-902-1ML)
	Diazepam-D5 (SIGMA-ALDRICH, Cat:D-902-1ML)
	Carbamazepine-D10 (SIGMA-ALDRICH, Cat:C-094-1ML)
	Secobarbital-D5 (SIGMA-ALDRICH, Cat:S-001-1ML)
	Diazinon-D10 (SIGMA-ALDRICH, Cat:74332-5MG)
	Phenobarbital-D5 (SIGMA-ALDRICH, Cat:P-018-1ML)
	1-Methyl-3-phenylpropylamine (SIGMA-ALDRICH, Cat:M70533-25G)
n-Alkane Standard	: C8-C40 Alkanes Calibration Standard (SIGMA-ALDRICH, Cat: 40147-U)
TFA derivatizing agent	: MBTFA

In addition, general pretreatment equipment, such as a centrifuge, is also required.
This product was developed jointly with the Department of Legal Medicine & Bioethics, Nagoya University Graduate School of Medicine.

List of Compounds (68 target compounds, six internal standard compounds, and two QC compounds)

Compound	Classification
Allobarbital	Barbiturates
Amobarbital	Barbiturates
Barbital	Barbiturates
Pentobarbital	Barbiturates
Phenobarbital	Barbiturates
Primidone	Barbiturates
Secobarbital	Barbiturates
Alprazolam	Benzodiazepines
Bromazepam	Benzodiazepines
Brotizolam	Benzodiazepines
Clobazam	Benzodiazepines
Clonazepam	Benzodiazepines
Clotiazepam	Benzodiazepines
Diazepam	Benzodiazepines
Estazolam	Benzodiazepines
Etizolam	Benzodiazepines
Fludiazepam	Benzodiazepines
Flunitrazepam	Benzodiazepines
Flurazepam	Benzodiazepines
Medazepam	Benzodiazepines
Nimetazepam	Benzodiazepines
Nitrazepam	Benzodiazepines
Oxazepam	Benzodiazepines
Prazepam	Benzodiazepines
Tofisopam	Benzodiazepines
Triazolam	Benzodiazepines
Acetylfentanyl	Drugs of Abuse
Cocaine	Drugs of Abuse
Diphenidine	Drugs of Abuse
Fentanyl	Drugs of Abuse
JWH-018	Drugs of Abuse
JWH-122	Drugs of Abuse
JWH-210	Drugs of Abuse
Ketamine	Drugs of Abuse
MAM2201	Drugs of Abuse
THC	Drugs of Abuse
Butamifos	Pesticides
Chlorpyrifos	Pesticides
Coumaphos	Pesticides
Cyanophos	Pesticides
Diazinon	Pesticides
Edifenphos	Pesticides
EPN	Pesticides
Etrimfos	Pesticides
Fenitrothion	Pesticides
Fenthion	Pesticides
Iprobenfos	Pesticides
Isofenphos	Pesticides
Isoxathion	Pesticides
Malathion	Pesticides
Methidathion	Pesticides
Phosalone	Pesticides
Terbufos	Pesticides
Amphetamine-TFA	Phenethylamines
MDA-TFA	Phenethylamines
MDMA-TFA	Phenethylamines
Methamphetamine-TFA	Phenethylamines
Sertraline	SSRI
Amitriptyline	Tri/Tetracyclics
Carbamazepine	Tri/Tetracyclics
Chlorpromazine	Tri/Tetracyclics
Clomipramine	Tri/Tetracyclics
Imipramine	Tri/Tetracyclics
Mianserin	Tri/Tetracyclics
Nortriptyline	Tri/Tetracyclics
Promethazine	Tri/Tetracyclics
Thioridazine	Tri/Tetracyclics
Trimipramine	Tri/Tetracyclics
1-Methyl-3-phenylpropylamine-TFA	ISTD
Alprazolam-d5	ISTD
Carbamazepine-d10	ISTD
Diazepam-d5	ISTD
Diazinon-d10	ISTD
Secobarbital-d5	ISTD
Phenobarbital-d5 (QC)	QC
Secobarbital-d5 (QC)	QC

Note

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.Quantitative information obtained using this system are quantitative values determined without using standard samples. To calculate more accurate quantitative values, be sure to perform tests using a standard sample.

3.To reliably identify substances registered with this database, perform measurement using the system requirements of the method file included with the product.

4.This database is intended for research purposes. It cannot be used for clinical diagnostic applications.

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