SHIMADZU
Excellence in Science

GC/MS Forensic Toxicology Screening System

Taking GC-MS to the Limit

GCMS-QP2010 Ultra

Gas Chromatograph Mass Spectrometer

Applications

1. Identification of abused drugs such as stimulants, narcotics and other illegal drugs
2. Detection and semi-quantitation of compounds related to poisoning incidents

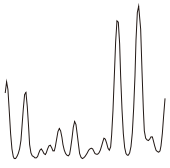
Features

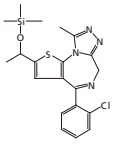
1. Optimized forensic and toxicology analysis method enables high-sensitivity scan measurement for simultaneous multi-compound analysis.
2. Retention time prediction function can estimate the retention times of target compounds without standards.
3. 1011 mass spectra of toxicology-related compounds, such as drugs of abuse, psychotropic drugs, and pesticides, are registered in the library. The semi-quantitation function can provide a rough quantitation result for compounds detected at poisoning incidents.
4. Deconvolution program enables quick data analysis.

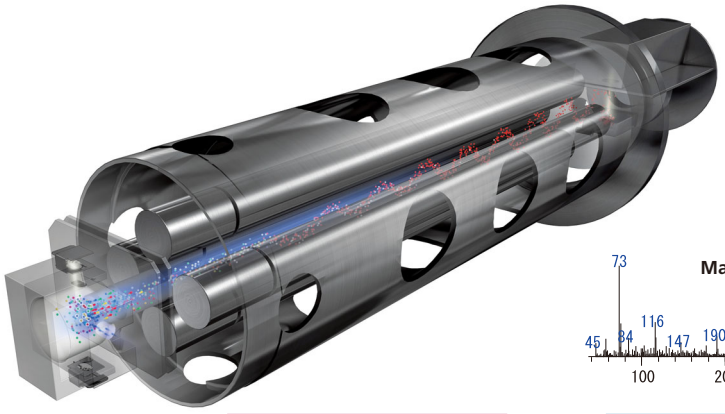
1. High-Speed Scanning for Simultaneous Multi-Compound Analysis

Pretreatment of unknown compounds

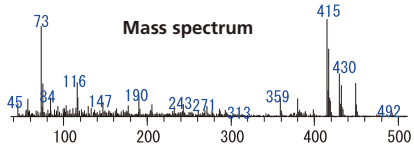
To GC-MS







Scan data acquisition for comprehensive measurement of fragment ions

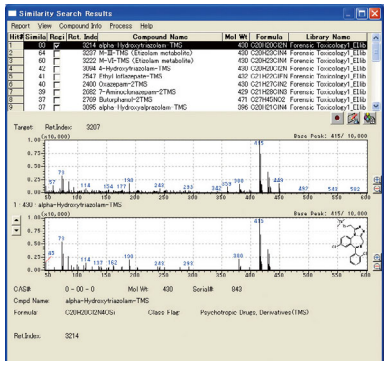


Reference with library

The Scan data acquisition method is traditionally used for GC/MS toxicology analysis. It is the common method for identifying illegal drugs and unknown poison compounds. Shimadzu's GC/MS forensic toxicology screening system optimizes all of the data acquisition analysis settings for improved identification of compounds.

1. EI mode generates fragment ions specific to the compound
2. Scan data acquisition method enables a mass spectrum, which is effective for identification of unknown compounds, to be obtained

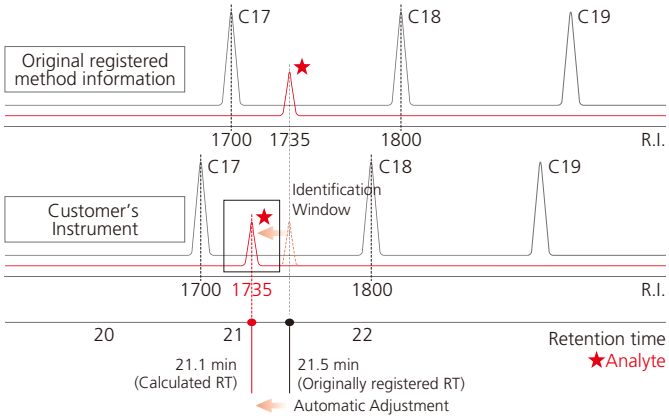
   (Comprehensive compound detection is possible without limiting the numbers of target compounds as compared to the selective ion measurement mode.)
3. Method file registers optimized GC conditions and compound information, such as retention indices
4. Specialized mass spectral toxicology library can be used simultaneously with general libraries



*** Please confirm qualitative and quantitative results through separate analysis using a standard mixture.**

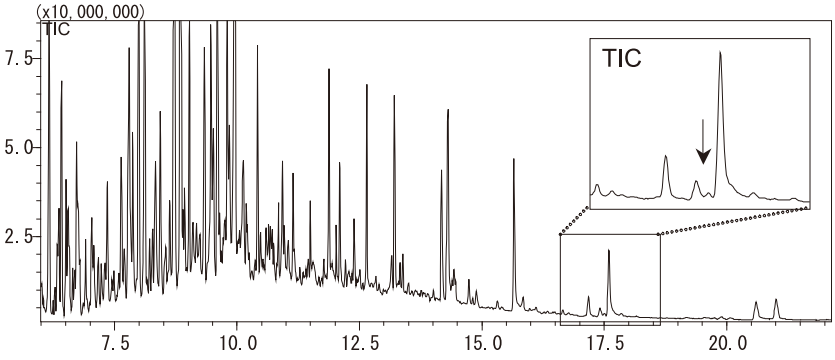
2. Identification Without Standards is Possible Using Retention Times

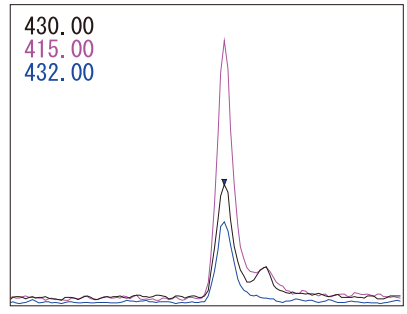
GCMSsolution Version 2.6 workstation software for GCMS-QP2010 Ultra provides versatile functionality using retention indices. For instance, searching the library using both retention indices and a mass spectrum, in combination with the AART (Automatic Adjustment of Retention Time) function, which estimates the retention times of target compounds, makes identification easier.



Compounds' retention indices and mass spectrums are registered in a method file. The AART function can estimate the retention times of target compounds accurately. The identification window (time range of the predicted retention time) provides quick and instant confirmation of the registered compounds.
Retention time adjustment can cover many points, from low to high boiling points, so accurate adjustment is possible over a wide range using an alkane standard mix.

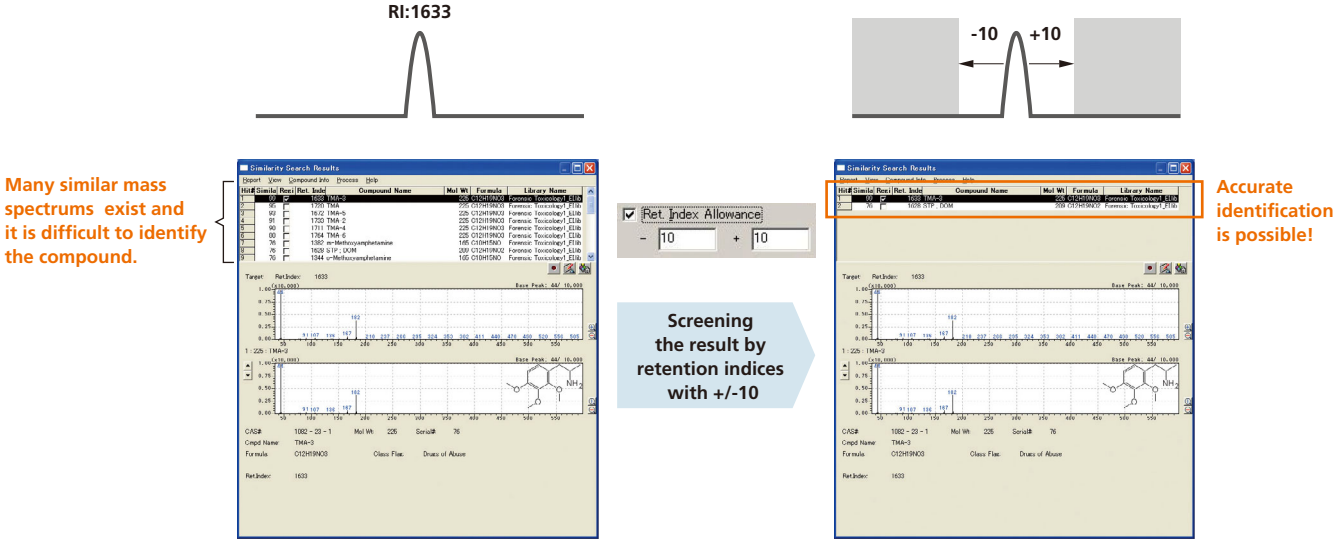
Analysis example of urine sample





Alpha-Hydroxytriazolam-TMS detection

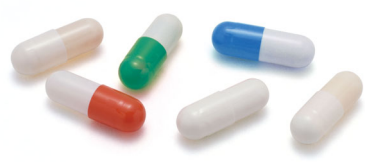
The above figure illustrates the measurement result of a urine sample using the database method. Confirming the peak at TIC is difficult, but alpha-hydroxytriazolam-TMS can be identified from the retention time predicted by AART and multiple *m/z* mass chromatograms registered in the method file.



Retention indices are registered in a mass spectral library. When compounds have similar mass spectral patterns, it may be difficult to identify target compounds by the degree of similarity.
GCMSsolution Ver. 2.6 software allows mass spectral similarity search using retention indices, resulting in more effective identification of target compounds.

3. Comprehensive Database Covers a Variety of Forensic and Toxicology-related Compounds

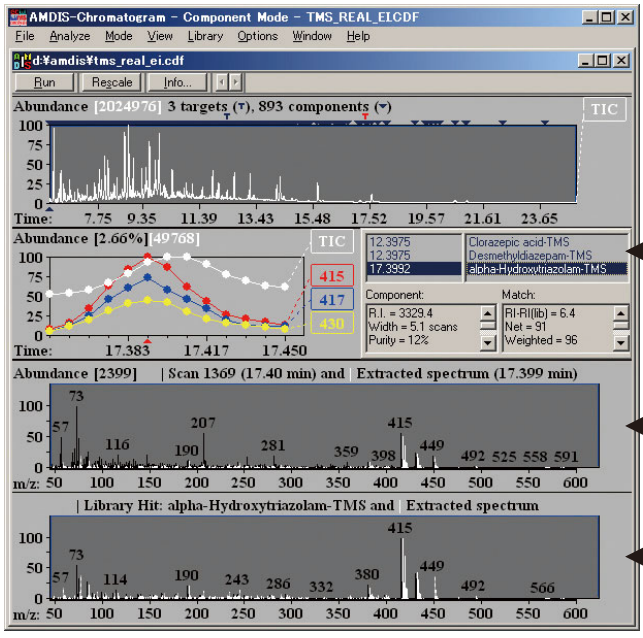
The Database contains 1011 spectra for 502 forensic and toxicology-related compounds, such as drugs of abuse, psychotropic drugs, general drugs, and pesticides, etc., including their free-, TMS-, and TFA-body types*.
The information registered in the analysis method file and mass spectral library can be used for identification of target compounds from retention times and mass spectra.
For compounds detected at poisoning incidents, the response factors related to internal standards are also registered and simple estimation of the quantitation value is possible.**



Category I	Spectral numbers	Category II	Spectral numbers
Drugs of Abuse	591	Free-body	208
		TMS-body	204
		TFA-body	179
Psychotropic Drugs	274	Free-body	156
		TMS-body	111
		TFA-body	7
General Drugs	110	Free-body	52
		TMS-body	58
Pesticides	36	TFA-body	36

*** : TMS-body is trimethylsilyl derivative and TFA-body is trifluoroacetyl derivative.**
****: The quantitation value may differ from the true value depending on instrument conditions and temperature. Please confirm the quantitative result through separate analysis using a standard mixture.**
When performing quantitative analysis, use solvent flush mode, which features simultaneous injection of sample solution and internal standard substances. When using solvent flush mode, be sure to combine the AOC-20i autoinjector with the AOC-20s autosampler.

4. Deconvolution Program Enables Quick Data Analysis



The mass spectral library contained in the database can be used as a library for AMDIS program analysis provided by NIST. The AMDIS program allows the identification of target compounds and the discovery of unknown components using a mass spectrum deconvolution function.
(The NIST Library must be purchased separately.)

Display a compound searched by AMDIS.

Display a mass spectrum where deconvolution is processed.

Compare with the mass spectrum registered in the library.

Mass spectral library in database → **Conversion** → **AMDIS deconvolution analysis library**

Additional registration is also possible.

In addition to the mass spectra and compound information registered in the library, the retention indices are also converted. Identification parameters in AMDIS using the retention indices can be used, resulting in more accurate automatic searches.

System Configuration and Measurement Parameters

GCMS-QP2010 Ultra

N-alkane
(C7-C13)

GC/MS Forensic
Toxicological Database

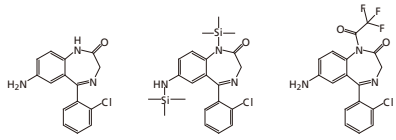
Inactivated splitless
wool insert (5 pcs.)

GC-MS	:GCMS-QP2010 Ultra
Workstation	:GCMSsolution Ver. 2.6
Injection port temp.	:260 °C
Carrier gas	:Constant linear velocity (45.6 cm/sec, He)
Column	:DB-5ms or Rxi® -5Sil MS (30 m x I.D 0.25 mm, df=0.25 µm)
Column temp.	:60 °C (2 min) - (10 °C/min) - 320 °C (10min)
Interface temp.	:280 °C
Ion source temp.	:200 °C
Measurement mode	:Scan
Injection volume	:1 µL
Insert	: Inactivated splitless wool insert (P/N: 221-48876-03)

Operation Procedure

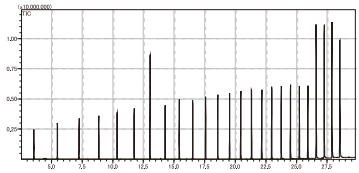
Step:01

Components are extracted from a urine or blood sample. The components undergo TMS- and TFA-derivatization if needed.



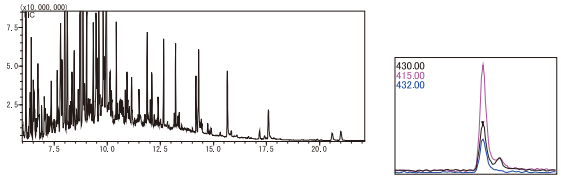
Step:02

Simple retention time adjustment is possible using n-alkane data measured in advance and the AART function.



Step:03

GC/MS analysis is conducted using a method downloaded from the GC/MS Forensic Toxicological Database. In the method, mass information of the monitored chromatogram (for both quantitation ion and confirmation ion) is registered and easy compound identification is possible.



Precautions:

1. The accuracy of information in the database and of the information value obtained from the analysis result is not guaranteed.
2. Confirm the qualitative and quantitative data obtained by this system through separate analysis using a standard mixture.
3. Analyze data in accordance with the instrument conditions of the method template file contained in this product in order to precisely identify registered compounds using this database.

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