SHIMADZU

Application News

Gas Chromatography Mass Spectrometry No.M266A

GC/MS Forensic Toxicological Database (Part 2)

■ Introduction

In recent years, abuse of stimulants and other illegal drugs, particularly hallucinogens, shows no signs of abating; crime and poisoning events due to medicines, agricultural chemicals, and psychotropic drugs are on the increase, presenting a growing and serious social problem. In crime laboratories and forensic research laboratories, these chemicals are analyzed using a gas chromatograph mass spectrometer (GC-MS).
The detection of these harmful drugs by GC-MS requires investigation to determine the optimum analytical conditions and data processing conditions specific to each of the drugs. To eliminate the need to conduct these cumbersome operations, Shimadzu has developed its own proprietary "GC/MS Forensic Toxicological Database," which contains critical information for more than 1000 drugs*, including psychotropic drugs, narcotics, stimulants, and pesticides. With emphasis on harmful drugs of abuse, difficult-to-obtain standard samples of these drugs and their metabolites are registered in the library, making the library ideal for forensic toxicological analysis. In addition, the database contains a library of mass spectra, method files containing the names, quantitation and reference ions, standard mass spectra, and retention indices specific to each of these drugs of abuse.
Here we introduce quick and easy techniques for detecting and conducting semi-quantitation of harmful drugs using method files.

* Includes derivatized compounds.

■ Content of Forensic Toxicological Method Files

Fig. 1 shows a view of the information contained in the GC/MS Forensic Toxicological Database, including chemical names, quantitation and reference ions, standard mass spectra, and retention indices. Furthermore, relative response factors are also included for specific toxic substances, which can be used to calculate rough estimates of their concentrations in real-world samples.

ID#	Name	Ret.Time	Ret. Index	m/z	Ref.Ions	STD Spec
300	Promethazine	21.363	2319	72.00	284.00-213.00	Registered
301	Biperiden	21.397	2323	98.00	218.00-112.00	Registered
302	Benzalkonium chloride art	21.414	2325	134.00	91.00-317.00	Registered
303	5-MeO-DALT	21.414	2325	110.00	270.00-160.00	Registered
304	5-MeO-DPT	21.414	2325	114.00	274.00-160.00	Registered
305	4-OH-DIPT	21.507	2336	114.00	260.00-146.00	Registered
306	6-MeO-DIPT	21.541	2340	114.00	160.00	Registered
307	Setiptiline	21.549	2341	261.00	217.00-202.00	Registered
308	Piroheptine	21.651	2353	288.00	303.00-215.00	Registered
309	Endosulfan sulfate	21.651	2353	272.00	387.00-274.00	Registered
310	Carbamazepine	21.693	2358	193.00	236.00-165.00	Registered
311	5-OH-DIPT	21.820	2373	114.00	160.00-146.00	Registered
312	Maprotiline	21.837	2375	277.00	203.00-191.00	Registered
313	Oxazepam	21.879	2380	269.00	239.00-268.00	Registered
314	Acetazolamide	21.913	2384	180.00	222.00-194.00	Registered
315	Profenamine	22.154	2413	100.00	180.00-312.00	Registered

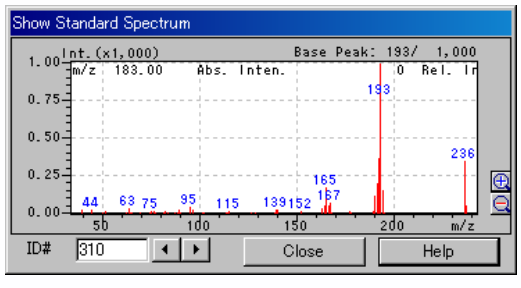

Fig. 1 Registered Information in Method File

Table 1 Analytical Conditions

Model	: GCMS-QP2010 Series
Workstation	: GCMSsolution Ver. 2.5 or later
Column	: DB-5 ms (30 m × 0.25 mm I.D. df = 0.25 µm) or Rxi®-5 Sil MS (30 m × 0.25 mm I.D. df = 0.25 µm)

-GC-		-MS-	
Column Temp.	: 60 °C (2 min)-10 °C/min-320 °C (10 min)	Interface Temp.	: 280 °C
Carrier Gas	: He (Constant Linear Velocity Mode)	Ion Source Temp.	: 200 °C
Linear Velocity	: 45.6 cm/sec	Scan Interval	: 0.3 sec
Injection Method	: Splitless		

■ Peak Detection Using Mass Chromatograms and Predicted Retention Time

Fig. 2 shows the screen used to analyze the data obtained from analysis of a drug-spiked urine sample using this method. When conducting actual analysis, it is very difficult to confirm the target peak associated with the drug of abuse because it is buried in the total ion current chromatogram (TICC), as shown in the upper part of the figure.
Use of this method file allows easy detection of the drug of abuse even in such cases of difficult-to-pinpoint target drug chromatographic peaks. First, the retention time of the target substance is predicted using the GCMSsolution AART (Automatic Adjustment of Retention Time) feature, based on the retention times of n-alkanes measured beforehand, in addition to the registered retention index for each of the toxic substances. Then, the target drug substance is detected from the mass chromatogram (shown at the lower left of Fig. 2) of the quantitation and reference ions in the vicinity of the predicted retention time. These operations can be performed using the automatic processing function of the GCMSsolution software. Moreover, the final result can be verified through comparison with the standard spectrum, which is registered in the method file; the standard spectrum is shown here in the middle tier.

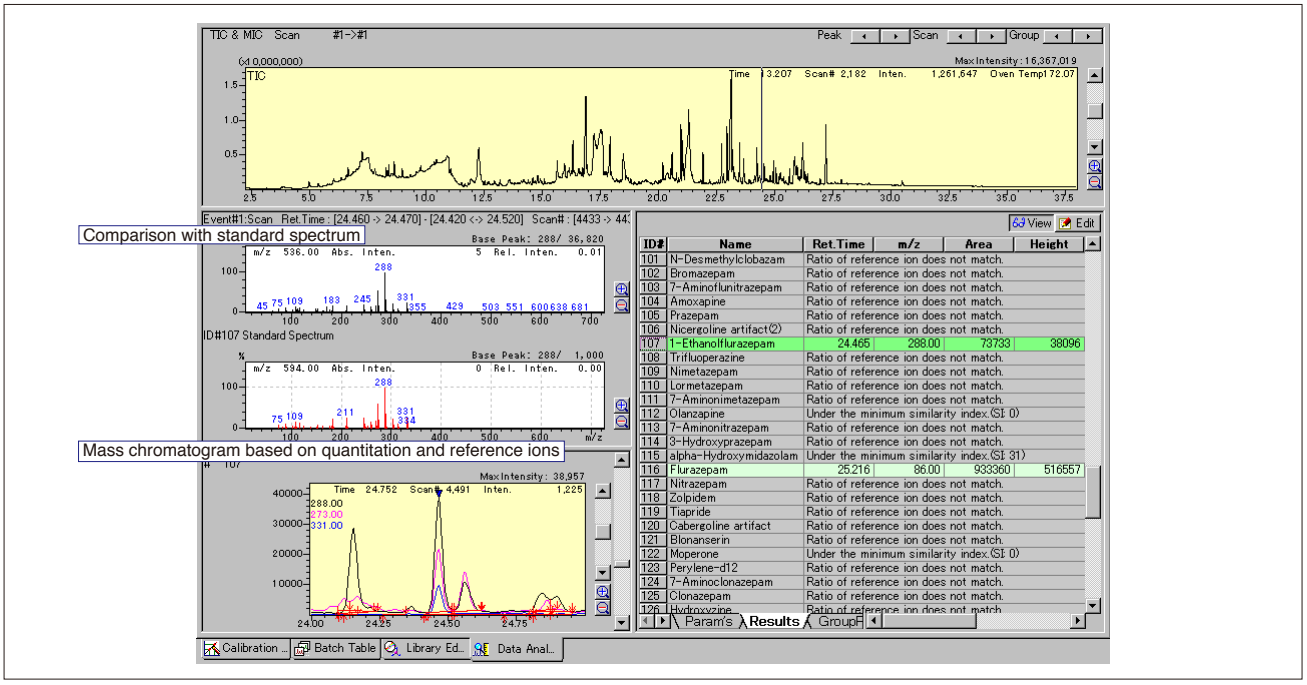

Fig. 2 Screen Capture of Data Processing Using GCMSsolution

■ Semi Quantitation-Calculation

This database method file contains relative response factors which are used for calculating semi-quantitative values for specific toxic drugs. As shown in Fig. 3, the drug concentration can be roughly calculated without generating a calibration curve.

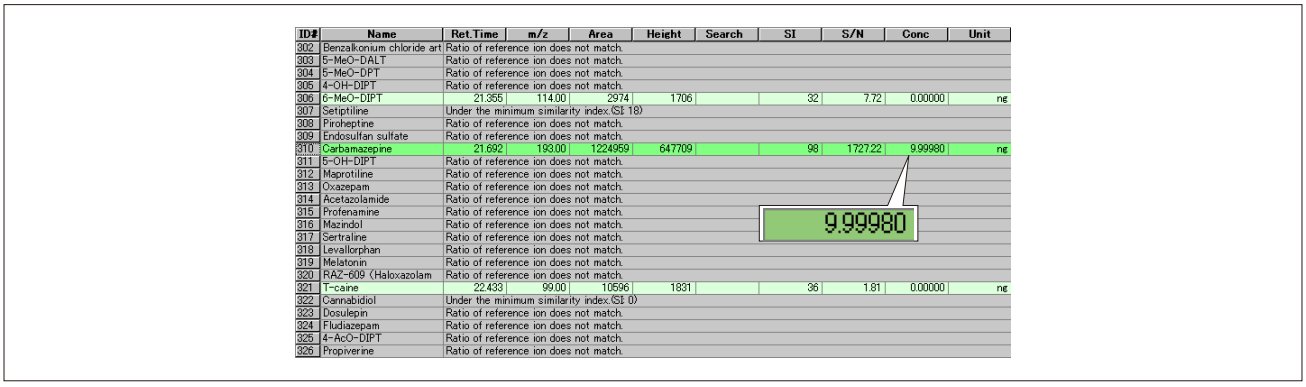

Fig. 3 Calculated Result Using Semi-Quantitation

■ Summary

The method file in the GC/MS Forensic Toxicological Database contains optimized analytical conditions, so toxic drug substances can be analyzed immediately. In addition, this method file contains various types of information for many toxic substances, permitting semi-quantitation values to be calculated from an automatically identified drug of abuse.

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