

Application News

Gas Chromatography Mass Spectrometry

No.M262

GC/MS Forensic Toxicological Database

■ 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 and agricultural medicines, including psychotropic drugs, are also on the increase, presenting a growing and serious social problem. In crime laboratories and forensic research laboratories at universities, these chemicals are analyzed using a gas chromatograph mass spectrometer (GC/MS).

The use of libraries of recorded retention indices and mass spectra is effective for identification and detection of these chemical substances. Shimadzu has developed its own proprietary "GC/MS Forensic Toxicological Database" containing more than 1000 retention indices and mass spectra for chemical

substances, including psychotropic drugs, narcotics, stimulants, and pesticides, including common derivatives. With emphasis on chemical substances of abuse, difficult-to-obtain standard samples of chemical substances and metabolites are registered in the database, making this library ideal for forensic toxicological analysis.

Moreover, method files containing compound information according to category are also included in this database, thereby eliminating such complicated tasks as investigating analytical conditions and settings.

This Application News introduces the usefulness of the forensic substance library in this GC/MS Forensic Toxicological Database.

■ Information Contained in Forensic Toxicological Database

The library in the GC/MS Forensic Toxicological Database contains not only mass spectra, but the retention indices obtained in analysis using the standard analytical conditions, as shown in Table 1. Additional information, including the compound name, CAS number, molecular weight, molecular formula and structural formula are also included.

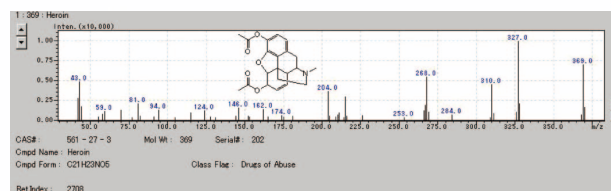


Fig. 1 Information Included for Registered Compounds

Table 1 Analytical Conditions

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

■ Effectiveness of Library Search Using Mass Spectra and Retention Indices

Since a typical library search is based solely on the mass spectrum, it is difficult to distinguish among compounds that present similar mass spectra, such as positional isomers and homologs. It is therefore not unusual for multiple compounds to be listed at higher

similarity indices in any given library search result. Using the GCMSsolution software (Ver. 2.5 or later), sorting of library match compounds can be conducted not only on the basis of mass spectrum, but on retention index as well.

Library Search for Isomers

Fig. 2(a) shows the results of a library search based on the data obtained from analysis of *m*-methoxyamphetamine. Since *o*-, *m*-, and *p*-isomers exist for methoxyamphetamine, these isomers appear in the library search results list with similarity indices of 90 or greater. Fig. 2(b) shows the search results in which the retention index (permissible width ± 10) is

added as a condition to the initial search conditions. It can be seen that there are no search results for the other (*o*- and *p*-) isomers, because these isomers elute outside the retention index window of ± 10 RI units. Thus, the reliability of the mass spectral library search result can be improved by using the mass spectrum together with the retention index.

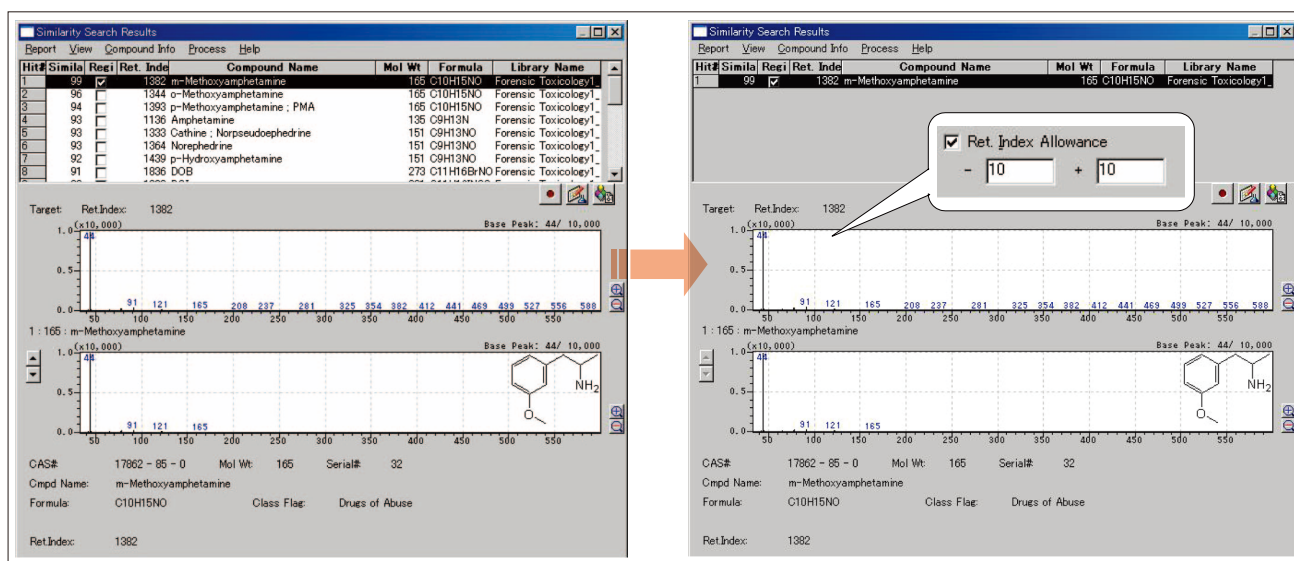


Fig. 2 Library Search Result for *m*-Methoxyamphetamine (a) Using only mass spectrum, (b) Using mass spectrum and retention index

Library Search for Phenethylamines

Fig. 3(a) shows the results of the library search based on data obtained in analysis of methamphetamine. Phenethylamines include many compounds that present similar mass spectra, and as in the isomer search results, many compounds appear in the search results list with similarity indices of 90 or greater. Fig. 3(b) shows the search results in which the retention index (permissible width ± 10) is added as a condition

to the initial search conditions, demonstrating that the compounds with a similarity index of 90 or greater are considerably diminished. These results show that not only in the case of isomers, but also when there are many compounds with similar mass spectra, highly reliable search results can be obtained by using a library search that combines retention index in the search conditions.

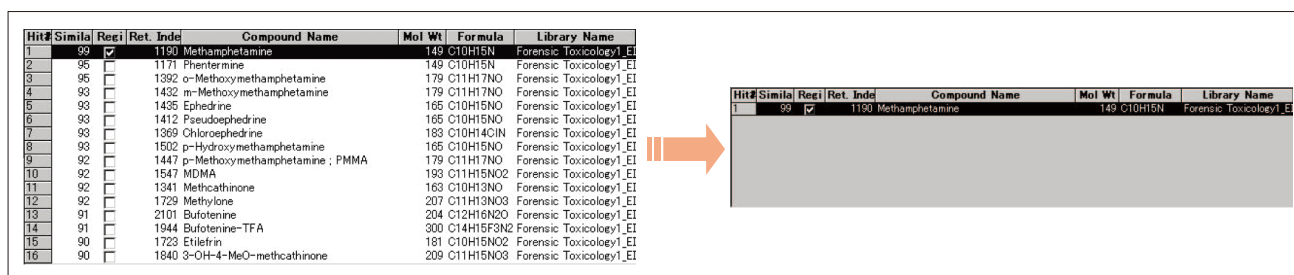


Fig. 3 Library Search Result for Methamphetamine (a) Using mass spectrum, (b) Using mass spectrum and retention index

Summary

The mass spectral library with retention indices of the GC/MS Forensic Toxicological Database is an effective library for identification of drugs of abuse. In particular, the ability to conduct identification using

retention indices is an effective means of distinguishing among compounds with similar mass spectra.



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