COMPOUND COMPOSER Database Software 2nd edition

GCMS-QP2010 Series Workstation Optional Software

Features

1. Rough quantitation values for hazardous chemicals can be confirmed without using a standard sample.
2. The retention times, mass spectra and calibration curves for 942 hazardous chemicals are registered in the database. In combination with the prediction of retention times using n-alkane, the database supports highly reliable compound identification.
3. Analysis and report generation are conducted using GCMSsolution for GCMS-QP2010 Series.

Applications

This system is effective for the following types of applications.

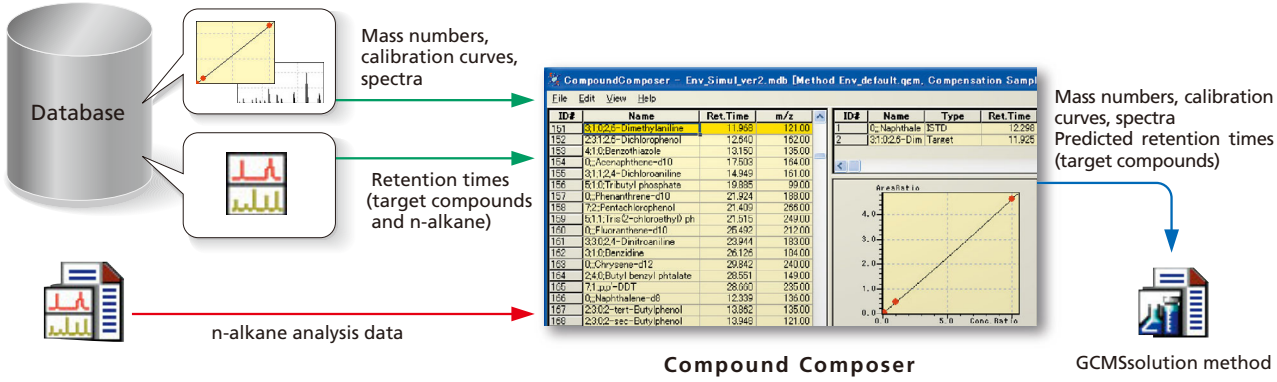
- For confirming the presence or the amount of both restricted and unrestricted hazardous chemicals.
- For grasping the approximate quantitation values of substances when difficult to obtain standard samples.
- For quick and easy identification and q uantitation of chemical substances in accidents and incidents.
- For prescreening substances to determine which substances should be quantitatively analyzed more precisely.

Compound Composer

Extract compound information from database for substance identification and quantitation

Compound Composer extracts the target mass numbers, mass spectra, calibration curves and other information required for quantitation of components of interest, and generates a GCMSsolution method. It also predicts the retention times of target components using the n-alkane retention time information in the database together with the n-alkane measurement data acquired under the instrumental conditions used for analysis, thereby enabling their identification and quantitation using GCMSsolution even without specifying other conditions. In addition, data on substances for verifying the instrument performance is also registered in the database, so that the GCMSsolution QA/QC function can be used to increase the reliability of identification and quantitation.

Category I	Number	Category II	Number
Compounds consisting of CH	194	Aliphatic compounds	31
		Benzenes	14
		Polycyclic compounds	79
		PCB	62
		Others	8
Compounds consisting of CHO	150	Ethers	11
		Ketones	6
		Phenols	50
		Phthalates	11
		Ester fatty acids	34
		Others	38
Compounds consisting of CHN (O)	113	Aromatic amines	43
		Quinoline	3
		Nitro compounds	42
		Nitrosoamines	5
		Others	20
Compounds consisting of CHS (NO)	12		12
Compounds consisting of CHP	8	Phosphoric esters	8
PPCPs	14		14
Pesticides	451	Insecticides	184
		Herbicides	118
		Fungicides	116
		Others	33
Total	942		942
Internal standard	8		



Compound Composer

Specifications

- **Applicable instrument** — **GCMS-QP2010 Series with GCMSsolution 2.21 or later**
- **Operation environment** — **Microsoft® Windows® XP Professional or Windows® 2000 Professional SP3 or greater**
  * If the OS is earlier than Windows 2000 SP3, please update the OS beforehand.
- **Product content** — **Database for Simultaneous Analysis (Environmental, 942 compounds), Compound Composer**

When using this database system, n-alkane, internal standard solutions and instrument performance evaluation substances must be obtained separately.

Cautions

1. Shimadzu makes no warranty regarding the accuracy of information included in the product or the usefulness of information obtained from using the product.
2. The database quantitation performance is adequate for screening if the GC/MS instruments including the column are appropriately adjusted. However, compared to the existing method in which a calibration curve is generated at the time of sample measurement, quantitation performance is inferior. For this reason, if strict quantitation results are required, be sure to measure a separately obtained standard solution, generate a calibration curve and then perform quantitation.
3. To identify registered substances with certainty using this database, conduct analysis using the instrument conditions in the method template file included with the product.
4. When analyzing compounds that easily adsorb or decompose, such as nitrogen-containing compounds, or carbamate or pyrethroid pesticides, quantitation results may differ greatly from the actual values depending on the conditions of the column and sample solution.
5. An analytical condition is fixed as follows,
   Column: DB-5ms [30m × 0.25mm I.D., df=0.25μm] J&W P/N 122-5532 Injection method: Splitless (Inj. Temp. 250°C, Sampling time 1.00 min)
   Carrier gas: He (Constant Linear Velocity mode: 40cm/sec) GC oven temperature program: 40°C (2min) → (8°C/min) → 310°C → (5min)

*** This system was jointly developed by Shimadzu and The University of Kitakyushu in Japan.**

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