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Application Data Sheet

No.80

GC-MS
Gas Chromatograph Mass Spectrometer

Analysis of PCBs and Organochlorinated Pesticides in River Water Using Simultaneous Scan/MRM Measurement in GC-MS/MS (3)

In recent years, incidents of the discharge of chemical substances have increased on a global scale, heightening demands for the identification of unanticipated chemical substances in order to investigate causes and take necessary measures. To this end, the Scan mode is effective as a means to accommodate as many chemical substances as possible, and to identify compounds from their mass spectral data.

The GCMS-TQ8030 GC-MS/MS system achieves simultaneous scan/MRM measurements using high-speed scan and high-speed MRM data acquisition technology.

This Application Data Sheet introduces an example of screening for environmental pollutants other than PCBs and chlorinated pesticides, which are targeted for MRM measurements, by applying Compound Composer Database Software to the scan data acquired in simultaneous scan/MRM measurements. Also introduced is an accurate trace quantitation analysis of PCBs and chlorinated pesticides with the MRM data acquired in simultaneous scan/MRM measurements in Application Data Sheets No. 78 and No. 79.

Compound Composer Database Software

Compound Composer Database Software consists of the Compound Composer software plus a database (environment) containing information on 942 environmental pollutants. The database is preregistered with information for the identification (retention indices and mass spectra) and semi-quantitation (internal standard corrected calibration curves) of each compound. Using the Compound Composer software, information on target compounds is extracted from the database, and method files are created for semi-quantitation.
The retention times for target compounds are simultaneously and reliably estimated, from low to high boiling points, using measurement data from an n-alkane standard mixture sample.

Since calibration curve information is stored in the database, it is possible to calculate the approximate concentrations (semi-quantitative values) by simply adding the internal standard substance to the sample and then taking measurements, without requiring a standard sample.

Table 1 shows the environmental pollutants contained in the database.

Table 1 Compounds Registered in the Database

Category 1	Num.	Category 2	Num.
Internal Standard	8		8
Compounds consisting of CH	194	Aliphatic Compounds	31
		Benzenes	14
		Polycyclic compounds	79
		PCB's	62
		Others	8
Compounds consisting of CHO	150	Ethers	11
		Ketones	6
		Phenols	50
		Phthalates	11
		Fatty acid esters	34
		Others	38
Compounds consisting of CHN(O)	113	Aromatic amines	43
		Quinoline	3
		Nitro compounds	42
		Nitrosoamines	5
		Others	20
CHS(NO)	12		12
CHP(NOS)	8	Phosphoric esters	8
*PPCP's	14		14
Pesticides	451	Insecticides	184
		Herbicides	118
		Fungicides	116
		Others	33
Total			942

*PPCP's: Pharmaceuticals and Personal Care Products

Experimental

For the river water pretreatment method, refer to Application Data Sheet No. 79. For the GC-MS/MS analysis conditions, refer to Application Data Sheet No. 78.

Results

Fig. 1 shows the scan total ion current chromatogram from the river water sample using simultaneous scan/MRM measurements, as well as mass chromatograms for typical environmental pollutants, detected using the Compound Composer Database Software. In addition, semi-quantitative results for the environmental pollutants detected are shown in Table 2. Using the Compound Composer Database Software, it was possible to identify and semi-quantitate 84 environmental pollutants, including the PPCPs (pharmaceuticals and personal care products) such as ibuprofen and pesticides such as fenobcarb and permethrin.

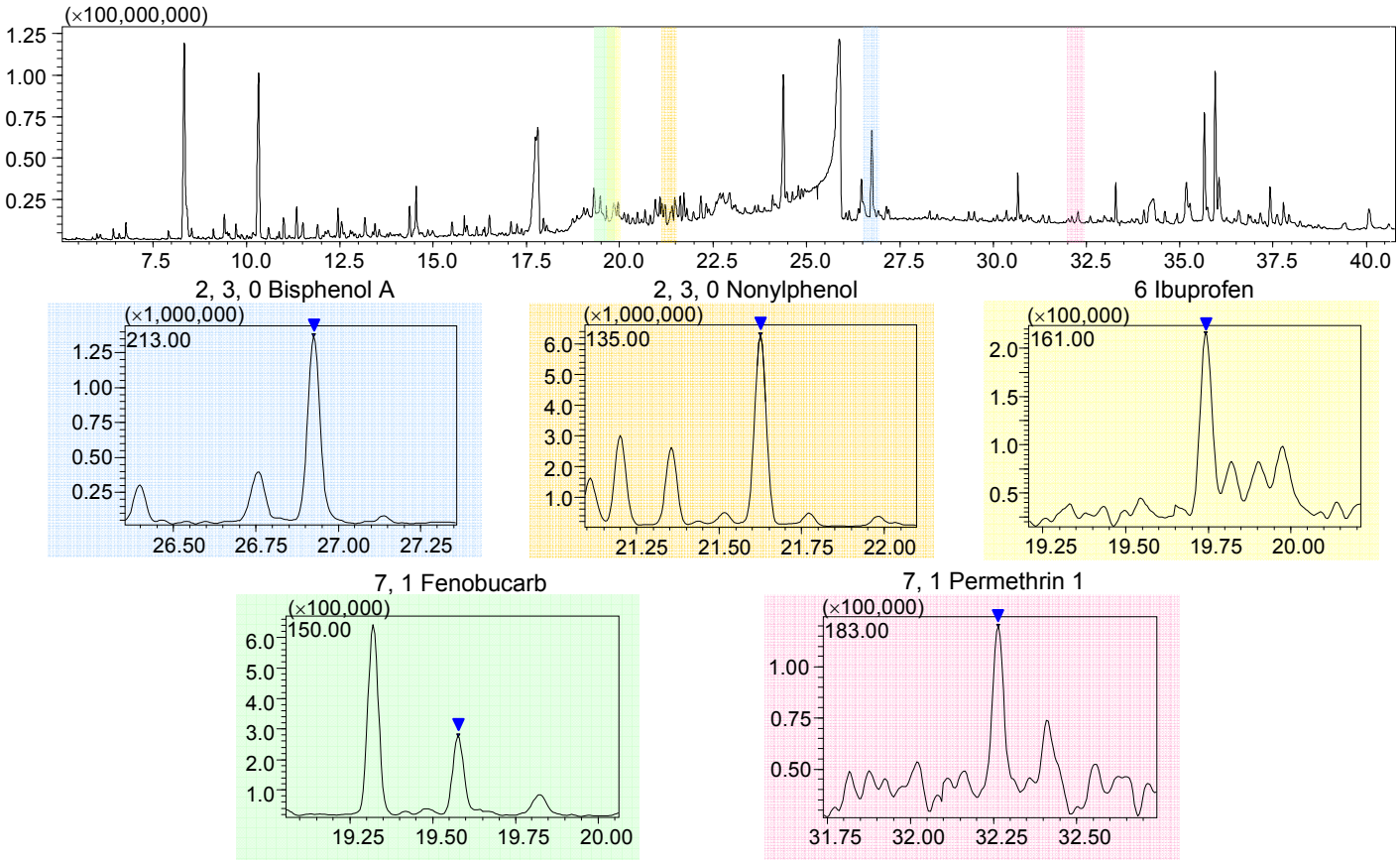

Fig. 1 Total Ion Current Chromatogram for a River Water Sample, and Mass Chromatograms for Detected Environmental Pollutants

* The numbers prefixed to the names indicate the category of detected compounds in the database.

Table 2 Semi-Quantitative Results for Detected Environmental Pollutants Using Compound Composer Database Software

Categ	Detected Compounds	Conc. (ng/L in water)	Categ	Detected Compounds	Conc. (ng/L in water)	Categ	Detected Compounds	Conc. (ng/L in water)
1	n-C11H24	62.7	1	Biphenyl	160.7	2	Coprostanol	14121.5
1	n-C12H26	120.1	1	Fluorene	44.6	2	Cyclohexanol	899.7
1	n-C13H28	241.3	1	Naphthalene	270.4	2	Ethanol, 2-phenoxy-	1989.0
1	n-C14H30	190.5	1	Phenanthrene	126.4	2	Phenylethyl alcohol	101.2
1	n-C15H32	188.6	2	Diphenyl ether	213.6	2	Stigmasterol	1697.2
1	n-C16H34	215.3	2	Isophorone	8601.1	2	1,3-Dichloro-2-propanol	304.5
1	n-C17H36	419.8	2	2-Methylphenol	506.7	3	2-Naphthylamine	93.4
1	n-C18H38	420.6	2	2-Naphthol	126.0	3	Acetamide, N-phenyl-	571.0
1	n-C19H40	435.1	2	2-Phenylphenol	52.4	3	2-Chloroaniline	533.5
1	n-C20H42	541.7	2	4-Methyl-2,6-di-t-butylphenol	167.6	3	3,4-Dichloroaniline	959.2
1	n-C21H44	677.3	2	4-tert-Octylphenol	155.4	3	Quinoline	175.4
1	n-C22H46	794.4	2	Bisphenol A	3169.6	4	2(3H)-Benzothiazolone	2544.3
1	n-C23H48	1118.2	2	Nonylphenol	9845.0	4	2-(Methylthio)-benzothiazol	277.7
1	n-C24H50	1505.7	2	2,4,5-Trichlorophenol	38.1	4	2-Acetyl-5-methylthiophene	65.4
1	n-C25H52	2383.4	2	2,4,6-Tribromophenol	3292.6	4	Benzothiazole	177.0
1	n-C26H54	1299.5	2	2,4,6-Trichlorophenol	44.7	5	Tris(1,3-dichloro-2-propyl) phosphate	677.0
1	n-C27H56	1392.3	2	Triclosan	211.3	6	Caffeine	1736.5
1	n-C28H58	966.2	2	Bis(2-ethylhexyl)phthalate	11036.3	6	Diethyltoluamide	345.0
1	n-C29H60	1445.2	2	Diethyl phthalate	2306.6	6	Ibuprofen	1596.3
1	n-C30H62	1625.2	2	Diisobutyl phthalate	914.1	6	L-Menthol	4281.0
1	n-C31H64	2393.8	2	Dimethyl phthalate	261.8	6	Thymol	223.1
1	n-C32H66	979.3	2	Di-n-butyl phthalate	807.1	6	Nicotine	846.2
1	n-C33H68	863.2	2	2-Butoxyethanol	4013.9	7	Fenobucarb	551.5
1	n-C9H20	152.0	2	2-Ethyl-1-hexanol	1628.3	7	Permethrin 1	661.7
1	4-Cymene	351.2	2	alpha-Terpineol	900.9	7	Permethrin 2	114.2
1	1,3-Dimethylnaphthalene	618.1	2	Benzyl alcohol	203.7	7	Piperonyl butoxide	85.7
1	2,6-Dimethylnaphthalene	403.9	2	beta-Sitosterol	3799.5	7	2-Phenylphenol (OPP)	63.9
1	2-Methylnaphthalene	100.9	2	Cholesterol	14408.1	7	Biphenyl	34.6

The river water sample was provided by Prof. Kadokami of the University of Kitakyushu.

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