

Application Data Sheet

No. 79

GC-MS

Gas Chromatograph Mass Spectrometer

Analysis of PCBs and Organochlorinated Pesticides in River Water Using Simultaneous Scan/MRM Measurement in GC-MS/MS (2)

This data sheet introduces an example of the accurate quantification of PCBs and chlorinated pesticides in river water using the analytical conditions for simultaneous scan/MRM measurements introduced in Application Data Sheet No. 78. It presents sensitivity and repeatability results for PCBs and chlorinated pesticides in MRM mode, acquired with simultaneous scan/MRM measurements, in Application Data Sheet No. 78. In addition, Application Data Sheet No. 80 introduces an example of the screening for environmental pollutants not suited to MRM measurement by applying Compound Composer Database Software to the scan data acquired with simultaneous scan/MRM measurements.

Experimental

Pretreatment stages are shown in Fig. 1.

1 mL of 1 mol/L phosphate buffer was added to 1 L of river water. 50 g of sodium chloride was then added. Liquid-liquid extraction was performed twice using 50 mL of dichloromethane, and the sample was concentrated to 1 mL after dehydration with anhydrous sodium sulfate. Afterwards, 100 μ L of the 10 μ g/mL internal standard solution was added to form the measurement sample. For the GC-MS/MS analysis conditions, refer to Application Data Sheet No. 78.

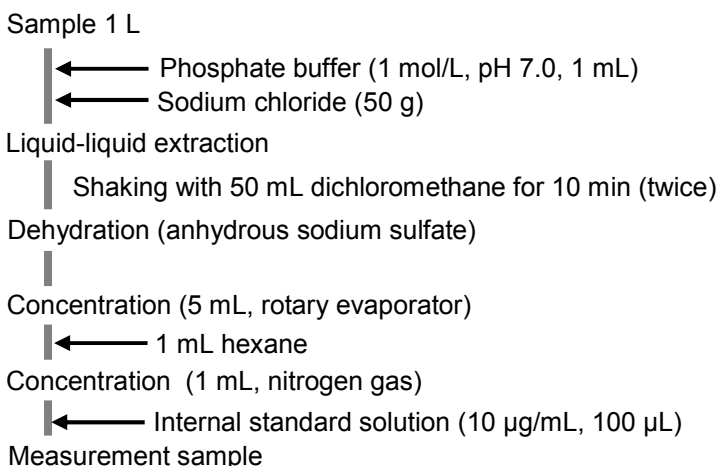


Fig. 1 River Water Pretreatment Flow

Results

The scan and MRM total ion chromatogram results acquired in simultaneous scan/MRM measurements of the sample extracted from river water are shown in Fig. 2. In the scan mode, a variety of impurities originating in the river water were detected. In the MRM mode, however, it was possible to eliminate almost all interfering impurities through a 2-stage mass separation, enabling the selective detection of PCBs and chlorinated pesticides.

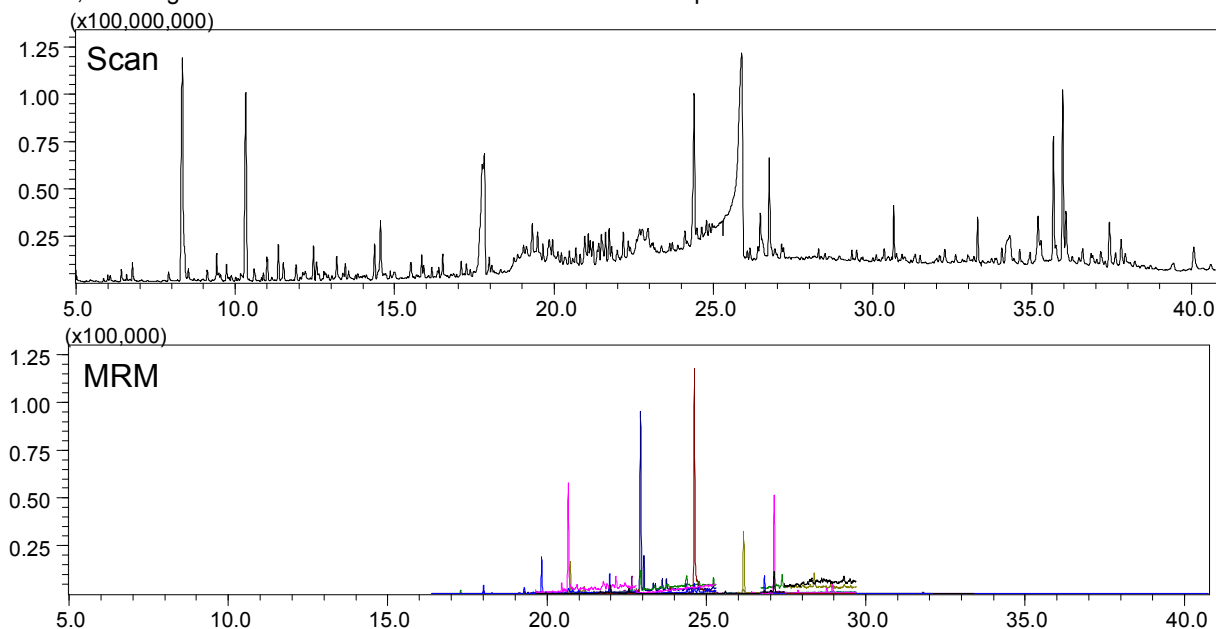


Fig. 2 Scan and MRM Total Ion Current Chromatogram from Simultaneous Scan/MRM Measurements of a River Water Sample

The river water sample was subjected to simultaneous scan/MRM measurements and SIM measurements. The MRM and SIM mass chromatograms for the detected compounds are shown in Fig. 3. Table 1 shows the quantitative values for the PCBs and chlorinated pesticides detected in the river water sample. In the SIM data, the impurities overlap, making peak detection difficult. With MRM, however, the impurities can be separated by mass with high sensitivity and high resolution to obtain quantification with favorable sensitivity, even for trace compounds at the ppq to ppt level.

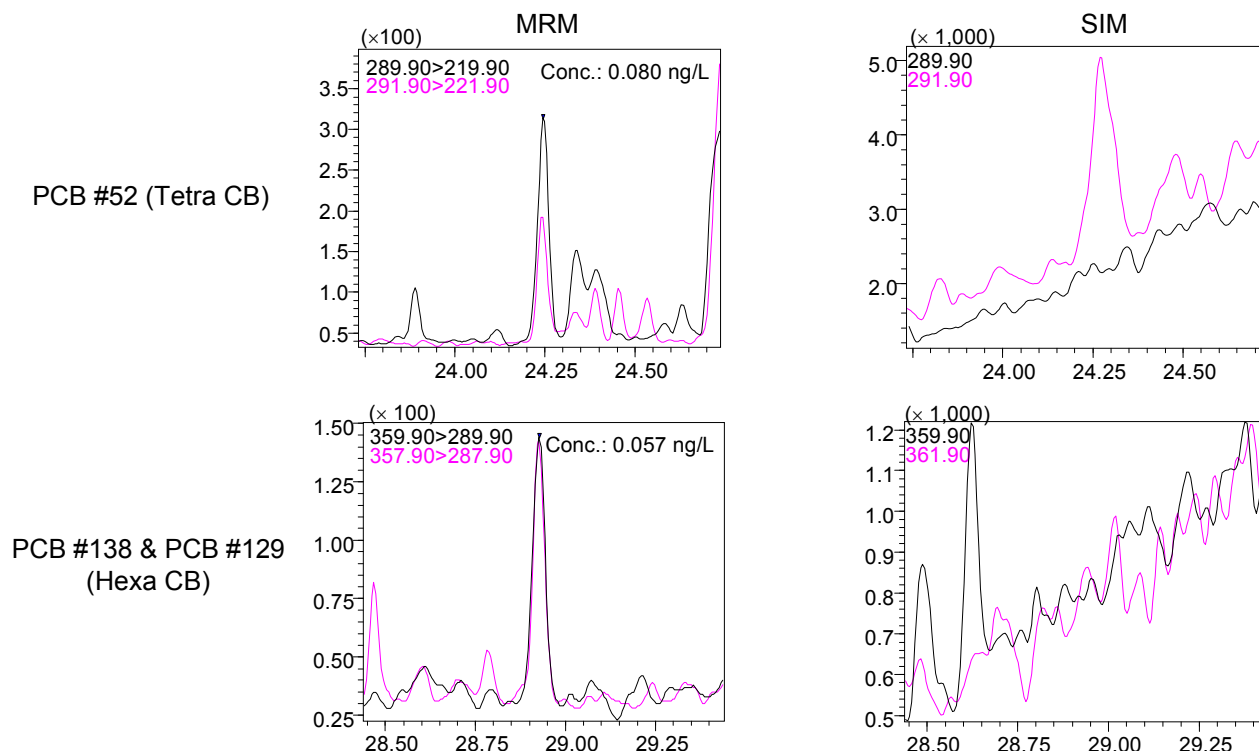


Fig. 3 MRM and SIM Mass Chromatograms for Compounds Detected in Measurements of a River Water Sample
(Left: MRM Mass Chromatogram, Right: SIM Mass Chromatogram)

Table 1 PCBs and Chlorinated Pesticides Detected in a River Water Sample (The detection concentrations indicate the concentrations in the river water.)

Compound Name	Conc. (pg/L in water)	Compound Name	Conc. (pg/L in water)
PCB #1 (Mono CB)	0.363	PCB #70 (Tetra CB)	0.159
PCB #3 (Mono CB)	0.401	PCB #66 (Tetra CB)	0.144
PCB #4 & #10 (Di CB)	0.194	PCB #101 + PCB #90 (Penta CB)	0.063
alpha-BHC	0.032	PCB #99 (Penta CB)	0.079
Hexachlorobenzene	0.403	PCB #119 (Penta CB)	0.028
PCB #8 (Di CB)	0.244	p,p'-DDE	0.306
PCB #19 (Tri CB)	0.026	PCB #110 (Penta CB)	0.381
PCB #18 (Tri CB)	0.111	PCB #149 (Hexa CB)	0.013
PCB #15 (Di CB)	0.116	PCB #153 & PCB #168 (Hexa CB)	0.081
delta-BHC	2.820	PCB #105 (Penta CB)	0.255
PCB #52 (Tetra CB)	0.080	PCB #138 & PCB #129 (Hexa CB)	0.057
PCB #49 (Tetra CB)	0.039	PCB #187 (Hepta CB)	0.006
PCB #44 (Tetra CB)	0.092	PCB #183 (Hepta CB)	0.007
PCB #41 (Tetra CB)	0.108	PCB #180 (Hepta CB)	0.011
PCB #74 (Tetra CB)	0.169	PCB #169 (Hexa CB)	0.026

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

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