

Analysis of Alkylphenols using LC-MS

Alkylphenols are found widely in the environment as raw materials or decomposed products of chemical compounds. Some alkylphenols are suspected of having endocrine disrupting properties, and investigations are being undertaken to monitor alkylphenols found in the environment.

As alkylphenols exhibit different characteristics depending on the side chain conformation, it is required to accurately determine each component. Here, LC-MS, which employs highly selective mass spectrometer as its detector, was

used to simultaneously analyze bisphenol A and alkylphenols (C₄-C₉).

Fig.1 shows the mass chromatogram in the scan mode. Alkylphenols give a deprotonated molecule through the negative ion Atmospheric Pressure Chemical Ionization (APCI) method, and the components can be accurately identified by performing mass chromatography with these mass numbers. Fig.2 shows the SIM chromatograms at 10ppb.

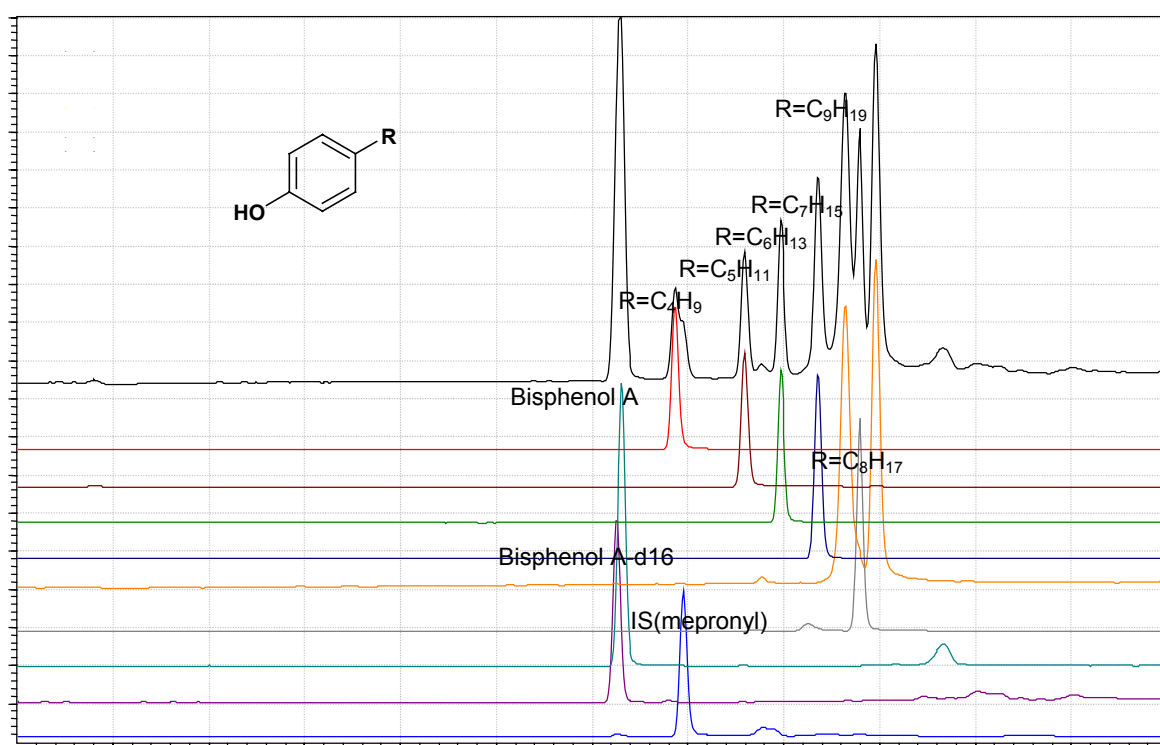


Fig. 1 Mass chromatograms of alkylphenols

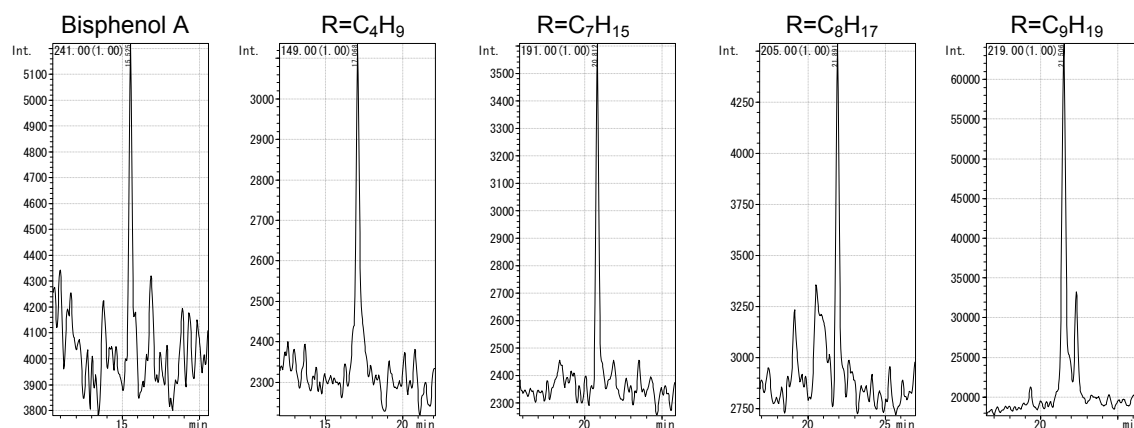


Fig. 2 SIM chromatograms of alkylphenols (10ppb)

Fig.3 shows the calibration curves (n=5) from 10 to 1000ppb obtained by the internal standard method using

mepronyl.

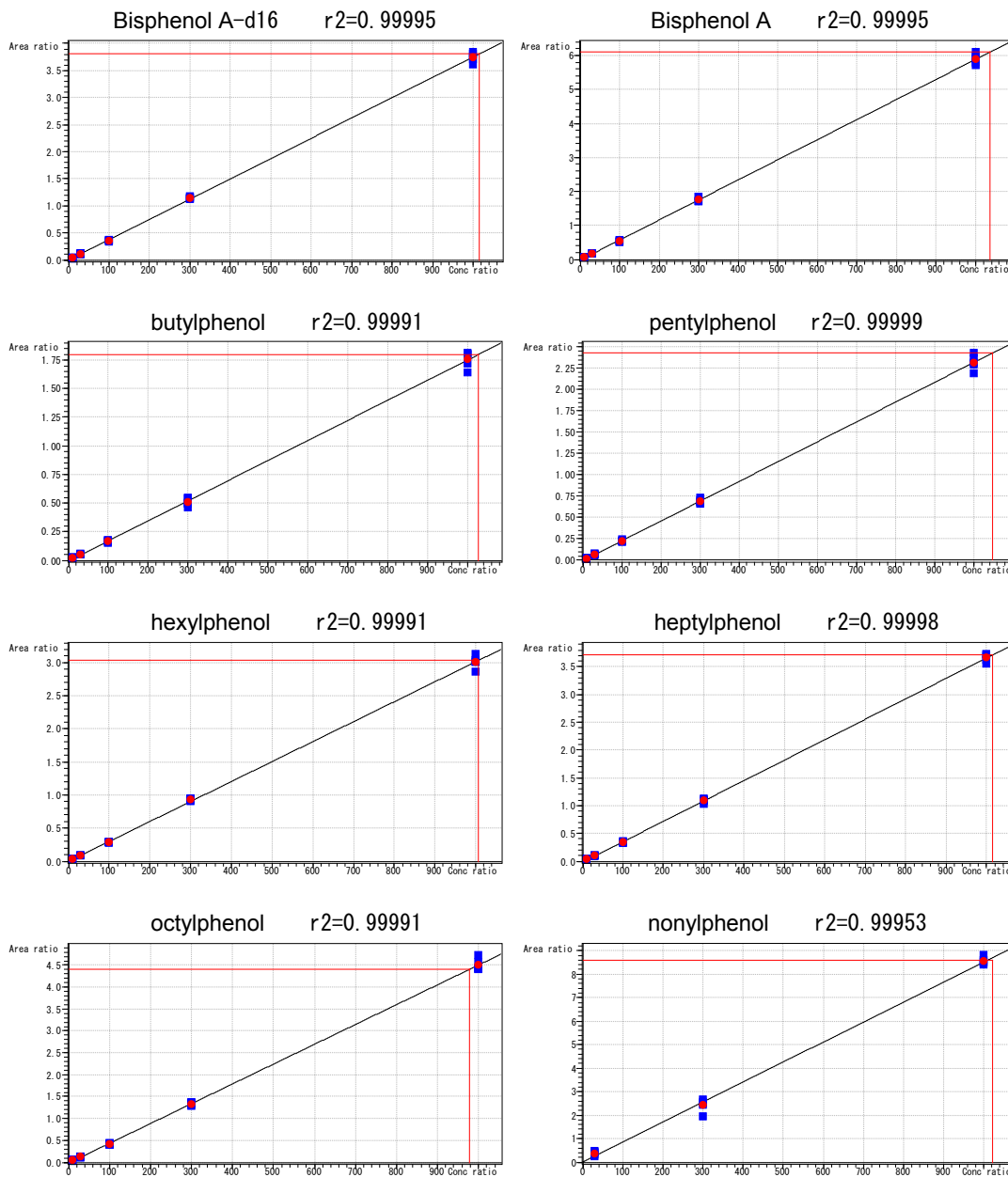


Fig. 3 calibration curves of alkylphenols

* This data has been acquired with the cooperation of Dr. Shigeru Suzuki from the Kawasaki Municipal Research Institute for Environmental Protection (now of the National Institute for Environmental Studies). We hereby express our appreciation for his cooperation.

Table 1 Analytical conditions for LC-MS

Column	: Shimadzu VP-ODS (2.0 mmI.D. x 150 mm)	Column temperature	: 40 degree C
Mobile phase A	: water	Block Heater temperature	: 200 degree C
Mobile phase B	: methanol	Q-array RF	: scan mode
Gradient program	: 20% B - 90%B(15min) - 90%B(30min) - 20%B(30.01-40min)		
Flow rate	: 0.2 mL/min		
Injection volume	: 10 uL		
Probe voltage	: -3.0 kV (APCI-Negative mode)		
Probe temperature	: 400 degree C		
CDL temperature	: 200 degree C		
Nebulizing gas flow	: 2.5 L/min		
CDL voltage	: +20 V		
Q-array DC voltage	: -25 V		
Scan range	: m/z 50 – 600 (1.0 sec/scan)		

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