SHIMADZU

LC-MS Application Data Sheet No. 032

Analysis of Bisphenol A and Nonylphenol using LC-MS

Previously, concerns about toxic chemicals in the environment focused on carcinogenic effects after long-term exposure. Recently, the effects of trace amounts of "endocrine disrupter compounds," on human health, wild animals, and the environment have been identified and research has been conducted into them.

Environmental studies are being conducted into Bisphenol A and Nonylphenol, which are suspected exogenous endocrine disrupter compounds. These phenols are generally derivatized using trimethylsilyl (TMS) reagent before analysis by GC-MS. However, this data sheet introduces the direct analysis of Bisphenol A and Nonylphenol using LC-MS, without derivatization.

Figure.1 shows the mass chromatogram made in the scan mode, and Figs. 2 and 3 show the mass spectra of Bisphenol A and Nonylphenol.

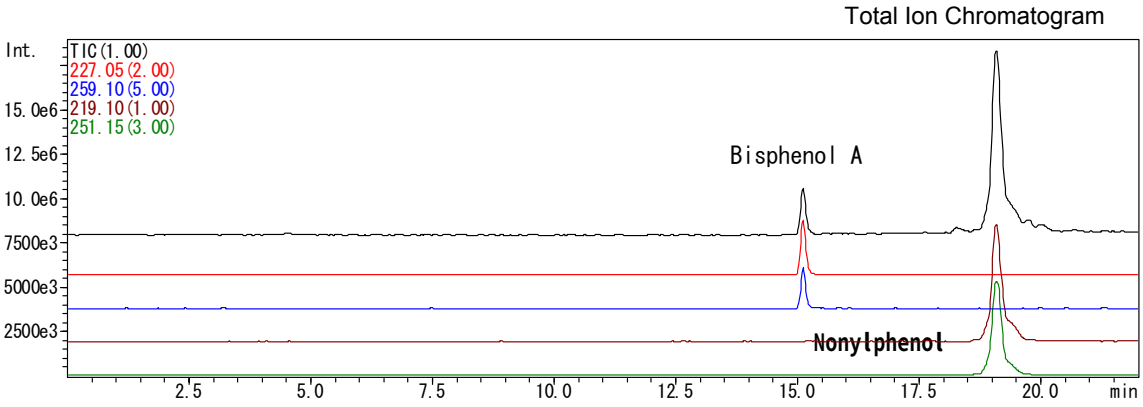
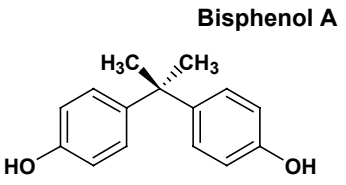


Fig. 1 Mass chromatograms of Bisphenol A and Nonylphenol



$C_{15}H_{16}O_2$
Exact Mass: 228.12
Mol. Wt.: 228.29

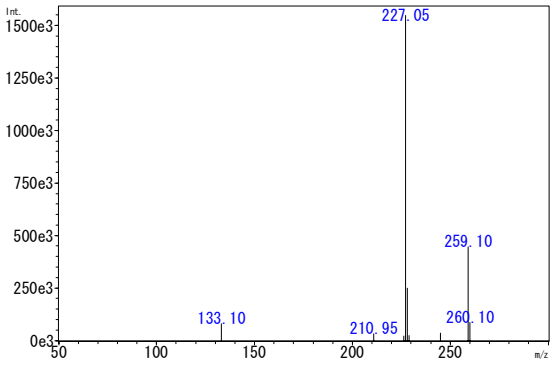
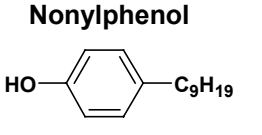


Fig. 2 Mass spectrum of Bisphenol A



$C_{15}H_{24}O$
Exact Mass: 220.18
Mol. Wt.: 220.35

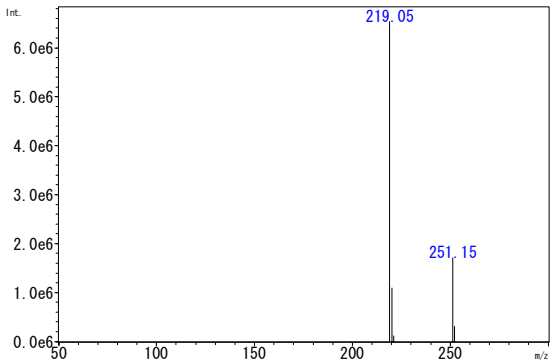


Fig. 3 Mass spectrum of Nonylphenol

Figs. 4 and 5 show the SIM chromatograms and calibration curves (n=5) of Bisphenol A and Nonylphenol. Good area count repeatability was obtained for standards from 0.1 to 5ppb with CV values from 2 to 7%.

(The peak near 20 minutes in Fig.5 has been identified as the BHT antioxidant.)

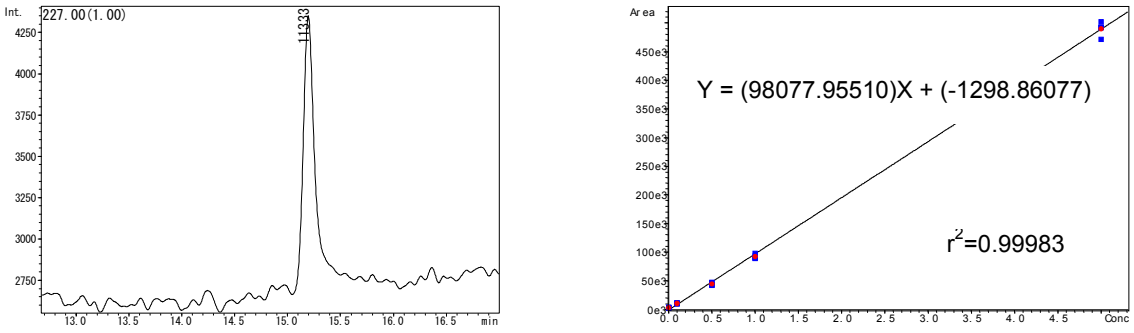


Fig. 4 SIM chromatogram (0.1ppb) and calibration curve for Bisphenol A

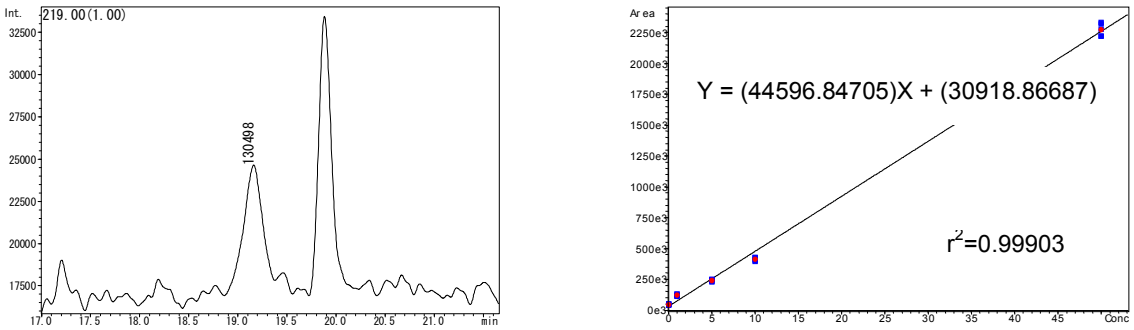


Fig. 5 SIM chromatogram (1ppb) and calibration curve of Nonylphenol

Table 1 Reproducibility of Bisphenol A

	1	2	3	4	5	Mean	SD	CV(%)
0.1ppb	10512	9883	10754	11819	11333	10860.20	746.7059	6.88
5ppb	47304	43464	47545	41723	41626	44332.40	2917.143	6.58
1ppb	90174	89287	90605	93377	97719	92232.40	3426.8685	3.72
5ppb	471945	491852	492773	501947	492953	490294.00	11046.734	2.25

Table 2 Reproducibility of Nonylphenol

	1	2	3	4	5	Mean	SD	CV(%)
1ppb	113838	118551	118066	130864	130498	122363.40	7812.1124	6.38
5ppb	250476	250893	229923	245356	231494	241628.40	10219.226	4.23
10ppb	403894	429939	425462	410675	396545	413303.00	14149.77	3.42
50ppb	2318916	2332011	2221520	2219802	2276594	2273768.60	52632.589	2.31

Table 3 Analytical conditions for LC-MS

Column	:Shimadzu VP-ODS (2.0 mmI.D. x 150 mm)		
Mobile phase A	:water	**Mobile phase B**	:methanol
Gradient program	:20% B－90%B (5-22min)		
Flow rate	:0.2 mL/min		
Injection volume	:500 uL	**Column temperature**	:40 °C
Probe voltage	:-3.0 kV (APCI-Negative mode)		
Probe temperature	:400 °C		
CDL temperature	:200 °C	**Block Heater temperature**	: 200 °C
Nebulizing gas flow	:2.5 L/min		
CDL voltage	:+15 V		
Q-array DC voltage	:-25 V	**Q-array RF**	: 130
Scan range	:m/z 50 – 500 (1.0 sec/scan)		

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