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Rapid quantitative analysis of semi-volatile organic compounds in indoor surface film using direct analysis in real time mass spectrometry: a case study on phthalates

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Table S1 The optimized MS/MS acquisition parameters of the selected phthalates.

Compounds	Precursor ions (*m/z*)	Product ions (*m/z*)	DP (volts)	CE (volts)
DEHP/DnOP	391.3	113.0	55	14
		149.1	55	23
		167.2	55	14
		261.1	55	11
		279.1	55	11
DiBP/DnBP	279.2	57.3	55	13
		149.1	55	20
		205.0	55	9

a: DP: declustering potential.

b: CE: collision energy.

Table S2 The optimized DAR-MS/MS acquisition parameters, regression equations and correlation coefficients for calibration curves for the four selected PAEs spiked on glass capillaries.

Compounds	Precursor ions (*m/z*)	Product ions[a] (*m/z*)	Calibration	r
DEHP	391.3	113.0	y=244710 x	0.997
		149.1	y=553054x	0.981
		167.2	y=320202x	0.996
		279.1	y=159683x	0.997
DnOP	391.3	149.1	y=470837x	0.993
		261.1	y=137084x	0.992
DiBP	279.2	57.3	y=246187x	0.993
		149.1	\	
		205.0	y=889277x	0.992
DnBP/DBP	279.2	149.1	\	
		205.0	y=760974x	0.993

a: Due to the intensities of some product ions being less than 8.5 % max intensities, data were not included.

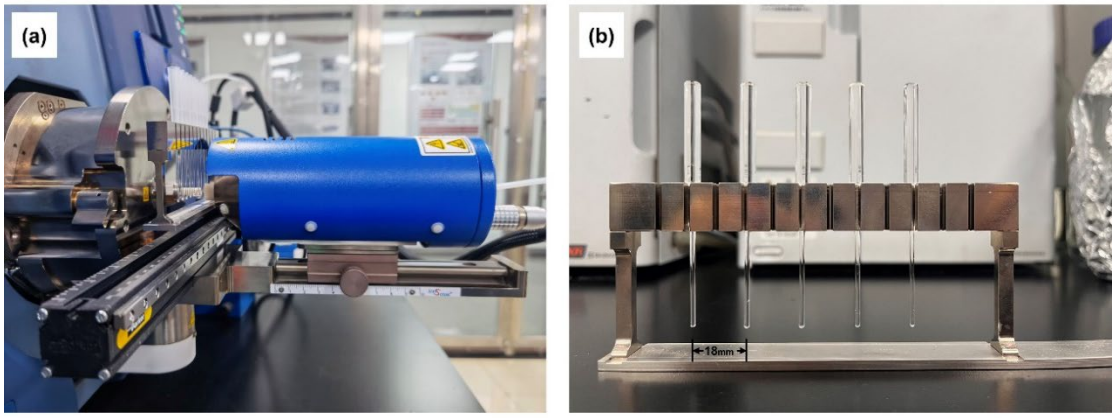

Figure S1 (a) DART-MS/MS set up during analysis. (b) Metal holder with six glass capillary tubes on a stainless steel stand. The center-to-center distance between two glass capillary tubes is 18 mm.

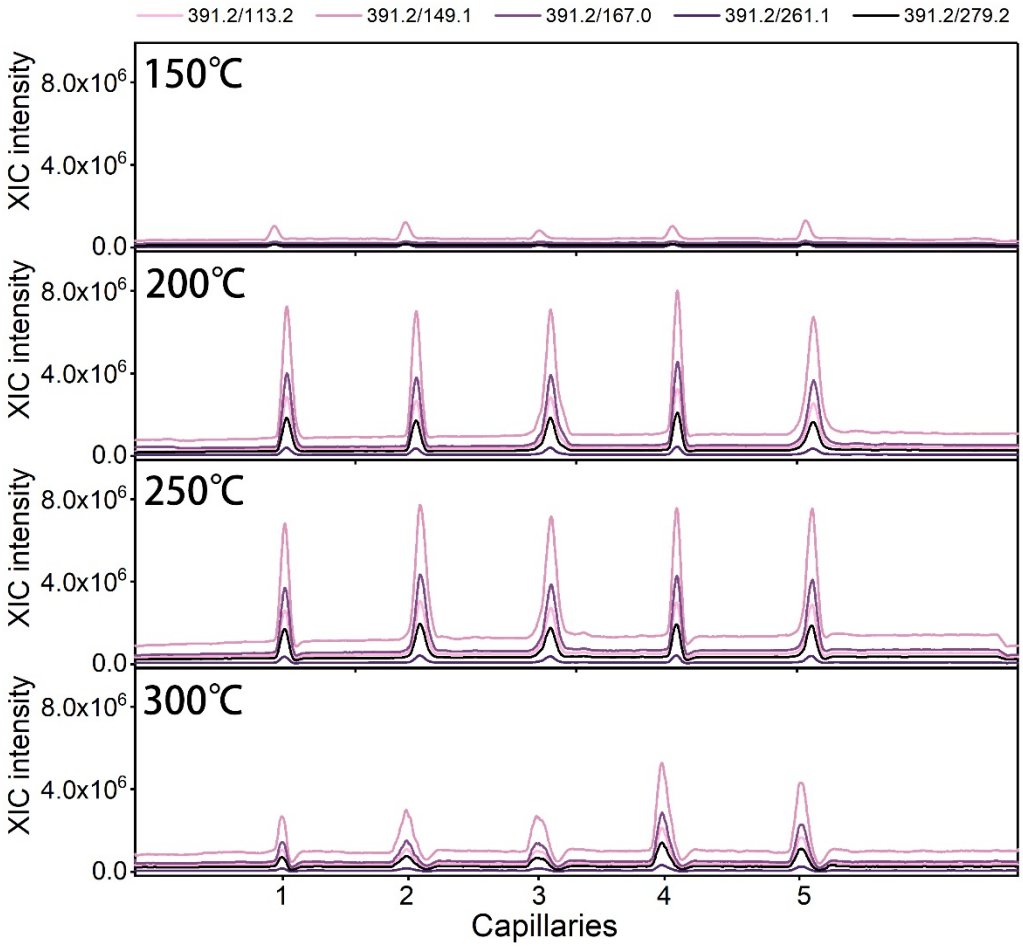

Figure S2 Temperature variations of the extracted ion chromatograms (XIC) obtained from 5 capillaries samples for spiked DEHP within 4 minutes. The He flux temperature was set at 150 ℃, 200 ℃, 250 ℃, and 300 ℃ due to the boiling points of DEHP were 384 ℃.