Supporting Information

Hydroxylated Metabolites of 4-Monochlorobiphenyl and Its Metabolic Pathway in Whole Poplar Plants

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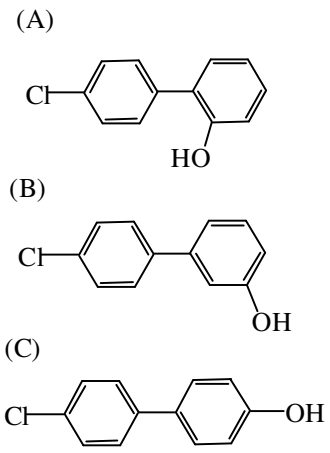

Fig. S1. Chemical structures of hydroxylated CB3 (A) 2'OH-CB3 (B) 3'OH-CB3, (C) 4'OH-CB3

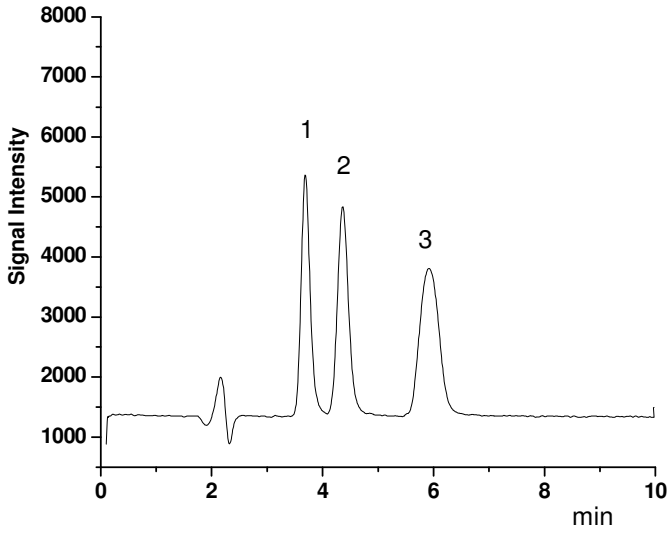

Fig. S2. Chromatograms of three OH-CB3s at the optimized conditions (1) 4'OH-CB3; (2) 3'OH-CB3; (3) 2'OH-CB3

Analytical performance. Table S1 shows the analytical performance data of this optimized HPLC-MS method. Compounds of 2'OH-CB3, 3'OH-CB3 and 4'OH-CB3 were baseline separated in less than 10 minutes. Linear calibration curves, based on peak areas to concentration, were obtained in the range of 1.0–100.0 ng ml^{-1}, with correlation coefficients of 0.9996, 0.9999 and 0.9996 (n=3) for 2'OH-CB3, 3'OH-CB3 and 4'OH-CB3, respectively. The relative standard deviations measured at the 10.0 ng ml^{-1} level for 2'OH-CB3 and 3'-OH-CB3 and the 5.0 ng ml^{-1} level for 4'OH-CB3 were in the range of 1.18-1.45% (n= 5). Calculated detection limits (*S/N* = 3) of 2'OH-CB3, 3'OH-CB3 and 4'OH-CB3 were 0.127, 0.117 and 0.034 ng ml^{-1}, respectively.

Table S1. Some analytical performance data of the proposed method.

Compound	Calibration curve	Correlation coefficient	Detection limit (ng ml^{-1})	RSD (%, n = 5)[a]
2'OH-CB3	$Y = 1.61\times10^4 X$	0.9996	0.127	1.18
3'OH-CB3	$Y = 1.42\times10^4 X$-1454	0.9999	0.117	1.45
4'OH-CB3	$Y = 2.33\times10^4 X$-1260	0.9996	0.034	1.21

[a], Standard concentration, 2'OH-CB3 and 3'OH-CB3 10.0 ng ml^{-1}; 4'OH-CB3 5.0 ng ml^{-1};

Table S2. Recoveries of OH-CB3s in hydroponic solution and different parts of blank poplars with spiked masses: 2'OH-CB3 0.4 μg, 3'OH-CB3 0.4 μg and 4'OH-CB3 0.2 μg (%, n = 3)

Compound	Hydroponic solution	Root	Wood	Bark	Leaf
2'OH-CB3	95.6±0.3	89.8±5.5	92.9±1.6	85.9±6.4	81.7±4.7
3'OH-CB3	88.2±0.5	83.5±4.2	84.3±3.5	81.0±4.3	76.4±3.9
4'OH-CB3	95.5±0.6	88.5±2.8	87.1±7.8	81.5±5.1	85.2±6.4