Supporting Information (SI)

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Title:

Enantioselective Biotransformation of Chiral PCBs in Whole Poplar Plants

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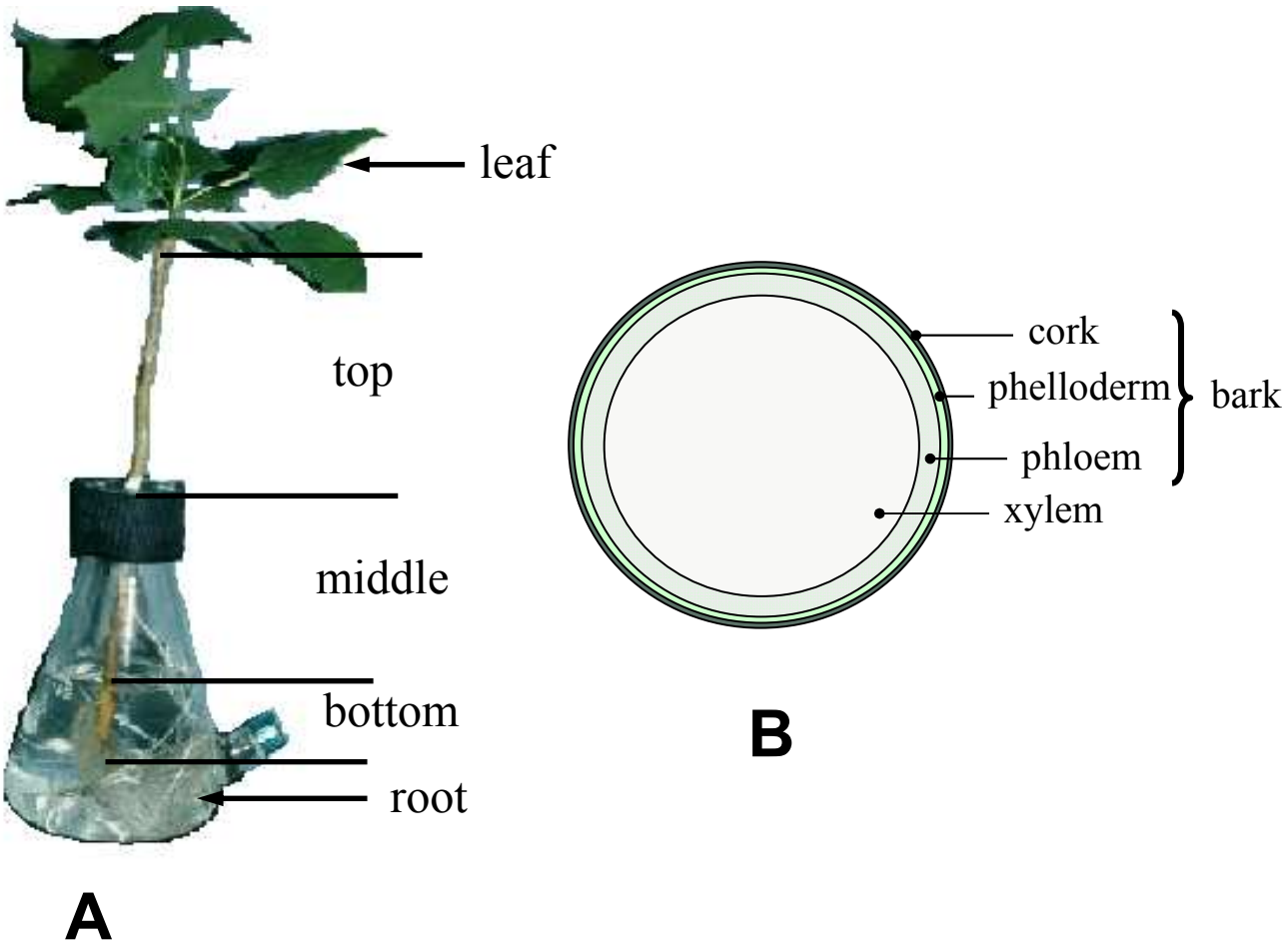

Figure S1: A) the exposure setup of PCBs and method to divide the different plant parts; B) the cross-section illustration of bark.

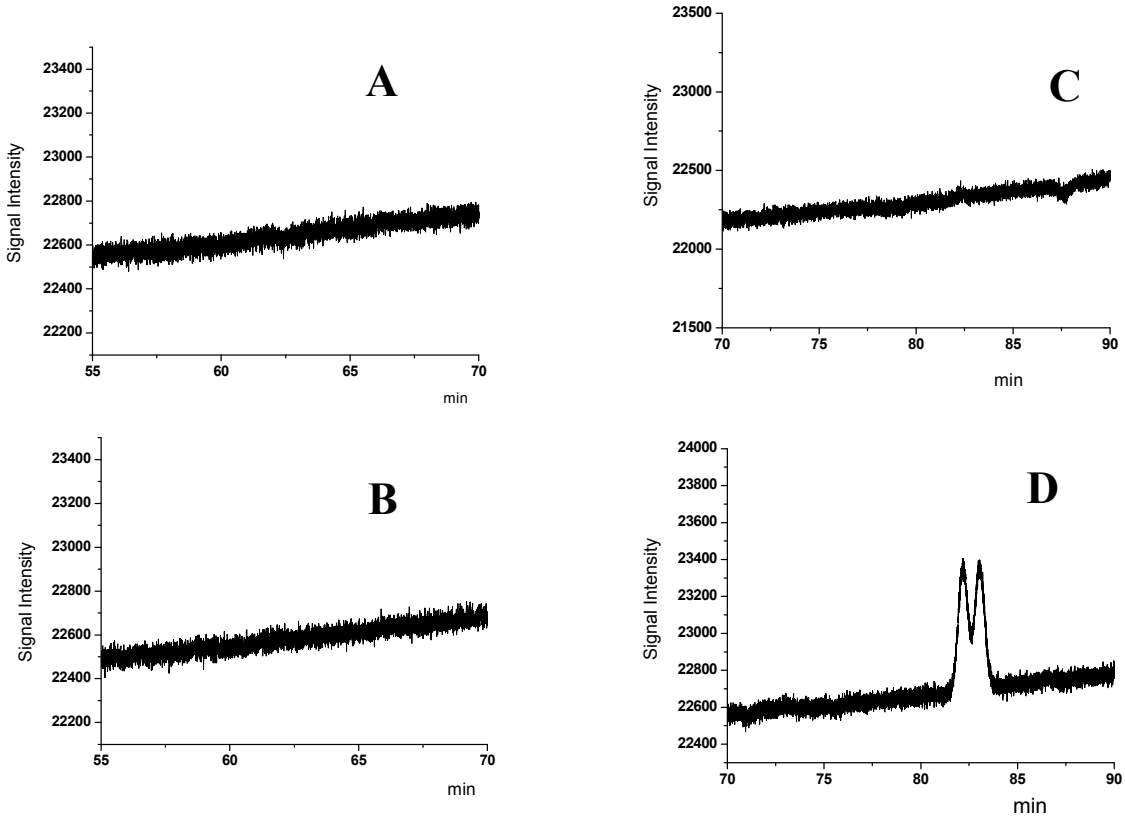

Figure S2: Signals of GC-ECD for selected parts of blank whole poplars; other parts have similar background signals. A) blank bark for PCB95; B) blank root for PCB95; C) blank bark for PCB136; D) signal of 5 ng mL^{-1} of PCB136 standard.

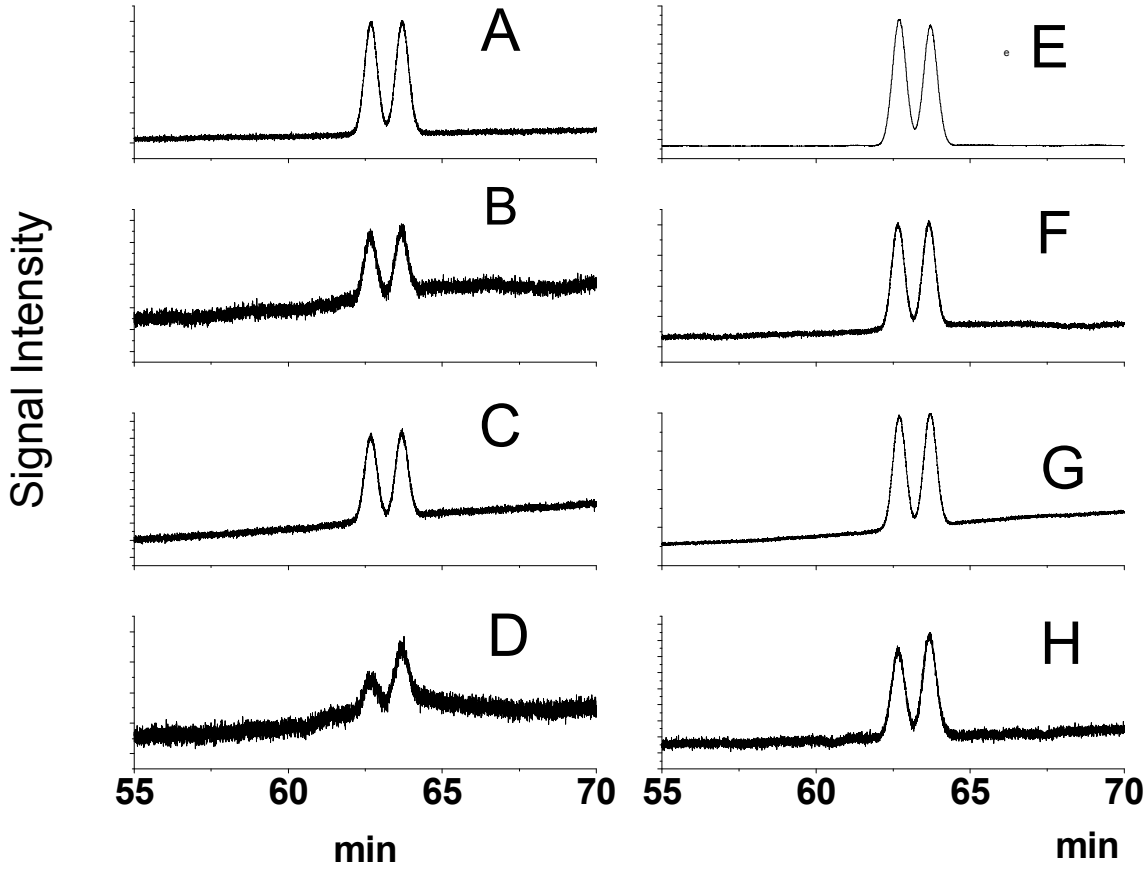

Figure S3: Some typical chromatograms of PCB95 on GC-ECD. A) 5 ng mL^{-1} of PCB95 standard; followed by PCB95 signals in treatments of : B) middle xylem at day 5; C) middle xylem at day 10; D) middle xylem at day 20; E) root-second sample at day 20; F) bottom xylem at day 5; G) bottom xylem at day 10; H) bottom xylem at day 20

Table S1. Masses (ng), concentrations (ng g^{-1} wet weight) and EFs of PCB136 in hydroponic solutions and different parts of dead poplar plants (n=3)

sample	day 5			day 10			day 20		
	ng	ng g^{-1}	EF [b]	ng	ng g^{-1}	EF	ng	ng g^{-1}	EF
middle xylem	ND	ND	ND	ND	ND		ND	ND	
middle bark	101±0.97	76.4±6.07	0.505±0.002	82.9±0.60	62.0±2.65	0.504±0.002	44.3±0.31	33.4±2.17	0.506±0.002
bottom xylem	11.9±0.05	3.53±0.26	0.504±0.007	13.6±0.31	3.82±0.34	0.505±0.003	26.8±0.50	7.39±0.68	0.515±0.006*
bottom bark	403±3.91	174±11.6	0.505±0.002	407±5.68	167±19.7	0.506±0.001	446±2.35	171±16.12	0.510±0.001*
solution	107±1.27	0.267±0.003	0.495±0.004*	113±0.29	0.282±0.001	0.498±0.003*	95.0±0.89	0.237±0.002	0.506±0.003
total recovery mass	623±5.75			617±6.25			612±3.70		
Recovery (%) [a]	77.9±0.7			77.1±0.8			76.5±0.5		

[a] Total added mass of PCB136 was 800 ng; [b] EF of PCB136 standard is 0.506±0.003 (n=12); * Significant difference of EFs from standard by one way ANOVA at $\alpha = 0.05$.

Table S2. Masses (ng), concentrations (ng g^{-1} wet weight) and EFs of PCB136 in hydroponic solutions and different parts of whole poplar plants (n=3)

sample		day 5			day 10			day 20		
		ng	ng g^{-1}	EF [e]	ng	ng g^{-1}	EF	ng	ng g^{-1}	EF
leaf		ND [d]	ND	ND	ND	ND	ND	ND	ND	ND
top xylem		ND	ND	ND	ND	ND	ND	ND	ND	ND
top bark		ND	ND	ND	ND	ND	ND	ND	ND	ND
middle xylem		ND	ND	ND	ND	ND	ND	1.03±0.22	0.30±0.04	0.480±0.009*
middle bark [a]	cork [b]	91.1±55.1	36.5±13.9	0.504±0.004	122±50.8	45.6±25.7	0.503±0.002	147.7±9.85	242±95.1	0.503±0.005
	phelloderm							2.92±1.05	5.65±1.74	0.500±0.009
	phloem							3.28±2.13	1.91±1.01	0.504±0.007
bottom xylem		2.92±1.01	0.97±0.34	0.506±0.002	3.79±2.22	1.00±0.56	0.502±0.001	3.36±0.49	0.87±0.26	0.507±0.010
bottom bark [a]	cork [b]	312±112	312±44.3	0.504±0.003	221±13.8	66.8±18.1	0.503±0.002	258±37.5	208±41.2	0.503±0.002
	phelloderm							9.43±5.03	11.7±6.39	0.504±0.002
	phloem							3.28±0.10	2.13±0.72	0.512±0.005*
root first		56.9±8.25	57.9±9.89	0.509±0.002	57.4±22.9	22.1±5.16	0.509±0.008	40.4±18.7	22.6±12.8	0.508±0.004
root second		140±44.9	143±47.5	0.509±0.003	204±13.6	85.2±28.3	0.509±0.006	147±25.5	77.2±19.6	0.509±0.003
solution		44.6±3.17	0.11±0.01	0.494±0.011*	24.4±8.91	0.06±0.02	0.492±0.008*	12.9±4.22	0.03±0.01	0.485±0.011*
total recovery mass		648±50.2			632±33.3			629±37.2		
Recovery (%) [c]		80.9±6.3			79.1±4.2			78.6±4.6		

[a] Middle bark and bottom bark at day 20 were divided three parts: cork, phelloderm and phloem (Figure S1); [b] The values in cork row at day 5 and 10 are the relative bark values; [c] total added mass of PCB136 was 800 ng; [d] ND=not detectable; [e] EF of PCB136 standard is 0.506±0.003 (n=12); * Significant difference of EFs from standard by one way ANOVA at $\alpha = 0.05$.

Metabolic Mechanisms of Chiral PCBs in Animals Potentially Applicable to Poplars. Many studies have suggested that cytochrome P-450 (CYP) enzymes could be the driver for the enantioselective metabolism of chiral PCBs, but they were focused on animal enzymes and animal species *(1,2*). Even though there is some proof to support the role of P-450 enzymes in metabolizing chiral PCBs enantioselectively, the complete metabolic pathway for transformation of chiral PCBs in biota is still sketchy. Kania-Korwel et al *(3)* found that (+)-PCB136 had more affinity to hepatic microsomal P450 enzymes (such as CYP2B and CYP3A) than did (-)-PCB136, suggesting it was binding, not metabolism which caused the enantioselective enrichment of the (+)-PCB136 atropisomer in tissues of mice. In addition, they *(4)* further proved that the metabolism of PCB136 by CYP2Bs in the liver was not a likely cause of the enantiomeric enrichment of chiral PCBs in mice. Thus, enantioselective binding to (hepatic) enzymes should be further investigated as the potential cause of the enantiomeric enrichment of PCB136 and other PCB congeners *in vivo*. Of course, one cannot exclude the other CYP subfamily as potentially responsible for the enantioselective biotransformation of PCB136.

Plants also contain a large group of cytochrome P450 systems *(5),* which have similar metabolic functions to those in animals. Therefore, the EF changes for PCB95 in whole poplar were most likely the consequence of enantioselective metabolism and enantioselective binding by cytochrome P450 in whole poplars. However, more enzymic experiments should be performed to confirm the enantioselective metabolic process in whole poplars, a model plant used in phytoremediation.

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