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Supporting Information

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Table S1 Monitored ions of derivatized hydroxylated PCBs observed in high-resolution gas chromatography/high-resolution mass spectrometry.

Homologue	Derivatized homologue	Selected fragment (*m/z*)
OH-HpCB	CH_3-HpCBs	423.8131 $[M+2]^+$
		425.8102 $[M+4]^+$
		380.7947 $[M+2-COCH_3]^+$
		373.8202 $[M+2-ClCH_3]^+$
OH-[$^{13}C_{12}$]-HpCB	CH_3-[$^{13}C_{12}$]-HpCB	433.8563 $[M]^+$

HpCB: heptachlorobiphenyl

Table S2 Retention times of methylated products from 2,2′,3,4,4′,5′,6-heptachlorobiphenyl (CB183) metabolites produced by human CYP2B6 and hydroxylated (OH)-CB183 standards.

MeOH-PCB[*1]		Retention time (min)		
		(+)[*2]	(–)[*3]	(±)
Authentic standard[*4]	S1			33.3
	S2			33.6
CB183 metabolite	M1	33.3	33.3	
	M2	33.7	33.7	

[*1]Methylated hydroxylated polychlorinated biphenyl

[*2]Retention times of methylated products of M1 and M2 that are produced by human CYP2B6 from (+)-CB183 as a substrate are represented.

[*3]Retention times of methylated products of M1 and M2 that are produced by human CYP2B6 from (–)-CB183 as a substrate are represented.

[*4]The authentic standards S1 and S2 are 3′-MeO-CB183 and 5-MeO-CB183, respectively.

Table S3 Isotope ratios of methylated products from 2,2′,3,4,4′,5′,6-heptachlorobiphenyl (CB183) metabolites produced by human CYP2B6 and hydroxylated (OH)-CB183 standards.

MeOH-PCB[*1]		Isotope ratio ($[M+2]^+$:$[M+4]^+$)			Theoretical ratio
		(+)[*2]	(–)[*3]	(±)	
Authentic standard[*4]	S1			1:1.02	1:097
	S2			1:1.12	
CB183 metabolite	M1	1:1.10	1:0.97		
	M2	1:1.04	1:1.09		

[*1]Methylated hydroxylated polychlorinated biphenyl

[*2]Isotope ratios of methylated products of M1 and M2 that are produced by human CYP2B6 from (+)-CB183 as a substrate are represented.

[*3]Isotope ratios of methylated products of M1 and M2 that are produced by human CYP2B6 from (–)-CB183 as a substrate are represented.

[*4]The authentic standards S1 and S2 are 3′-MeO-CB183 and 5-MeO-CB183, respectively.

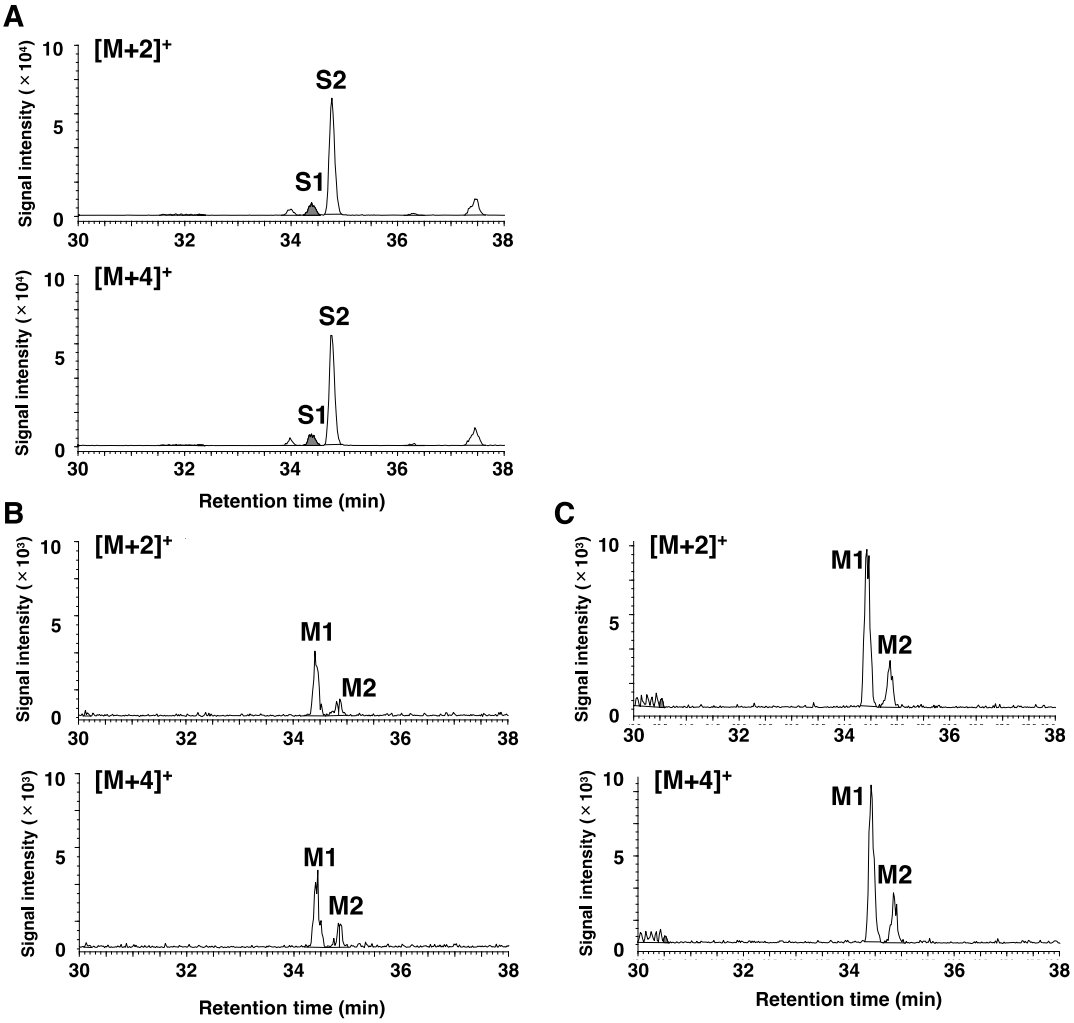

Figure S1 Isotope ratios ([M+2]$^+$ and [M+4]$^+$) of hydroxylated heptachloro metabolites of CB183 by human CYP2B6 analyzed by high-resolution gas chromatography/ high-resolution mass spectrometry.

(A): Authentic standards S1 (3′-MeO-CB183) and S2 (5-MeO-CB183). (B) and (C): Hydroxylated heptachloro metabolites of (+)-CB183 and (–)-CB183, respectively.

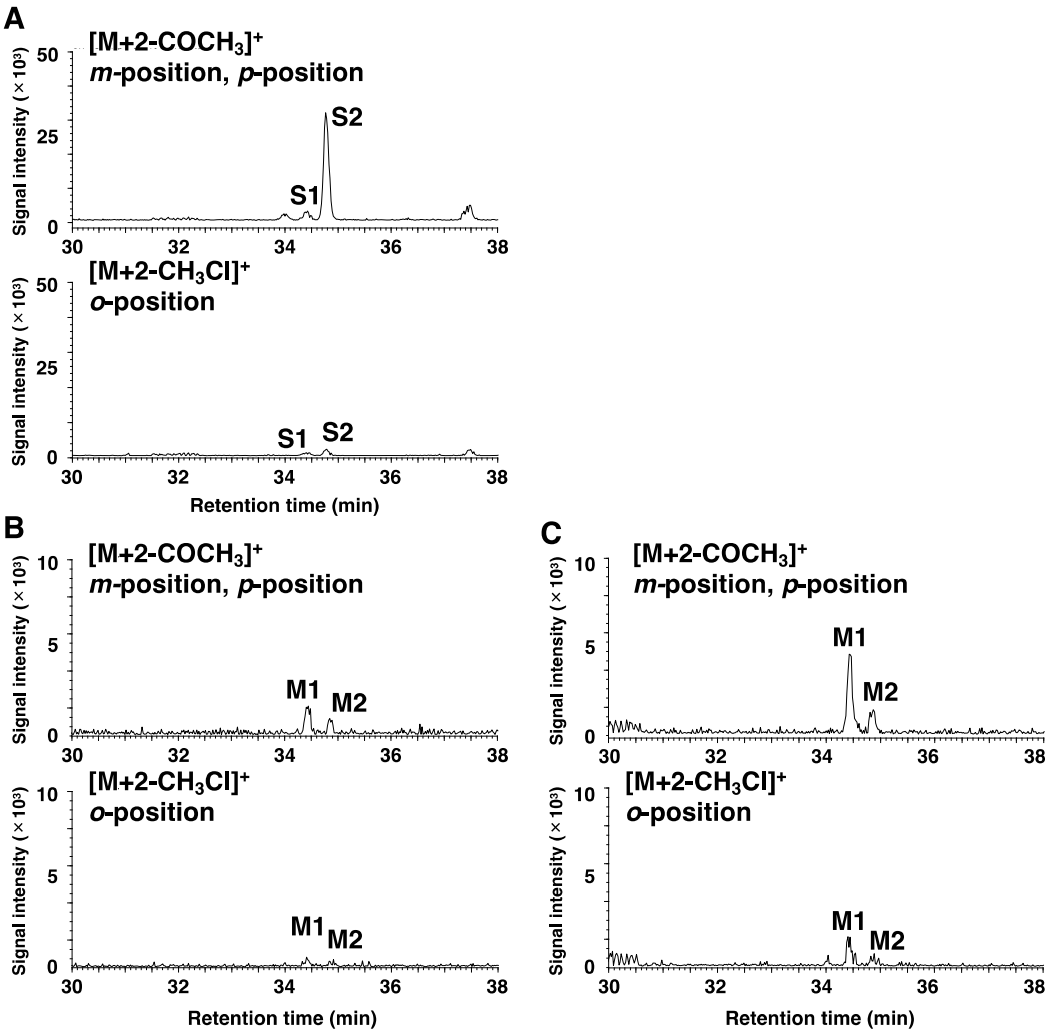

Figure S2 Pattern of fragment ions ($[M+2-COCH_3]^+$ and $[M+2-CH_3Cl]^+$) of hydroxylated heptachloro metabolites of CB183 by human CYP2B6 analyzed by high-resolution gas chromatography/ high-resolution mass spectrometry.

(A) Authentic standards S1 (3′-MeO-CB183) and S2 (5-MeO-CB183). (B) and (C): Hydroxylated heptachloro metabolites of (+)-CB183 and (–)-CB183, respectively.

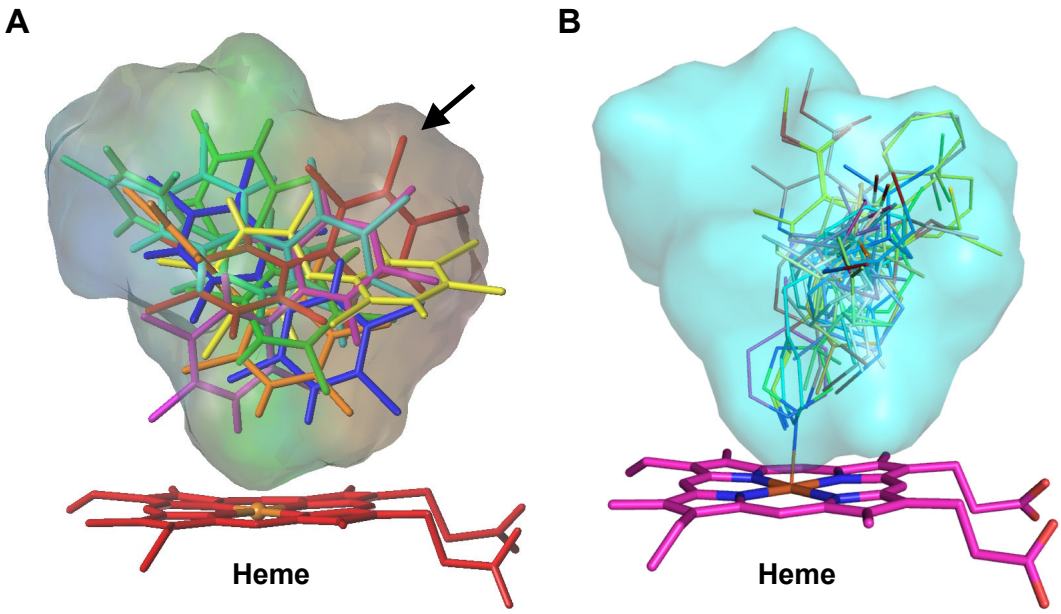

Figure S3 Docking models of CB183 with human CYP2B6.
(A): Eight conformations of CB183 were docked into the substrate-binding cavity of human CYP2B6 (PDB: 3IBD). The arrow indicates the plausible conformation of CB183 in the cavity. (B): Thirteen crystal structures of human CYP2B6 (mentioned under Materials and Methods) superimposed to show sixteen ligands in their substrate-binding cavities.

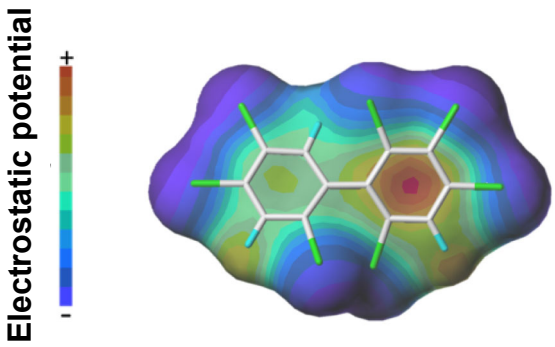

Figure S4 Electrostatic potential map of CB183. Blue portion indicates region of high electron density.