

Table S1. Organic compound list and codes used in PCA development

	<i>Compound</i>	<i>PCA code</i>	
PAHs	Anthracene	P1	
	Fluoranthene	P2	
	Pyrene	P3	
	Benz[a]anthracene	P4	
	Chrysene +Trif	P5	
	Benz[k]fluoranthene	P6	
	Benz[b]fluoranthene	P7	
	Benz[a]fluoranthene	P8	
	Benz[e]pyrene	P9	
	Benz[a]pyrene	P10	
	Benz[ghi]perylene	P11	
	Indeno[1,2,3-cd]pyrene	P12	
	Coronene	P13	
Oxy-PAHs	9-Fluorenone	O1	
	1,8-Naphthalic anhydride	O2	
	4H-Cyclopenta[def]phenanthrene-4-one	O3	
	1,4-Phenanthrenedione	O4	
	9,10-Anthracene-dione	O5	
	9,10-Phenanthrenequinone	O6	
	Benz[a]fluorenone	O7	
	1,9-Benz-10-anthrone	O8	
	Benzo[a]anthracene-7,12-dione	O9	
Nitro-PAHs	2-N-Fluorene	N1	
	2-N-Anthracene	N2	
	2-N-Phenanthrene	N3	
	3-N- Phenanthrene	N4	
	9-N- Anthracene	N5	
	9-N- Phenanthrene	N6	
	2-N-Fluoranthene	N7	
	1-N-Pyrene	N8	
	3-N-Fluoranthene	N9	
	7-N-benz[a]anthracene	N10	
			<i>Abbreviation</i>
PCBs	2,4,4'-Trichlorobiphenyl	PB28	PCB28
	2,3,3',4,4'-Pentachlorobiphenyl	PB105	PCB105
	3,3',4,4',5-Pentachlorobiphenyl	PB126	PCB126
	2,2',3,4,4',5'-Hexachlorobiphenyl	PB138	PCB138
	2,2',3,4',5,5'-Hexachlorobiphenyl	PB146	PCB146
	2,2',3,5,5',6-Hexachlorobiphenyl	PB151	PCB151
	2,3,3',4,4',5-Hexachlorobiphenyl	PB156	PCB156
	2,3,3',4,4',5'-Hexachlorobiphenyl	PB157	PCB157
	2,3',4,4',5,5'-Hexachlorobiphenyl	PB167	PCB167
	3,3',4,4',5,5'-Hexachlorobiphenyl	PB169	PCB169
	2,2',3,3',4,4',5-Heptachlorobiphenyl	PB170	PCB170
	2,2',3,3',4',5,6-Heptachlorobiphenyl	PB177	PCB177
	2,2',3,4,4',5',6-Heptachlorobiphenyl	PB183	PCB183
	2,2',3,4',5,5',6-Heptachlorobiphenyl	PB187	PCB187
	2,3,3',4,4',5,6-Heptachlorobiphenyl	PB190	PCB190
PBDEs	2,4,4'-Tribromodiphenyl ether	B28	BDE28
	2,2',4,4'-Tetrabromodiphenyl ether	B47	BDE47
	2,2',4,5'-Tetrabromodiphenyl ether	B49	BDE49
	2,2',4,4',5-Pentabromodiphenyl ether	B99	BDE99
	2,2',4,4',6-Pentabromodiphenyl ether	B100	BDE100
	2,2',4,4',5,5'-Hexabromodiphenyl ether	B153	BDE153
	2,2',3,4,4',5',6-Heptabromodiphenyl ether	B183	BDE183
NBFRs	2,4-Dibromophenol	NB1	2,4-DBP
	2,6-Dibromophenol	NB2	2,6-DBP
	2,4,6-Tribromophenol	NB3	TBP
	Allyl-2,4,6-tribromophenyl ether	NB4	ATE
	1,2-dibromo-4-(1,2-dibromoethyl) cyclohexane	NB5	TBECH

2,3,4,5,6-pentabromoethylbenzene	NB6	PBEB
2,3-dibromopropyl-2, 4, 6-tribromophenylether	NB7	DPTE
Hexabromobenzene	NB8	HBB
2-Ethylhexyl-2,3,4,5-tetrabrombenzoate	NB9	TBB
1,2-bis(2,4,6-tribromophenoxy) ethane	NB10	BTBPE
bis (2-ethylhexyl)-3,4,5,6-tetrabromophthalate	NB11	TBPH

Table S2. PAH parameters for carcinogenic risk assessment

	<i>Compound</i>	<i>DET (h)^a</i>	<i>EF (d)</i>	<i>ED(y)</i>	<i>AT (y)</i>	<i>IUR (µg/m³)^{1,2}</i>
PAHs	Anthracene	8	350	30	70	1,10E-05
	Fluoranthene	8	350	30	70	1,10E-06
	Pyrene	8	350	30	70	1,10E-06
	Benz[a]anthracene	8	350	30	70	1,10E-04
	Chrysene +Trif	8	350	30	70	1,10E-05
	Benz[b]fluoranthene	8	350	30	70	1,10E-04
	Benz[a]fluoranthene	8	350	30	70	1,10E-04 ^b
	Benz[e]pyrene	8	350	30	70	1,10E-03 ^c
	Benz[a]pyrene	8	350	30	70	1,10E-03
	Indeno[1,2,3-cd]pyrene	8	350	30	70	1,10E-04
	Benz[ghi]perylene	8	350	30	70	1,10E-05

^a Daily working hours; ^b Benz[b]fluoranthene value (see par. 2.3); ^c Benz[a]pyrene value (see par. 2.3)

Table S3. Oxy-PAH parameters for carcinogenic risk assessment

	<i>Compound</i>	<i>DET (h)</i>	<i>EF (d)</i>	<i>ED(y)</i>	<i>AT (y)</i>	<i>IUR (µg/m³)³</i>
Oxy-PAHs	9-Fluorenone	8	350	30	70	8,70E-05
	1,8-Naphthalic anhydride	8	350	30	70	8,70E-05
	4H-Cyclopenta[def]phenanthrene-4-one	8	350	30	70	8,70E-05
	1,4-Phenanthrenedione	8	350	30	70	8,70E-05
	9,10-Anthracene-dione	8	350	30	70	8,70E-05
	9,10-Phenanthrenequinone	8	350	30	70	8,70E-05
	Benz[a]fluorenone	8	350	30	70	8,70E-05
	1,9-Benz-10-anthrone	8	350	30	70	8,70E-05
	Benzo[a]anthracene-7,12-dione	8	350	30	70	8,70E-05

Table S4. Nitro-PAH parameters for carcinogenic risk assessment

	<i>Compound</i>	<i>DET (h)</i>	<i>EF (d)</i>	<i>ED(y)</i>	<i>AT (y)</i>	<i>IUR (µg/m³)³</i>
Nitro-PAHs	2-N-Fluorene	8	350	30	70	8,70E-05
	2-N-Anthracene	8	350	30	70	8,70E-05
	2-N-Phenanthrene	8	350	30	70	8,70E-05
	3-N- Phenanthrene	8	350	30	70	8,70E-05
	9-N- Anthracene	8	350	30	70	8,70E-05
	9-N- Phenanthrene	8	350	30	70	8,70E-05
	2-N-Fluoranthene	8	350	30	70	8,70E-05
	1-N-Pyrene	8	350	30	70	8,70E-05
	3-N-Fluoranthene	8	350	30	70	8,70E-05
	7-N-benz[a]anthracene	8	350	30	70	8,70E-05

Table S5. PCB parameters for carcinogenic risk assessment

	<i>Compound</i>	<i>DET (h)</i>	<i>EF (d)</i>	<i>ED(y)</i>	<i>AT (y)</i>	<i>IUR (µg/m³)^d</i>
PCBs	PB105	8	350	30	70	1,10E-03
	PB126	8	350	30	70	3,80E+00
	PB156	8	350	30	70	1,10E-03
	PB157	8	350	30	70	1,10E-03
	PB167	8	350	30	70	1,10E-03
	PB169	8	350	30	70	1,10E+00
	PB187	8	350	30	70	1,10E-03

Table S6. PBDE parameters for non-carcinogenic risk assessment

	<i>Compound</i>	<i>DET (h)</i>	<i>EF (d)</i>	<i>ED(y)</i>	<i>AT (y)</i>	<i>RFC (µg/m³)^e</i>
PBDEs	BDE28	8	350	30	25	1,10E-02 ^d
	BDE47	8	350	30	25	1,10E-02 ^d
	BDE49	8	350	30	25	1,10E-02 ^d
	BDE99 ^e	8	350	30	25	7,00E-03
	BDE100 ^e	8	350	30	25	7,00E-03
	BDE153	8	350	30	25	7,00E-03
	BDE183	8	350	30	25	1,10E-02 ^d

^d as a precautionary approach, the highest value associated with PBDEs was chosen (see par. 4.4)

Table S7. NBFR parameters non carcinogenic risk assessment

	<i>Compound</i>	<i>DET (h)</i>	<i>EF (d)</i>	<i>ED(y)</i>	<i>AT (y)</i>	<i>RFC (µg/m³)^e</i>
NBFRs	HBCD	8	350	30	25	1,10E-02
	TBB	8	350	30	25	1,10E-02
	TBCO	8	350	30	25	1,10E-02
	TBPH	8	350	30	25	1,10E-02

^e as a precautionary approach, the highest value associated with PBDEs was chosen (see par. 4.4)

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