In Silico Approach To Identify Potential Thyroid Hormone Disruptors among Currently Known Dust Contaminants and Their Metabolites

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Table S1. TTR dataset used for development of QSAR model (Weiss et al.[1])

Compound[1]	CAS No[2]	Activity[3]	Model Class[4]
Thyroxine	51-48-9	binder	Train
PCB 5	16605-91-7	binder	Train
3'-OH PCB 138	149589-59-3	binder	Train
3'-OH PCB 180	158076-69-8	binder	Train
3'-OH PCB 182	941713-67-3	binder	Train
3'-OH PCB 203	941713-71-9	binder	Train
4-OH PCB 146	145413-90-7	binder	Train
5-OH PCB 183	1337921-25-1	binder	Train
4-OH PCB 14	1137-59-3	binder	Train
4'-OH PCB 35	124882-64-0	binder	Train
4-OH PCB 50	666747-64-4	binder	Train
4-OH PCB 56	150975-82-9	binder	Train
4'-OH PCB 61	67651-34-7	binder	Train
4'-OH PCB 69	189578-00-5	binder	Train
4'-OH PCB 79	111810-41-4	binder	Train
4'-OH PCB 82	150975-83-0	binder	Train
4-OH PCB 93	527696-88-4	binder	Train
4-OH PCB 106*	1070202-09-3	binder	Train
4'-OH PCB 108	149589-55-9	binder	Train
4-OH PCB 112*	499130-25-5	binder	Train
4'-OH PCB 121	190271-92-2	binder	Train
4-OH PCB 127	157956-69-9	binder	Train
4'-OH PCB 130	158076-62-1	binder	Train
4-OH-PCB 187	158076-68-7	binder	Train
4-OH PCB 201	941713-70-8	binder	Train
4,4'-OH PCB 80	13049-13-3	binder	Train
4,4'-OH PCB 111	150975-84-1	binder	Train
4,4-OH PCB 202	21647-18-7	binder	Train
5-OH PCB 77	42208-08-2	binder	Train
5-OH PCB 105	118024-68-3	binder	Train
PBDE 190	189084-68-2	binder	Train
2'-OH PBDE 3*	300560-92-3	binder	Train
2'-OH PBDE 7*	602326-09-0	binder	Train
2'-OH PBDE 28	4656-58-0	binder	Train
2'-OH PBDE 66	184174-87-6	binder	Train
2'-OH PBDE 68	80246-25-9	binder	Train
3'-OH PBDE 7*	602326-18-1	binder	Train
3'-OH PBDE 28*	24949-30-2	binder	Train
3-OH PBDE 154*	1171030-72-0	binder	Train
4-OH PBDE 42	602326-22-7	binder	Train
4'-OH PBDE 49	602326-23-8	binder	Train
5-OH PBDE 47	602326-30-7	binder	Train
6-OH PBDE 85*	35162-01-7	binder	Train
Tribromobisphenol A	6386-73-8	binder	Train
2,4,6-Tribromophenol	118-79-6	binder	Train

Table S1. TTR dataset used for development of QSAR model

Compound[1]	CAS No[2]	Activity[3]	Model Class[4]
Pentabromophenol	608-71-9	binder	Train
2,4,6-Trichlorophenol	88-06-2	binder	Train
Pentachlorophenol	87-86-5	binder	Train
2,6-Dibromo-4-(2,4,6-tribromo-phenoxy) phenol	91370-78-4	binder	Train
2,4-Dinitrophenol*	51-28-5	binder	Train
4-(2,4,6-Tribromo-phenoxy) phenol	218303-99-2	binder	Train
5,7-Dihydroxy-3-(4-hydroxyphenyl)chromen-4-one*	446-72-0	binder	Train
2,2-Bis[3,5-dibromo-4-(2,3-dibromopropoxy)phenyl]propane	21850-44-2	binder	Train
4-OH-Heptachlorostyrene	77212-81-8	binder	Train
Hexachlorophene*	70-30-4	binder	Train
2-Hydroxy-1,3,7,8-tetrachlorodibenzo-p-dioxin	82019-03-2	binder	Train
2-Hydroxy-3,7,8-trichlorodibenzo-p-dioxin	82019-04-3	binder	Train
2,6,7,8-Tetrachloro-3-Dibenzofuranol	150975-86-3	binder	Train
5-[(E)-2-(4-Hydroxyphenyl)ethenyl]benzene-1,3-diol	501-36-0	binder	Train
Perfluoroheptanoic acid	375-85-9	binder	Train
Perfluorooctanoic acid	335-67-1	binder	Train
Perfluorononanoic acid	375-95-1	binder	Train
Perfluorodecanoic acid	335-76-2	binder	Train
Perfluorotridecanoic acid	72629-94-8	binder	Train
Perfluorohexanesulfonic acid	355-46-4	binder	Train
Perfluorooctanesulfonic acid	1763-23-1	binder	Train
2H-Perfluoro-2-octenoic acid	70887-88-6	binder	Train
7H-Dodecafluoroheptanoic acid	1546-95-8	binder	Train
Perfluorooctansulfinate	647-29-0	binder	Train
Perfluorooctane sulfonamide	754-91-6	binder	Train
Alpha-HBCDD	3194-55-6	nonbinder	Train
Acetochlor	34256-82-1	nonbinder	Train
Alachlor	15972-60-8	nonbinder	Train
Benzene*	71-43-2	nonbinder	Train
Bisphenol A	80-05-7	nonbinder	Train
Bisphenol A bis (2,3-dihydroxypropyl) ether	5581-32-8	nonbinder	Train
Bisphenol A bis (3-chloro-2-hydroxypropyl) ether	4809-35-2	nonbinder	Train
Bisphenol A diglycidyl ether	1675-54-3	nonbinder	Train
Dibromo bisphenol A	29426-78-6	nonbinder	Train
Diphenylsulfone	127-63-9	nonbinder	Train
1,2-Dichlorobenzene*	95-50-1	nonbinder	Train
2,6-Dichlorophenol	87-65-0	nonbinder	Train
2,4,6-Tribromaniline	147-82-0	nonbinder	Train
2,3,5,6-Tetrabrom-p-xylene	23488-38-2	nonbinder	Train
2,3,4,5,6-Pentabromtoluene	87-83-2	nonbinder	Train
Hexabrombenzene	87-82-1	nonbinder	Train
Phenol	108-95-2	nonbinder	Train
Octylphenol	1806-26-4	nonbinder	Train
4-Nonylphenol	104-40-5	nonbinder	Train
4-Phenoxyphenol	831-82-3	nonbinder	Train
4-(1,1,3,3-Tetramethylbutyl)-phenol	140-66-9	nonbinder	Train

Table S1. TTR dataset used for development of QSAR model

Compound[1]	**CAS No**[2]	**Activity**[3]	**Model Class**[4]
4-Tertpentylphenol	80-46-6	nonbinder	Train
Celestolide	13171-00-1	nonbinder	Train
Galaxolide	1222-05-5	nonbinder	Train
Phantolide	15323-35-0	nonbinder	Train
Tonalide	21145-77-7	nonbinder	Train
Traseolide	68857-95-4	nonbinder	Train
Musk Ambrette	123-69-3	nonbinder	Train
Musk ketone	81-14-1	nonbinder	Train
PCB 14*	34883-41-5	nonbinder	Train
PCB 19	38444-73-4	nonbinder	Train
PCB 28	7012-37-5	nonbinder	Train
PCB 51	68194-04-7	nonbinder	Train
PCB 52	35693-99-3	nonbinder	Train
PCB 53	41464-41-9	nonbinder	Train
PCB 95	38379-99-6	nonbinder	Train
PCB 100	39485-83-1	nonbinder	Train
PCB 101	37680-73-2	nonbinder	Train
PCB 104	56558-16-8	nonbinder	Train
PCB 125	74472-39-2	nonbinder	Train
PCB 128	38380-07-3	nonbinder	Train
PCB 136	38411-22-2	nonbinder	Train
PCB 153	35065-27-1	nonbinder	Train
PCB 168	59291-65-5	nonbinder	Train
PCB 190	41411-64-7	nonbinder	Train
PCB 38*	53555-66-1	nonbinder	Train
PCB 77	32598-13-3	nonbinder	Train
PCB 80	33284-52-5	nonbinder	Train
PCB 105	32598-14-4	nonbinder	Train
PCB 111*	39635-32-0	nonbinder	Train
PCB 126	57465-28-8	nonbinder	Train
PCB 138	35065-28-2	nonbinder	Train
PCB 169*	32774-16-6	nonbinder	Train
PBDE 19	147217-73-0	nonbinder	Train
PBDE 39	407606-57-9	nonbinder	Train
PBDE 49	243982-82-3	nonbinder	Train
PBDE 100	189084-64-8	nonbinder	Train
PBDE 127	446254-86-0	nonbinder	Train
PBDE 155	35854-94-5	nonbinder	Train
PBDE 169	446255-18-1	nonbinder	Train
PBDE 183	207122-16-5	nonbinder	Train
PBDE 206	63387-28-0	nonbinder	Train
PBDE 209	1163-19-5	nonbinder	Train
o,p'-DDT	789-02-6	nonbinder	Train
p,p'-DDE	72-55-9	nonbinder	Train
p,p'-DDT	50-29-3	nonbinder	Train
Triclocarban	101-20-2	nonbinder	Train

Table S1. TTR dataset used for development of QSAR model

Compound[1]	CAS No[2]	Activity[3]	Model Class[4]
Tri (2-chloro-ethyl) phosphate	115-96-8	nonbinder	Train
Triphenyl phosphate	115-86-6	nonbinder	Train
Tris(2-ethylhexyl) phosphate	78-42-2	nonbinder	Train
Cresyl diphenyl phosphate	26444-49-5	nonbinder	Train
Butylbenzyl phthalate	85-68-7	nonbinder	Train
di-n-Butylphthalate	84-74-2	nonbinder	Train
Methoprene*	40596-69-8	nonbinder	Train
Perfluorobutanoic acid	375-22-4	nonbinder	Train
Perfluorododecanoic acid	307-55-1	nonbinder	Train
Heptacosafluorotetradecanoic acid	376-06-7	nonbinder	Train
1-Perfluorobutanesulfonic acid	375-73-5	nonbinder	Train
Perfluorodecanesulfonate	335-77-3	nonbinder	Train
2-(Perfluorohexyl)ethane-1-sulfonic acid	27619-97-2	nonbinder	Train
2-Perfluorooctyl ethanol	678-39-7	nonbinder	Train
2-(N-methylperfluoro-1-octanesulfonamido)	24448-09-7	nonbinder	Train
2-(N-ethylperfluoro-1-octanesulfonamido)	1691-99-2	nonbinder	Train
n,n-Dimethyl perfluorooctanesulfonamid	213181-78-3	nonbinder	Train
n-Methyl perfluorooctanesulfonamid	31506-32-8	nonbinder	Train
n-Ethyl perfluorooctansulfonamide	4151-50-2	nonbinder	Train
2-Methyl-4-(1,1,3,3-tetramethylbutyl)-phenol	2219-84-3	nonbinder	Train
Mono(2-ethyl-5-oxohexyl)phthalate	40321-98-0	nonbinder	Train
Mono(5-carboxy-2-ethylpentyl)phthalate	40809-41-4	nonbinder	Train
Mono-2-ethyl-5-hydroxyhexylphthalate	40321-99-1	nonbinder	Train
Bis(2-ethylhexyl)phthalate	117-81-7	nonbinder	Train
Tris(2-chloro-1-(chloromethyl)ethyl)phosphate	13674-87-8	nonbinder	Train
Tri-o-cresyl phosphate	78-30-8	nonbinder	Train
Triisobutyl phosphate	126-71-6	nonbinder	Train
Tris(2-butoxyethyl) phosphate	78-51-3	nonbinder	Train
Bisphenol A diphosphate	75805-15-1	nonbinder	Train
Resorcinol tetraphenyl diphosphate	57583-54-7	nonbinder	Train
9,10-Dihydro-9-oxa-10-phosphaphenanthren 10-oxide	35948-25-5	nonbinder	Train
Lauric acid	143-07-7	nonbinder	Train
Myristic acid	544-63-8	nonbinder	Train
Stearic acid	57-11-4	nonbinder	Train
Octanoic acid (Caprylic acid)	124-07-2	nonbinder	Train
Hexaethyleneglycol monododecyl ether	3055-96-7	nonbinder	Train
4-Phenylmethyl phenol	101-53-1	nonbinder	Train
4-OH Biphenyl	92-69-3	nonbinder	Train
2,3-Dichloro-7-hydroxydibenzo-p-dioxin	97741-80-5	nonbinder	Train
2,3-Dichlorophenol	576-24-9	nonbinder	Train
p,p'-DDOH*	2642-82-2	nonbinder	Train
2-Bromo-4-(2,4,6-tribromo-phenoxy) phenol	218303-98-1	binder	Valid
2,4-Dibromphenol	615-58-7	binder	Valid
2,4,5-Trichlorophenol	95-95-4	binder	Valid
3,3',5,5'-Tetrachlorobisphenol A	79-95-8	binder	Valid
3,3',5,5'-Tetrabromobisphenol A	79-94-7	binder	Valid

Table S1. TTR dataset used for development of QSAR model

Compound[1]	**CAS No**[2]	**Activity**[3]	**Model Class**[4]
PCB 127*	39635-33-1	binder	Valid
2-OH PCB 105	42208-07-1	binder	Valid
4-OH PCB 107	152969-11-4	binder	Valid
4'-OH PCB 109*	192190-10-6	binder	Valid
4'-OH PCB 172	849833-74-5	binder	Valid
3-OH PBDE 47	24949-31-3	binder	Valid
PBDE 181	189084-67-1	binder	Valid
PBDE 185	405237-86-7	binder	Valid
4'-OH PBDE 17*	602326-21-6	binder	Valid
6-OH PBDE 47	79755-43-4	binder	Valid
Triclosan	3380-34-5	binder	Valid
Perfluoro-n-pentanoic acid	2706-90-3	binder	Valid
Perfluorohexanoic acid	307-24-4	binder	Valid
2-Chlorophenol*	95-57-8	nonbinder	Valid
3-Chlorophenol*	108-43-0	nonbinder	Valid
Decanoic acid (Capric acid)	334-48-5	nonbinder	Valid
Hexanoic acid	142-62-1	nonbinder	Valid
2-Hydroxy-7,8-dichlorodibenzofuran	74423-77-1	nonbinder	Valid
8-Hydroxy-2,3,4-trichlorodibenzofuran	103124-63-6	nonbinder	Valid
Monobromobisphenol A	6073-11-6	nonbinder	Valid
o,p'-DDD	53-19-0	nonbinder	Valid
3-OH PCB 30	70792-94-8	nonbinder	Valid
PCB 47	2437-79-8	nonbinder	Valid
PCB 74	32690-93-0	nonbinder	Valid
PCB 110*	38380-03-9	nonbinder	Valid
PCB 118	31508-00-6	nonbinder	Valid
PCB 122	76842-07-4	nonbinder	Valid
PCB 162*	39635-34-2	nonbinder	Valid
PCB 170	35065-30-6	nonbinder	Valid
PCB 180	35065-29-3	nonbinder	Valid
PBDE 28	41318-75-6	nonbinder	Valid
PBDE 38	337513-54-9	nonbinder	Valid
PBDE 47	5436-43-1	nonbinder	Valid
PBDE 79	446254-48-4	nonbinder	Valid
PBDE 99	60348-60-9	nonbinder	Valid
PBDE 153	68631-49-2	nonbinder	Valid
Squalene	111-02-4	nonbinder	Valid
Perfluoroundecanoic acid	2058-94-8	nonbinder	Valid
2-Perfluorohexyl ethanol	647-42-7	nonbinder	Valid

[1]Chemical name or commonly used abbreviation or trade name; [2]Chemical Abstracts Service numbers; [3]Binders were defined as compounds with IC_{50} for human TTR < 10 μM and for nonbinders ≥10 μM; [4]Data set was divided in a training set (Train) for model development and a validation set (Valid) for external model validation.*Chemicals were not tested in the assay described in *Lans et al*.[2]

Table S2. Organic contaminants identified in indoor dust with Chemical Abstracts Service numbers (CAS No), chemical name, abbreviation or trade name, chemical class, and references

Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
Acetone	67-64-1	VOC	[3]
Ambralux	54464-57-2	VOC	[4]
Benzaldehyde	100-52-7	VOC	[3]
2-Butenal	4170-30-3	VOC	[3]
Decanal	112-31-2	VOC	[3]
Dibutylhydroxytoluene	128-37-0	VOC	[3, 5]
2-Furaldehyde	98-01-1	VOC	[3]
Furfuryl alcohol	98-00-0	VOC	[3]
Heptanal	111-71-7	VOC	[3]
Heptenal	29381-66-6	VOC	[3]
Hexanal	66-25-1	VOC	[3]
Hexenal	56-29-1	VOC	[3]
3-Methyl-butanal	590-86-3	VOC	[3]
2-Methyl-propenal	78-85-3	VOC	[3]
Nonanal	124-19-6	VOC	[3]
Nonenal	30551-15-6	VOC	[3]
Octanal	124-13-0	VOC	[3]
Octenal	25447-69-2	VOC	[3]
Pentanal	110-62-3	VOC	[3]
Pentylfuran	64079-01-2	VOC	[3]
Pyrrole	109-97-7	VOC	[3]
2-Benzoyl-5-methoxyphenol	131-57-7	UV filter	[6]
2,2'-Dihydroxy-4-methoxybenzophenone	131-53-3	UV filter	[6]
2,4-Dihydroxybenzophenone	131-56-6	UV filter	[3, 6]
4-Hydroxybenzophenone	1137-42-4	UV filter	[6]
2,4,2',4'-Tetrahydroxybenzophenone	131-55-5	UV filter	[6]
2-Aminobenzothiazole	136-95-8	UV filter	[6]
1H-Benzotriazole	95-14-7	UV filter	[6]
Benzothiazole	95-16-9	UV filter	[6]
5-Chlorobenzotriazole	94-97-3	UV filter	[6]
5,6-Dimethylbenzotriazole	4184-79-6	UV filter	[6]
1-Hydroxybenzotriazole	2592-95-2	UV filter	[6]
2-Hydroxybenzothiazole	934-34-9	UV filter	[6]
2-[2-Hydroxy-3,5-di-(1,1-dimethylbenzyl)]-2H-benzotriazole (Tinuvin 234)	70321-86-7	UV filter	[7]
2-(Methylthio)benzothiazole	615-22-5	UV filter	[6]
4-Methylbenzotriazole	29878-31-7	UV filter	[6]
5-Methylbenzotriazole	136-85-6	UV filter	[6]
2-(Thiocyanomethylthio)benzothiazole	21564-17-0	UV filter	[6]
2-(2-Hydroxy-3,5-di-tert-butylphenyl)benzotriazole (Tinuvin 320)	3846-71-7	UV filter	[7]
2-(2'-Hydroxy-3'-tert-butyl-5'-methylphenyl)-5-chlorobenzotriazole (Tinuvin 326)	3896-11-5	UV filter	[7, 8]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
2-(2-Hydroxy-3,5-di-tert-butylphenyl)-5-chlorobenzotriazole (Tinuvin 327)	3864-99-1	UV filter	[7, 8]
2-(2-Hydroxy-3,5-di-tert-pentylphenyl)benzotriazole (Tinuvin 328)	25973-55-1	UV filter	[7, 8]
2-(2-Hydroxy-5-methphenyl) benzotriazole (Tinuvin P)	2440-22-4	UV filter	[8]
2,3,7,8-Tetrabromodibenzodioxin	50585-41-6	PXDD/F	[9]
1,2,3,7,8-Pentabromodibenzodioxin	109333-34-8	PXDD/F	[9]
1,2,3,4,7,8-Hexabromodibenzodioxin	110999-44-5	PXDD/F	[9]
1,2,3,4,6,7,8-Heptabromodibenzodioxin	110999-47-8	PXDD/F	[9]
Octabromodibenzodioxin	2170-45-8	PXDD/F	[9]
2,3,7,8-Tetrachlorodibenzodioxin	1746-01-6	PXDD/F	[9-11]
1,2,3,7,8-Pentachlorodibenzodioxin	40321-76-4	PXDD/F	[9-11]
1,2,3,4,7,8-Hexachlorodibenzodioxin	39227-28-6	PXDD/F	[9-11]
1,2,3,6,7,8-Hexachlorodibenzodioxin	57653-85-7	PXDD/F	[9-11]
1,2,3,7,8,9-Hexachlorodibenzodioxin	19408-74-3	PXDD/F	[9-11]
1,2,3,4,6,7,8-Heptachlorodibenzodioxin	35822-46-9	PXDD/F	[9-11]
Octachlorodibenzodioxin	3268-87-9	PXDD/F	[9-11]
2,3,7,8-Tetrabromodibenzofuran	67733-57-7	PXDD/F	[9]
2,3,4,7,8-Pentabromodibenzofuran	131166-92-2	PXDD/F	[9]
1,2,3,4,7,8-Hexabromodibenzofuran	129880-08-6	PXDD/F	[9]
1,2,3,4,6,7,8-Heptabromodibenzofuran	107555-95-3	PXDD/F	[9]
2,3,7,8-Tetrachlorodibenzofuran	51207-31-9	PXDD/F	[9-11]
1,2,3,7,8-Pentachlorodibenzofuran	57117-41-6	PXDD/F	[9-11]
1,2,3,4,8-Pentachlorodibenzofuran	67517-48-0	PXDD/F	[9]
2,3,4,7,8-Pentachlorodibenzofuran	57117-31-4	PXDD/F	[9-11]
1,2,3,4,7,8-Hexachlorodibenzofuran	70648-26-9	PXDD/F	[9-11]
1,2,3,4,7,9-Hexachlorodibenzofuran	91538-84-0	PXDD/F	[9]
1,2,3,6,7,8-Hexachlorodibenzofuran	57117-44-9	PXDD/F	[9-11]
1,2,3,7,8,9-Hexachlorodibenzofuran	72918-21-9	PXDD/F	[9-11]
2,3,4,6,7,8-Hexachlorodibenzofuran	60851-34-5	PXDD/F	[9-11]
1,2,3,4,6,7,8-Heptachlorodibenzofuran	67562-39-4	PXDD/F	[9-11]
1,2,3,4,7,8,9-Heptachlorodibenzofuran	55673-89-7	PXDD/F	[9-11]
Octachlorodibenzofuran	39001-02-0	PXDD/F	[9-11]
Benzyl 2-ethylhexyl phthalate	27215-22-1	Phthalate	[12]
Benzylbutyl phthalate	85-68-7	Phthalate	[3, 5, 12-26]
Bis(2-ethylhexyl)2,3,4,5-tetrabromophthalate	26040-51-7	Phthalate	[27-35]
Bis(2-n-butoxyethyl)phthalate	117-83-9	Phthalate	[16]
Di(2-ethoxyethyl) phthalate	605-54-9	Phthalate	[16]
Di(2-ethylhexyl) terephthalate	6422-86-2	Phthalate	[36]
Di-2-ethylhexyl phthalate	117-81-7	Phthalate	[3, 5, 12-26]
Dibenzyl phthalate	523-31-9	Phthalate	[12]
Dicyclohexyl phthalate	84-61-7	Phthalate	[3, 12, 15, 16, 18, 19, 24]
Diethyl phthalate	84-66-2	Phthalate	[3, 12-26]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	**CAS No**	**Chemical Class**[2]	**References**[3]
Di-iso-butyl phthalate	84-69-5	Phthalate	[3, 5, 12-16, 18, 20, 22, 24-26]
Di-iso-decyl phthalate	26761-40-0	Phthalate	[12, 13, 18, 23, 24]
Diisoheptyl phthalate	71888-89-6	Phthalate	[12]
Diisononyl phthalate	28553-12-0	Phthalate	[5, 12, 13, 22-26]
Dimethyl phthalate	131-11-3	Phthalate	[3, 12-16, 18-21, 23-26]
Dimethylglycol phthalate	117-82-8	Phthalate	[16, 18, 25, 26]
Di-n-butyl phthalate	84-74-2	Phthalate	[3, 5, 12-26]
Di-n-hexyl phthalate	84-75-3	Phthalate	[3, 12, 15, 16, 18, 19]
Di-n-nonylphthalate	84-76-4	Phthalate	[16, 18]
Di-n-octyl phthalate	117-84-0	Phthalate	[3, 15, 16, 18, 19, 21, 23]
Di-n-pentyl phthalate	131-18-0	Phthalate	[16, 24]
Dipropyl phthalate	131-16-8	Phthalate	[3]
Diundecyl phthalate	3648-20-2	Phthalate	[12]
Hexyl 2-ethylhexyl phthalate	75673-16-4	Phthalate	[16]
1,2-Benzenedicarboxylic acid	68515-40-2	Phthalate	[12]
Phenol	108-95-2	Phenol	[3]
2,4-Dichlorophenol	120-83-2	Phenol	[3]
4-Cumylphenol	599-64-4	Phenol	[3]
4-Octylphenol	1806-26-4	Phenol	[3]
4-Nonylphenol	104-40-5	Phenol	[3]
Nonyl phenols	25154-52-3	Phenol	[3]
o-Phenylphenol	90-43-7	Phenol	[3]
p-Phenylphenol	92-69-3	Phenol	[3]
4-Nitrophenol	100-02-7	Phenol	[3]
4-Tert-butylphenol	98-54-4	Phenol	[3]
Bisphenol A	80-05-7	Phenol	[3, 25, 37, 38]
Bisphenol B	77-40-7	Phenol	[38]
Bisphenol F	2467-02-9	Phenol	[38]
Bisphenol M	13595-25-0	Phenol	[25]
Bisphenol P	2167-51-3	Phenol	[38]
Bisphenol S	80-09-1	Phenol	[38]
Bisphenol Z	843-55-0	Phenol	[38]
Bisphenol AF	1478-61-1	Phenol	[38]
Bisphenol AP	1571-75-1	Phenol	[38]
Bisphenol A bis(2,3-dihydroxypropyl) ether	5581-32-8	Phenol	[39]
Bisphenol A (3-chloro-2-hydroxypropyl) (2,3-dihydroxypropyl) ether	227947-06-0	Phenol	[39]
Bisphenol A (2,3-dihydroxypropyl) glycidyl ether	76002-91-0	Phenol	[39]
Bisphenol A diglycidyl ether	1675-54-3	Phenol	[25, 39]
4-Nonylphenol monoethoxylate	104-35-8	Phenol	[3]
4-Octylphenol monoethoxylate	51437-89-9	Phenol	[3]
4-Nonylphenol diethoxylate	20427-84-3	Phenol	[3]
Octylphenol diethoxylate	51437-90-2	Phenol	[3]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
Nonylphenol ethoxycarboxylate	3115-49-9	Phenol	[3]
3-Biphenylol	580-51-8	Phenol	[3]
4,4'-Biphenyldiol	92-88-6	Phenol	[3]
4,4'-Methylenediphenol	620-92-8	Phenol	[3]
Bis(3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanol) hydrogen phosphate (4:2 diPAP)	135098-69-0	PFAS	[40]
Bis[2-(perfluorohexyl)ethyl] Phosphate (6:2 diPAP)	57677-95-9	PFAS	[40]
Bis[2-(perfluorooctyl)ethyl] Phosphate (8:2 diPAP)	678-41-1	PFAS	[40]
Bis(3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanol) hydrogen phosphate (10:2 diPAP)	1895-26-7	PFAS	[40]
2-(N-Methylperfluoro-1-octanesulfonamido)- ethanol	24448-09-7	PFAS	[3, 41-43]
2-(N-Ethylperfluoro-1-octanesulfonamido)-ethanol	1691-99-2	PFAS	[3, 41-44]
2-(Perfluorobutyl)ethanol	2043-47-2	PFAS	[45]
2-(Perfluorohexyl)ethanol	647-42-7	PFAS	[3, 40-43, 45]
2-(Perfluorooctyl)ethanol	678-39-7	PFAS	[3, 40-43, 45]
2-(Perfluorodecyl)ethanol	865-86-1	PFAS	[3, 40-43, 45]
5:3 Fluorotelomer saturated carboxylic acid	914637-49-3	PFAS	[42]
6:2 Fluorotelomer unsaturated carboxylic acid	70887-88-6	PFAS	[42, 44]
8:2 Fluorotelomer unsaturated carboxylic acid	70887-84-2	PFAS	[42, 44]
10:2 Fluorotelomer unsaturated carboxylic acid	70887-94-4	PFAS	[42]
Perfluorobutanoic acid	375-22-4	PFAS	[42, 43, 46, 47]
Perfluorohexanoic acid	307-24-4	PFAS	[3, 41-44, 46-48]
Perfluoroheptanoic acid	375-85-9	PFAS	[3, 41-44, 47-49]
Perfluorooctanoic acid	335-67-1	PFAS	[3, 41-51]
Perfluorononanoic acid	375-95-1	PFAS	[3, 41-44, 46-49]
Perfluorodecanoic acid	335-76-2	PFAS	[3, 41-44, 46-49]
Perfluorododecanoic acid	307-55-1	PFAS	[3, 41-44, 47-49]
Perfluoropentanoic acid	2706-90-3	PFAS	[42-44, 47]
Perfluoroundecanoic acid	2058-94-8	PFAS	[3, 41-43, 47-49]
Perfluorotridecanoic acid	72629-94-8	PFAS	[42-44, 48]
Perfluorotetradecanoic acid	376-06-7	PFAS	[42-44, 48]
Perfluro-n-tetradecanoic acid	16517-11-6	PFAS	[41]
Perfluorohexane hosphonic acid	40143-76-8	PFAS	[40]
Perfluorooctane hosphonic acid	40143-78-0	PFAS	[40]
Perfluorodecane hosphonic acid	52299-26-0	PFAS	[40]
Perfluorooctane sulfonamide	754-91-6	PFAS	[3, 44, 49]
N-Ethylperfluorooctane sulfonamide	4151-50-2	PFAS	[3, 41, 42, 44]
N-Methylperfluorooctane sulfonamide	31506-32-8	PFAS	[41, 42, 44]
Perfluorobutane sulfonate	375-73-5	PFAS	[3, 42-44, 46, 47]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	**CAS No**	**Chemical Class**[2]	**References**[3]
Perfluorohexane sulfonate	355-46-4	PFAS	[3, 42-44, 46, 47, 49, 51]
Perfluoroheptane sulfonate	375-92-8	PFAS	[44, 47]
Perfluorooctane sulfonate	1763-23-1	PFAS	[3, 40-47, 49-51]
Perfluorononane sulfonate	68259-12-1	PFAS	[47]
Perfluorodecane sulfonate	335-77-3	PFAS	[42, 44, 47, 49]
Perfluoropentane sulfonate	2706-91-4	PFAS	[47]
Perfluoro-p-ethylcyclohexane sulfonate	646-83-3	PFAS	[40]
6:2 Fluorotelomer sulfonate	27619-97-2	PFAS	[44, 47]
8:2 Fluorotelomer sulfonate	39108-34-4	PFAS	[44, 47]
N-Methyl perfluorooctane sulfonamidethylacrylate	25268-77-3	PFAS	[3]
PCN 1	90-13-1	PCN	[9]
PCN 2	91-58-7	PCN	[9]
PCN 3	2050-69-3	PCN	[9]
PCN 4	2198-75-6	PCN	[9]
PCN 5	1825-31-6	PCN	[9]
PCN 6	1825-30-5	PCN	[9]
PCN 7	2050-72-8	PCN	[9]
PCN 8	2050-73-9	PCN	[9]
PCN 9	2050-74-0	PCN	[9]
PCN 10	2050-75-1	PCN	[9]
PCN 11	2065-70-5	PCN	[9]
PCN 12	2198-77-8	PCN	[9]
PCN 13	50402-52-3	PCN	[9]
PCN 14	50402-51-2	PCN	[9]
PCN 15	55720-33-7	PCN	[9]
PCN 16	51570-44-6	PCN	[9]
PCN 17	55720-34-8	PCN	[9]
PCN 18	55720-35-9	PCN	[9]
PCN 19	51570-43-5	PCN	[9]
PCN 20	55720-36-0	PCN	[9]
PCN 21	55720-37-1	PCN	[9]
PCN 22	55720-38-2	PCN	[9]
PCN 23	2437-55-0	PCN	[9]
PCN 24	2437-54-9	PCN	[9]
PCN 25	55720-39-3	PCN	[9]
PCN 26	55720-40-6	PCN	[9]
PCN 28	53555-63-8	PCN	[9]
PCN 29	149864-78-8	PCN	[9]
PCN 33	51570-45-7	PCN	[9]
PCN 34	67922-21-8	PCN	[9]
PCN 35	6529-87-9	PCN	[9]
PCN 36	67922-22-9	PCN	[9]
PCN 37	67922-23-0	PCN	[9]
PCN 38	149864-80-2	PCN	[9]
PCN 40	67922-24-1	PCN	[9]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
PCN 41	149864-82-4	PCN	[9]
PCN 42	53555-64-9	PCN	[9]
PCN 43	31604-28-1	PCN	[9]
PCN 44	55720-42-8	PCN	[9]
PCN 45	150224-15-0	PCN	[9]
PCN 47	55720-43-9	PCN	[9]
PCN 49	67922-25-2	PCN	[9]
PCN 50	67922-26-3	PCN	[9]
PCN 51	150224-18-3	PCN	[9]
PCN 52	53555-65-0	PCN	[9]
PCN 53	150224-24-1	PCN	[9]
PCN 54	150224-16-1	PCN	[9]
PCN 55	150224-23-0	PCN	[9]
PCN 56	150205-21-3	PCN	[9]
PCN 57	150224-20-7	PCN	[9]
PCN 58	150224-19-4	PCN	[9]
PCN 59	150224-25-2	PCN	[9]
PCN 60	150224-17-2	PCN	[9]
PCN 61	150224-22-9	PCN	[9]
PCN 62	150224-21-8	PCN	[9]
PCN 63	58877-88-6	PCN	[9]
PCN 64	67922-27-4	PCN	[9]
PCN 65	103426-93-3	PCN	[9]
PCN 66	103426-96-6	PCN	[9]
PCN 67	103426-97-7	PCN	[9]
PCN 68	103426-95-5	PCN	[9]
PCN 69	103426-94-4	PCN	[9]
PCN 70	17062-87-2	PCN	[9]
PCN 71	90948-28-0	PCN	[9]
PCN 72	103426-92-2	PCN	[9]
PCN 73	58863-14-2	PCN	[9]
PCN 74	58863-15-3	PCN	[9]
PCN 75	2234-13-1	PCN	[9]
PCB 10	33146-45-1	PCB	[3]
PCB 15	2050-68-2	PCB	[3]
PCB 18	37680-65-2	PCB	[52]
PCB 28	7012-37-5	PCB	[25, 33, 52, 53]
PCB 31	16606-02-3	PCB	[3, 25, 33]
PCB 33	38444-86-9	PCB	[3]
PCB 37	38444-90-5	PCB	[52]
PCB 44	41464-39-5	PCB	[3, 52]
PCB 49	41464-40-8	PCB	[52]
PCB 52	35693-99-3	PCB	[3, 22, 25, 26, 33, 52, 53]
PCB 70	32598-11-1	PCB	[3, 52]
PCB 74	32690-93-0	PCB	[33, 52]
PCB 77	32598-13-3	PCB	[3, 9, 10, 25, 52]

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Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
PCB 81	70362-50-4	PCB	[9, 10, 52]
PCB 87	38380-02-8	PCB	[3, 52]
PCB 95	38379-99-6	PCB	[3, 33]
PCB 99	38380-01-7	PCB	[33, 52]
PCB 101	37680-73-2	PCB	[3, 22, 25, 26, 33, 52, 53]
PCB 105	32598-14-4	PCB	[3, 9, 10, 25, 26, 33, 52-55]
PCB 110	38380-03-9	PCB	[3, 33]
PCB 114	74472-37-0	PCB	[9, 10, 53]
PCB 118	31508-00-6	PCB	[3, 9, 10, 22, 25, 26, 33, 52-54, 56, 57]
PCB 119	56558-17-9	PCB	[52]
PCB 123	65510-44-3	PCB	[9, 10, 52]
PCB 126	57465-28-8	PCB	[3, 9, 10, 25, 52]
PCB 128	38380-07-3	PCB	[33, 52]
PCB 132	38380-05-1	PCB	[3]
PCB 138	35065-28-2	PCB	[3, 22, 25, 26, 33, 52-57]
PCB 144	68194-14-9	PCB	[52]
PCB 149	38380-04-0	PCB	[3, 33]
PCB 151	52663-63-5	PCB	[52]
PCB 153	35065-27-1	PCB	[3, 22, 25, 26, 33, 52-57]
PCB 156	38380-08-4	PCB	[9, 10, 33, 52, 53, 57]
PCB 157	69782-90-7	PCB	[9, 10, 52, 53]
PCB 158	74472-42-7	PCB	[52]
PCB 167	52663-72-6	PCB	[9, 10, 52, 53]
PCB 168	59291-65-5	PCB	[52]
PCB 169	32774-16-6	PCB	[3, 9, 10, 52]
PCB 170	35065-30-6	PCB	[33, 52, 55-57]
PCB 177	52663-70-4	PCB	[52]
PCB 180	35065-29-3	PCB	[3, 22, 25, 26, 33, 52-57]
PCB 183	52663-69-1	PCB	[33, 52, 57]
PCB 187	52663-68-0	PCB	[33, 52, 57]
PCB 189	39635-31-9	PCB	[9, 10, 52, 53]
PCB 194	35694-08-7	PCB	[33, 52, 53]
PCB 199	52663-75-9	PCB	[33, 52]
PCB 206	40186-72-9	PCB	[33]
PCB 209	2051-24-3	PCB	[3, 33, 53]
Methyl paraben	99-76-3	Paraben	[3, 39, 58]
Ethyl paraben	120-47-8	Paraben	[3, 39, 58]
Propyl paraben	94-13-3	Paraben	[3, 39, 58]
Iso-propyl paraben	4191-73-5	Paraben	[58]
Butyl paraben	94-26-8	Paraben	[3, 39, 58]
Heptyl paraben	1085-12-7	Paraben	[39]
Benzyl paraben	94-18-8	Paraben	[39]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	**CAS No**	**Chemical Class**[2]	**References**[3]
Acenaphthene	83-32-9	PAH	[3, 25, 59-61]
Acenaphthylene	208-96-8	PAH	[3, 59-61]
Anthracene	120-12-7	PAH	[3, 25, 26, 59-62]
Benzo(a)anthracene	56-55-3	PAH	[3, 54, 59-63]
Benzo(a)pyrene	50-32-8	PAH	[3, 22, 25, 26, 54, 59-63]
Benzo(b)fluoranthene	205-99-2	PAH	[3, 54, 59-63]
Benzo(e)pyrene	192-97-2	PAH	[3]
Benzo(ghi)perylene	191-24-2	PAH	[3, 59-62]
Benzo(k)fluoranthene	207-08-9	PAH	[3, 54, 59-63]
Chrysene	218-01-9	PAH	[3, 54, 59-63]
Coronene	191-07-1	PAH	[3, 63]
Cyclopenta(cd)pyrene	27208-37-3	PAH	[3]
Dibenzo(a,e)pyrene	192-65-4	PAH	[63]
Dibenzo(a,h)anthracene	53-70-3	PAH	[3, 54, 59-63]
Fluoranthene	206-44-0	PAH	[3, 22, 25, 26, 59-62]
Fluorene	86-73-7	PAH	[3, 25, 26, 60, 61]
Indeno(1,2,3-cd)pyrene	193-39-5	PAH	[3, 54, 59-63]
Naphthalene	91-20-3	PAH	[3, 59-61]
Phenanthrene	85-01-8	PAH	[3, 22, 25, 26, 59-62]
Pyrene	129-00-0	PAH	[3, 22, 25, 26, 59-62]
Squalene	111-02-4	PAH	[64]
Monobutyltin	78763-54-9	Organotin	[3]
Monooctyltin	15231-57-9	Organotin	[3]
Dibutyltin	14488-53-0	Organotin	[3]
Dioctyltin	60004-29-7	Organotin	[3]
Tributyltin	36643-28-4	Organotin	[3]
Triphenyltin	668-34-8	Organotin	[3]
Decamethylcyclopentasiloxane	541-02-6	Organosiloxane	[65]
Decamethyltetrasiloxane	141-62-8	Organosiloxane	[65]
Docosamethyldecasiloxane	556-70-7	Organosiloxane	[65]
Dodecamethylcyclohexasiloxane	540-97-6	Organosiloxane	[65]
Dodecamethylpentasiloxane	141-63-9	Organosiloxane	[65]
Eicosamethylnonasiloxane	2652-13-3	Organosiloxane	[65]
Hexacosamethyldodecasiloxane	2471-08-1	Organosiloxane	[65]
Hexadecamethylheptasiloxane	541-01-5	Organosiloxane	[65]
Octadecamethyloctasiloxane	556-69-4	Organosiloxane	[65]
Octamethylcyclotetrasiloxane	556-67-2	Organosiloxane	[65]
Tetracosamethylhendecasiloxane	107-53-9	Organosiloxane	[65]
Tetradecamethylcycloheptasiloxane	107-50-6	Organosiloxane	[65]
Tetradecamethylhexasiloxane	107-52-8	Organosiloxane	[65]
Tetradecasiloxane	2471-10-5	Organosiloxane	[65]
Tridecasiloxane	2471-09-2	Organosiloxane	[65]
Diphenylethylhexyl phosphates	1241-94-7	Organophosphate	[13, 14, 66]
Trimethyl phosphate	512-56-1	Organophosphate	[67]
Triethyl phosphates	78-40-0	Organophosphate	[13, 14, 29, 33, 67, 68]
Tri-n-propyl phosphate	513-08-6	Organophosphate	[13, 29, 33]

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Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
Triisopropyl phosphates	513-02-0	Organophosphate	[13]
Tri-n-butyl-phosphate	126-73-8	Organophosphate	[3, 13, 14, 22, 25, 26, 28-30, 33, 66-69]
Triisobutyl phosphate	126-71-6	Organophosphate	[3, 13, 14, 29, 33, 66, 68]
Tripentyl Phosphates	2528-38-3	Organophosphate	[13, 14]
Trihexyl phosphates	2528-39-4	Organophosphate	[13, 14]
Triphenyl phosphate	115-86-6	Organophosphate	[3, 13, 14, 28-30, 33, 66-70]
Tricresyl phosphate	78-32-0	Organophosphate	[13, 14, 29, 30, 33, 67-69]
Tris(2-ethylhexyl) phosphate	78-42-2	Organophosphate	[13, 14, 67]
Tris(2-butoxyethyl) phosphate	78-51-3	Organophosphate	[3, 13, 14, 28-30, 33, 66-69]
Tris(2-chloroethyl) phosphate	115-96-8	Organophosphate	[3, 12-14, 29, 30, 33, 35, 66-69]
Tris(chloropropyl) phosphate	6145-73-9	Organophosphate	[67]
Tris(1,3-dichloropropyl) phosphate	40120-74-9	Organophosphate	[29, 30, 33, 35, 69, 70]
Tris(2,3-dichloropropyl) phosphate	78-43-3	Organophosphate	[68]
Tris(2-chloroisopropyl) phosphate	13674-84-5	Organophosphate	[3, 13, 14, 29, 30, 33, 35, 66, 68, 69]
Tri(1,3-dichloroisopropyl) phosphates	13674-87-8	Organophosphate	[3, 13, 14, 66, 67]
2,2-Bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	38051-10-4	Organophosphate	[12]
Triphenyl phosphine oxide	791-28-6	Organophosphate	[3]
Celestolide	13171-00-1	Musk	[3, 4, 71]
Galaxolide	1222-05-5	Musk	[3, 4, 22, 25, 26, 71, 72]
Galaxolidone	256393-37-0	Musk	[4, 72]
Traesolide	68140-48-7	Musk	[3, 4, 71]
Musk ambrette	83-66-9	Musk	[4]
Musk indanone	33704-61-9	Musk	[3]
Musk ketone	81-14-1	Musk	[3, 4, 71, 72]
Musk moskene	116-66-5	Musk	[3, 4, 72]
Musk phantolide	15323-35-0	Musk	[3, 4, 71]
Musk tonalide	21145-77-7	Musk	[3, 4, 22, 25, 26, 71, 72]
Musk xylene	81-15-2	Musk	[3, 4, 71, 72]
Biphenyl	92-52-4	Miscellaneous	[3]
Cholesterol	57-88-5	Miscellaneous	[64]
Di-(2-ethylhexyl) adipate	103-23-1	Miscellaneous	[3, 5]
1,4-Dioxacycloheptadecane-5,17-dione	105-95-3	Miscellaneous	[4]
Diisononyl cyclohexane-1,2-dicarboxylate	166412-78-8	Miscellaneous	[36]
4-Hydroxybenzoic acid	99-96-7	Miscellaneous	[39]
Octabromotrimethylphenylindane	155613-93-7	Miscellaneous	[73, 74]
1,2-Dichlorobenzene	95-50-1	Chlorinatedbenzene	[3]
1,3-Dichlorobenzene	541-73-1	Chlorinatedbenzene	[3]
1,4-Dichlorobenzene	106-46-7	Chlorinatedbenzene	[3]
1,2,3-Trichlorobenzene	87-61-6	Chlorinatedbenzene	[3]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
1,2,4-Trichlorobenzene	120-82-1	Chlorinatedbenzene	[3]
1,2,3,4-Tetrachlorobenzene	634-66-2	Chlorinatedbenzene	[3]
1,2,4,5-Tetrachlorobenzene	95-94-3	Chlorinatedbenzene	[3]
Pentachlorobenzene	608-93-5	Chlorinatedbenzene	[3]
Hexachlorobenzene	118-74-1	Chlorinatedbenzene	[3, 33, 57, 75]
Alachlore	15972-60-8	Biocide	[3]
Aldrin	309-00-2	Biocide	[3, 22, 25, 76]
Allethrin	584-79-2	Biocide	[3, 77]
Bendiocarb	22781-23-3	Biocide	[3]
Bifenthrin	82657-04-3	Biocide	[3, 77]
Carbaryl	63-25-2	Biocide	[3]
Chlordane	5103-71-9	Biocide	[3, 22, 25, 33, 76]
Chlorothalonil	1897-45-6	Biocide	[3]
Chlorpyrifos	2921-88-2	Biocide	[3, 22, 25, 26, 76, 78]
1-[(2,4-Dichlorophenyl)aminocarbonyl]-1-cyclopropanecarboxylic acid (Cyclanilide)	113136-77-9	Biocide	[79]
Cyfluthrin	68359-37-5	Biocide	[3, 22, 76, 77]
Cyhalothrin	68085-85-8	Biocide	[3, 77]
Cypermethrin	52315-07-8	Biocide	[3, 22, 25, 26, 77]
Cyphenothrin	39515-40-7	Biocide	[3]
Deltamethrin	52918-63-5	Biocide	[3, 26, 77]
Diazinon	333-41-5	Biocide	[3, 22, 25, 76]
Dicamba	1918-00-9	Biocide	[76]
Dichlorvos	62-73-7	Biocide	[25, 78]
2,4-Dichlorophenoxyacetic acid	94-75-7	Biocide	[3, 76]
Dicofol	115-32-2	Biocide	[3]
Dieldrin	60-57-1	Biocide	[3, 22, 25, 26, 76]
Endosulfan	959-98-8	Biocide	[25]
Endrin	72-20-8	Biocide	[3, 25, 76]
Esfenvalerate	66230-04-4	Biocide	[3, 77]
Fenpropathrin	39515-41-8	Biocide	[77]
Heptachlor	76-44-8	Biocide	[3, 22, 25, 76]
Hexachlorocyclohexane	58-89-9	Biocide	[3, 22, 25, 26, 33, 57, 75, 76]
Imiprothrin	72963-72-5	Biocide	[77]
Methoxychlore	72-43-5	Biocide	[3]
Methyl parathion	298-00-0	Biocide	[3]
Oxadiazon	19666-30-9	Biocide	[26]
Oxychlordane	27304-13-8	Biocide	[28, 33, 57]
o,p'-DDD*	53-19-0	Biocide	[33]
o,p'-DDE*	3424-82-6	Biocide	[33, 75]
o,p'-DDT*	789-02-6	Biocide	[33, 57, 75]
p,p'-DDD*	72-54-8	Biocide	[3, 33, 57, 75]
p,p'-DDE*	72-55-9	Biocide	[3, 22, 26, 33, 56, 57, 75]
p,p'-DDT*	50-29-3	Biocide	[3, 22, 25, 26, 33, 57, 75, 76]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
Pentachlorophenol	87-86-5	Biocide	[3]
Permethrin	52645-53-1	Biocide	[3, 22, 25, 26, 76, 77]
Phenothrin	26002-80-2	Biocide	[3, 77]
Piperonyl butoxide	51-03-6	Biocide	[3]
Prallethrin	23031-36-9	Biocide	[77]
Prometon	1610-18-0	Biocide	[3]
Propoxur	114-26-1	Biocide	[3]
Resmethrin	10453-86-8	Biocide	[3, 77]
Tetramethrin	7696-12-0	Biocide	[3, 22, 25, 26, 77]
Transfluthrin	118712-89-3	Biocide	[3]
Trans-nonachlor	39765-80-5	Biocide	[28, 33, 57, 75]
Triclosan	3380-34-5	Biocide	[3]
2,4,5-Trichlorophenoxyacetic acid	93-76-5	Biocide	[76]
3,5,6-Trichloro-2-pyridinol	6515-38-4	Biocide	[3]
1,2-Bis(2,4,6-tribromophenoxy)ethane	37853-59-1	BFR	[3, 27-30, 32-34, 74, 80]
2,3-Dibromopropyl 2,4,6-tribromophenyl ether	35109-60-5	BFR	[73]
2,3-Dibromo-1-propanol	96-13-9	BFR	[3]
2-Ethylhexyl-2,3,4,5-tetrabromobenzoate	183658-27-7	BFR	[27-35]
2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5-triazine	25713-60-4	BFR	[81]
1,2,5,6-Tetrabromocyclooctane	3194-57-8	BFR	[73]
Tetrabromobisphenol A	79-94-7	BFR	[35, 46, 68, 82]
Tetrabromobisphenol A bis(2,3-dibromopropylether)	21850-44-2	BFR	[27]
Tetrabromoethylcyclohexane	3322-93-8	BFR	[73]
Decabromodiphenylethane	84852-53-9	BFR	[3, 27-30, 32, 33, 69, 74, 80]
Dechlorane plus	13560-89-9	BFR	[3]
Hexabromobenzene	87-82-1	BFR	[80]
Hexabromocyclododecane	3194-55-6	BFR	[3, 29, 30, 32-35, 46, 74, 82-84]
Hexachlorocyclopentadienyl-Dibromocyclooctane	1068659-48-2	BFR	[3, 29, 33]
Polybrominated biphenyl 153	59080-40-9	BFR	[80]
Polybrominated biphenyl 209	13654-09-6	BFR	[80]
PBDE 17	147217-75-2	BFR	[3, 85-88]
PBDE 28	41318-75-6	BFR	[3, 25, 29, 32, 33, 46, 57, 83-95]
PBDE 32	189084-60-4	BFR	[91]
PBDE 33	147217-78-5	BFR	[3, 85, 90, 92]
PBDE 35	147217-80-9	BFR	[32]
PBDE 47	5436-43-1	BFR	[3, 25, 27, 29, 32-35, 46, 54, 57, 69, 74, 80, 83-93, 95-97]
PBDE 49	243982-82-3	BFR	[3, 32, 84-88, 90, 92]
PBDE 66	189084-61-5	BFR	[3, 32, 35, 80, 84-92]
PBDE 71	189084-62-6	BFR	[3, 91]

Table S2. Organic contaminants identified in indoor dust

Chemical Name[1]	CAS No	Chemical Class[2]	References[3]
PBDE 75	189084-63-7	BFR	[3, 90, 92]
PBDE 85	182346-21-0	BFR	[3, 25, 26, 32, 35, 80, 84-90, 92]
PBDE 99	60348-60-9	BFR	[3, 22, 25-27, 29, 32-35, 46, 54, 57, 69, 80, 83-93, 95-97]
PBDE 100	189084-64-8	BFR	[3, 22, 25, 26, 29, 32-35, 46, 54, 57, 80, 84-93, 95-97]
PBDE 119	189084-66-0	BFR	[25]
PBDE 138	182677-30-1	BFR	[3, 88, 90, 92]
PBDE 153	68631-49-2	BFR	[3, 25, 29, 32, 33, 35, 46, 54, 57, 80, 83-93, 95, 97]
PBDE 154	207122-15-4	BFR	[3, 25, 29, 32, 33, 35, 46, 54, 57, 80, 84-93, 95]
PBDE 155	35854-94-5	BFR	[3, 35, 90-92]
PBDE 156	405237-85-6	BFR	[3]
PBDE 179	446255-25-0	BFR	[91]
PBDE 183	207122-16-5	BFR	[3, 27-29, 32-35, 46, 54, 57, 69, 74, 80, 83-85, 87-93, 95]
PBDE 184	117948-63-7	BFR	[3, 32]
PBDE 190	189084-68-2	BFR	[3, 88, 91]
PBDE 191	446255-30-7	BFR	[3]
PBDE 196	446255-39-6	BFR	[3, 32, 33, 46, 80, 87, 90-92]
PBDE 197	117964-21-3	BFR	[3, 27, 32, 33, 46, 80, 83-85, 87, 90-92]
PBDE 201	446255-50-1	BFR	[3, 34, 80, 90-92]
PBDE 202	67797-09-5	BFR	[80, 91]
PBDE 203	337513-72-1	BFR	[3, 32, 33, 46, 80, 84, 85, 87, 91]
PBDE 204	446255-54-5	BFR	[3]
PBDE 206	63387-28-0	BFR	[3, 32, 34, 74, 80, 83-85, 87, 90-92]
PBDE 207	437701-79-6	BFR	[3, 32, 34, 74, 80, 83-85, 90-92]
PBDE 208	437701-78-5	BFR	[3, 32, 34, 80, 83-85, 90-92]
PBDE 209	1163-19-5	BFR	[3, 25, 27-29, 32-35, 46, 50, 54, 57, 68, 69, 74, 80, 83-85, 87-93, 95]

[1]Chemical name or commonly used abbreviation or trade name; [2]Chemical class according to Mercier et al 2011 (2) with additions; VOC: Volatile organic compounds; UV filter: UV filter related chemicals; PXDD/F: Polyhalogenated dibenzodioxins and dibenzofurans; PFAS: Poly and perfluorinated compounds; PCN: Polychlorinated naphthalenes; PCB: Polychlorinated biphenyls; PAH: Polycyclic aromatic hydrocarbons; BFR: Brominated flame retardants; [3]References published after Mercier et al 2011 (2)

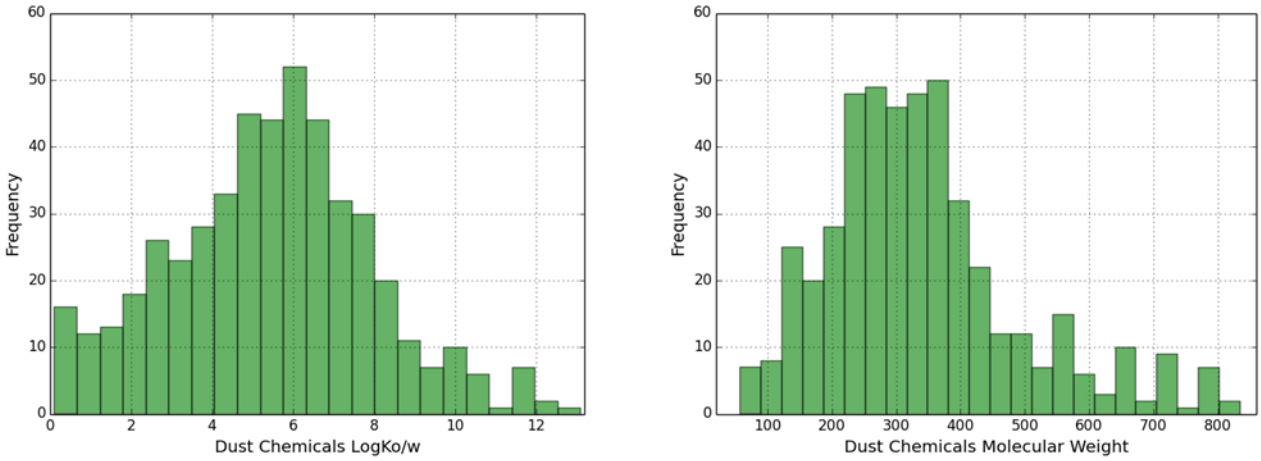


Figure S1. Histogram of the logarithm of the octanol/water partition coefficient (log Kow) and the molecular weight (g/mol) of organic contaminants in indoor dust

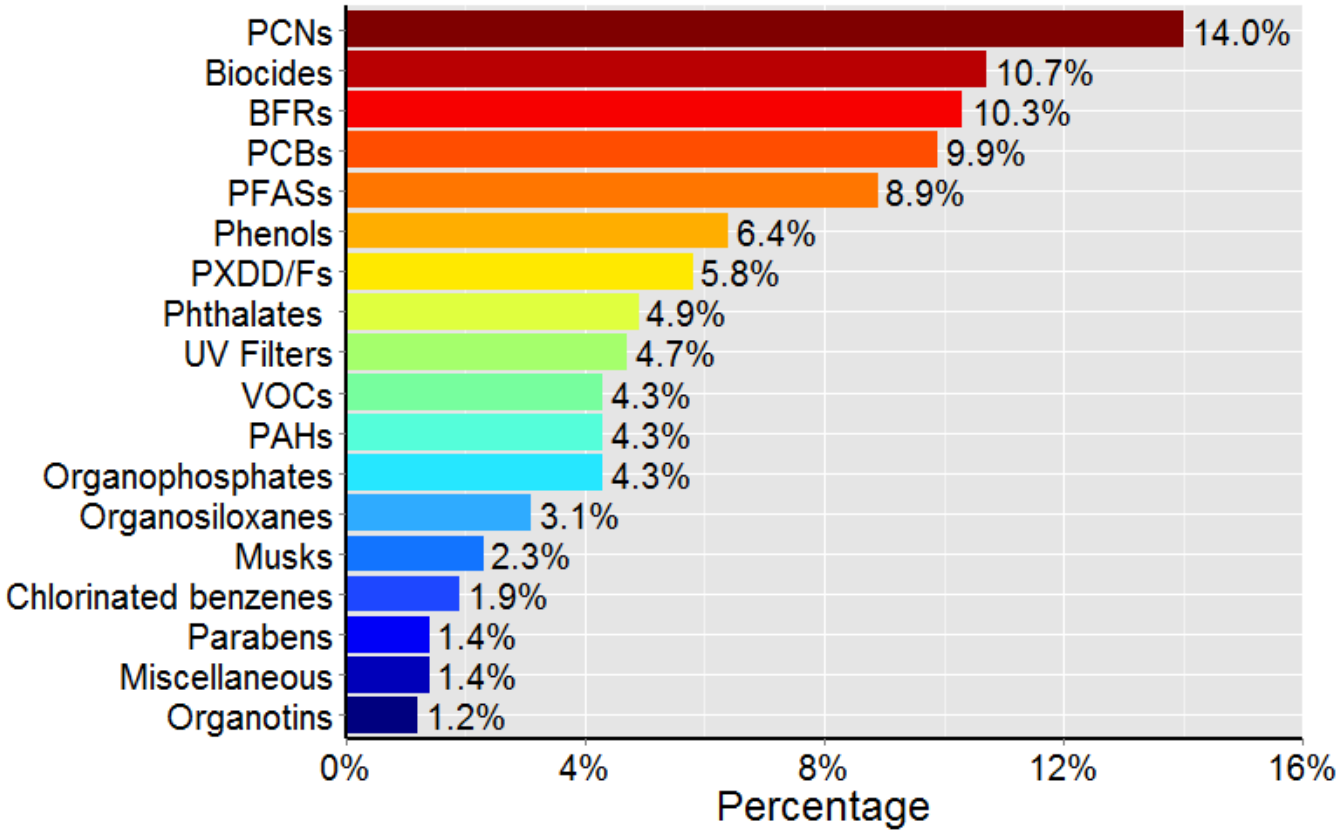


Figure S2. The chemical composition of indoor dust contaminants (in percentages). Chemical class abbreviations are given in Table S2 of the Supporting Information.

Description of Kennard Stone partition algorithm and the three modeling methods

Part 1 Kennard-stone

The Kennard Stone partition algorithm was performed as the following procedures:[98]

(1) The descriptors were firstly normalized (Eq 1) and Euclidean distances between any two chemicals were calculated with Eq 2. The two chemicals with the largest differences were selected as the anchor chemicals into the training set.

$$\text{Eq 1: } X_{\text{norm}}^{\text{d}} = \frac{X - \bar{d}}{SD_{\text{d}}}$$

Where X_{norm}^{d} and X are the normalized and original descriptor values for descriptor k, and $\bar{d}$ and SD_d are the mean and standard deviation for descriptor k for the overall set.

$$\text{Eq 2: } E_{distance\ a\_b} = \sqrt{\sum_{k=1}^{Descriptors} \left(X_{norm}^{a\ k} - X_{norm}^{b\ k}\right)^2}$$

Where $X_{norm}^{a\ k}$ and $X_{norm}^{b\ k}$ are the normalized descriptor values for descriptor k for chemicals a and b.

(2) The chemicals that have the smallest and largest distances from the two anchor chemicals were stored into the training set. This step was looped until 80% of the compounds in the original experimental data set were stored into the training set. The rest 20% would serve as the test set.

The training set was used to select molecular descriptors and to build the classification models. Molecules of the test set were used just to evaluate the predictive ability of the trained models.

Part 2 three modeling methods

In the kNN method, the class of a chemical is decided by considering the majority class of its k nearest neighbors in the chemical space.[99] In this study, Euclidean metric was used to describe the distances among chemicals. The optimal k value (k equals to 4) was determined by cross-validation to return the lowest classification error.

SVM as used for classification defined by a separating hyperplane, maps the data into a high-dimensional space in which the data points become linearly separable.[100] A kernel function (a radial basis function in this study) is used by the algorithm (C-SVC in LIB-SVM for this study) to find out the support vectors that give the best separating hyperplane. The algorithm also helps determine the most suitable hyperplane with the maximal margin of all possible ones. The hyperplane grant the most generalized solution to the classification problem.

PLS-DA searches relations between molecular descriptors and compound classes by calculating latent variables (LVs), which are orthogonal linear combinations of the original molecular descriptors.[101] In this study, we used three LVs that were optimized by cross-validation to reach the highest model correctness.

Description of Mutual Information-Differential Shannon Entropy (MI-DSE) calculation

The MI-DSE approach was designed to identify the descriptors providing the greatest amount of class-specific information in an imbalanced data set.[102] This method quantifies the ability of the studied descriptors to distinguish between compounds belonging to different classes (e.g. TTR binders and non-binders in our project). The MI-DSE avoids problems arising from weight-difference introduced by class size variation and is hence preferred to other methods measuring class information contents such as Shannon Entropy (SE) .[102]

SE was introduced to estimate the descriptor variance. The method allows comparing various descriptors since it considers relative information content of each descriptor.[103] The SE of a descriptor is defined as

Eq. 3: $H(D) = -\sum_{i=1}^{n} P_i log_2 P_i$

where n is the number of descriptors and P is the probability of their appearance.

Mutual information (MI) describes the class-specific information contents of a descriptor. It is equal to the difference between the SE of the descriptor for two combined classes and the conditional SE of the descriptor for the class of interest (Eq. 4).[102]

Eq. 4: $MI(D, C) = H(D) - H(D|C)$

where D and C are the descriptor and class, and H(D) and H(D|C) are the SE and the conditional SE, respectively.

The conditional SE of the descriptor is given by Eq. 3.

Eq 5: $H(D|C) = H_A(D) * P(C_A) + H_B(D) * P(C_B)$

$P(C_A)$ and $P(C_B)$ are the probabilities that a compound belongs to class A (binders) and B(non-binders), respectively; $H_A(D)$ and $H_B(D)$ are the SE value of a descriptor in class A and B, respectively. By setting the probabilities to 0.5, the descriptor was assumed to be distributed equally in both classes. This changed Eq. 3 to

Eq. 6: $MI(D, C) = H(D) - \frac{H_A(D) - H_B(D)}{2}$

The equation normalizes the MI(D,C) scores such that they are always between 0 and 1.

A modified DSE score (MI-DSE) was calculated using normalized SE— $H_{norm}(D)$ values to eliminate class size-dependent weights from the frequency calculations;

Eq. 7: $MI - DSE(D) = H_{norm}(D) - \frac{H_A(D) - H_B(D)}{2}$

A score of 0 shows that the descriptor captures no class-specific information, whereas a score of 1 indicates that it discriminates perfectly between classes A and B. The calculations above were written in Python (version 2.7.5).

Table S3. Comparison of the outcomes of different isoform settings in MetaSite with the results of incubation experiments

Chemicals	CYP1A1	CYP1A2	CYP2B6	Liver	Major Metabolite[1]	References
PBDE-47	6-OH PBDE47	4'-OH-BDE17	6-OH PBDE47	5-OH PBDE47	3-OH-PBDE47	[104]
PBDE-99	6'-OH-PBDE99	4'-OH-PBDE48	6'-OH-PBDE99	5'-OH-PBDE99	5'-OH-PBDE99	[104]
PCB-3	4'-OH-PCB3	4'-OH-PCB3	4'-OH-PCB3	4'-OH-PCB3	4'-OH-PCB3	[105]
PCB-15	3-OH-PCB15	3-OH-PCB15	3-OH-PCB15	3-OH-PCB15	3-OH-PCB15	[106]
PCB-77	6-OH PCB77	6-OH PCB77	6-OH PCB77	6-OH PCB77	5-OH-PCB77	[107]
PCB 136	5-OH-PCB136	4-OH-PCB136	5-OH-PCB136	4-OH-PCB136	4-OH-PCB136	[108]
PCB-153	4'-OH-PCB101	3-OH-PCB153	3-OH-PCB153	3-OH-PCB153	3-OH-PCB153	[109]
PCB-187	4-OH-PCB187	4-OH-PCB187	4-OH-PCB187	4-OH-PCB187	4-OH-PCB187	[110]

[1] Major metabolite determined in incubation experiments.

Table S4. Description of the 14 selected descriptors and their Mutual Information-Differential Shannon entropy (MI-DSE) value

Descriptor Name	MI-DSE	Description
TPSA	0.320	Polar surface area (Å2) calculated using group contributions to approximate the polar surface area from connection table information only.
a_don	0.310	Number of hydrogen bond donor atoms (not counting basic atoms but counting atoms that are both hydrogen bond donors and acceptors such as -OH).
a_nOH	0.301	Number of hydroxyl groups.
nX	0.240	Number of halogen atoms.
PEOE_VSA_FNEG	0.236	Fractional negative van der Waals surface area. This is the sum of the vi such that qi is negative divided by the total surface area. The vi is calculated using a connection table approximation.
PEOE_RPC-	0.231	Relative negative partial charge: the smallest negative qi divided by the sum of the negative qi.
density	0.224	Molecular mass density: Weight divided by van der Waals volume (amu/Å3).
PEOE_RPC+	0.200	Relative positive partial charge: the largest positive qi divided by the sum of the positive qi. Q_RPC+ is identical to RPC+ which has been retained for compatibility.
diameter	0.177	Largest value in the distance matrix.
PEOE_PC+	0.157	Total positive partial charge: the sum of the positive qi.
vsa_hyd	0.150	Approximation to the sum of van der Waals surface areas of hydrophobic atoms.
KierFlex	0.1407	Kier molecular flexibility index.
logP(o/w)	0.116	Log of the octanol/water partition coefficient.
opr_brigid	0.114	Number of rigid bonds.

Table S5. Dust contaminants (Parent AD) and metabolites (Metabolite AD) defined as out of the models' applicability domain or defined as persistent by MetaSite.

Chemical Name[1]	CAS No[2]	Chemical Class[3]	Parent AD[4]	Metabolite AD[4]
Acetone	67-64-1	VOC	Moderate	Persistent
Ambralux	54464-57-2	VOC	Moderate	In
3-Methyl-butanal	590-86-3	VOC	Moderate	In
2-Methyl-propenal	78-85-3	VOC	Moderate	Moderate
Pentanal	110-62-3	VOC	Moderate	In
Pyrrole	109-97-7	VOC	In	Persistent
2-[2-Hydroxy-3,5-di-(1,1-dimethylbenzyl)]-2H-benzotriazole (Tinuvin 234)	70321-86-7	UV filter	Moderate	Moderate
Diundecyl phthalate	3648-20-2	Phthalate	Moderate	Moderate
Bisphenol A bis(2,3-dihydroxypropyl) ether	5581-32-8	Phenol	Moderate	Severe
Bis(3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanol) hydrogen phosphate (4:2 diPAP)	135098-69-0	PFAS	Moderate	In
Bis[2-(perfluorohexyl)ethyl] Phosphate (6:2 diPAP)	57677-95-9	PFAS	Severe	In
Bis[2-(perfluorooctyl)ethyl] Phosphate (8:2 diPAP)	678-41-1	PFAS	Severe	In
Bis(3,3,4,4,5,5,6,6,6-nonafluoro-1-hexanol) hydrogen phosphate (10:2 diPAP)	1895-26-7	PFAS	Severe	Severe
2-(N-Methylperfluoro-1-octanesulfonamido)- ethanol	24448-09-7	PFAS	Moderate	Moderate
2-(N-Ethylperfluoro-1-octanesulfonamido)-ethanol	1691-99-2	PFAS	Moderate	Moderate
2-(Perfluorodecyl)ethanol	865-86-1	PFAS	Moderate	Moderate
6:2 Fluorotelomer unsaturated carboxylic acid	70887-88-6	PFAS	In	Persistent
8:2 Fluorotelomer unsaturated carboxylic acid	70887-84-2	PFAS	In	Persistent
10:2 Fluorotelomer unsaturated carboxylic acid	70887-94-4	PFAS	Moderate	Persistent
Perfluorobutanoic acid	375-22-4	PFAS	In	Persistent
Perfluorohexanoic acid	307-24-4	PFAS	In	Persistent
Perfluoroheptanoic acid	375-85-9	PFAS	In	Persistent
Perfluorooctanoic acid	335-67-1	PFAS	In	Persistent
Perfluorononanoic acid	375-95-1	PFAS	Moderate	Persistent
Perfluorodecanoic acid	335-76-2	PFAS	Moderate	Persistent
Perfluorododecanoic acid	307-55-1	PFAS	Severe	Persistent
Perfluoropentanoic acid	2706-90-3	PFAS	In	Persistent
Perfluoroundecanoic acid	2058-94-8	PFAS	Severe	Persistent
Perfluorotridecanoic acid	72629-94-8	PFAS	Severe	Persistent
Perfluorotetradecanoic acid	376-06-7	PFAS	Severe	Persistent
Perfluro-n-tetradecanoic acid	16517-11-6	PFAS	Severe	Persistent
Perfluorohexane phosphonic acid	40143-76-8	PFAS	In	Persistent
Perfluorooctane phosphonic acid	40143-78-0	PFAS	Moderate	Persistent
Perfluorodecane phosphonic acid	52299-26-0	PFAS	Severe	Persistent

Table S5. Dust contaminants and metabolites defined as outliers or persistent

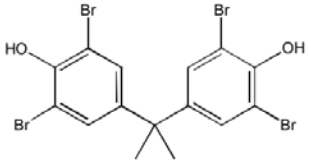
Chemical Name[1]	CAS No[2]	Chemical Class[3]	Parent AD[4]	Metabolite AD[4]
Perfluorooctane sulfonamide	754-91-6	PFAS	Moderate	Persistent
N-Ethylperfluorooctane sulfonamide	4151-50-2	PFAS	Moderate	Moderate
N-Methylperfluorooctane sulfonamide	31506-32-8	PFAS	Moderate	Moderate
Perfluorobutane sulfonate	375-73-5	PFAS	In	Persistent
Perfluorohexane sulfonate	355-46-4	PFAS	In	Persistent
Perfluoroheptane sulfonate	375-92-8	PFAS	In	Persistent
Perfluorooctane sulfonate	1763-23-1	PFAS	Moderate	Persistent
Perfluorononane sulfonate	68259-12-1	PFAS	Moderate	Persistent
Perfluorodecane sulfonate	335-77-3	PFAS	Severe	Persistent
Perfluoropentane sulfonate	2706-91-4	PFAS	In	Persistent
Perfluoro-p-ethylcyclohexane sulfonate	646-83-3	PFAS	Moderate	Persistent
6:2 Fluorotelomer sulfonate	27619-97-2	PFAS	In	Moderate
8:2 Fluorotelomer sulfonate	39108-34-4	PFAS	Moderate	Severe
N-Methyl perfluorooctane sulfonamidethylacrylate	25268-77-3	PFAS	In	Moderate
Benzo(ghi)perylene	191-24-2	PAH	Moderate	In
Coronene	191-07-1	PAH	Severe	Moderate
Dibenzo(a,e)pyrene	192-65-4	PAH	Moderate	Moderate
Indeno(1,2,3-cd)pyrene	193-39-5	PAH	Moderate	In
Squalene	111-02-4	PAH	Moderate	In
Monobutyltin	78763-54-9	Organotin	In	Persistent
Monooctyltin	15231-57-9	Organotin	In	Persistent
Dibutyltin	14488-53-0	Organotin	Moderate	Persistent
Dioctyltin	60004-29-7	Organotin	In	Persistent
Tributyltin	36643-28-4	Organotin	In	Persistent
Triphenyltin	668-34-8	Organotin	In	Persistent
Decamethylcyclopentasiloxane	541-02-6	Organosiloxane	Moderate	Persistent
Decamethyltetrasiloxane	141-62-8	Organosiloxane	Moderate	Persistent
Docosamethyldecasiloxane	556-70-7	Organosiloxane	Severe	Persistent
Dodecamethylcyclohexasiloxane	540-97-6	Organosiloxane	Moderate	Persistent
Dodecamethylpentasiloxane	141-63-9	Organosiloxane	Moderate	Persistent
Eicosamethylnonasiloxane	2652-13-3	Organosiloxane	Severe	Persistent
Hexacosamethyldodecasiloxane	2471-08-1	Organosiloxane	Severe	Persistent
Hexadecamethylheptasiloxane	541-01-5	Organosiloxane	Severe	Persistent
Octadecamethyloctasiloxane	556-69-4	Organosiloxane	Severe	Persistent
Octamethylcyclotetrasiloxane	556-67-2	Organosiloxane	Moderate	Persistent
Tetracosamethylhendecasiloxane	107-53-9	Organosiloxane	Severe	Persistent
Tetradecamethylcycloheptasiloxane	107-50-6	Organosiloxane	Severe	Persistent
Tetradecamethylhexasiloxane	107-52-8	Organosiloxane	Severe	Persistent
Tetradecasiloxane	2471-10-5	Organosiloxane	Severe	Persistent
Tridecasiloxane	2471-09-2	Organosiloxane	Severe	Persistent
Tris(2-butoxyethyl) phosphate	78-51-3	Organophosphate	Moderate	Moderate
2,2-Bis(chloromethyl)trimethylene bis(bis(2-chloroethyl)phosphate)	38051-10-4	Organophosphate	Moderate	Moderate
Musk indanone	33704-61-9	Musk	Moderate	In
Cholesterol	57-88-5	Miscellaneous	Moderate	Moderate
1-[(2,4-Dichlorophenyl)aminocarbonyl]-1-	113136-77-9	Biocide	In	Persistent

Table S5. Dust contaminants and metabolites defined as outliers or persistent

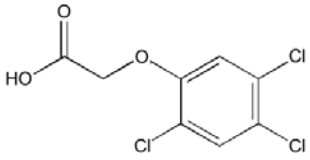
cyclopropanecarboxylic acid (Cyclanilide)				
Hexachlorocyclohexane	58-89-9	Biocide	In	Persistent
2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5-triazine	25713-60-4	BFR	Severe	Severe
Dechlorane plus	13560-89-9	BFR	Moderate	In

[1]Chemical name or commonly used abbreviation or trade name; [2]Chemical Abstracts Service numbers; [3]Chemical class according to Mercier et al 2011 (1) with additions; VOC: Volatile organic compounds; UV filter: UV filter related chemicals; PXDD/F: Polyhalogenated dibenzodioxins and dibenzofurans; PFAS: Poly and perfluorinated compounds; PCN: Polychlorinated naphthalenes; PCB: Polychlorinated biphenyls; PAH: Polycyclic aromatic hydrocarbons; BFR: Brominated flame retardants; [4]Outliers are defined as "Moderate" if >95% and "Severe" if >99% of the confidence interval. "In" refers to compounds in the applicability domain but their parent or metabolite was defined either as outliers according to the model applicability domain or as "Persistent" by MetaSite.

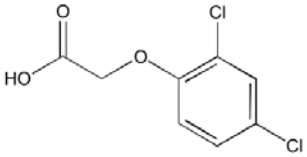
Table S6. Predicted potential TTR-binders in organic dust contaminants based on QSAR model



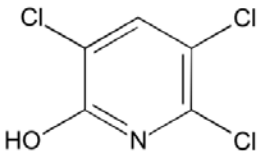
CAS_No: 79-94-7
Chemical Name: Tetrabromobisphenol A
Chemical Class: BFR



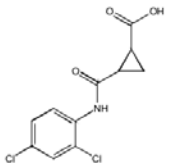
CAS_No: 93-76-5
Chemical Name: 2,4,5-Trichlorophenoxyacetic acid
Chemical Class: Biocide



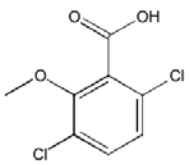
CAS_No: 94-75-7
Chemical Name: 2,4-Dichlorophenoxyacetic acid
Chemical Class: Biocide



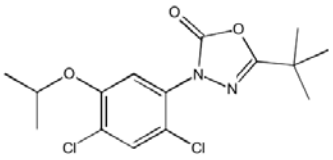
CAS_No: 6515-38-4
Chemical Name: 3,5,6-Trichloro-2-pyridinol
Chemical Class: Biocide



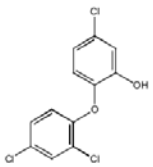
CAS_No: 113136-77-9
Chemical Name: Cyclanilide
Chemical Class: Biocide



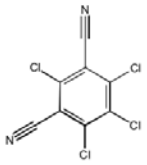
CAS_No: 1918-00-9
Chemical Name: Dicamba
Chemical Class: Biocide



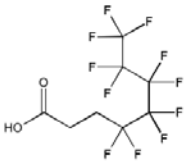
CAS_No: 19666-30-9
Chemical Name: Oxadiazon
Chemical Class: Biocide



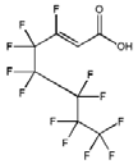
CAS_No: 3380-34-5
Chemical Name: Triclosan
Chemical Class: Biocide



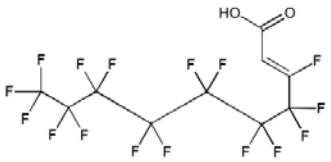
CAS_No: 1897-45-6
Chemical Name: Chlorothalonil
Chemical Class: Biocide



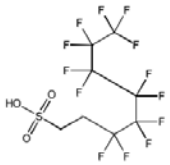
CAS_No: 914637-49-3
Chemical Name: 5:3 Fluorotelomer saturated carboxylic acid
Chemical Class: PFAS



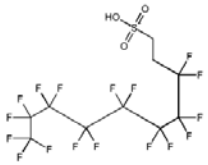
CAS_No: 70887-88-6
Chemical Name: 6:2 Fluorotelomer unsaturated carboxylic acid
Chemical Class: PFAS



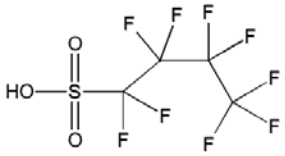
CAS_No: 70887-84-2
Chemical Name: 8:2 Fluorotelomer unsaturated carboxylic acid
Chemical Class: PFAS



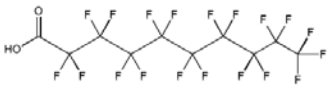
CAS_No: 27619-97-2
Chemical Name: 6:2 Fluorotelomer sulfonate
Chemical Class: PFAS



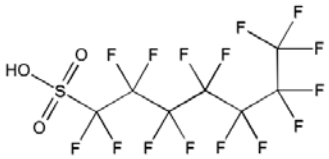
CAS_No: 39108-34-4
Chemical Name: 8:2 Fluorotelomer sulfonate
Chemical Class: PFAS



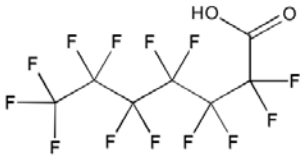
CAS_No: 375-73-5
Chemical Name: Perfluorobutanesulfonic acid
Chemical Class: PFAS



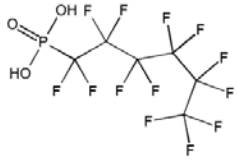
CAS_No: 335-76-2
Chemical Name: Perfluorodecanoic acid
Chemical Class: PFAS



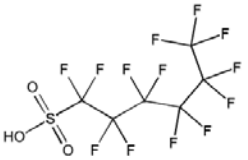
CAS_No: 375-92-8
Chemical Name: Perfluoroheptanesulfonic acid
Chemical Class: PFAS



CAS_No: 375-85-9
Chemical Name: Perfluoroheptanoic acid
Chemical Class: PFAS

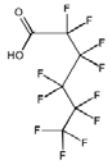


CAS_No: 40143-76-8
Chemical Name: Perfluorohexane phosphonate
Chemical Class: PFAS



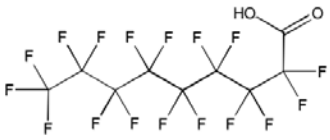
CAS_No: 355-46-4
Chemical Name: Perfluorohexanesulfonic acid
Chemical Class: PFAS

Table S6. Predicted potential TTR-binders in organic dust contaminants based on QSAR model

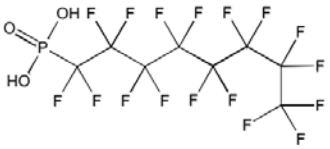


CAS_No: 307-24-4
Chemical Name: Perfluorohexanoic acid
Chemical Class: PFAS

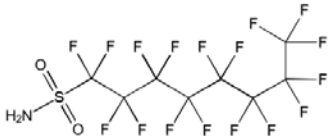
CAS_No: 68259-12-1
Chemical Name: Perfluorononanesulfonic acid
Chemical Class: PFAS



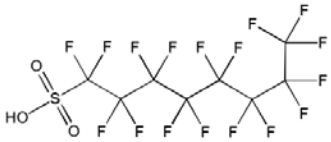
CAS_No: 375-95-1
Chemical Name: Perfluorononanoic acid
Chemical Class: PFAS



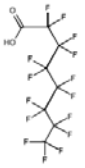
CAS_No: 40143-78-0
Chemical Name: Perfluorooctane phosphonate
Chemical Class: PFAS



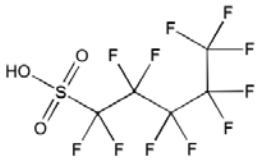
CAS_No: 754-91-6
Chemical Name: Perfluorooctane sulfonamide
Chemical Class: PFAS



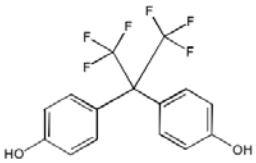
CAS_No: 1763-23-1
Chemical Name: Perfluorooctanesulfonic acid
Chemical Class: PFAS



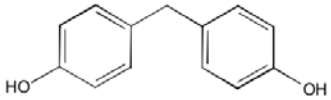
CAS_No: 335-67-1
Chemical Name: Perfluorooctanoic acid
Chemical Class: PFAS



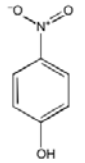
CAS_No: 2706-91-4
Chemical Name: Perfluoropentanesulfonic acid
Chemical Class: PFAS



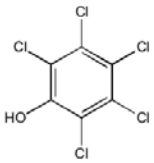
CAS_No: 1478-61-1
Chemical Name: Bisphenol AF
Chemical Class: Phenol



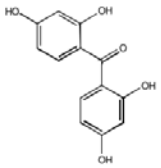
CAS_No: 620-92-8
Chemical Name: 4,4'-Methylenediphenol
Chemical Class: Phenol



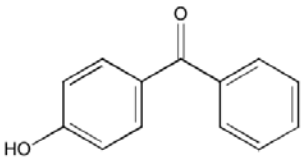
CAS_No: 100-02-7
Chemical Name: 4-Nitrophenol
Chemical Class: Phenol



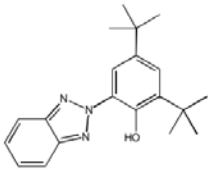
CAS_No: 87-86-5
Chemical Name: Pentachlorophenol
Chemical Class: Phenol



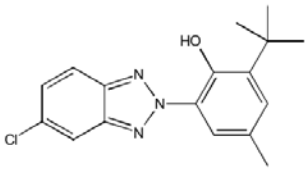
CAS_No: 131-55-5
Chemical Name: 2,4,2',4'-Tetrahydroxybenzophenone
Chemical Class: UV Filter



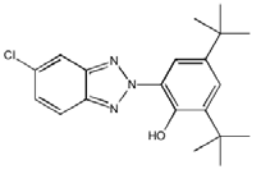
CAS_No: 1137-42-4
Chemical Name: 4-Hydroxybenzophenone
Chemical Class: UV Filter



CAS_No: 3846-71-7
Chemical Name: Tinuvin 320
Chemical Class: UV Filter

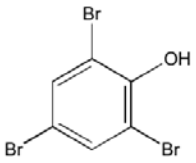


CAS_No: 3896-11-5
Chemical Name: Tinuvin 326
Chemical Class: UV Filter

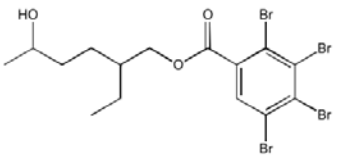


CAS_No: 3864-99-1
Chemical Name: Tinuvin 327
Chemical Class: UV Filter

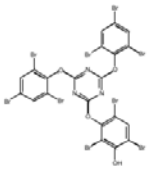
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



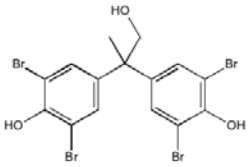
Parent CAS_No: 35109-60-5
Parent Chemical Name: 2,3-Dibromopropyl 2,4,6-tribromophenyl ether
Parent Chemical Class: BFR



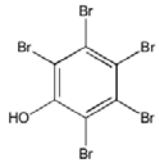
Parent CAS_No: 183658-27-7
Parent Chemical Name: 2-Ethylhexyl-2,3,4,5-tetrabromobenzoate
Parent Chemical Class: BFR



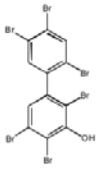
Parent CAS_No: 25713-60-4
Parent Chemical Name: 2,4,6-Tris(2,4,6-tribromophenoxy)-1,3,5-triazine
Parent Chemical Class: BFR



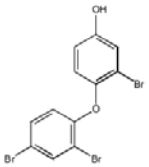
Parent CAS_No: 79-94-7
Parent Chemical Name: Tetrabromobisphenol A
Parent Chemical Class: BFR



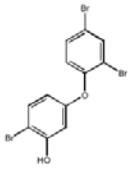
Parent CAS_No: 87-82-1
Parent Chemical Name: Hexabromobenzene
Parent Chemical Class: BFR



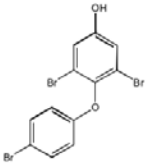
Parent CAS_No: 59080-40-9
Parent Chemical Name: Polybrominated biphenyl 153
Parent Chemical Class: BFR



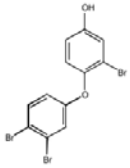
Parent CAS_No: 147217-75-2
Parent Chemical Name: PBDE 17
Parent Chemical Class: BFR



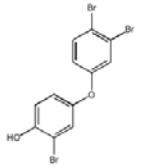
Parent CAS_No: 41318-75-6
Parent Chemical Name: PBDE 28
Parent Chemical Class: BFR



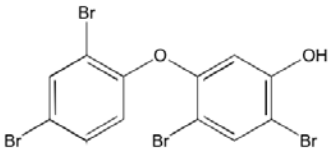
Parent CAS_No: 189084-60-4
Parent Chemical Name: PBDE 32
Parent Chemical Class: BFR



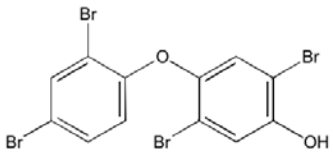
Parent CAS_No: 147217-78-5
Parent Chemical Name: PBDE 33
Parent Chemical Class: BFR



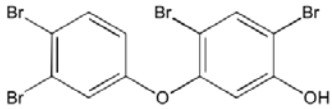
Parent CAS_No: 147217-80-9
Parent Chemical Name: PBDE 35
Parent Chemical Class: BFR



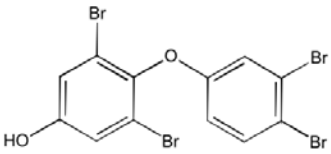
Parent CAS_No: 5436-43-1
Parent Chemical Name: PBDE 47
Parent Chemical Class: BFR



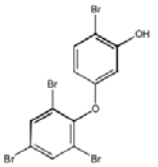
Parent CAS_No: 243982-82-3
Parent Chemical Name: PBDE 49
Parent Chemical Class: BFR



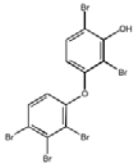
Parent CAS_No: 189084-61-5
Parent Chemical Name: PBDE 66
Parent Chemical Class: BFR



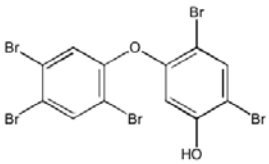
Parent CAS_No: 189084-62-6
Parent Chemical Name: PBDE 71
Parent Chemical Class: BFR



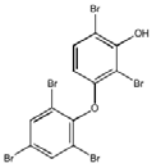
Parent CAS_No: 189084-63-7
Parent Chemical Name: PBDE 75
Parent Chemical Class: BFR



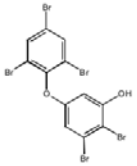
Parent CAS_No: 182346-21-0
Parent Chemical Name: PBDE 85
Parent Chemical Class: BFR



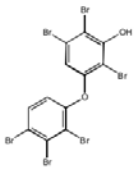
Parent CAS_No: 60348-60-9
Parent Chemical Name: PBDE 99
Parent Chemical Class: BFR



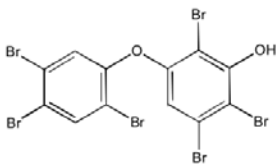
Parent CAS_No: 189084-64-8
Parent Chemical Name: PBDE 100
Parent Chemical Class: BFR



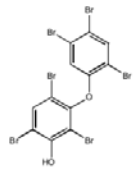
Parent CAS_No: 189084-66-0
Parent Chemical Name: PBDE 119
Parent Chemical Class: BFR



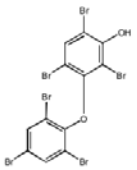
Parent CAS_No: 182677-30-1
Parent Chemical Name: PBDE 138
Parent Chemical Class: BFR



Parent CAS_No: 68631-49-2
Parent Chemical Name: PBDE 153
Parent Chemical Class: BFR

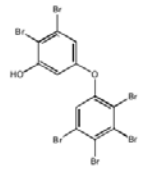


Parent CAS_No: 207122-15-4
Parent Chemical Name: PBDE 154
Parent Chemical Class: BFR

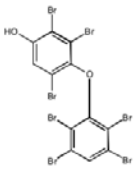


Parent CAS_No: 35854-94-5
Parent Chemical Name: PBDE 155
Parent Chemical Class: BFR

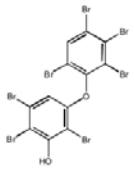
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



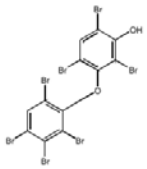
Parent CAS_No: 405237-85-6
Parent Chemical Name: PBDE 156
Parent Chemical Class: BFR



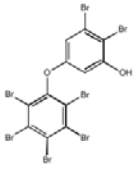
Parent CAS_No: 446255-25-0
Parent Chemical Name: PBDE 179
Parent Chemical Class: BFR



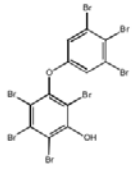
Parent CAS_No: 207122-16-5
Parent Chemical Name: PBDE 183
Parent Chemical Class: BFR



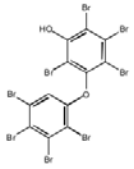
Parent CAS_No: 117948-63-7
Parent Chemical Name: PBDE 184
Parent Chemical Class: BFR



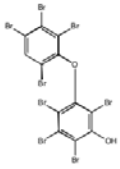
Parent CAS_No: 189084-68-2
Parent Chemical Name: PBDE 190
Parent Chemical Class: BFR



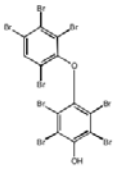
Parent CAS_No: 446255-30-7
Parent Chemical Name: PBDE 191
Parent Chemical Class: BFR



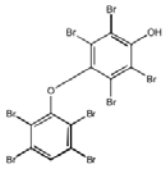
Parent CAS_No: 446255-39-6
Parent Chemical Name: PBDE 196
Parent Chemical Class: BFR



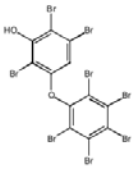
Parent CAS_No: 117964-21-3
Parent Chemical Name: PBDE 197
Parent Chemical Class: BFR



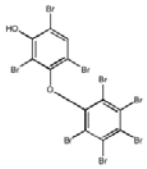
Parent CAS_No: 446255-50-1
Parent Chemical Name: PBDE 201
Parent Chemical Class: BFR



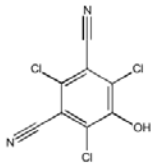
Parent CAS_No: 67797-09-5
Parent Chemical Name: PBDE 202
Parent Chemical Class: BFR



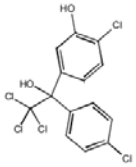
Parent CAS_No: 337513-72-1
Parent Chemical Name: PBDE 203
Parent Chemical Class: BFR



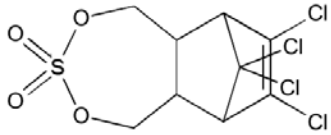
Parent CAS_No: 446255-54-5
Parent Chemical Name: PBDE 204
Parent Chemical Class: BFR



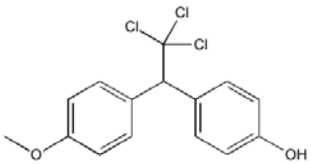
Parent CAS_No: 1897-45-6
Parent Chemical Name: Chlorothalonil
Parent Chemical Class: Biocide



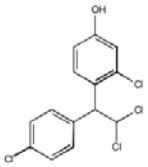
Parent CAS_No: 115-32-2
Parent Chemical Name: Dicofol
Parent Chemical Class: Biocide



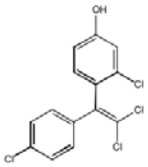
Parent CAS_No: 959-98-8
Parent Chemical Name: Endosulfan
Parent Chemical Class: Biocide



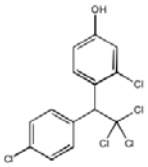
Parent CAS_No: 72-43-5
Parent Chemical Name: Methoxychlore
Parent Chemical Class: Biocide



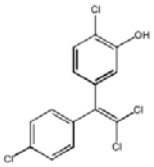
Parent CAS_No: 53-19-0
Parent Chemical Name: o,p'-DDD
Parent Chemical Class: Biocide



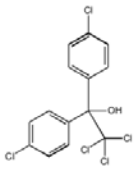
Parent CAS_No: 3424-82-6
Parent Chemical Name: o,p'-DDE
Parent Chemical Class: Biocide



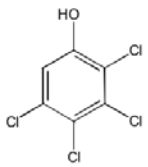
Parent CAS_No: 789-02-6
Parent Chemical Name: o,p'-DDT
Parent Chemical Class: Biocide



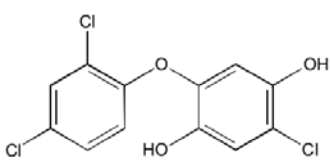
Parent CAS_No: 72-55-9
Parent Chemical Name: p,p'-DDE
Parent Chemical Class: Biocide



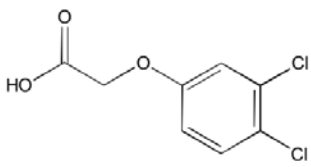
Parent CAS_No: 50-29-3
Parent Chemical Name: p,p'-DDT
Parent Chemical Class: Biocide



Parent CAS_No: 87-86-5
Parent Chemical Name: Pentachlorophenol
Parent Chemical Class: Biocide

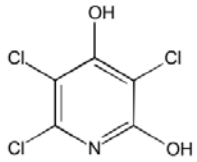


Parent CAS_No: 3380-34-5
Parent Chemical Name: Triclosan
Parent Chemical Class: Biocide

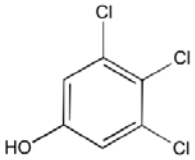


Parent CAS_No: 93-76-5
Parent Chemical Name: 2,4,5-Trichlorophenoxyacetic acid
Parent Chemical Class: Biocide

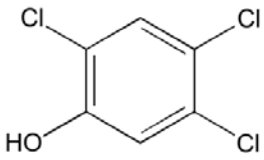
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



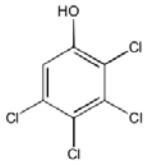
Parent CAS_No: 6515-38-4
Parent Chemical Name: 3,5,6-Trichloro-2-pyridinol
Parent Chemical Class: Biocide



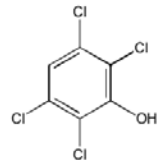
Parent CAS_No: 87-61-6
Parent Chemical Name: 1,2,3-Trichlorobenzene
Parent Chemical Class: Chlorinatedbenzene



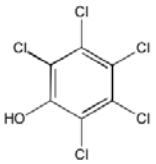
Parent CAS_No: 120-82-1
Parent Chemical Name: 1,2,4-Trichlorobenzene
Parent Chemical Class: Chlorinatedbenzene



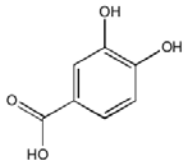
Parent CAS_No: 634-66-2
Parent Chemical Name: 1,2,3,4-Tetrachlorobenzene
Parent Chemical Class: Chlorinatedbenzene



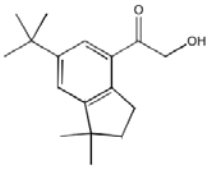
Parent CAS_No: 95-94-3
Parent Chemical Name: 1,2,4,5-Tetrachlorobenzene
Parent Chemical Class: Chlorinatedbenzene



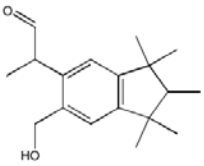
Parent CAS_No: 608-93-5
Parent Chemical Name: Pentachlorobenzene
Parent Chemical Class: Chlorinatedbenzene



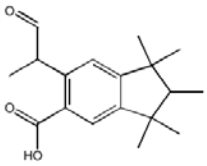
Parent CAS_No: 99-96-7
Parent Chemical Name: 4-Hydroxybenzoic acid
Parent Chemical Class: Miscellaneous



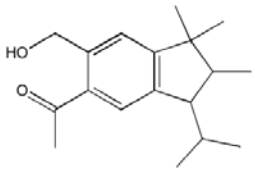
Parent CAS_No: 13171-00-1
Parent Chemical Name: Celestolide
Parent Chemical Class: Musk



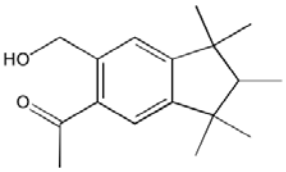
Parent CAS_No: 1222-05-5
Parent Chemical Name: Galaxolide
Parent Chemical Class: Musk



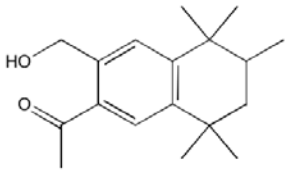
Parent CAS_No: 256393-37-0
Parent Chemical Name: Galaxolidone
Parent Chemical Class: Musk



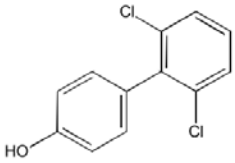
Parent CAS_No: 68140-48-7
Parent Chemical Name: Traesolide
Parent Chemical Class: Musk



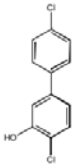
Parent CAS_No: 15323-35-0
Parent Chemical Name: Musk phantolide
Parent Chemical Class: Musk



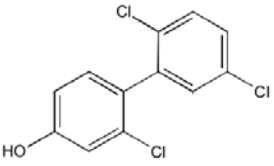
Parent CAS_No: 21145-77-7
Parent Chemical Name: Musk tonalid
Parent Chemical Class: Musk



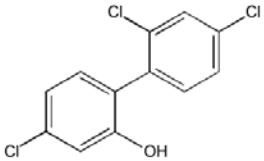
Parent CAS_No: 33146-45-1
Parent Chemical Name: PCB 10
Parent Chemical Class: PCB



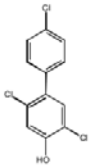
Parent CAS_No: 2050-68-2
Parent Chemical Name: PCB 15
Parent Chemical Class: PCB



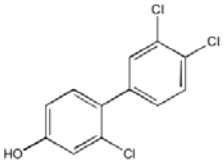
Parent CAS_No: 37680-65-2
Parent Chemical Name: PCB 18
Parent Chemical Class: PCB



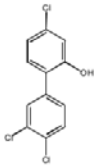
Parent CAS_No: 7012-37-5
Parent Chemical Name: PCB 28
Parent Chemical Class: PCB



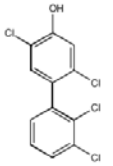
Parent CAS_No: 16606-02-3
Parent Chemical Name: PCB 31
Parent Chemical Class: PCB



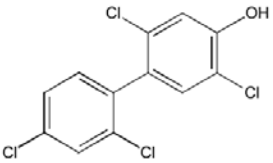
Parent CAS_No: 38444-86-9
Parent Chemical Name: PCB 33
Parent Chemical Class: PCB



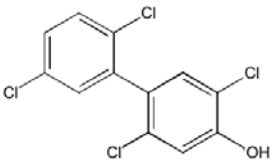
Parent CAS_No: 38444-90-5
Parent Chemical Name: PCB 37
Parent Chemical Class: PCB



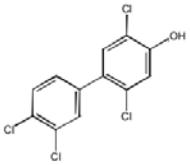
Parent CAS_No: 41464-39-5
Parent Chemical Name: PCB 44
Parent Chemical Class: PCB



Parent CAS_No: 41464-40-8
Parent Chemical Name: PCB 49
Parent Chemical Class: PCB

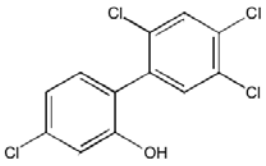


Parent CAS_No: 35693-99-3
Parent Chemical Name: PCB 52
Parent Chemical Class: PCB

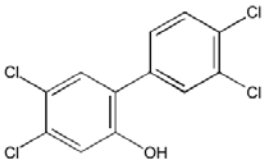


Parent CAS_No: 32598-11-1
Parent Chemical Name: PCB 70
Parent Chemical Class: PCB

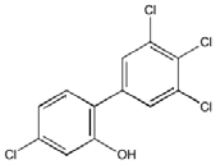
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



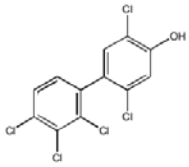
Parent CAS_No: 32690-93-0
Parent Chemical Name: PCB 74
Parent Chemical Class: PCB



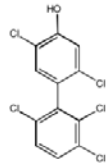
Parent CAS_No: 32598-13-3
Parent Chemical Name: PCB 77
Parent Chemical Class: PCB



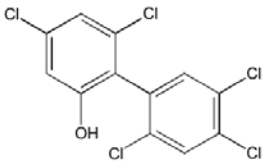
Parent CAS_No: 70362-50-4
Parent Chemical Name: PCB 81
Parent Chemical Class: PCB



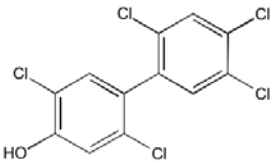
Parent CAS_No: 38380-02-8
Parent Chemical Name: PCB 87
Parent Chemical Class: PCB



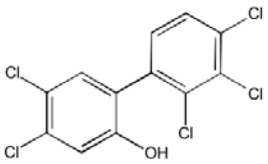
Parent CAS_No: 38379-99-6
Parent Chemical Name: PCB 95
Parent Chemical Class: PCB



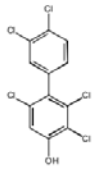
Parent CAS_No: 38380-01-7
Parent Chemical Name: PCB 99
Parent Chemical Class: PCB



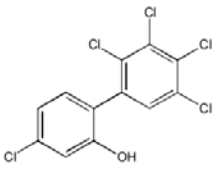
Parent CAS_No: 37680-73-2
Parent Chemical Name: PCB 101
Parent Chemical Class: PCB



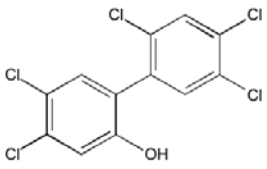
Parent CAS_No: 32598-14-4
Parent Chemical Name: PCB 105
Parent Chemical Class: PCB



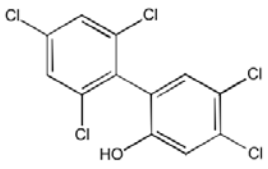
Parent CAS_No: 38380-03-9
Parent Chemical Name: PCB 110
Parent Chemical Class: PCB



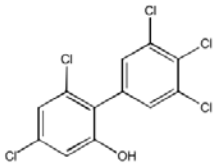
Parent CAS_No: 74472-37-0
Parent Chemical Name: PCB 114
Parent Chemical Class: PCB



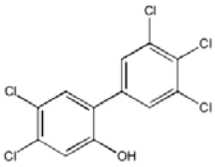
Parent CAS_No: 31508-00-6
Parent Chemical Name: PCB 118
Parent Chemical Class: PCB



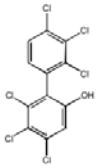
Parent CAS_No: 56558-17-9
Parent Chemical Name: PCB 119
Parent Chemical Class: PCB



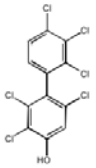
Parent CAS_No: 65510-44-3
Parent Chemical Name: PCB 123
Parent Chemical Class: PCB



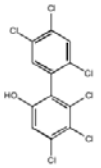
Parent CAS_No: 57465-28-8
Parent Chemical Name: PCB 126
Parent Chemical Class: PCB



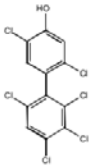
Parent CAS_No: 38380-07-3
Parent Chemical Name: PCB 128
Parent Chemical Class: PCB



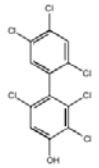
Parent CAS_No: 38380-05-1
Parent Chemical Name: PCB 132
Parent Chemical Class: PCB



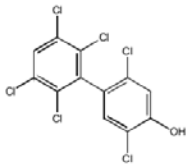
Parent CAS_No: 35065-28-2
Parent Chemical Name: PCB 138
Parent Chemical Class: PCB



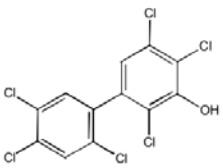
Parent CAS_No: 68194-14-9
Parent Chemical Name: PCB 144
Parent Chemical Class: PCB



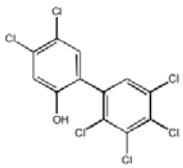
Parent CAS_No: 38380-04-0
Parent Chemical Name: PCB 149
Parent Chemical Class: PCB



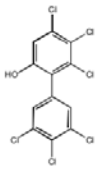
Parent CAS_No: 52663-63-5
Parent Chemical Name: PCB 151
Parent Chemical Class: PCB



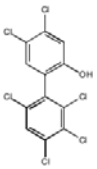
Parent CAS_No: 35065-27-1
Parent Chemical Name: PCB 153
Parent Chemical Class: PCB



Parent CAS_No: 38380-08-4
Parent Chemical Name: PCB 156
Parent Chemical Class: PCB

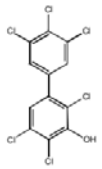


Parent CAS_No: 69782-90-7
Parent Chemical Name: PCB 157
Parent Chemical Class: PCB

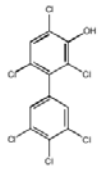


Parent CAS_No: 74472-42-7
Parent Chemical Name: PCB 158
Parent Chemical Class: PCB

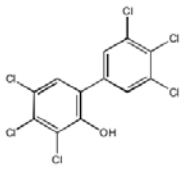
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



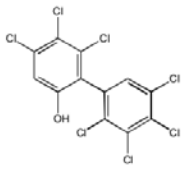
Parent CAS_No: 52663-72-6
Parent Chemical Name: PCB 167
Parent Chemical Class: PCB



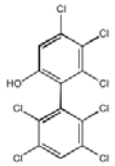
Parent CAS_No: 59291-65-5
Parent Chemical Name: PCB 168
Parent Chemical Class: PCB



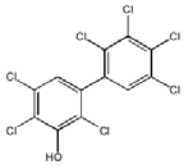
Parent CAS_No: 32774-16-6
Parent Chemical Name: PCB 169
Parent Chemical Class: PCB



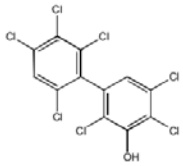
Parent CAS_No: 35065-30-6
Parent Chemical Name: PCB 170
Parent Chemical Class: PCB



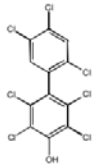
Parent CAS_No: 52663-70-4
Parent Chemical Name: PCB 177
Parent Chemical Class: PCB



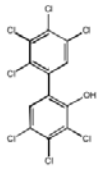
Parent CAS_No: 35065-29-3
Parent Chemical Name: PCB 180
Parent Chemical Class: PCB



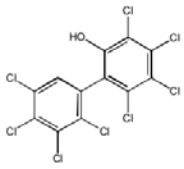
Parent CAS_No: 52663-69-1
Parent Chemical Name: PCB 183
Parent Chemical Class: PCB



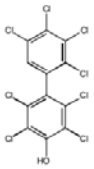
Parent CAS_No: 52663-68-0
Parent Chemical Name: PCB 187
Parent Chemical Class: PCB



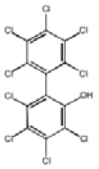
Parent CAS_No: 39635-31-9
Parent Chemical Name: PCB 189
Parent Chemical Class: PCB



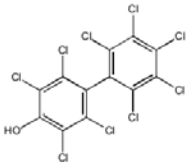
Parent CAS_No: 35694-08-7
Parent Chemical Name: PCB 194
Parent Chemical Class: PCB



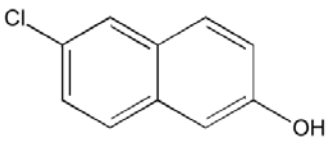
Parent CAS_No: 52663-75-9
Parent Chemical Name: PCB 199
Parent Chemical Class: PCB



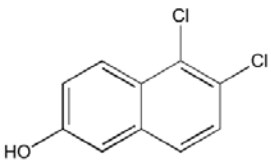
Parent CAS_No: 40186-72-9
Parent Chemical Name: PCB 206
Parent Chemical Class: PCB



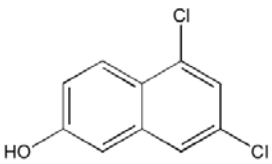
Parent CAS_No: 2051-24-3
Parent Chemical Name: PCB 209
Parent Chemical Class: PCB



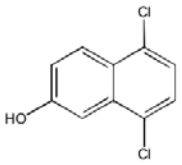
Parent CAS_No: 91-58-7
Parent Chemical Name: PCN 2
Parent Chemical Class: PCN



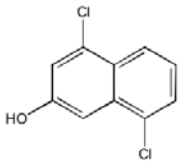
Parent CAS_No: 2050-69-3
Parent Chemical Name: PCN 3
Parent Chemical Class: PCN



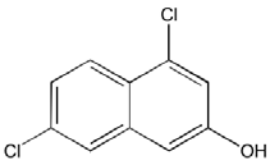
Parent CAS_No: 2198-75-6
Parent Chemical Name: PCN 4
Parent Chemical Class: PCN



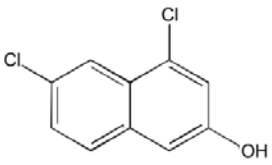
Parent CAS_No: 1825-31-6
Parent Chemical Name: PCN 5
Parent Chemical Class: PCN



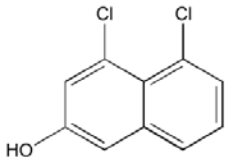
Parent CAS_No: 1825-30-5
Parent Chemical Name: PCN 6
Parent Chemical Class: PCN



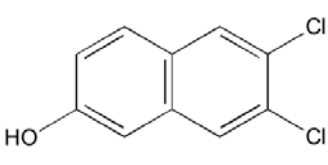
Parent CAS_No: 2050-72-8
Parent Chemical Name: PCN 7
Parent Chemical Class: PCN



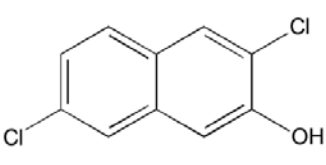
Parent CAS_No: 2050-73-9
Parent Chemical Name: PCN 8
Parent Chemical Class: PCN



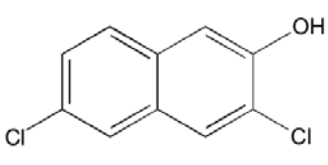
Parent CAS_No: 2050-74-0
Parent Chemical Name: PCN 9
Parent Chemical Class: PCN



Parent CAS_No: 2050-75-1
Parent Chemical Name: PCN 10
Parent Chemical Class: PCN

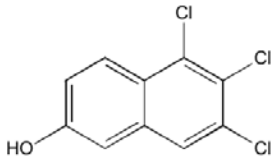


Parent CAS_No: 2065-70-5
Parent Chemical Name: PCN 11
Parent Chemical Class: PCN

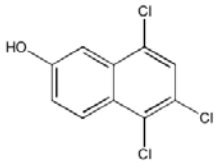


Parent CAS_No: 2198-77-8
Parent Chemical Name: PCN 12
Parent Chemical Class: PCN

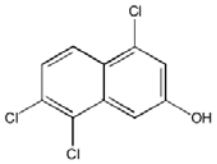
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



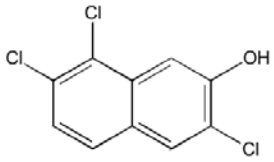
Parent CAS_No: 50402-52-3
Parent Chemical Name: PCN 13
Parent Chemical Class: PCN



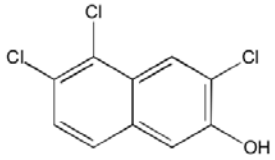
Parent CAS_No: 50402-51-2
Parent Chemical Name: PCN 14
Parent Chemical Class: PCN



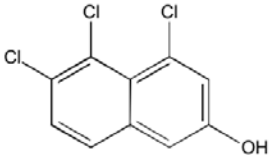
Parent CAS_No: 55720-33-7
Parent Chemical Name: PCN 15
Parent Chemical Class: PCN



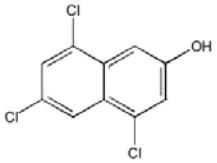
Parent CAS_No: 51570-44-6
Parent Chemical Name: PCN 16
Parent Chemical Class: PCN



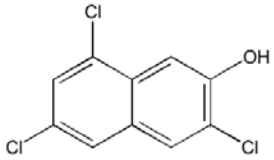
Parent CAS_No: 55720-34-8
Parent Chemical Name: PCN 17
Parent Chemical Class: PCN



Parent CAS_No: 55720-35-9
Parent Chemical Name: PCN 18
Parent Chemical Class: PCN



Parent CAS_No: 51570-43-5
Parent Chemical Name: PCN 19
Parent Chemical Class: PCN



Parent CAS_No: 55720-36-0
Parent Chemical Name: PCN 20
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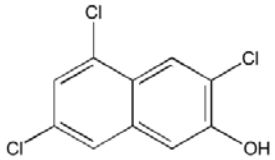
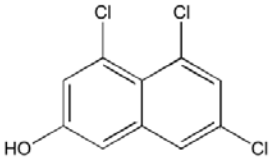
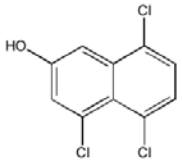


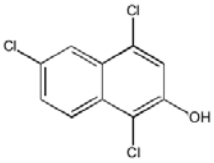
Parent CAS_No: 55720-37-1
Parent Chemical Name: PCN 21
Parent Chemical Class: PCN



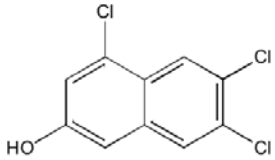
Parent CAS_No: 55720-38-2
Parent Chemical Name: PCN 22
Parent Chemical Class: PCN



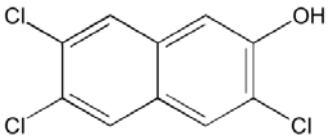
Parent CAS_No: 2437-55-0
Parent Chemical Name: PCN 23
Parent Chemical Class: PCN



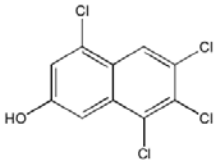
Parent CAS_No: 2437-54-9
Parent Chemical Name: PCN 24
Parent Chemical Class: PCN



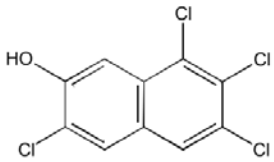
Parent CAS_No: 55720-39-3
Parent Chemical Name: PCN 25
Parent Chemical Class: PCN



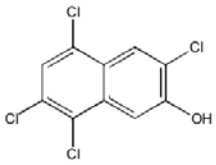
Parent CAS_No: 55720-40-6
Parent Chemical Name: PCN 26
Parent Chemical Class: PCN



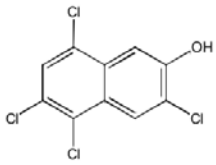
Parent CAS_No: 53555-63-8
Parent Chemical Name: PCN 28
Parent Chemical Class: PCN



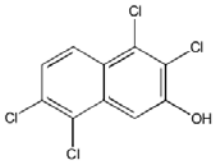
Parent CAS_No: 149864-78-8
Parent Chemical Name: PCN 29
Parent Chemical Class: PCN



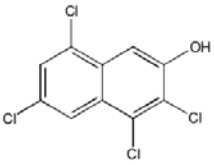
Parent CAS_No: 51570-45-7
Parent Chemical Name: PCN 33
Parent Chemical Class: PCN



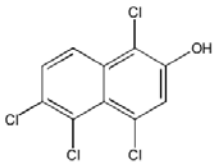
Parent CAS_No: 67922-21-8
Parent Chemical Name: PCN 34
Parent Chemical Class: PCN



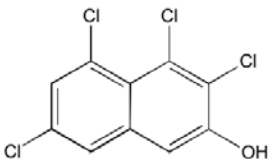
Parent CAS_No: 67922-22-9
Parent Chemical Name: PCN 36
Parent Chemical Class: PCN



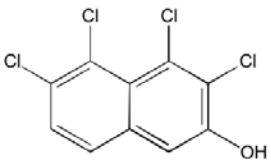
Parent CAS_No: 67922-23-0
Parent Chemical Name: PCN 37
Parent Chemical Class: PCN



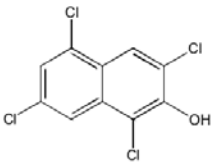
Parent CAS_No: 149864-80-2
Parent Chemical Name: PCN 38
Parent Chemical Class: PCN



Parent CAS_No: 67922-24-1
Parent Chemical Name: PCN 40
Parent Chemical Class: PCN

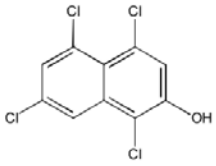


Parent CAS_No: 149864-82-4
Parent Chemical Name: PCN 41
Parent Chemical Class: PCN

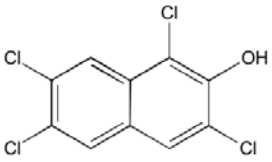


Parent CAS_No: 53555-64-9
Parent Chemical Name: PCN 42
Parent Chemical Class: PCN

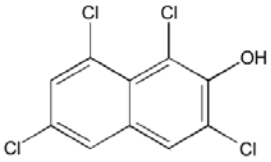
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



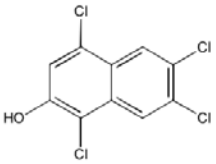
Parent CAS_No: 31604-28-1
Parent Chemical Name: PCN 43
Parent Chemical Class: PCN



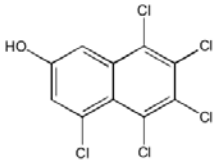
Parent CAS_No: 55720-42-8
Parent Chemical Name: PCN 44
Parent Chemical Class: PCN



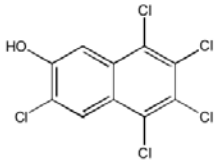
Parent CAS_No: 150224-15-0
Parent Chemical Name: PCN 45
Parent Chemical Class: PCN



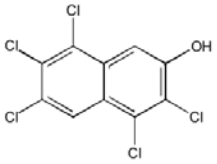
Parent CAS_No: 55720-43-9
Parent Chemical Name: PCN 47
Parent Chemical Class: PCN



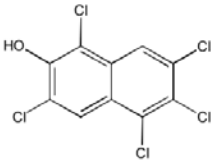
Parent CAS_No: 67922-25-2
Parent Chemical Name: PCN 49
Parent Chemical Class: PCN



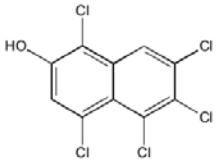
Parent CAS_No: 67922-26-3
Parent Chemical Name: PCN 50
Parent Chemical Class: PCN



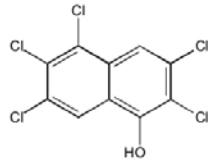
Parent CAS_No: 150224-18-3
Parent Chemical Name: PCN 51
Parent Chemical Class: PCN



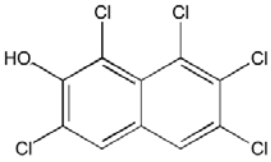
Parent CAS_No: 53555-65-0
Parent Chemical Name: PCN 52
Parent Chemical Class: PCN



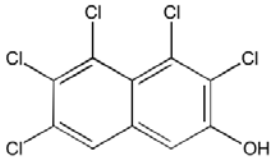
Parent CAS_No: 150224-24-1
Parent Chemical Name: PCN 53
Parent Chemical Class: PCN



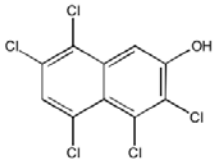
Parent CAS_No: 150224-16-1
Parent Chemical Name: PCN 54
Parent Chemical Class: PCN



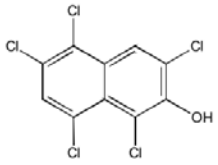
Parent CAS_No: 150224-23-0
Parent Chemical Name: PCN 55
Parent Chemical Class: PCN



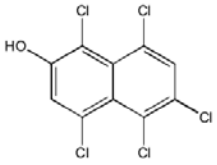
Parent CAS_No: 150205-21-3
Parent Chemical Name: PCN 56
Parent Chemical Class: PCN



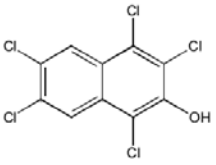
Parent CAS_No: 150224-20-7
Parent Chemical Name: PCN 57
Parent Chemical Class: PCN



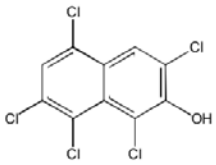
Parent CAS_No: 150224-19-4
Parent Chemical Name: PCN 58
Parent Chemical Class: PCN



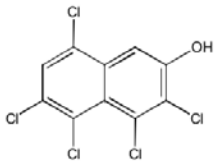
Parent CAS_No: 150224-25-2
Parent Chemical Name: PCN 59
Parent Chemical Class: PCN



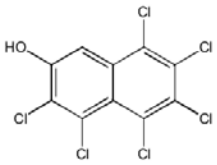
Parent CAS_No: 150224-17-2
Parent Chemical Name: PCN 60
Parent Chemical Class: PCN



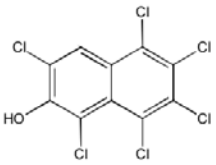
Parent CAS_No: 150224-22-9
Parent Chemical Name: PCN 61
Parent Chemical Class: PCN



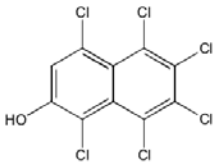
Parent CAS_No: 150224-21-8
Parent Chemical Name: PCN 62
Parent Chemical Class: PCN



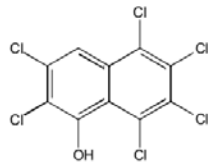
Parent CAS_No: 58877-88-6
Parent Chemical Name: PCN 63
Parent Chemical Class: PCN



Parent CAS_No: 67922-27-4
Parent Chemical Name: PCN 64
Parent Chemical Class: PCN



Parent CAS_No: 103426-93-3
Parent Chemical Name: PCN 65
Parent Chemical Class: PCN



Parent CAS_No: 103426-96-6
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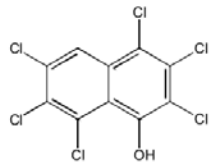
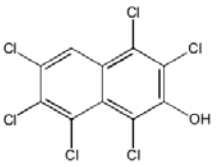
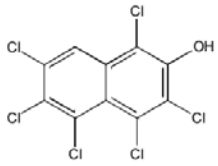


Parent CAS_No: 103426-97-7
Parent Chemical Name: PCN 67
Parent Chemical Class: PCN

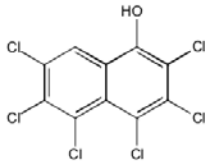


Parent CAS_No: 103426-95-5
Parent Chemical Name: PCN 68
Parent Chemical Class: PCN

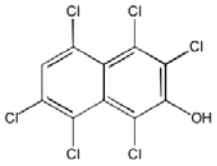
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



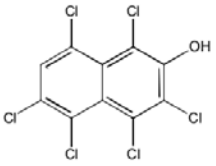
Parent CAS_No: 103426-94-4
Parent Chemical Name: PCN 69
Parent Chemical Class: PCN



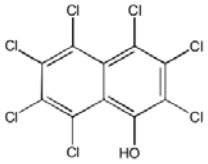
Parent CAS_No: 17062-87-2
Parent Chemical Name: PCN 70
Parent Chemical Class: PCN



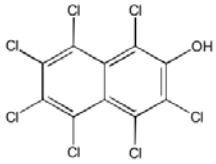
Parent CAS_No: 90948-28-0
Parent Chemical Name: PCN 71
Parent Chemical Class: PCN



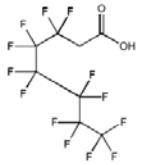
Parent CAS_No: 103426-92-2
Parent Chemical Name: PCN 72
Parent Chemical Class: PCN



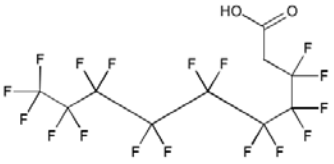
Parent CAS_No: 58863-14-2
Parent Chemical Name: PCN 73
Parent Chemical Class: PCN



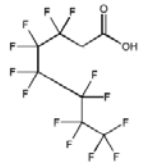
Parent CAS_No: 58863-15-3
Parent Chemical Name: PCN 74
Parent Chemical Class: PCN



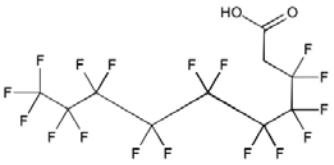
Parent CAS_No: 57677-95-9
Parent Chemical Name:
Bis[2-(perfluorohexyl)ethyl] Phosphate
Parent Chemical Class: PFAS



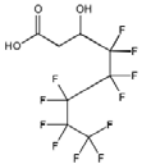
Parent CAS_No: 678-41-1
Parent Chemical Name:
Bis[2-(perfluorooctyl)ethyl] Phosphate
Parent Chemical Class: PFAS



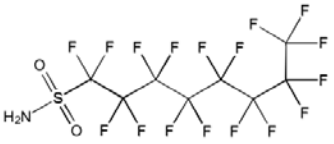
Parent CAS_No: 647-42-7
Parent Chemical Name:
2-(Perfluorohexyl)ethanol
Parent Chemical Class: PFAS



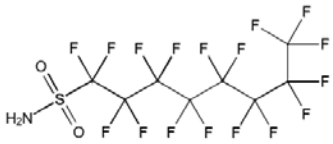
Parent CAS_No: 678-39-7
Parent Chemical Name:
2-(Perfluorooctyl)ethanol
Parent Chemical Class: PFAS



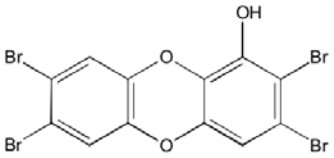
Parent CAS_No: 914637-49-3
Parent Chemical Name: 5:3
Fluorotelomer saturated carboxylic acid
Parent Chemical Class: PFAS



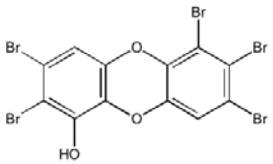
Parent CAS_No: 4151-50-2
Parent Chemical Name: N-
Ethylperfluorooctane sulfonamide
Parent Chemical Class: PFAS



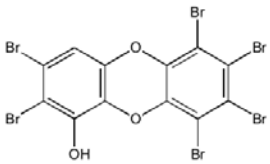
Parent CAS_No: 31506-32-8
Parent Chemical Name: N-
Methylperfluorooctane sulfonamide
Parent Chemical Class: PFAS



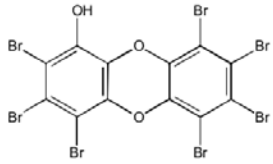
Parent CAS_No: 50585-41-6
Parent Chemical Name: 2,3,7,8-
Tetrabromodibenzodioxin
Parent Chemical Class: PXDD/F



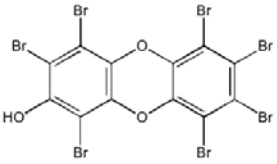
Parent CAS_No: 109333-34-8
Parent Chemical Name: 1,2,3,7,8-
Pentabromodibenzodioxin
Parent Chemical Class: PXDD/F



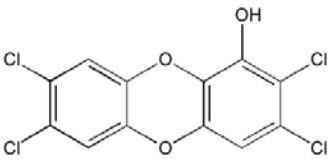
Parent CAS_No: 110999-44-5
Parent Chemical Name: 1,2,3,4,7,8-
Hexabromodibenzodioxin
Parent Chemical Class: PXDD/F



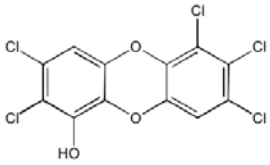
Parent CAS_No: 110999-47-8
Parent Chemical Name: 1,2,3,4,6,7,8-
Heptabromodibenzodioxin
Parent Chemical Class: PXDD/F



Parent CAS_No: 2170-45-8
Parent Chemical Name:
Octabromodibenzodioxin
Parent Chemical Class: PXDD/F

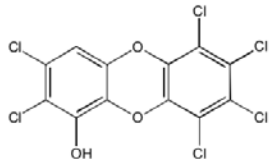


Parent CAS_No: 1746-01-6
Parent Chemical Name: 2,3,7,8-
Tetrachlorodibenzodioxin
Parent Chemical Class: PXDD/F

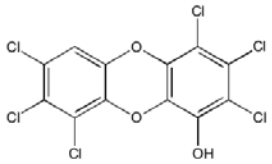


Parent CAS_No: 40321-76-4
Parent Chemical Name: 1,2,3,7,8-
Pentachlorodibenzodioxin
Parent Chemical Class: PXDD/F

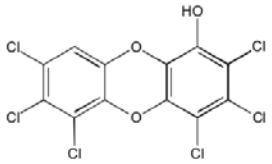
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



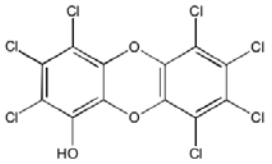
Parent CAS_No: 39227-28-6
Parent Chemical Name: 1,2,3,4,7,8-Hexachlorodibenzodioxin
Parent Chemical Class: PXDD/F



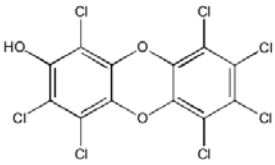
Parent CAS_No: 57653-85-7
Parent Chemical Name: 1,2,3,6,7,8-Hexachlorodibenzodioxin
Parent Chemical Class: PXDD/F



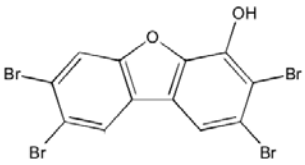
Parent CAS_No: 19408-74-3
Parent Chemical Name: 1,2,3,7,8,9-Hexachlorodibenzodioxin
Parent Chemical Class: PXDD/F



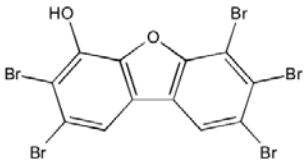
Parent CAS_No: 35822-46-9
Parent Chemical Name: 1,2,3,4,6,7,8-Heptachlorodibenzodioxin
Parent Chemical Class: PXDD/F



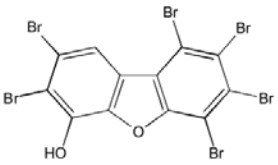
Parent CAS_No: 3268-87-9
Parent Chemical Name: Octachlorodibenzodioxin
Parent Chemical Class: PXDD/F



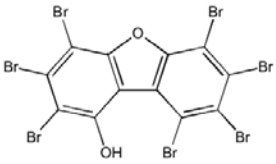
Parent CAS_No: 67733-57-7
Parent Chemical Name: 2,3,7,8-Tetrabromodibenzofuran
Parent Chemical Class: PXDD/F



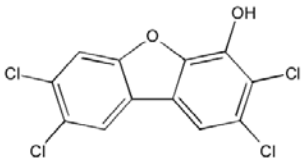
Parent CAS_No: 131166-92-2
Parent Chemical Name: 2,3,4,7,8-Pentabromodibenzofuran
Parent Chemical Class: PXDD/F



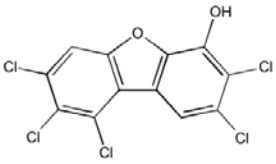
Parent CAS_No: 129880-08-6
Parent Chemical Name: 1,2,3,4,7,8-Hexabromodibenzofuran
Parent Chemical Class: PXDD/F



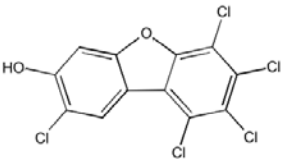
Parent CAS_No: 107555-95-3
Parent Chemical Name: 1,2,3,4,6,7,8-Heptabromodibenzofuran
Parent Chemical Class: PXDD/F



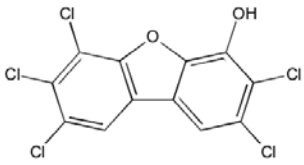
Parent CAS_No: 51207-31-9
Parent Chemical Name: 2,3,7,8-Tetrachlorodibenzofuran
Parent Chemical Class: PXDD/F



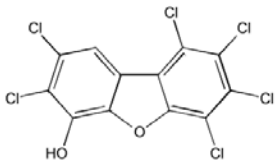
Parent CAS_No: 57117-41-6
Parent Chemical Name: 1,2,3,7,8-Pentachlorodibenzofuran
Parent Chemical Class: PXDD/F



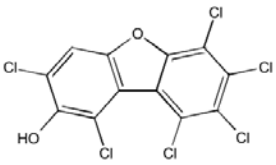
Parent CAS_No: 67517-48-0
Parent Chemical Name: 1,2,3,4,8-Pentachlorodibenzofuran
Parent Chemical Class: PXDD/F



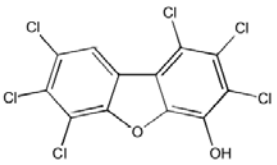
Parent CAS_No: 57117-31-4
Parent Chemical Name: 2,3,4,7,8-Pentachlorodibenzofuran
Parent Chemical Class: PXDD/F



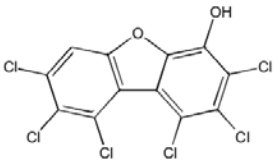
Parent CAS_No: 70648-26-9
Parent Chemical Name: 1,2,3,4,7,8-Hexachlorodibenzofuran
Parent Chemical Class: PXDD/F



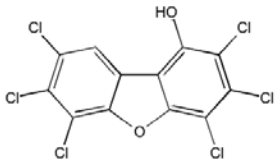
Parent CAS_No: 91538-84-0
Parent Chemical Name: 1,2,3,4,7,9-Hexachlorodibenzofuran
Parent Chemical Class: PXDD/F



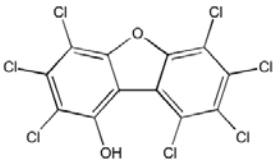
Parent CAS_No: 57117-44-9
Parent Chemical Name: 1,2,3,6,7,8-Hexachlorodibenzofuran
Parent Chemical Class: PXDD/F



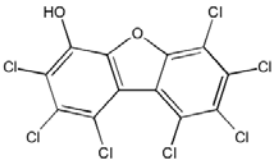
Parent CAS_No: 72918-21-9
Parent Chemical Name: 1,2,3,7,8,9-Hexachlorodibenzofuran
Parent Chemical Class: PXDD/F



Parent CAS_No: 60851-34-5
Parent Chemical Name: 2,3,4,6,7,8-Hexachlorodibenzofuran
Parent Chemical Class: PXDD/F

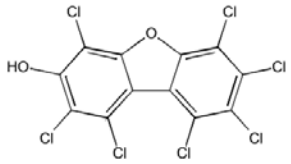


Parent CAS_No: 67562-39-4
Parent Chemical Name: 1,2,3,4,6,7,8-Heptachlorodibenzofuran
Parent Chemical Class: PXDD/F

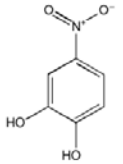


Parent CAS_No: 55673-89-7
Parent Chemical Name: 1,2,3,4,7,8,9-Heptachlorodibenzofuran
Parent Chemical Class: PXDD/F

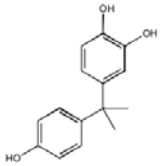
Table S7. Predicted TTR-binders in the metabolites of organic dust contaminants based on QSAR model



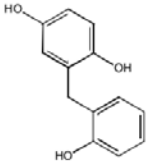
Parent CAS_No: 39001-02-0
Parent Chemical Name: Octachlorodibenzofuran
Parent Chemical Class: PXDD/F



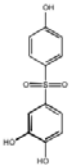
Parent CAS_No: 100-02-7
Parent Chemical Name: 4-Nitrophenol
Parent Chemical Class: Phenol



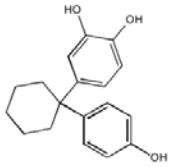
Parent CAS_No: 80-05-7
Parent Chemical Name: Bisphenol A
Parent Chemical Class: Phenol



Parent CAS_No: 2467-02-9
Parent Chemical Name: Bisphenol F
Parent Chemical Class: Phenol



Parent CAS_No: 80-09-1
Parent Chemical Name: Bisphenol S
Parent Chemical Class: Phenol



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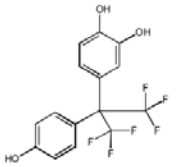

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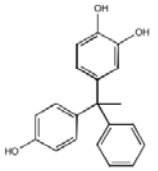

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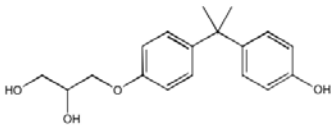

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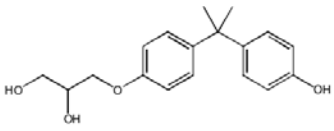
Parent Chemical Class: Phenol



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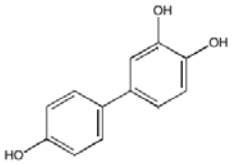
Parent Chemical Class: Phenol



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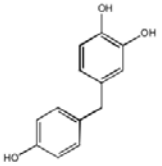

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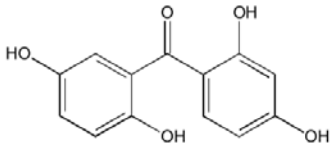
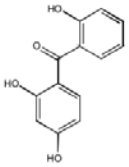
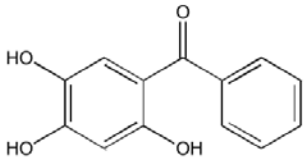
Parent Chemical Class: Phenol



Parent CAS_No: 131-57-7
Parent Chemical Name: 2-Benzoyl-5-methoxyphenol
Parent Chemical Class: UV filter



Parent CAS_No: 131-53-3
Parent Chemical Name: 2,2'-Dihydroxy-4-methoxybenzophenone
Parent Chemical Class: UV filter



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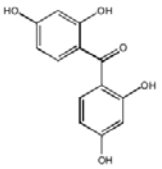

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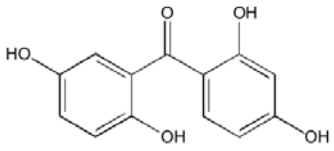
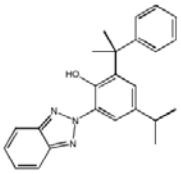
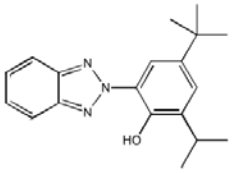
Parent Chemical Name: 4-Hydroxybenzophenone
Parent Chemical Class: UV filter



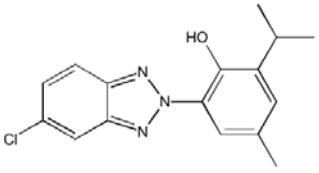
Parent CAS_No: 131-55-5
Parent Chemical Name: 2,4,2',4'-Tetrahydroxybenzophenone
Parent Chemical Class: UV filter



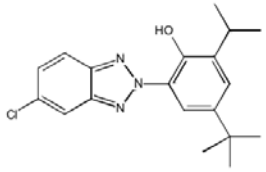
Parent CAS_No: 70321-86-7
Parent Chemical Name: 2-[2-Hydroxy-3,5-di-(1,1-dimethylbenzyl)]-2H-benzotriazole
Parent Chemical Class: UV filter



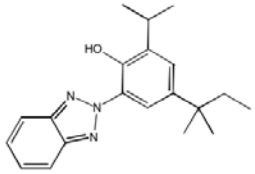
Parent CAS_No: 3846-71-7
Parent Chemical Name: 2-(2-Hydroxy-3,5-di-tert-butylphenyl)benzotriazole
Parent Chemical Class: UV filter



Parent CAS_No: 3896-11-5
Parent Chemical Name: 2-(2'-Hydroxy-3'-tert-butyl-5'-methylphenyl)-5-chlorobenzotriazole (Tinuvin 326)
Parent Chemical Class: UV filter



Parent CAS_No: 3864-99-1
Parent Chemical Name: 2-(2-Hydroxy-3,5-di-tert-butylphenyl)-5-chlorobenzotriazole (Tinuvin 327)
Parent Chemical Class: UV filter



Parent CAS_No: 25973-55-1
Parent Chemical Name: 2-(2-Hydroxy-3,5-di-tert-pentylphenyl)benzotriazole
Parent Chemical Class: UV filter

Table S8. Information of the chemicals tested in the bioassay

Chemical Name	CAS No.	Purity (%)	Provider
Mono-[2-(perfluorohexyl)ethyl] Phosphate	57678-01-0	98	Toronto Research Chemicals (Toronto, Canada)
Mono [2-(perfluorooctyl)ethyl] Phosphate	57678-03-2	97	Toronto Research Chemicals (Toronto, Canada)
Sodium bis(1H, 1H, 2H, 2H-perfluorodecyl)phosphate	678-41-1	96	Toronto Research Chemicals (Toronto, Canada)
Sodium bis(1H, 1H, 2H, 2H-perfluorooctyl)phosphate	57677-95-9	98	Toronto Research Chemicals (Toronto, Canada)
Perfluorohexylphosphonic acid	40143-76-8	98	Wellington Laboratories Inc. (Guelph, Ontario, Canada)
Perfluoroheptanesulfonic acid	375-92-8	98	Wellington Laboratories Inc. (Guelph, Ontario, Canada)
Perfluorodecylphosphonic acid	52299-26-0	98	Wellington Laboratories Inc. (Guelph, Ontario, Canada)
2,2',4,4'-Tetrahydroxybenzophenone (BP-2)	131-55-5	97	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
2-(2'-Hydroxy-3'-tert-butyl-5'-methylphenyl)-5-chlorobenzotriazole (Tinuvin 326)	3896-11-05	98	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
2-(2-Hydroxy-3,5-di-tert-butylphenyl)-5-chlorobenzotriazole (Tinuvin 327)	3864-99-1	98	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
2,4,5-Trichlorophenoxyacetic acid	93-76-5	98	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
3,5,6-Trichloro-2-pyridinol	6515-38-4	99.6	AccuStandard (New Haven, CT, USA)

2-Tert-butyl-4-(2,4-dichloro-5-isopropoxyphenyl)-5-oxo-1,3,4-oxadiazoline (Oxadiazon)	19666-30-9	100	AccuStandard (New Haven, CT,USA)
1-[(2,4-Dichlorophenyl)aminocarbonyl]-1-cyclopropanecarboxylic acid (Cyclanilide)	113136-77-9	98	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
3,6-Dichloro-2-methoxybenzoic acid (Dicamba)	1918-00-9	98	AccuStandard (New Haven, CT, USA)
4-Nitrophenol	100-02-7	96	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
Tris(isobutyl) phosphate	126-71-6	99	Merck Chemicals and Life Science AB (Solna, Sweden)
Tris(2-butoxyethyl) phosphate	78-51-3	94	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
Tris(1-chloro-2-propyl) phosphate	13674-84-5	99.5	Dr Ehrenstorfer GmbH (Augsburg, Germany)
Methyl paraben	99-76-3	99	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
Ethyl paraben	120-47-8	99	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
Butyl paraben	94-26-8	99	Sigma-Aldrich Sweden AB (Stockholm, Sweden)
Propyl paraben	94-13-3	99	Sigma-Aldrich Sweden AB (Stockholm, Sweden)

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