Polybrominated dibenzo-p-dioxins and dibenzofurans and mixed polybrominated/chlorinated dibenzo-p-dioxins and dibenzofurans

Additional information relating to the draft risk profile

February 2025

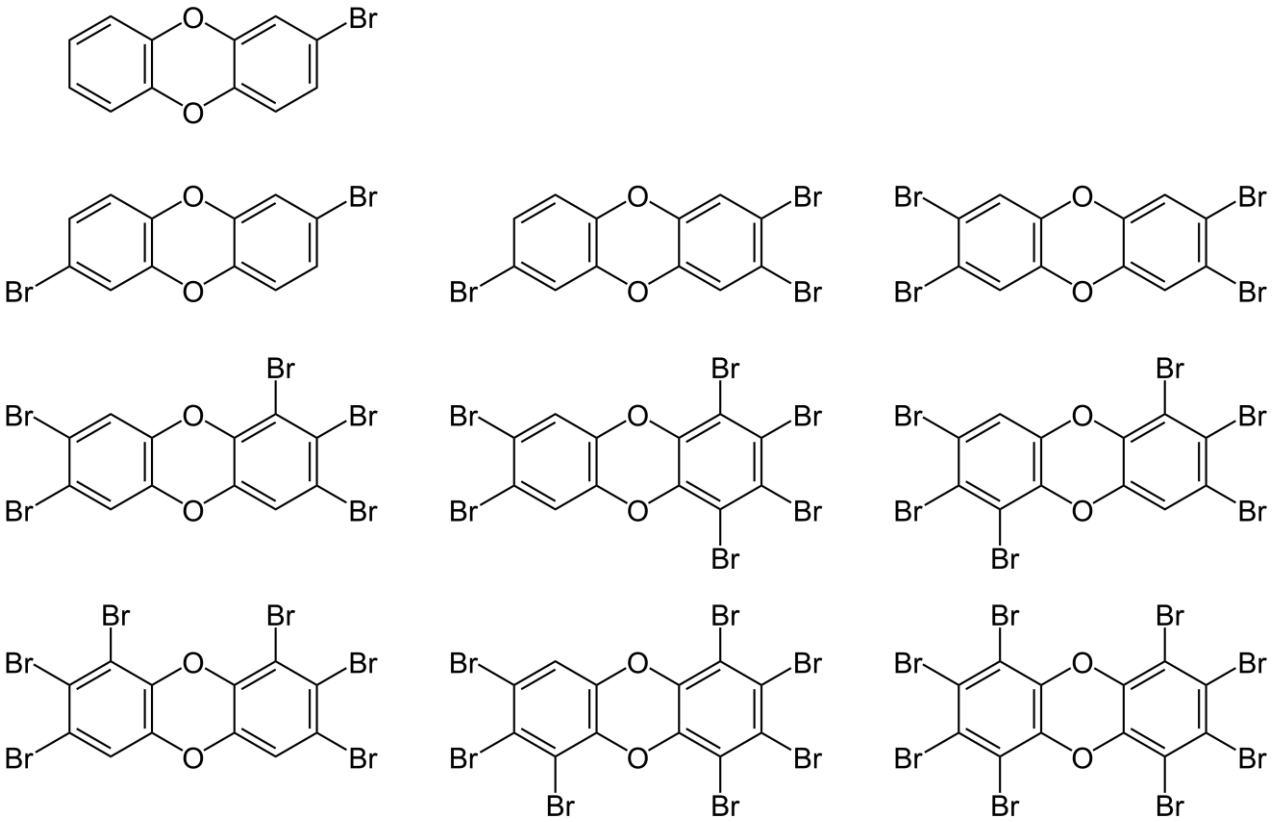

Figure 1. Structural formulae of the PBDD congeners contained in Table 1 of (UNEP/POPS/POPRC.21/#).

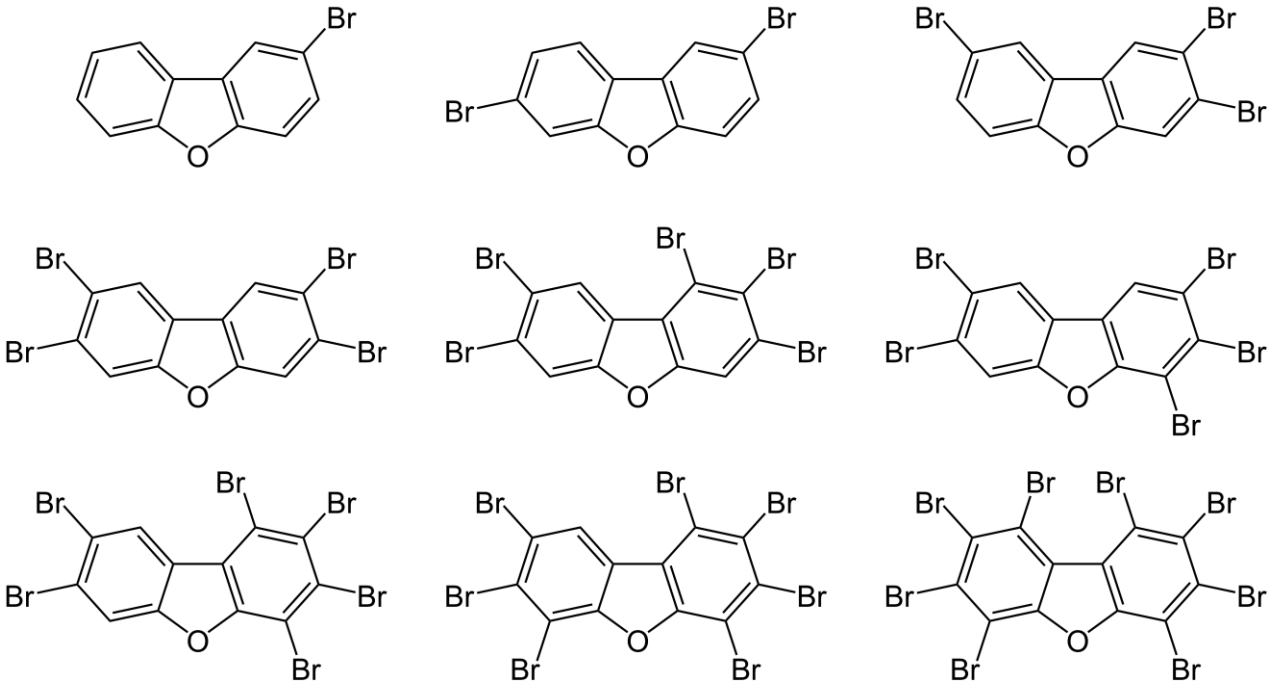

Figure 2. Structural formulae of the PBDF congeners contained in Table 1 of (UNEP/POPS/POPRC.21/#).

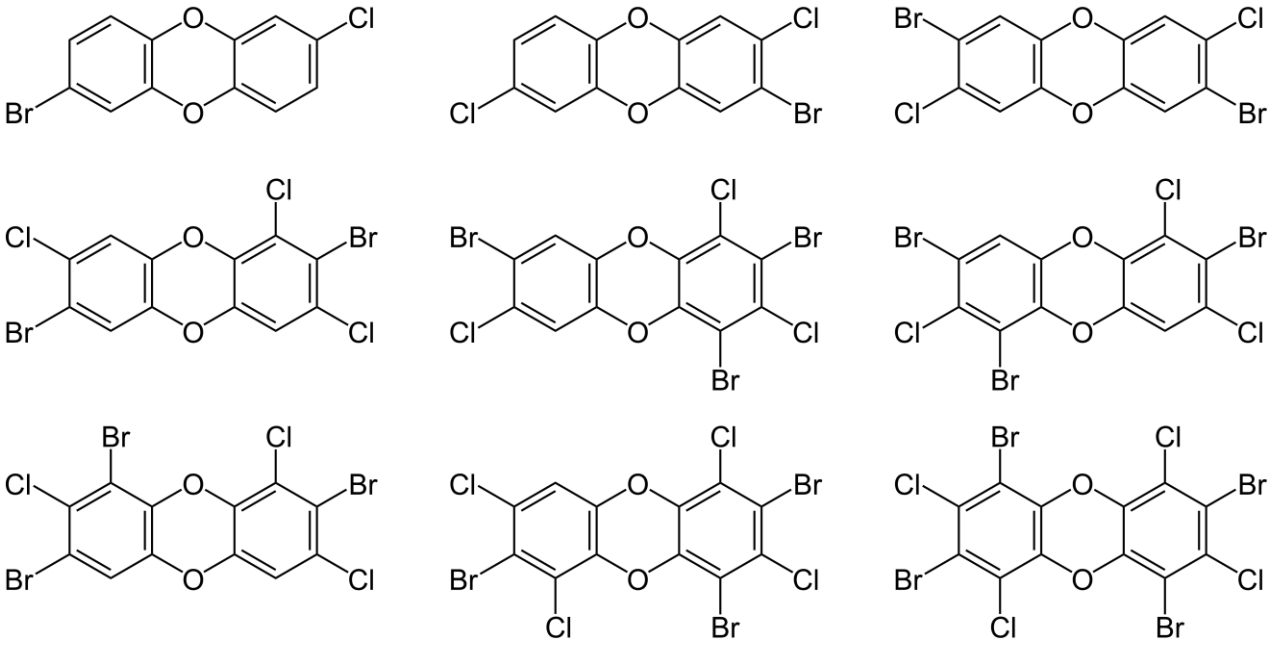

Figure 3. Structural formulae of PBCDD congeners with alternating chloro and bromo substituents. The substitution patterns correspond to those of the PBDD congeners in Table 1 of (UNEP/POPS/POPRC.21/#).

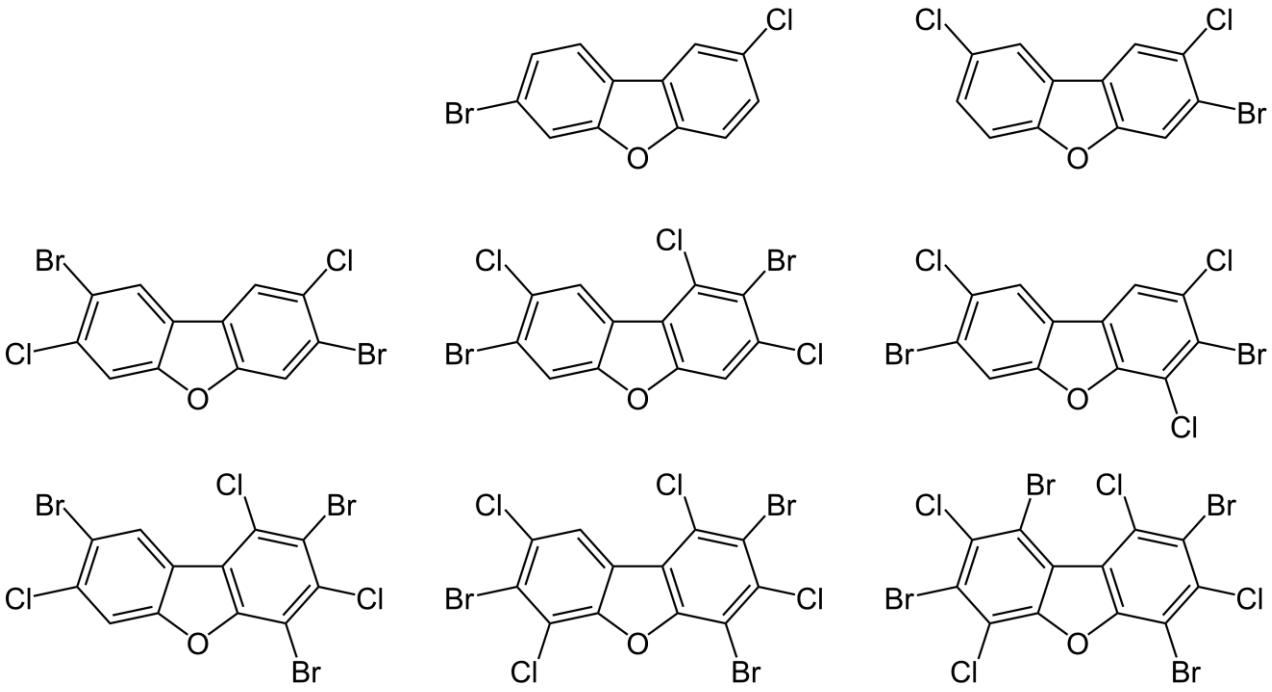

Figure 4. Structural formulae of PBCDF congeners with alternating chloro and bromo substituents. The substitution patterns correspond to those of the PBDF congeners in Table 1 of (UNEP/POPS/POPRC.21/#).

Table 1. Half-lives of PBDD/F and PBCDD/F congeners in water (values in days): Estimated based on the BIOWIN3 scores derived using the BIOWIN v4.10 module implemented in EPI Suite and the equation from Scheringer et al. (2012) and multiplied by a factor of 1.85 (Boethling et al. 1995). For comparison, half-lives of PCDD/F congeners estimated by same procedure as well as half-lives derived by Sinkonen & Paasivirta (2000).

	Converted from BIOWIN3			Sinkkonen & Paasivirta (2000)
	Br	**Cl/Br**	**Cl**	**Cl**
2-MoXDD	41	n.a.	39	–
2,7-DiXDD	73	70	66	–
2,3,7-TrXDD	130	117	112	–
2,3,7,8-TeXDD	230	208	188	167
1,2,3,7,8-PeXDD	408	350	316	300
1,2,3,4,7,8-HxXDD	723	620	533	617
1,2,3,6,7,8-HxXDD	723	620	533	617
1,2,3,7,8,9-HxXDD	723	620	533	617
1,2,3,4,6,7,8-HpXDD	1280	1044	897	1250
OXDD	2267	1850	1509	3292
2-MoXDF	35	n.a.	33	–
2,7-DiXDF	62	59	56	–
2,3,8-TrXDF	109	99	94	–
2,3,7,8-TeXDF	194	175	158	267
1,2,3,7,8-PeXDF	343	295	266	550
2,3,4,7,8-PeXDF	343	295	266	550
1,2,3,4,7,8-HxXDF	608	522	448	1167
1,2,3,4,6,7,8-HpXDF	1078	879	755	2667
OXDF	1909	1557	1270	8000

n.a.: not applicable

Table 2. Half-lives of PBDD/F and PBCDD/F congeners in soil (values in days): Estimated based on the BIOWIN3 scores derived using the BIOWIN v4.10 module implemented in EPI Suite and the equation from Scheringer et al. (2012) and multiplied by a factor of 1.85 (Boethling et al. 1995). For comparison, half-lives of PCDD/F congeners estimated by same procedure as well as half-lives derived by Sinkonen & Paasivirta (2000) and Terzaghi et al. (2020).

	Converted from BIOWIN3			Sinkkonen & Paasivirta (2000)	Terzaghi et al. (2020)
	Br	Cl/Br	Cl	Cl	Cl
2-MoXDD	77	n.a.	73	–	–
2,7-DiXDD	136	129	123	–	–
2,3,7-TrXDD	241	217	207	–	–
2,3,7,8-TeXDD	426	385	348	37500	927–1628
1,2,3,7,8-PeXDD	755	648	585	41667	1354–2113
1,2,3,4,7,8-HxXDD	1337	1148	985	100000	646–1095
1,2,3,6,7,8-HxXDD	1337	1148	985	22917	894–1606
1,2,3,7,8,9-HxXDD	1337	1148	985	29167	1325–3048
1,2,3,4,6,7,8-HpXDD	2368	1932	1659	37500	814–3230
OXDD	4195	3422	2792	54167	1219–1343
2-MoXDF	65	n.a.	61	–	–
2,7-DiXDF	114	109	103	–	–
2,3,8-TrXDF	203	183	174	–	–
2,3,7,8-TeXDF	359	324	293	22917	1573–2964
1,2,3,7,8-PeXDF	635	545	493	18750	1226–1967
2,3,4,7,8-PeXDF	635	545	493	22917	1456–2362
1,2,3,4,7,8-HxXDF	1125	966	829	25000	1314–2263
1,2,3,4,6,7,8-HpXDF	1994	1626	1396	14583	1186–3665
OXDF	3531	2881	2350	10416	960–2548

n.a.: not applicable

Table 3. QSAR predictions of probability of fast degradation in water using BIOWIN2 (nonlinear probability model)

BIOWIN2	*p* value		
	Br	Cl/Br	Cl
2,3,7-TrXDD	0.029	0.051	0.0676
2,3,7,8-TeXDD	0.0018	0.0033	0.0059
1,2,3,7,8-PeXDD	0.0001	0.0003	0.0005
1,2,3,4,7,8-HxXDD	0	0	0
1,2,3,6,7,8-HxXDD	0	0	0
OXDD	0	0	0
2,3,7,8-TeXDF	0.0002	0.0004	0.0008
1,2,3,7,8-PeXDF	0	0	0.0001
2,3,4,7,8-PeXDF	0	0	0.0001
1,2,3,4,7,8-HxXDF	0	0	0
1,2,3,4,6,7,8-HpXDF	0	0	0
OXDF	0	0	0

Does not biodegrade fast (probability <0.5), does biodegrade fast (probability >0.5)

Table 4. QSAR predictions of probability of readily biodegradable in water using BIOWIN6 (MITI non-linear model prediction)

Substance	Probability from BIOWIN6
2,3,7-TrBDD	0.0702
2,3,7,8-TeBDD	0.0332
1,2,3,7,8-PeBDD	0.0153
1,2,3,4,7,8-HxBDD	0.007
1,2,3,6,7,8-HxBDD	0.007
OBDD	0.0015
2,3,7,8-TeBDF	0.0262
1,2,3,7,8-PeBDF	0.0121
2,3,4,7,8-PeBDF	0.0121
1,2,3,4,7,8-HxBDF	0.0055

1,2,3,4,6,7,8-HpBDF	0.0025
OBDF	0.0011

Does not biodegrade fast (probability <0.5), does biodegrade fast (probability >0.5)

Table 5. Log K_{OW} of PBDD/F and PBCDD/F congeners estimated using the KOWWIN v1.69 module implemented in EPI Suite. Estimated log K_{OW} of PCDD/F congeners for comparison.

	Log K_{OW}		
	Br	**Cl/Br**	**Cl**
2-MoXDD	5.2	n.a.	5.0
2,7-DiXDD	6.1	5.9	5.6
2,3,7-TrXDD	7.0	6.5	6.3
2,3,7,8-TeXDD	7.9	7.4	6.9
1,2,3,7,8-PeXDD	8.8	8.1	7.6
1,2,3,4,7,8-HxXDD	9.7	9.0	8.2
1,2,3,6,7,8-HxXDD	9.7	9.0	8.2
1,2,3,7,8,9-HxXDD	9.7	9.0	8.2
1,2,3,4,6,7,8-HpXDD	10.6	9.6	8.9
OXDD	11.5	10.5	9.5
2-MoXDF	4.9	n.a.	4.7
2,7-DiXDF	5.8	5.6	5.3
2,3,8-TrXDF	6.7	6.2	6.0
2,3,7,8-TeXDF	7.6	7.1	6.6
1,2,3,7,8-PeXDF	8.5	7.8	7.3
2,3,4,7,8-PeXDF	8.5	7.8	7.3
1,2,3,4,7,8-HxXDF	9.4	8.7	7.9
1,2,3,4,6,7,8-HpXDF	10.3	9.3	8.6
OXDF	11.2	10.2	9.2

n.a.: not applicable

Table 6. Gas-phase half-lives of PBDD/F and PBCDD/F congeners obtained from the AOPWIN v1.92 module implemented in EPI Suite, based on estimated second-order rate constants for the reaction with OH radicals. Estimated half-lives of PCDD/F congeners for comparison.

	Gas-phase half-life (days)		
	Br	**Cl/Br**	**Cl**
2-MoXDD	1.8	n.a.	1.7
2,7-DiXDD	2.9	2.8	2.6
2,3,7-TrXDD	6.4	5.7	5.7
2,3,7,8-TeXDD	16	14	14
1,2,3,7,8-PeXDD	26	22	22
1,2,3,4,7,8-HxXDD	61	52	51
1,2,3,6,7,8-HxXDD	43	38	34
1,2,3,7,8,9-HxXDD	43	38	34
1,2,3,4,6,7,8-HpXDD	99	79	77
OXDD	256	205	197
2-MoXDF	2.4	n.a.	2.3
2,7-DiXDF	4.0	3.8	3.5
2,3,8-TrXDF	9.9	8.6	8.3
2,3,7,8-TeXDF	25	23	22
1,2,3,7,8-PeXDF	44	38	36
2,3,4,7,8-PeXDF	45	39	37
1,2,3,4,7,8-HxXDF	110	94	91
1,2,3,4,6,7,8-HpXDF	208	167	163
OXDF	504	435	389

n.a.: not applicable