Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting information

Sponge-derived polybrominated diphenyl ethers and dibenzo-*p*-dioxins, irreversible inhibitors of the bacterial α-D-galactosidase

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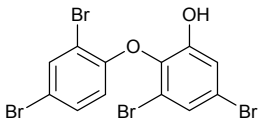
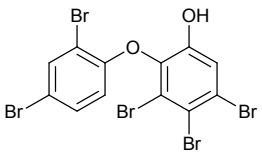
Table S1. ^{1}H, ^{13}CNMR data of compounds**1-3** (^{1}H NMR, 300 MHz; ^{13}C NMR, 75 MHz)

	1(DMSO-d_6)		**2**(DMSO-d_6)		**3**(DMSO-d_6)	
position	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1	152.1		150.8		148.8	
2	138.3		139.4		139.8	
3	118.7		121.6		117.2	
4	125.1	7.40 (1H, *d*, 2.4)	116.0		125.2	
5	118.0		121.6		119.8	
6	119.5	7.15 (1H, *d*,2.4)	120.5	7.45(1H, s)	115.8	
1′	152.6		152.3		152.0	
2′	111.6		111.8		112.1	
3′	135.0	7.88 (1H, *d*, 2.4)	135.1	7.90(1H, *d*, 2.4)	135.0	7.79 (1H, *d*, 2.4)
4′	114.0		114.0		114.3	
5′	131.3	7.40 (1H, *dd*, 9.0, 2.4)	131.7	7.40(1H, *dd*, 8.8, 2.4)	131.6	7.29 (1H, *dd*, 8.8, 2.4)
6′	116.1	6.46 (1H, *d*, 9.0)	115.9	6.51(1H, *d*, 8.8)	116.1	6.42 (1H, *d*, 8.8)
		10.80 (1H, brs, OH)		10.96 (1H, brs, OH)		10.94(1H, brs, OH)





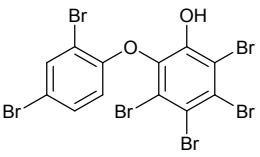
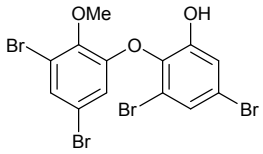


Table S2. ^{1}H, ^{13}CNMR data of compounds**4** and **5** (^{1}H NMR, 300 MHz; ^{13}C NMR, 75 MHz,)

	4		**5**(DMSO-d_6)	
position	δ_C(DMSO-d_6)	δ_H (J in Hz)($CDCl_3$)	δ_C	δ_H (J in Hz)
1	151.5		148.8	
2	137.7		139.4	
3	117.5		125.5	
4	125.0	7.45 (1H, *d*, 2.0)	120.4	
5	118.4		117.4	
6	119.6	7.18 (1H, *d*,2.0)	115.7	
1′	150.8		145.8	
2′	144.8		144.0	
3′	118.1		111.2	
4′	127.8	7.45 (1H, *d*, 2.0)	128.5	7.29 (1H, *d*, 2.4)
5′	115.5		109.4	
6′	116.3	6.77 (1H, *d*, 2.0)	115.5	6.42 (1H, *d*, 2.4)
OCH_3	60.40	4.03(*s*)		
		6.65 (*s*. OH)		10.91(br*s*, OH)



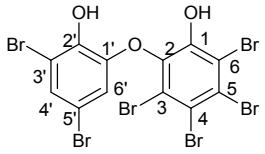
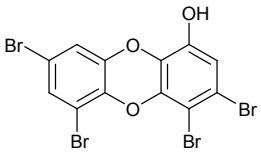
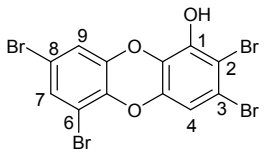
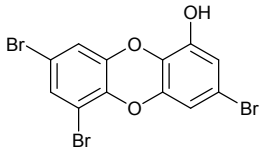


Table S3. ^{1}H, ^{13}CNMR data of compounds **6-8** (^{1}H NMR, 300 MHz; ^{13}C NMR, 75 MHz,)

	6(DMSO-d_6)		**7**(DMSO-d_6)		**8**(DMSO-d_6)	
position	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)	δ_C	δ_H (*J* in Hz)
1	146.8		144.1		145.7	
2	115.6	6.73 (1H, *d*,2.1)	109.7		116.3	6.93 (1H, *s*)
3	114.7		117.9		117.9	
4	109.7	6.64 (1H, *d*,2.1)	111.1	6.94 (1H, *s*)	101.3	
4a	142.3		140.9		140.2	
10a	129.2		129.9		129.7	
5a	138.3		138.2		138.4	
6	110.2		110.3		110.3	
7	129.5	7.43 (1H, *d*,2.4)	129.8	7.14 (1H, *d,* 2.2)	129.7	7.17 (1H, *d*, 2.1)
8	115.4		115.4		115.9	
9	118.9	7.18 (1H, *d*, 2.4)	118.8	7.47 (1H, *d*, 2.2)	118.7	7.43 (1H, *d*, 2.1)
9a	142.8		142.4		142.4	







^{1}H NMR and ^{13}C NMR spectra were recorded on a Bruker AVANCE DPX-300 MHz NMR spectrometer