

## Supplementary Information

Table S1: Initial screening gradient.

Time (min)	% A (CO <sub>2</sub> )	% B (MeOH)	Flow Rate (mL/min.)
Initial	98	2	2
5.00	70	30	2
5.50	70	30	2
5.60	98	2	2

Table S2: Final chromatographic gradient.

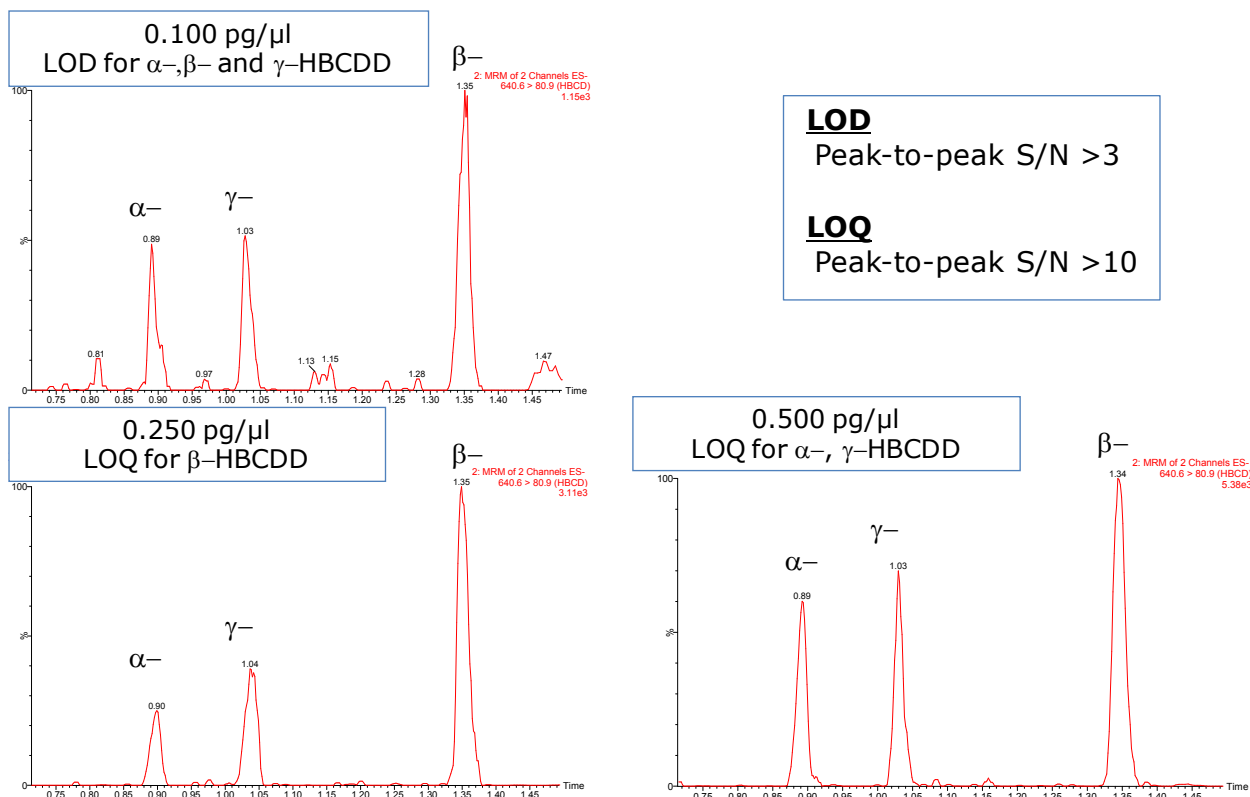
Time (min)	% A (CO <sub>2</sub> )	% B (MeOH)	Flow Rate (mL/min.)
Initial	98	2	2
2	90	10	2
2.01	90	10	2.5
2.3	98	2	2.5
2.31	98	2	2

Table S3: RPLC gradient, from Shi et al. <sup>7</sup>

Time (min)	% A (water)	% B (1:1 MeOH:MeCN)	Flow Rate (mL/min.)
Initial	50	50	0.2
1	50	50	0.2
5	90	10	0.2
8	90	10	0.2
10	100	0	0.2
12	50	50	0.2

Table S4: MRM transitions used for MS/MS analysis, where the two transitions are the Br<sup>81</sup> and Br<sup>79</sup> isotopes, respectively.

Compound	Parent (m/z)	Daughter (m/z)	Dwell Time (s)	Cone (V)	Collision Energy (V)
α-,β- and γ-HBCDD	640.6	78.9	0.05	30	20
α-,β- and γ-HBCDD	640.6	80.9	0.05	30	20



**LOD**  
Peak-to-peak S/N > 3

**LOQ**  
Peak-to-peak S/N > 10

Figure S1: Quantitative transition MRMs for  $\alpha$ -,  $\beta$ - and  $\gamma$ -HBCDD at their respective LODs and LOQs, as determined by calculated peak-to-peak S/N ratios.