Table S1 Structures of PBDEs that are mentioned in the introduction

References	Molecules	Structure
[9]	BDE-28	
	BDE-47	
[10]	BDE-209	
[12]	BDE-3	
	BDE-8	
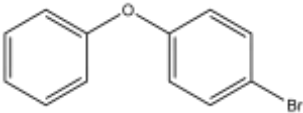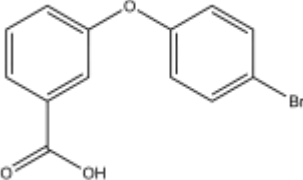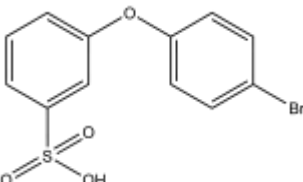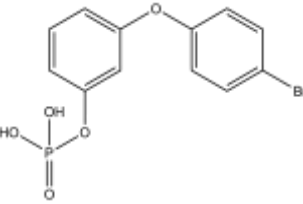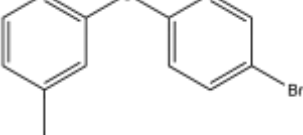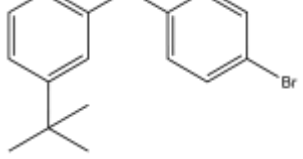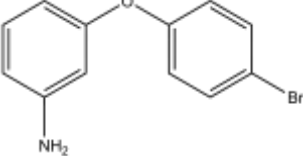
Table S2 References on comprehensive evaluation of pollutant properties using mathematical methods
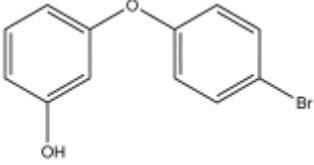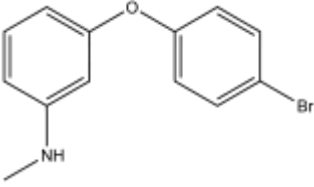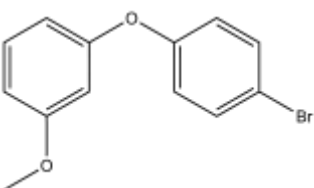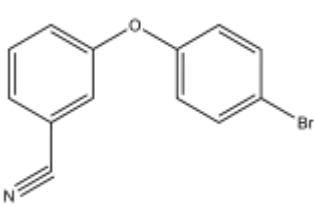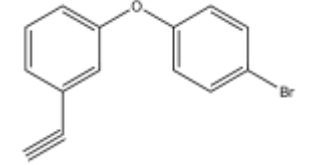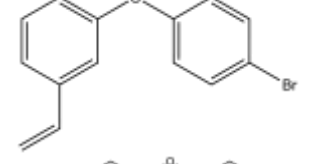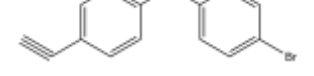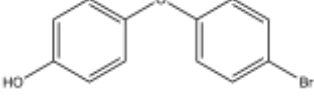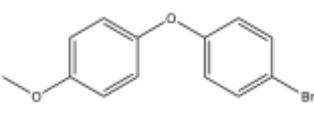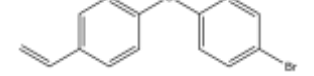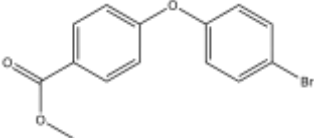
References	Method
[S1]	Averaging method
[S2]	Threshold Method
[S3]	Variation Weighting Method
[S4]	Simplified formula method
[S5]	Fuzzy comprehensive evaluation

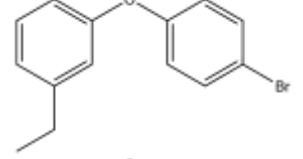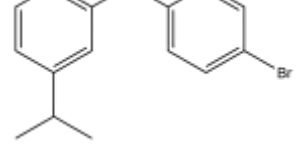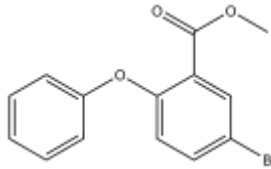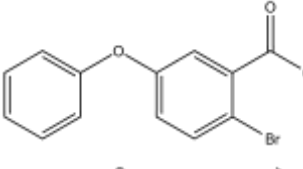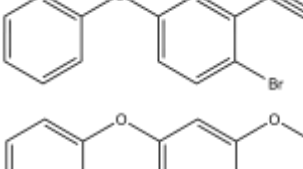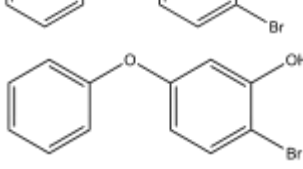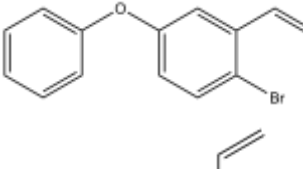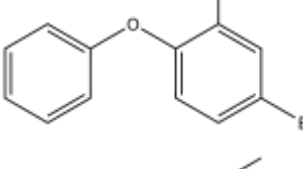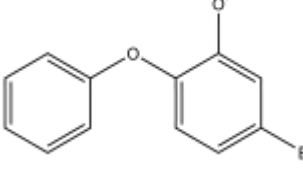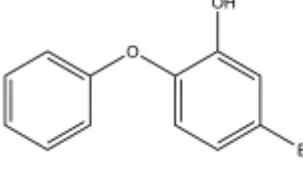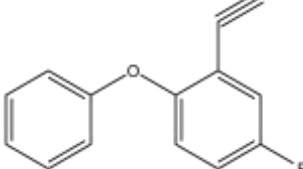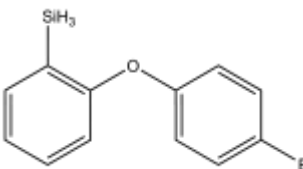**Table S3** Horizontal comparison of model parameters

References	Model	q^2 (>0.5)	$r^2 pred$ (>0.6)
[S1]	CoMSIA	0.535	0.773
[S2]	CoMFA	0.760	0.650
[S3]	CoMFA	0.767	0.967
[S4]	CoMFA	0.691	0.833
	CoMSIA	0.828	0.838
[S5]	CoMFA	0.560	0.692

Table S4 Molecular information of PBDEs derivatives

No.	Structural formula	Structure	Molar mass (g/mol)
BDE-3	$C_{12}H_9BrO$		249.10
BDE-3-1	$C_{13}H_9BrO_3$		293.11
BDE-3-2	$C_{12}H_9BrO_4S$		329.17
BDE-3-3	$C_{12}H_{10}BrO_5P$		345.08
BDE-3-4	$C_{13}H_{11}BrO$		263.13
BDE-3-5	$C_{14}H_{13}BrO$		277.16
BDE-3-6	$C_{15}H_{15}BrO$		291.18
BDE-3-7	$C_{16}H_{17}BrO$		305.21
BDE-3-8	$C_{12}H_{10}BrNO$		264.12

BDE-3-9	$C_{12}H_9BrO_2$		265.10
BDE-3-10	$C_{13}H_{12}BrNO$		278.14
BDE-3-11	$C_{13}H_{11}BrO_2$		279.13
BDE-3-12	$C_{13}H_8BrNO$		274.11
BDE-3-13	$C_{14}H_9BrO$		273.12
BDE-3-14	$C_{14}H_{11}BrO$		275.14
BDE-3-15	$C_{14}H_9BrO$		273.12
BDE-3-16	$C_{12}H_9BrO2$		265.10
BDE-3-17	$C_{13}H_{11}BrO_2$		279.13
BDE-3-18	$C_{14}H_{11}BrO$		275.14
BDE-3-19	$C_{14}H_{11}BrO_3$		307.14

BDE-3-20	$C_{14}H_{11}BrO_3$		307.14
BDE-3-21	$C_{14}H_{11}BrO_3$		307.14
BDE-3-22	$C_{14}H_9BrO$		273.12
BDE-3-23	$C_{13}H_{11}BrO_2$		279.13
BDE-3-24	$C_{12}H_9BrO_2$		265.10
BDE-3-25	$C_{14}H_{11}BrO$		275.14
BDE-3-26	$C_{14}H_{11}BrO$		275.14
BDE-3-27	$C_{13}H_{11}BrO_2$		279.13
BDE-3-28	$C_{12}H_9BrO_2$		265.10
BDE-3-29	$C_{14}H_9BrO$		273.12
BDE-3-30	$C_{12}H_{11}BrOSi$		279.20

Table S5-1 Toxicokinetic prediction and assessment of BDE before and after modification using TOPKAT module

| No. | Ames mutagenicity | NTP Rodent Carcinogenicity | | | | | FDA Rodent Carcinogenicity | | |
		Male rat	Female rat	Male mouse	Female mouse	Male rat Non vs. Carc	Male rat Single vs. Mult	Female rat Non vs. Carc	Female rat Single vs. Mult
BDE-3	0.6454/Non	0.6695/Carc	0.5620/Carc	0.8748/Carc	0.7095/Carc	0.3204/Non	Needless	0.2630/Non	Needless
BDE-3-4	0.6996/Non	0.6127/Carc	0.5333/Carc	0.7729/Carc	0.5946/Non	0.2811/Non	Needless	0.2361/Non	Needless
BDE-3-5	0.6472/Non	0.5567/Non	0.5142/Non	0.8151/Carc	0.7558/Carc	0.3223/Non	Needless	0.2471/Non	Needless
BDE-3-7	0.6455/Non	0.6587/Carc	0.5277/Non	0.5574/Non	0.3541/Non	0.3042/Non	Needless	0.2196/Non	Needless
BDE-3-13	0.4206/Non	0.5420/Non	0.5059/Carc	0.7859/Carc	0.6016/Carc	0.3047/Non	Needless	0.2385/Non	Needless
BDE-3-19	0.6418/Non	0.4707/Non	0.5010/Non	0.8600/Carc	0.5851/Non	0.2935/Non	Needless	0.2492/Non	Needless

Probability value

Table S5-2 Toxicokinetic predictions of BDE before and after modification using TOPKAT module

No.	Probability value				Rat chronic oral LOAEL[*] g/kg	Rat oral LD50[*] g/kg	Rat maximum tolerated dose-feed/Water g/kg	Rat maximum tolerated dose-gavage g/kg	Rat inhalational LC50 [*] mg/m³/h
	FDA Rodent Carcinogenicity								
	Male mouse Non vs. Carc	Male mouse Single vs. Mult	Female mouse Non vs. Carc	Female mouse Single vs. Mult					
BDE-3	0.3056/Carc	0.1464/Single	0.2758/Carc	0.4973/Mult	0.1490/Mod	0.7420/Low	0.0727/Mod	0.0006/Hyper	3310.7200/High
BDE-3-4	0.2822/Carc	0.1457/Single	0.2795/Carc	0.4941/Mult	0.1342/Mod	0.4853/Low	0.2464/Mod	0.0002/Hyper	3475.5200/High
BDE-3-5	0.2884/Carc	0.1458/Single	0.3146/Carc	0.4444/Mult	0.0426/High	2.2460/Non	0.0946/Mod	0.0010/Hyper	5211.2700/High
BDE-3-7	0.2118/Non	Needless	0.2101/Non	Needless	0.0620/Mod	4.5981/Non	0.1444/High	0.0004/Hyper	8941.2300/Mod
BDE-3-13	0.2615/Carc	0.1500/Single	0.2159/Non	Needless	0.0174/High	0.7351/Low	0.1437/Mod	0.0001/Hyper	466.9520/Hyper
BDE-3-19	0.2841/Carc	0.1456/Single	0.2547/Carc	0.5429/Mult	0.0969/Mod	0.9813/Low	0.2464/Mod	0.0002/Hyper	3475.5200/High

* Assessment finished based on "Acute Oral, Inhalation and Percutaneous Toxicity Classification for Rats" (Table S4-2), cited form the Guidelines for the Hazard Evaluation of New Chemical Substances (HJ/T154-2004), Ministry of Ecology and Environment of the People's Republic of China, April 13, 2004.

Table S5-3 Toxicokinetic predictions of BDE before and after modification using TOPKAT module

No.	Fathead minnow LC50 [*] g/L	Daphnia EC50 [*] mg/L	Probability value					
			Developmental toxicity potential (DTP)	Skin irritancy	Skin sensitization NON vs. SENS	Skin sensitization (MLD/MOD) vs. SEV	Ocular irritancy (Non/Mild) vs. (Mod/Sev)	Ocular irritancy MOD vs. SEV
BDE-3	0.0019/Hyper	0.1466/Hyper	0.6253/Yes	0.9635/Non	0.8855/SENS	0.9866/SEV	0.7970/Mild	Needless
BDE-3-4	0.0014/High	0.1218/Hyper	0.6590/Yes	0.9633/Non	0.8433/SENS	0.9894/SEV	0.8146/(Mod/Sev)	0.6743/Mod
BDE-3-5	0.0022/Hyper	0.2380/Hyper	0.6551/Yes	0.9568/Non	0.8792/SENS	0.9837/SEV	0.7238/Mild	Needless
BDE-3-7	0.0020/Hyper	0.2376/Hyper	0.6549/Yes	0.9688/Non	0.8767/SENS	0.9917/SEV	0.7758/Mild	Needless
BDE-3-13	0.0058/High	0.1118/Hyper	0.5659/Yes	0.9506/Non	0.8797/SENS	0.9875/SEV	0.8372/(Mod/Sev)	0.6974/Sev
BDE-3-19	0.0034/High	0.1510/Hyper	0.6587/Yes	0.9554/Non	0.8501/SENS	0.9926/SEV	0.8491/(Mod/Sev)	0.6816/Sev

[*] Assessment finished based on "Ecotoxicological Hazard Classification" (Table S4-3), cited form the Guidelines for the Hazard Evaluation of New Chemical Substances (HJ/T154-2004), Ministry of Ecology and Environment of the People's Republic of China, April 13, 2004.

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