Supporting Information

Identification of novel tetrabromobisphenol A byproducts in industrial chemicals and environment near a manufacturing site: An overlooked source of novel pollutants

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Text S1. Samples pretreatment.

River water samples (200 mL) were filtered through a 0.45 μm glass fiber membrane filter, and added the isotope-labeled surrogate ($^{13}C_{12}$-BPA, 5 ng). The water samples were liquid-liquid extracted four times with 160 mL DCM. The combined extracts were rotary evaporated and re-dissolved in 1 mL of MeOH.[1]

The soil/sediment samples (3.0 g, dry weight), which had been mixed with isotope-labeled surrogate ($^{13}C_{12}$-BPA, 5 ng), were extracted with DCM (25 mL) for 30 min by ultrasonic extraction three times. The extracts were combined, concentrated with a rotary evaporator, solvent exchanged to 1 mL of DCM/hexane (1/1, v/v), and further cleaned by gel permeation chromatography (GPC, biobeads S-X3, 20 × 2.0 cm i.d.). Then, the GPC column was eluted with DCM/hexane (1/1, v/v). The initial 15 mL eluted were discarded, and the following 75 mL were collected and concentrated by rotary evaporator. The purified substances were re-dissolved in MeOH/ultrapure water (5%, v/v) and further purified by HLB (Waters Oasis, 200 mg, 6cc) solid phase extraction cartridges. The HLB cartridges were pre-conditioned with 5 mL MeOH and 5 mL MeOH/ultrapure water (5%, v/v). After loading sample solution, the cartridges were washed with 5 mL MeOH/ultrapure water (5%, v/v) to eliminate interferences, then vacuumed for 2 min to remove most of the water. Finally, the cartridges were eluted with 12 mL of MeOH, and concentrated to 1 mL before HPLC-MS/MS analysis.[2,3]

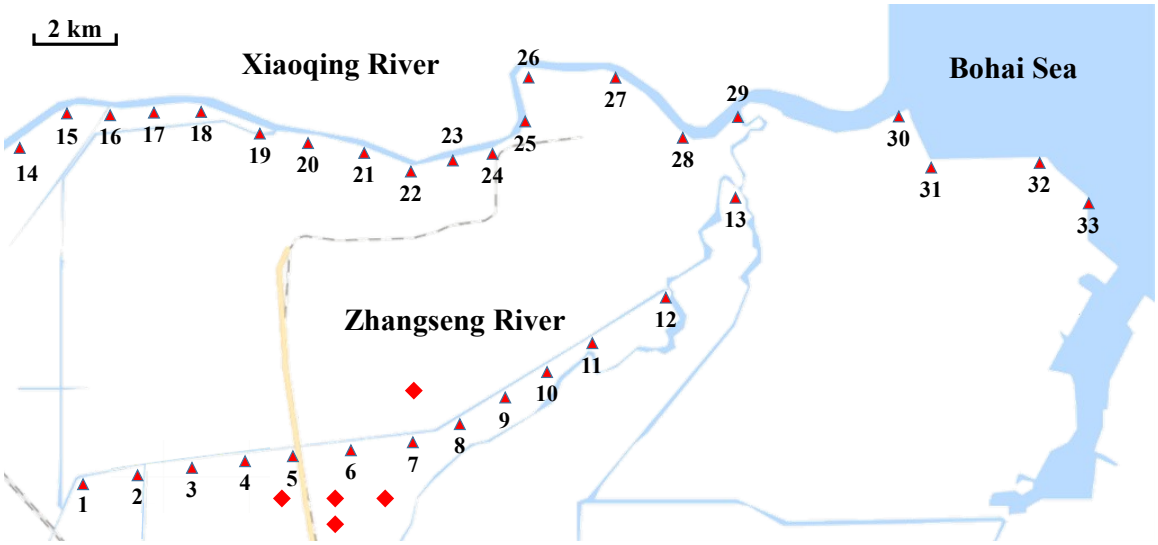

Figure S1. Sampling sites (1-33).[4]

▲: sampling site; ◆: the location of brominated flame retardant plant.

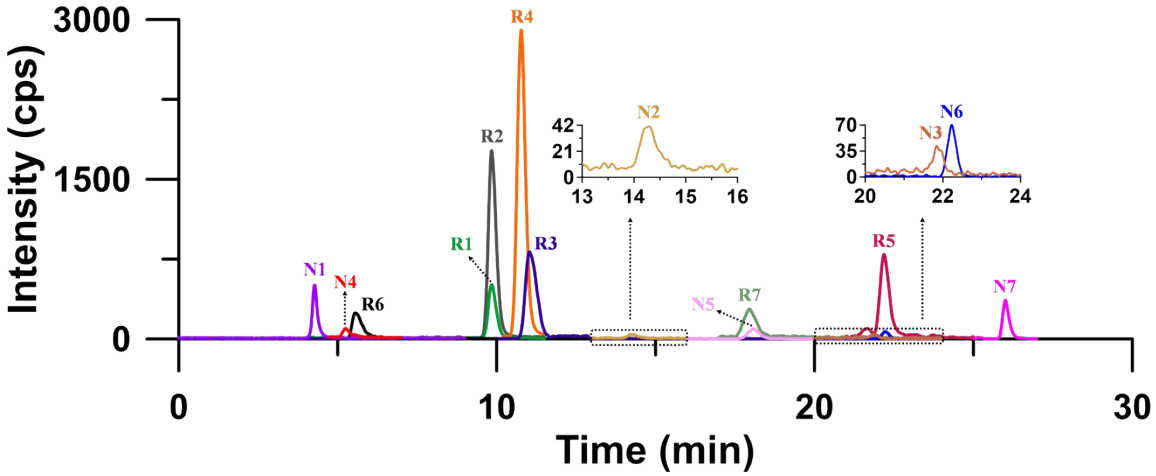

Figure S2. Chromatograms of TBBPA byproducts detected by HPLC-ITMS (Chemical information of R1-R7 and N1-N7 were listed in Table S2 and S6).

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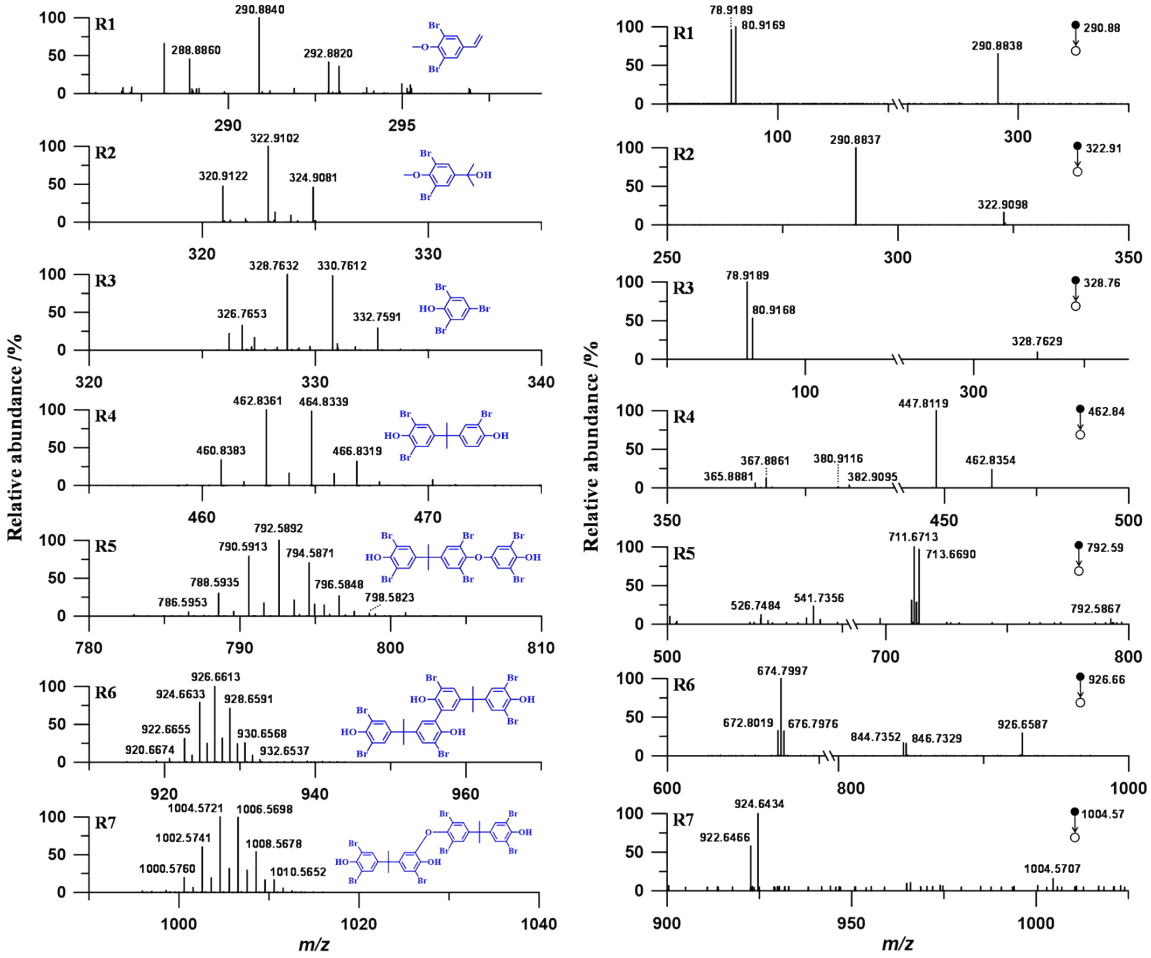


Figure S3. MS (left) and MS/MS (right) spectra of TBBPA byproducts (R1-R7) in industrial-grade TBBPA chemicals (Nantong Reform Petrochemical Co., Ltd.) detected by HPLC-Orbitrap HRMS.

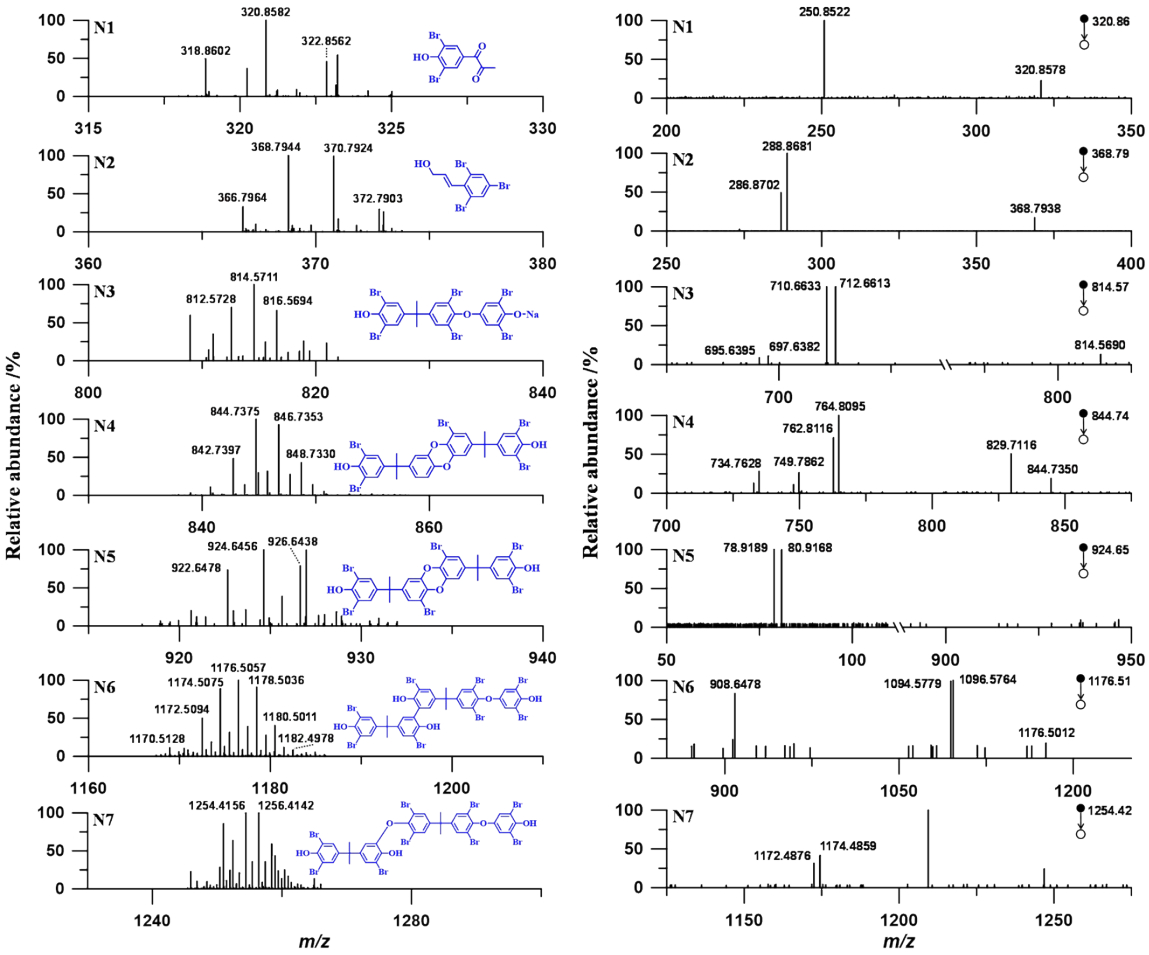


Figure S4. MS (left) and MS/MS (right) spectra of novel TBBPA byproducts (N1-N7) in industrial-grade TBBPA chemicals (Shandong Duoju Chemical Co., Ltd. and Foshan Nanhai Yincheng Trading Co., Ltd.) detected by HPLC-Orbitrap HRMS.

Table S1. The gradient elution conditions of HPLC-ITMS.

Time (min)	MeOH (%)	Ultrapure water (%)
0	90	10
8	90	10
11	100	0
36	100	0
39	90	10
56	90	10

Table S2. The MS/MS conditions and fragmentation paths of TBBPA byproducts (**R1-R7** and **N1-N7**) in industrial-grade TBBPA chemicals detected by HPLC-ITMS.

Precursor ions (*m/z*)	Retention time (min)	CID[a] collision energy (%)	Product ions (*m/z*)	Lost fragments
R1 (290.8)	9.84	29	276.9	$\bullet CH_2\bullet$
			260.9	CH_2O
			247.1	CH_2=CH-OH
			236.9	[•CHO, $\bullet C_2H$]
			210.9	$H^{79}Br$
			208.9	$H^{81}Br$
R2 (322.8)	9.84	18	290.8	CH_4O
			264.0	$\bullet C_3H_7O$
			242.9	$H^{79}Br$
			240.8	$H^{81}Br$
			232.9	[$\bullet C_3H_7O$, $\bullet OCH_3$]
R3 (328.7)	11.03	32	313.3	CH_4
			312.3	•OH
			248.9	$H^{79}Br$
			247.0	$H^{81}Br$
R4 (462.7)	10.77	26	447.7	$\bullet CH_3$
			382.9	$H^{79}Br$
			380.9	$H^{81}Br$

			367.9	$[H^{79}Br, \bullet CH_3]$
			365.9	$[H^{81}Br, \bullet CH_3]$
R5 (792.4)	22.19	22	777.4	$\bullet CH_3$
			713.5	$\bullet^{79}Br$
			712.6	$H^{79}Br$
			711.5	$\bullet^{81}Br$
			710.6	$H^{81}Br$
			697.5	$[H^{79}Br, \bullet CH_3]$
			695.5	$[H^{81}Br, \bullet CH_3]$
			541.6	$\bullet C_6H_3O^{79}Br^{81}Br$
			526.6	$[\bullet C_6H_3O^{79}Br^{81}Br, \bullet CH_3]$
R6 (926.5)	5.55	20	846.6	$H^{79}Br$
			844.6	$H^{81}Br$
			676.7	$C_6H_4O^{79}Br_2$
			674.7	$C_6H_4O^{79}Br^{81}Br$
			672.7	$C_6H_4O^{81}Br_2$
R7 (1004.4)	17.96	18	986.4	H_2O
			974.4	$[\bullet CH_3, \bullet CH_3]$
			924.4	$H^{79}Br$
			922.4	$H^{81}Br$
N1 (320.8)	4.27	25	306.2	$\bullet CH_3$
			303.0	H_2O
			291.0	CH_2O

			277.8	$\bullet C_2H_3O$
			250.8	$\bullet C_3H_2O_2\bullet$
			240.9	$H^{79}Br$
			238.9	$H^{81}Br$
N2 (368.8)	14.29	25	354.1	$\bullet CH_3$
			351.2	H_2O
			341.1	C_2H_4
			336.8	CH_4O
			328.9	C_3H_4
			325.1	CH_2=CH-OH
			315.0	[•CHO, $\bullet C_2H$]
			288.9	$H^{79}Br$
			286.9	$H^{81}Br$
N3 (814.5)	21.84	18	774.5	NaOH
			760.8	CH_3ONa
			712.5	$Na^{79}Br$
			710.5	$Na^{81}Br$
			697.5	[$Na^{79}Br$, $\bullet CH_3$]
			695.5	[$Na^{81}Br$, $\bullet CH_3$]
N4 (844.6)	5.24	32	829.5	$\bullet CH_3$
			812.5	CH_4O
			764.6	$H^{79}Br$
			762.6	$H^{81}Br$

			749.6	[$H^{79}Br$, $\bullet CH_3$]
			747.6	[$H^{81}Br$, $\bullet CH_3$]
			734.6	[$H^{79}Br$, $\bullet CH_3$, $\bullet CH_3$]
			732.5	[$H^{81}Br$, $\bullet CH_3$, $\bullet CH_3$]
N5 (461.8)	18.07	22	844.6	$H^{79}Br$
			842.5	$H^{81}Br$
			831.3	[$\bullet CH_2{}^{79}Br$]
			830.6	$CH_3{}^{79}Br$
			829.5	[$\bullet CH_2{}^{81}Br$] / [$H^{79}Br$, $\bullet CH_3$]
			828.5	$CH_3{}^{81}Br$
			827.5	[$H^{81}Br$, $\bullet CH_3$]
N6 (1176.3)	22.23	19	1096.3	$H^{79}Br$
			1094.3	$H^{81}Br$
			910.6	$C_6H_4O_2{}^{79}Br_2$
			908.4	$C_6H_4O_2{}^{79}Br^{81}Br$
			906.5	$C_6H_4O_2{}^{81}Br_2$
N7 (626.7)	26.01	18	1175.2	$\bullet{}^{79}Br$
			1174.2	$H^{79}Br$
			1173.3	$\bullet{}^{81}Br$
			1172.3	$H^{81}Br$
			1093.3	[$H^{79}Br$, $\bullet CH_3$, $\bullet CH_3$, $\bullet CH_3$, H_2O, H_2O]
			1091.3	[$H^{81}Br$, $\bullet CH_3$, $\bullet CH_3$, $\bullet CH_3$, H_2O, H_2O]

[a] CID means collision induced dissociation.

Table S3. The gradient elution conditions of HPLC-Orbitrap HRMS.

Time (min)	MeOH (%)	Ultrapure water (%)
0	90	10
8	90	10
11	100	0
23	100	0
26	90	10
37	90	10

Table S4. The MS/MS conditions and fragmentation paths of TBBPA byproducts (**R1-R7** and **N1-N7**) in industrial-grade TBBPA chemicals detected by HPLC-Orbitrap HRMS.

Precursor ions (*m/z*)	Retention time (min)	Collision type	Collision energy (%)	Collision time (ms)	Product ions (*m/z*)	Lost fragments
R1 (290.88)	9.56	HCD[a]	90	40	80.9169	
					78.9189	
R2 (322.91)	9.56	CID	25	25	290.8837	CH_4O
R3 (328.76)	11.49	HCD	120	40	80.9168	
					78.9189	
R4 (462.84)	10.52	CID	55	60	447.8119	$\bullet CH_3$
					382.9095	$H^{79}Br$
					380.9116	$H^{81}Br$
					367.8861	$[H^{79}Br, \bullet CH_3]$
					365.8881	$[H^{81}Br, \bullet CH_3]$
R5 (792.59)	19.37	CID	52	40	713.6690	$\bullet^{79}Br$
					712.6615	$H^{79}Br$
					711.6713	$\bullet^{81}Br$
					710.6633	$H^{81}Br$
					541.7356	$\bullet C_6H_3O^{79}Br^{81}Br$
					526.7484	$[\bullet C_6H_3O^{79}Br^{81}Br, \bullet CH_3]$
R6 (926.66)	6.05	CID	36	25	846.7329	$H^{79}Br$
					844.7352	$H^{81}Br$

					676.7976	$C_6H_4O^{79}Br_2$
					674.7997	$C_6H_4O^{79}Br^{81}Br$
					672.8019	$C_6H_4O^{81}Br_2$
R7 (1004.57)	17.83	CID	18	25	924.6434	$H^{79}Br$
					922.6646	$H^{81}Br$
N1 (320.86)	3.92	CID	48	30	250.8522	$\bullet C_3H_2O_2\bullet$
N2 (368.79)	14.73	CID	42	30	288.8681	$H^{79}Br$
					286.8702	$H^{81}Br$
N3 (814.57)	19.41	CID	50	30	712.6613	$Na^{79}Br$
					710.6633	$Na^{81}Br$
					697.6382	$[Na^{79}Br, \bullet CH_3]$
					695.6395	$[Na^{81}Br, \bullet CH_3]$
N4 (844.74)	5.37	CID	68	65	829.7116	$\bullet CH_3$
					764.8095	$H^{79}Br$
					762.8116	$H^{81}Br$
					749.7862	$[H^{79}Br, \bullet CH_3]$
					747.7887	$[H^{81}Br, \bullet CH_3]$
					734.7628	$[H^{79}Br, \bullet CH_3, \bullet CH_3]$
					732.7649	$[H^{81}Br, \bullet CH_3, \bullet CH_3]$
N5 (924.65)	17.78	HCD	70	40	80.9168	
					78.9189	
N6 (1176.51)	19.24	CID	20	30	1096.5764	$H^{79}Br$
					1094.5779	$H^{81}Br$

					908.6478	$C_6H_4O_2{}^{79}Br^{81}Br$
N7 (1254.42)	21.81	CID	33	30	1174.4859	$H^{79}Br$
					1172.4876	$H^{81}Br$

[a] HCD means high energy collision dissociation.

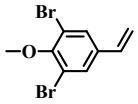
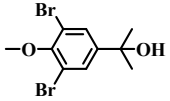
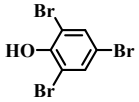
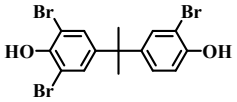
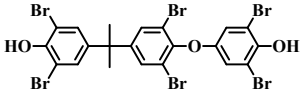
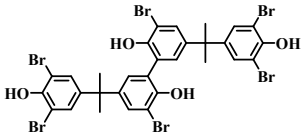
Table S5. The analytical performance of TriBP and TriBBPA in environmental samples detected by HPLC-Orbitrap HRMS.

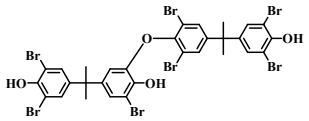
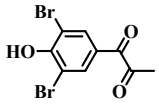
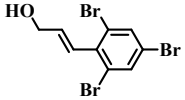
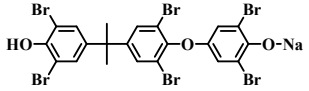
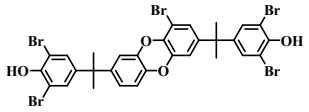
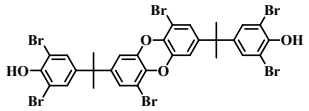
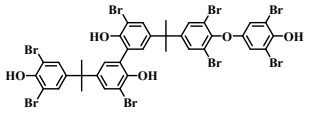
Compound	Recovery (%)			LOD[a]			ME[b] (%)		
	Water	Soil	Sediment	Water (ng L^{-1})	Soil (ng g^{-1} dw)	Sediment (ng g^{-1} dw)	Water	Soil	Sediment
TriBP	100	91	94	0.59	0.04	0.04	4	6	7
TriBBPA	102	105	96	0.68	0.05	0.05	9	4	5

[a] LOD means limit of detection.

[b] ME means matrix effect.

Table S6. Chemical information of TBBPA byproducts identified in industrial-grade TBBPA chemicals.

Byproduct	Name [abbreviation]	Structure	Formula	SMILES
R1	4-ethenyl-2,6-dibromoanisole		$C_9H_8OBr_2$	BrC1=CC(C=C)=CC(Br)=C1OC
R2	4-(2-hydroxyisopropyl)-2,6-dibromoanisole		$C_{10}H_{12}O_2Br_2$	CC(C)(O)C1=CC(Br)=C(OC)C(Br)=C1
R3	2,4,6-tribromophenol [TriBP]		$C_6H_3OBr_3$	BrC1=CC(Br)=CC(Br)=C1O
R4	Tribromobisphenol A [TriBBPA]		$C_{15}H_{13}O_2Br_3$	BrC1=CC(C(C)(C)C2=CC=C(O)C(Br)=C2)=CC(Br)=C1O
R5	TBBPA mono(3,5-dibromophenol ether)		$C_{21}H_{14}O_3Br_6$	BrC1=CC(C(C)(C2=CC(Br)=C(OC3=CC(Br)=C(O)C(Br)=C3)C(Br)=C2)C)=CC(Br)=C1O
R6	2,2′-dihydroxy-3,3′-dibromo-5,5′-di(3,5-dibromo-4-hydroxycumyl)-biphenyl		$C_{30}H_{24}O_4Br_6$	BrC1=CC(C(C)(C)C2=CC(Br)=C(O)C(C3=C(O)C(Br)=CC(C(C)(C)C4=CC(Br)=C(O)C(Br)=C4)=C3)=C2)=CC(Br)=C1O

R7	TBBPA mono(TriBBPA ether)		$C_{30}H_{23}O_4Br_7$	BrC1=CC(C(C)(C2=CC(Br)=C(O)C(Br)=C2)C)=CC(Br)=C1OC3=CC(C(C)(C)C4=CC(Br)=C(O)C(Br)=C4)=CC(Br)=C3O
N1	1-(3,5-dibromo-4-hydroxyphenyl)propane-1,2-dione		$C_9H_6O_3Br_2$	OC1=C(Br)C=C(C(C(C)=O)=O)C=C1Br
N2	2,4,6-tribromo-1-(3-(1-hydroxy-2-propenyl))-benzene		$C_9H_7OBr_3$	BrC1=CC(Br)=CC(Br)=C1/C=C/CO
N3	TBBPA mono(sodium 3,5-dibromophenolate ether)		$C_{21}H_{13}O_3Br_6Na$	BrC1=CC(C(C)(C2=CC(Br)=C(OC3=CC(Br)=C(O[Na])C(Br)=C3)C(Br)=C2)C)=CC(Br)=C1O
N4	1-bromo-3,8-di(3,5-dibromo-4-hydroxycumyl)-dibenzo[*b*,*e*][1,4]dioxine		$C_{30}H_{23}O_4Br_5$	BrC1=CC(C(C)(C)C2=CC=C(OC3=C(O4)C(Br)=CC(C(C)(C)C5=CC(Br)=C(O)C(Br)=C5)=C3)C4=C2)=CC(Br)=C1O
N5	1,6-dibromo-3,8-di(3,5-dibromo-4-hydroxycumyl)-dibenzo[*b*,*e*][1,4]dioxine		$C_{30}H_{22}O_4Br_6$	BrC1=CC(C(C)(C)C2=CC(Br)=C(OC3=C(O4)C(Br)=CC(C(C)(C)C5=CC(Br)=C(O)C(Br)=C5)=C3)C4=C2)=CC(Br)=C1O
N6	[2,2′-dihydroxy-3,3′-dibromo-5,5′-di(3,5-dibromo-4-hydroxycumyl)-biphenyl] mono(3,5-dibromophenol ether)		$C_{36}H_{26}O_5Br_8$	BrC1=CC(C(C)(C)C2=CC(Br)=C(O)C(C3=C(O)C(Br)=CC(C(C)(C)C4=CC(Br)=C(OC5=CC(Br)=C(O)C(Br)=C5)C(Br)=C4)=C3)=C2)=CC(Br)=C1O

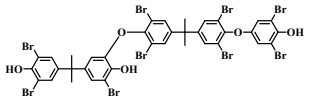
N7	2,6-dibromo-4-(2-(3-bromo-5-(TBBPA mono(3,5-dibromophenol ether))-4-hydroxyphenyl)isopropyl)phenol		$C_{36}H_{25}O_5Br_9$	BrC1=CC(C(C)(C2=CC(Br)=C(OC3=CC(Br)=C(O)C(Br)=C3)C(Br)=C2)C)=CC(Br)=C1OC4=CC(C(C)(C)C5=CC(Br)=C(O)C(Br)=C5)=CC(Br)=C4O

Table S7. Single-point energies of possible structures of R7.

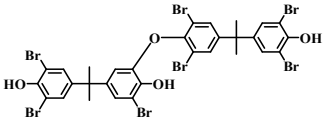
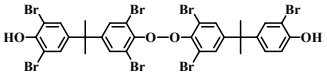
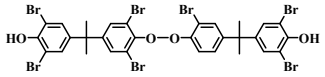
Compound	Structure	Single-point energy (a.u.)
R7-1		-19458.5611
R7-2		-19458.4906
R7-3		-19458.4917

Table S8. The results of TBBPA byproducts analyzed by HPLC-Orbitrap HRMS.

Byproduct	Detected *m/z*	Theoretical *m/z*	Formula	Error (ppm)	Isotope ratio
R1	290.8840	290.8849	$[C_9H_7OBr_2]^-$	-2.980	1:2:1
R2	322.9102	322.9111	$[C_{10}H_{11}O_2Br_2]^-$	-2.637	1:2:1
R3	328.7632	328.7641	$[C_6H_2OBr_3]^-$	-2.583	1:3:3:1
R4	462.8361	462.8372	$[C_{15}H_{12}O_2Br_3]^-$	-2.407	1:3:3:1
R5	792.5892	792.5909	$[C_{21}H_{13}O_3Br_6]^-$	-2.111	1:6:15:20:15:6:1
R6	926.6613	926.6641	$[C_{30}H_{23}O_4Br_6]^-$	-2.977	1:6:15:20:15:6:1
R7	1004.5721	1004.5746	$[C_{30}H_{22}O_4Br_7]^-$	-2.509	1:7:21:35:35:21:7:1
N1	320.8582	320.8591	$[C_9H_5O_3Br_2]^-$	-2.543	1:2:1
N2	368.7944	368.7954	$[C_9H_6OBr_3]^-$	-2.656	1:3:3:1
N3	814.5711	814.5729	$[C_{21}H_{12}O_3Br_6Na]^-$	-2.109	1:6:15:20:15:6:1
N4	844.7375	844.7400	$[C_{30}H_{22}O_4Br_5]^-$	-2.962	1:5:10:10:5:1
N5	924.6456	924.6484	$[C_{30}H_{21}O_4Br_6]^-$	-3.015	1:6:15:20:15:6:1
N6	1176.5057	1176.5093	$[C_{36}H_{25}O_5Br_8]^-$	-3.027	1:8:28:56:70:56:28:8:1
N7	1254.4156	1254.4198	$[C_{36}H_{24}O_5Br_9]^-$	-3.328	1:9:36:84:126:126:84:36:9:1

Table S9. Quantitative and semi-quantitative concentrations (μg g^{-1}) of byproducts in industrial-grade TBBPA chemicals.[a]

Byproduct	Pulov	Duoju	Goldchem	Reform	Yincheng	DF[b] (%)
R1 (*m/z* 290.88)	6.79×10^2	7.57×10^2	8.35×10^2	1.14×10^3	1.15×10^3	100
R2 (*m/z* 322.91)	8.01×10^3	8.77×10^3	9.95×10^3	1.04×10^4	1.35×10^4	100
R3 (*m/z* 328.76)	3.55×10^3	5.13×10^3	3.87×10^3	3.89×10^3	1.91×10^3	100
R4 (*m/z* 462.84)	1.37×10^4	1.68×10^4	1.55×10^4	2.29×10^4	2.01×10^4	100
R5 (*m/z* 792.59)	90.2	1.26×10^2	1.41×10^2	2.30×10^2	2.00×10^2	100
R6 (*m/z* 926.66)	4.77×10^2	<LOD[c]	67.1	1.99×10^3	1.93×10^3	80
R7 (*m/z* 1004.57)	14.8	13.5	<LOD	20.8	24.6	80
N1 (*m/z* 320.86)	6.64×10^2	9.89×10^2	6.12×10^2	<LOD	<LOD	60
N2 (*m/z* 368.79)	<LOD	<LOD	<LOD	<LOD	1.40×10^2	20
N3 (*m/z* 814.57)	11.6	18.0	17.4	43.7	27.5	100
N4 (*m/z* 844.74)	<LOD	<LOD	<LOD	10.8	9.20	40
N5 (*m/z* 924.65)	<LOD	<LOD	<LOD	33.1	38.3	40
N6 (*m/z* 1176.51)	<LOD	<LOD	<LOD	15.9	10.9	40
N7 (*m/z* 1254.42)	<LOD	2.77	<LOD	3.62	3.94	60

[a] Byproducts R3 and R4 were quantified by using their standard solution, and other TBBPA byproducts were semi-quantitatively analyzed by comparing with the TriBBPA standard solution.

[b] DF means detection frequency.

[c] <LOD means below the limit of detection.

Table S10. Concentrations of TBBPA byproducts in river water (ng L^{-1}), soil (ng g^{-1} dw), and sediment (ng g^{-1} dw).

	R1	R2	R3	R4	R5	R6	R7	N1	N2	N3	N4	N5	N6	N7
Water-1	52.5	28.2	2.27×10^2	7.90	<LOD[a]	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-2	13.4	4.53	36.9	2.33	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-3	32.0	14.1	94.9	9.96	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-4	27.5	4.42	1.13×10^2	6.00	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-5	17.1	2.05	1.20×10^2	7.38	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-6	22.3	24.1	1.44×10^2	14.6	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-7	27.6	20.4	1.52×10^2	10.8	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-8	23.7	33.9	1.11×10^2	12.5	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-9	45.0	75.1	2.10×10^2	19.5	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-10	49.0	1.39×10^2	4.57×10^2	31.1	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-11	58.2	2.22×10^2	4.08×10^2	25.1	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-12	20.1	39.7	1.13×10^2	1.73	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-13	2.24	2.84	44.5	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-14	<LOD	<LOD	8.65	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-15	<LOD	<LOD	1.87	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-16	<LOD	<LOD	12.1	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD

	R1	R2	R3	R4	R5	R6	R7	N1	N2	N3	N4	N5	N6	N7
Water-17	<LOD	<LOD	8.61	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-18	0.84	<LOD	1.10	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-19	<LOD	<LOD	47.1	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-20	<LOD	<LOD	11.8	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-21	<LOD	<LOD	11.6	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-22	<LOD	<LOD	6.76	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-23	<LOD	<LOD	7.45	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-24	<LOD	<LOD	3.39	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-25	<LOD	<LOD	4.96	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-26	<LOD	<LOD	17.2	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-27	<LOD	<LOD	10.0	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-28	<LOD	<LOD	12.5	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-29	<LOD	<LOD	5.36	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-30	<LOD	<LOD	9.32	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-31	<LOD	<LOD	8.54	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-32	<LOD	<LOD	3.37	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Water-33	<LOD	<LOD	3.72	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-1	<LOD	<LOD	3.52	0.49	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD

	R1	R2	R3	R4	R5	R6	R7	N1	N2	N3	N4	N5	N6	N7
Soil-2	<LOD	0.08	0.46	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-3	<LOD	0.08	14.2	1.57	<LOD	<LOD	<LOD	0.08	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-4	<LOD	0.19	10.8	5.40	<LOD	<LOD	<LOD	0.23	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-5	0.06	<LOD	4.25	1.92	<LOD	<LOD	<LOD	0.06	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-6	0.09	0.80	27.6	6.52	<LOD	<LOD	<LOD	0.14	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-7	<LOD	<LOD	6.66	0.12	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-8	<LOD	<LOD	7.94	0.37	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-9	0.12	<LOD	9.72	0.40	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-10	<LOD	<LOD	7.07	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-11	0.15	<LOD	2.63	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-12	<LOD	<LOD	1.33	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-13	<LOD	<LOD	8.00	0.38	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-14	<LOD	<LOD	0.43	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-15	<LOD	<LOD	0.92	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-16	<LOD	<LOD	0.86	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-17	<LOD	<LOD	0.65	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-18	<LOD	<LOD	1.35	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-19	<LOD	<LOD	1.01	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD

	R1	R2	R3	R4	R5	R6	R7	N1	N2	N3	N4	N5	N6	N7
Soil-21	<LOD	<LOD	0.77	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-23	<LOD	<LOD	3.51	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-24	0.12	<LOD	1.17	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-25	<LOD	<LOD	0.78	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-26	<LOD	<LOD	1.19	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-28	0.13	<LOD	1.86	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-29	<LOD	<LOD	0.59	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-30	<LOD	<LOD	1.39	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Soil-31	<LOD	<LOD	1.00	0.10	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Sediment-5	0.70	0.07	1.56×10^{2}	6.04	<LOD	<LOD	<LOD	0.60	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Sediment-7	2.85	<LOD	12.2	2.11	<LOD	<LOD	<LOD	0.05	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD
Sediment-8	0.31	0.08	11.8	2.53	<LOD	<LOD	<LOD	0.13	<LOD	<LOD	<LOD	<LOD	<LOD	<LOD

[a] <LOD means below the limit of detection.

Table S11. The prediction results of carcinogenicity (binary and trinary), eye corrosion, eye irritation, and acute oral toxicity.

Byproduct	Carcinogenicity (binary)		Carcinogenicity (trinary)		Eye corrosion		Eye irritation		Acute Oral Toxicity (-log mol/kg)
	Value	Probability	Value	Probability	Value	Probability	Value	Probability	
R1	-[a]	0.5537	Warning	0.4345	+[b]	0.7742	+	0.9654	1.733
R2	-	0.6450	Non-required	0.5131	-	0.6819	+	0.9697	1.431
R3	-	0.5626	Non-required	0.5232	+	0.9873	+	0.9950	1.674
R4	-	0.6187	Non-required	0.5936	-	0.9259	+	0.9826	1.629
R5	-	0.6348	Non-required	0.5021	-	0.9684	+	0.7511	1.605
R6	-	0.6258	Non-required	0.4667	-	0.9826	-	0.6641	1.716
R7	-	0.7059	Non-required	0.4336	-	0.9847	-	0.7168	1.699
N1	-	0.6458	Non-required	0.4789	+	0.8840	+	0.9777	1.932
N2	-	0.5584	Non-required	0.6591	+	0.8403	+	0.9934	0.908
N3	-	0.6209	Non-required	0.4864	-	0.9329	+	0.5269	1.729
N4	-	0.8869	Danger	0.4341	-	0.9858	-	0.6355	1.714
N5	-	0.8869	Danger	0.4341	-	0.9858	-	0.6383	2.156
N6	-	0.6396	Non-required	0.4040	-	0.9868	-	0.8475	1.820
N7	-	0.7059	Non-required	0.4336	-	0.9847	-	0.8537	1.813

Table S12. The prediction results of ames mutagenesis, hERG, micronuclear, hepatotoxicity, and skin sensitization.

Compound	Ames mutagenesis		hERG[c]		Micronuclear		Hepatotoxicity		skin sensitisation	
	Value	Probability	Value	Probability	Value	Probability	Value	Probability	Value	Probability
R1	-	0.8700	-	0.5493	-	0.7610	+	0.6625	+	0.6785
R2	-	0.8200	-	0.5588	-	0.7999	+	0.5284	-	0.5389
R3	-	0.9700	-	0.8167	-	0.6651	+	0.7875	+	0.9120
R4	-	0.9100	-	0.5450	-	0.6700	+	0.7750	+	0.7030
R5	-	0.8400	+	0.8154	-	0.6400	+	0.6000	-	0.5908
R6	-	0.8700	+	0.8852	-	0.5800	+	0.7500	-	0.7716
R7	-	0.8600	+	0.9024	-	0.6300	+	0.5625	-	0.7258
N1	-	0.8100	-	0.8404	+	0.6664	+	0.8875	+	0.7265
N2	-	0.7500	-	0.7534	-	0.7533	+	0.5928	+	0.8137
N3	-	0.7800	+	0.7189	-	0.7226	+	0.5875	-	0.6988
N4	-	0.7500	+	0.9087	+	0.5900	+	0.6000	-	0.8054
N5	-	0.8000	+	0.9205	+	0.5900	+	0.7000	-	0.8054
N6	-	0.7900	+	0.7878	-	0.6100	+	0.5125	-	0.8455
N7	-	0.7900	+	0.8769	-	0.6300	+	0.5375	-	0.7258

Table S13. The prediction results of respiratory, reproductive, mitochondrial, acute oral toxicity, and nephrotoxicity.

Compound	Respiratory toxicity		Reproductive toxicity		Mitochondrial toxicity		Nephrotoxicity		Acute Oral Toxicity (c)	
	Value	Probability	Value	Probability	Value	Probability	Value	Probability	Value	Probability
R1	-	0.7778	+	0.7333	-	0.9000	-	0.8437	III	0.8566
R2	-	0.7444	-	0.5778	-	0.8000	-	0.7990	III	0.5939
R3	-	0.7222	+	0.9392	-	0.8875	-	0.8459	III	0.5271
R4	-	0.6000	-	0.7889	-	0.7000	-	0.7819	IV	0.5893
R5	-	0.6667	-	0.6778	-	0.6875	-	0.8370	IV	0.5053
R6	-	0.6556	-	0.7444	-	0.6625	-	0.8021	IV	0.5412
R7	-	0.5333	-	0.6889	-	0.6750	-	0.8201	III	0.5137
N1	-	0.6556	+	0.6222	-	0.6250	-	0.8112	III	0.8913
N2	-	0.5889	-	0.5778	-	0.9000	-	0.7918	III	0.8196
N3	-	0.6667	-	0.6222	-	0.7000	-	0.8688	III	0.5447
N4	-	0.6667	+	0.6000	-	0.5750	-	0.8436	III	0.5813
N5	-	0.6333	+	0.6000	-	0.5750	-	0.8771	III	0.5813
N6	-	0.6333	-	0.7000	-	0.6750	-	0.8073	IV	0.5206
N7	-	0.5222	-	0.6889	-	0.6750	-	0.7937	III	0.5137

Table S14. The prediction results of estrogen, androgen, thyroid, glucocorticoid receptor binding, and aromatase binding.

Compound	Estrogen receptor binding		Androgen receptor binding		Thyroid receptor binding		Glucocorticoid receptor binding		Aromatase binding	
	Value	Probability	Value	Probability	Value	Probability	Value	Probability	Value	Probability
R1	-	0.6093	-	0.7967	-	0.6491	-	0.8413	-	0.8021
R2	+	0.6298	-	0.8368	-	0.6062	-	0.6479	-	0.5979
R3	+	0.5557	-	0.5535	-	0.5952	-	0.6566	-	0.7773
R4	+	0.8564	+	0.7607	+	0.6684	+	0.8952	+	0.8899
R5	+	0.8762	+	0.5792	+	0.7588	+	0.7491	+	0.7986
R6	+	0.8708	+	0.7701	+	0.7472	+	0.7923	+	0.7796
R7	+	0.7987	+	0.6177	+	0.6177	+	0.7547	+	0.6670
N1	-	0.4916	-	0.6002	-	0.7184	-	0.5315	-	0.6802
N2	-	0.5074	-	0.5535	-	0.5000	-	0.5095	-	0.6782
N3	+	0.7818	-	0.5141	+	0.7327	+	0.7114	+	0.7771
N4	+	0.8058	+	0.7077	+	0.6802	+	0.7718	+	0.6659
N5	+	0.8002	+	0.6010	+	0.6669	+	0.7505	+	0.6555
N6	+	0.7850	+	0.7037	+	0.6704	+	0.6882	+	0.7040
N7	+	0.7917	+	0.5948	+	0.6486	+	0.6843	+	0.6518

Table S15. The prediction results of PPAR gamma, biodegradation, honey bee, crustacea aquatic, and fish aquatic toxicity.

Compound	PPAR gamma		Honey bee toxicity		Biodegradation		Crustacea aquatic toxicity		Fish aquatic toxicity	
	Value	Probability	Value	Probability	Value	Probability	Value	Probability	Value	Probability
R1	-	0.6244	-	0.8536	-	0.7250	+	0.6000	+	0.9904
R2	-	0.5510	-	0.9676	-	0.5500	+	0.7000	+	0.9491
R3	-	0.5000	-	0.9741	+	0.7000	+	0.6500	+	0.9565
R4	+	0.8475	-	0.9758	-	0.8250	+	0.7600	+	0.9940
R5	+	0.8764	-	0.9184	-	0.8500	+	0.7000	+	0.9965
R6	+	0.8404	-	0.9664	-	0.8750	+	0.6500	+	1.0000
R7	+	0.7110	-	0.9314	-	0.9250	+	0.6851	+	0.9964
N1	-	0.7480	-	0.9790	+	0.5750	-	0.7000	+	0.9748
N2	+	0.5777	-	0.9391	-	0.6250	-	0.6200	+	0.9673
N3	+	0.8172	-	0.8446	-	0.8750	+	0.7400	+	0.9969
N4	+	0.6987	-	0.9471	-	0.9500	+	0.7000	+	0.9763
N5	+	0.6995	-	0.9497	-	0.9250	+	0.6600	+	0.9763
N6	+	0.7194	-	0.8877	-	0.8750	+	0.6600	+	1.0000
N7	+	0.7104	-	0.8881	-	0.9250	+	0.6951	+	0.6951

[a] "-" means negative.

[b] "+" means positive.

[c] hERG means the ability to block the human Ether-a-go-go-Related Gene Salubrinal channel and its analogs.

Table S16. Calculated physical-chemical constants of TBBPA byproducts[a].

Byproduct	log K_{ow}[b]	log K_{oa}[c]	log K_{oc}[d]	BCF[e]
R1	4.76	7.74	3.61	638
R2	3.81	10.64	2.68	151
R3	4.13	9.97	3.38	247
R4	6.31	16.94	4.75	6800
R5	10.20	23.68	6.96	360
R6	12.40	34.11	8.45	30.2
R7	13.22	31.89	8.79	11.9
N1	2.41	12.99	1.97	18.1
N2	4.51	10.90	3.01	245
N3	7.51	20.74	5.47	7480
N4	13.05	27.94	8.48	14.4
N5	13.94	29.23	8.97	5.28
N6	15.39	39.56	10.16	3.16
N7	16.22	37.35	10.51	3.16

[a] Calculated by EPI Suite™ v4.11.

[b] octanol-water partition coefficient.

[c] octanol-air partition coefficient.

[d] soil absorption coefficient.

[e] bioconcentration factor (L/kg, wet-wt).

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