Electronic supplementary material for Article

Binary mixtures of selected bisphenols in the environment: their toxicity in relationship to individual constituents

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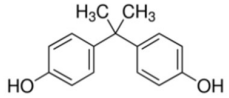
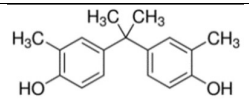
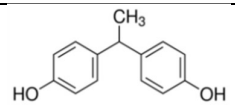
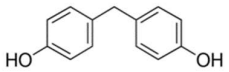
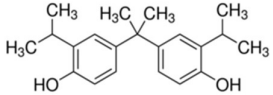
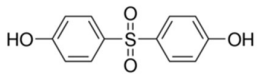
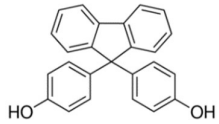
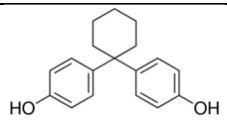
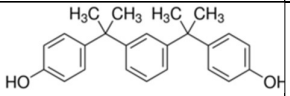
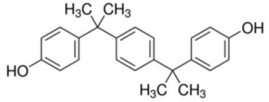
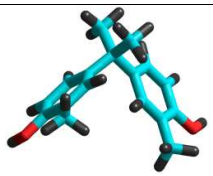
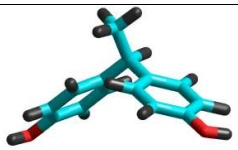
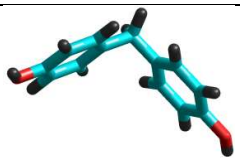
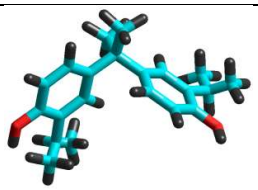
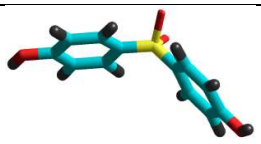
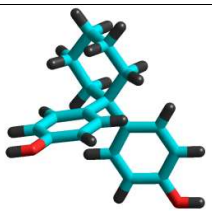
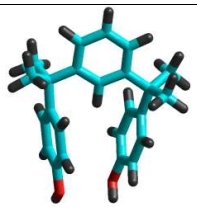
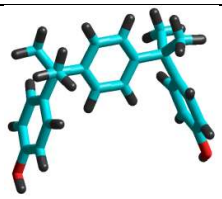
Supplementary Table S1. Basic information about analytes studied

Analyte /CAS no./ molecular weight [g/mol]	Structure	IUPAC name	Application (if known)
BPA / 80-05-7/ 228.29		2,2-bis(4-hydroxyphenyl) propane	Food packaging coatings, plastic bottles, plastic items (toys, every-day use products) [I]
BPC /79-97-0/ 256.34		2,2-bis(4-hydroxy-3-methylphenyl) propane	Used as intermediate in pesticide and pharmaceuticals production [II]
BPE /2081-08-5/ 214.26		1,1-bis(4-hydroxyphenyl) ethane	Polymer production, flame retardants resin composite, heat sensitive recording material [III, IV]
BPF /620-92-8/ 200.23		4,4′-methylenediphenol	BPA substitute, plastic items (toys, every-day use products)
BPG /127-54-8/ 312.45		2,2-bis(4-hydroxy-3-isopropylphenyl) propane	Thermally responsive recording materials [V]
BPS /80-09-1/ 250.27		4,4′-sulfonyldiphenol	Dental sealants, thermal papers production, electronics [VI]
BPFL /3236-71-3/ 350.41		4,4′-(9-fluorenylidene)diphenol	Photosensitive resins [VII]

BPZ /843-55-0/ 268.35		4,4′-cyclohexylidene-bisphenol	Polycarbonates plastic production, thermosensitive materials, optical composites [VIII, IX]
BPM /13595-25-0/ 346.46		4,4′-(1,3-phenylenediisopro-pylidene)bisphenol	Flame retardants, polycarbonate plastics production, aromatic co-polyesters manufacturing, thermosensitive materials [X, XI]
BPP /2167-51-3/ 346.46		4,4′-(1,4-phenylenediisopropylidene) bisphenol	Found in food packaging, polycarbonate plastics production, flame retardant production, thermoplastic resins production [XII, XIII, XIV]

Supplementary Table S2. Structural parameters of bisphenol analogs calculated with molecular dynamics

Analyte	Structure	Distance [Å]		Angle [°]
		O-C[1]	O-O[2]	O-C-O[3]
BPA		5.74	9.25	107.26
BPC		5.74	9.19	106.38
BPE		5.72	9.29	108.47
BPF		5.71	9.29	109.00
BPG		5.74	9.19	106.55
BPS		5.67	10.26	129.41
BPFL		5.74	9.70	115.40
BPZ		5.76	9.11	104.36

BPM		5.92	3.50	34.41
BPP		6.38	9.73	99.2

[1] Distance between central carbon atom and left branch oxygen atom forming phenol
[2] Distance between both branches oxygen atoms forming phenols.
[3] The angle between phenolic rings

Supplementary Table S3. Comparison of the polynomial models for BPs studied with Microtox®

BPs binary combination y/x	Regression coefficients: a, b, c	Correlation R^2	Mode of action
BPA/BPC	0.06; -0.16; 0.71	0.97	IA
BPC/BPA	0.07; -0.21; 0.72	0.98	
BPA/BPE	0.12; -0.44; 0.84	0.94	IA
BPE/BPA	0.08; -0.34; 0.52	0.97	
BPA/BPF	0.07; -0.27; 0.93	0.98	IA
BPF/BPA	0.06; -0.21; 0.85	0.98	
BPA/BPG	0.005; 0.08; 0.58	0.97	IA
BPG/BPA	0.007; 0.12; 0.61	1.00	
BPA/BPS	0.11; -0.42; 0.87	0.97	IA
BPS/BPA	0.11; -0.12; 0.36	0.96	
BPA/BPFL	0.06; -0.17; 075	0.98	IA
BPFL/BPA	0.04; -0.27; 0.16	0.98	
BPC/BPE	0.03; 0.002; 0.48	0.96	IA
BPE/BPC	0.07; 0.05; 0.60	0.94	
BPC/BPF	0.04; -0.06; 0.66	0.96	IA
BPF/BPC	0.05; -0.12; 0.73	0.97	
BPC/BPG	-0.003; 0.17;0.36	0.99	Different from IA
BPG/BPC	0.05; -0.16; 0.39	0.97	

BPC/BPS	0.06; -0.19; 0.66	0.94	IA
BPS/BPC	0.08; -0.24; 0.65	0.97	
BPC/BPFL	-0.007; 0.16; 0.49	*0*.99	IA
BPFL/BPC	-0.005; 0.26; 0.36	0.99	
BPE/BPF	0.05; -0.15; 0.75	0.97	IA
BPF/BPE	0.05; -0.14; 0.72	0.97	
BPE/BPG	0.02; 0.02; 0.55	0.99	IA
BPG/BPE	0.03; 0.11; 0.49	0.99	
BPE/BPS	0.07; -0.24; 0.79	0.96	IA
BPS/BPG	0.07; -0.18; 0.65	0.96	
BPE/BPFL	0.07; -0.19;0.73	0.98	IA
BPFL/BPE	0.06; -0.11; 0.62	0.99	
BPF/BPG	0.04; -0.10; 0.72	0.99	IA
BPG/BPF	0.04; -0.15; 0.92	0.99	
BPF/BPS	0.15; -0.48;0.58	0.95	IA
BPS/BPF	0.11; -0.25; 0,41	0.96	
BPF/BPFL	0.12; -0.32; 0.34	0.99	IA
BPFL/BPF	0.08; -0.33; 0.92	0.99	
BPG/BPS	0.06; -0.22; 0.92	0.77	Different from IA
BPS/BPG	0.07; -0.20; 0.68	0.98	
BPG/BPFL	-0.02; 0.22; 0.38	0.99	IA
BPFL/BPG	-0.01; 0.59; -0.005	0.99	
BPS/BPFL	0.05; -0.11; 0.53	0.86	Different from IA
BPFL/BPS	0.01; 0.10; 0.34	0.99	

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