toxics

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Supplementary materials

An Integrated Approach of Bioassays and Non-Target Screening for the Assessment of Endocrine-Disrupting Activities in Tap Water and Identification of Novel Endocrine-Disrupting Chemicals

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Table S1. Information on 43 external standards.

Name	Formula	CAS number	Reported bioactivity	References
Diethyl phthalate	C12H14O4	84-66-2	ER↑	[75]
Dibutyl phthalate	C16H22O4	84-74-2	ER↑, ER↓	[76, 77]
Diisobutyl phthalate	C16H22O4	84-69-5	ER↑	[76]
Dipentyl phthalate	C18H26O4	131-18-0	ER↑, ER↓	[76]
Dioctyl phthalate	C24H38O4	117-84-0	ER↑	[78]
Dinonyl phthalate	C26H42O4	84-76-4	ER↑	[78]
Dicyclohexyl phthalate	C20H26O4	84-61-7	ER↑, ER↓	[76]
Diphenyl phthalate	C20H14O4	84-62-8	-	
Benzyl butyl phthalate	C19H20O4	85-68-7	ER↑, ER↓	[76, 77]
Dimethylglycol phthalate	C14H18O6	117-82-8	-	
Diethoxyethyl phthalate	C16H22O6	605-54-9	-	
Bis(2-butoxyethyl) phthalate	C20H30O6	117-83-9	-	
Pentachlorophenol	C6HCl5O	87-86-5	ER↑, ER↓, PR↓	[79]
Tetrabromobisphenol A	C15H12Br4O2	79-94-7	ER↑, PR↓	[79]
Phenol	C6H6O	108-95-2	-	
Parathion-methyl	C8H10NO5PS	298-00-0	-	
Malathion	C10H19O6PS2	121-75-5	ER↑, GR↓	[80, 81]
Dimethoate	C5H12NO3PS2	60-51-5	ER↑, MR↓	[82, 83]
Bentazone	C10H12N2O3S	25057-89-0	-	
Perfluoropentanoic acid	C5HF9O2	2706-90-3	-	
Perfluorohexanoic acid	C6HF11O2	307-24-4	-	
Perfluoroheptanoic acid	C7HF13O2	375-85-9	-	
Pentadecafluorooctanoic acid	C8HF15O2	335-67-1	ER↑	[84]
Nonafluorobutane-1-sulfonic acid	C4HF9O3S	375-73-5	-	
Perfluorohexane-1-sulphonic acid	C6HF13O3S	355-46-4	ER↑	[85]
Perfluoroheptanesulfonic acid	C7HF15O3S	375-92-8	-	
Perfluorooctanesulfonic acid	C8HF17O3S	1763-23-1	ER↑	[85]
Imidacloprid	C9H10ClN5O2	138261-41-3	ER↑	[86]
Imidaclothiz	C7H8ClN5O2S	105843-36-5	-	
Thiamethoxam	C8H10ClN5O3S	153719-23-4	-	
Clothianidin	C6H8ClN5O2S	210880-92-5	-	
Thiacloprid	C10H9ClN4S	111988-49-9	ER↑	[86]
Acetamiprid	C10H11ClN4	135410-20-7	-	
Dinotefuran	C7H14N4O3	165252-70-0	-	
Nitenpyram	C11H15ClN4O2	150824-47-8	-	
Thiacloprid-amide	C10H11ClN4OS	676228-91-4	-	
N-desmethyl-acetamiprid	C9H9ClN4	190604-92-3	-	
Flonicamid	C9H6F3N3O	158062-67-0	-	
Benzo[a]pyrene	C20H12	50-32-8	ER↑, ER↓, PR↑, GR↓	[87]
Benzo[b]fluoranthene	C20H12	205-99-2	-	
Benzo[k]fluoranthene	C20H12	207-08-9	-	
3-phenoxy benzoic acid	C13H10O3	3739-38-6	GR↓	[11]
4-fluoro-3-phenoxy benzoic acid	C13H9FO3	77279-89-1	-	

All external standards were obtained from Tan-Mo Technology Co., Ltd. (Changzhou, China). ER: estrogen receptor. PR: progesterone receptor. GR: glucocorticoid receptor. MR: mineralocorticoid receptor. ↑: agonistic activity. ↓: antagonistic activity. - represents no agonistic or antagonistic activity in ER, PR, GR, or MR assays reported in the literature.

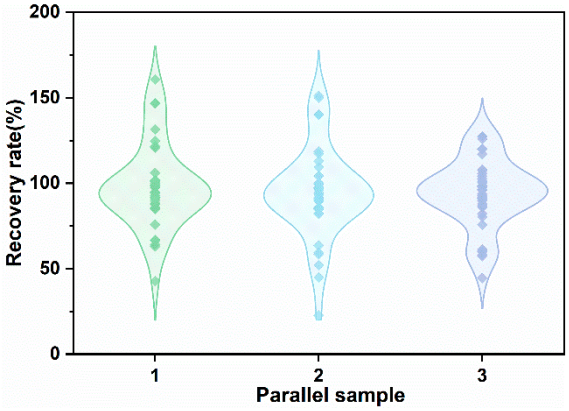

Figure S1. Violin plot of recovery rates of 43 external standards.

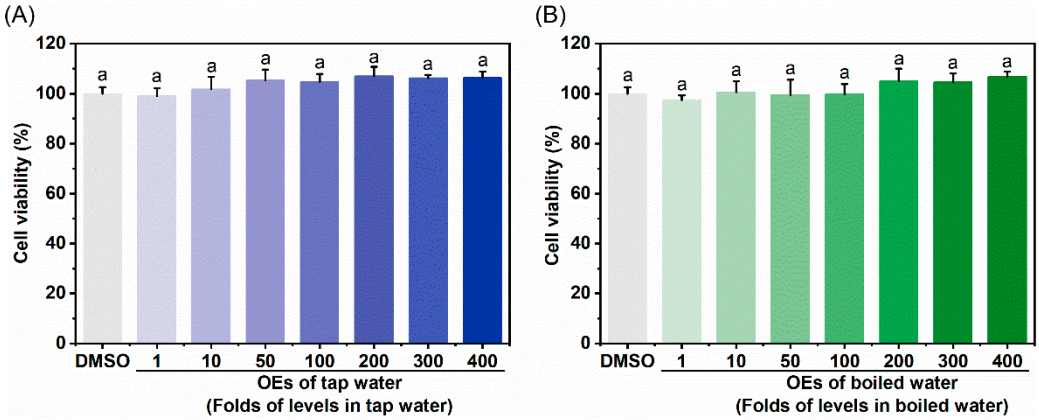

Figure S2. The viability of CHO-K1 cells exposed to OEs from tap water without or with boiling. **(A)** The cytotoxicity of OEs of tap water to CHO-K1 cells. CHO-K1 cells were exposed to the OEs of tap water or 1% DMSO (as vehicle control) for 24h. **(B)** The cytotoxicity of OEs of boiled water to CHO-K1 cells. CHO-K1 cells were exposed to the OEs of boiled water or 1% DMSO (as vehicle control) for 24h. Results were expressed as percent of control. Data are shown as mean±SD (n=6). Different letters on bars indicate significant differences among treatments (p<0.05).

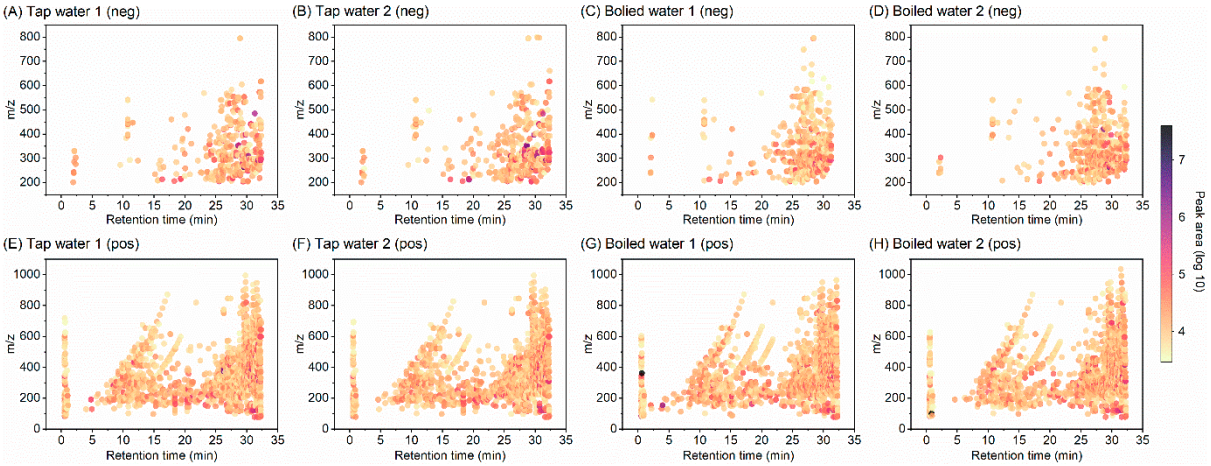

Figure S3. Plots of m/z and retention time of the non-target features detected per sample for negative **(A, B, C, D)** and positive **(E, F, G, H)** ionization. The color presents the peak area of a certain feature.

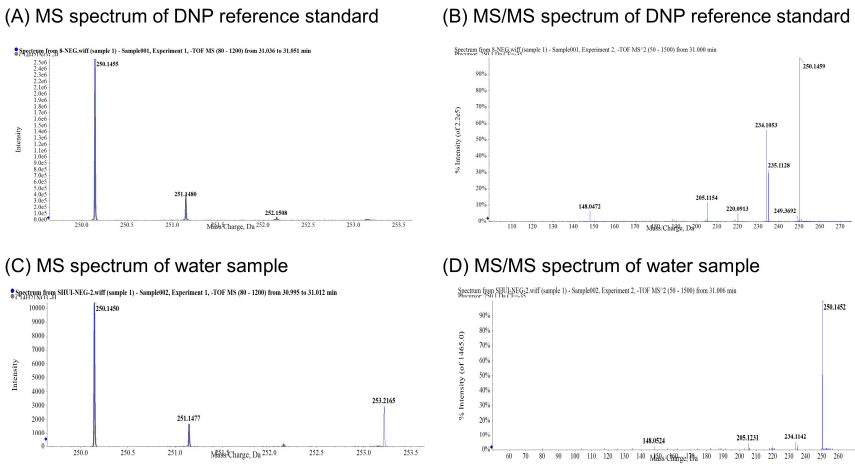

Figure S4 MS and MS/MS spectrum of DNP (precursor *m*/*z* 250.1) identified in the water sample.

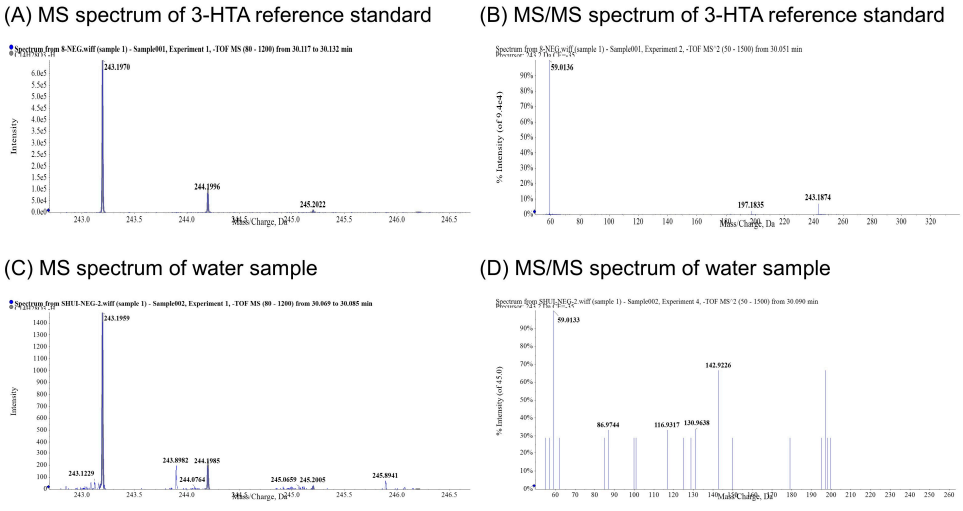

Figure S5 MS and MS/MS spectrum of 3-HTA (precursor *m*/*z* 243.2) identified in the water sample.

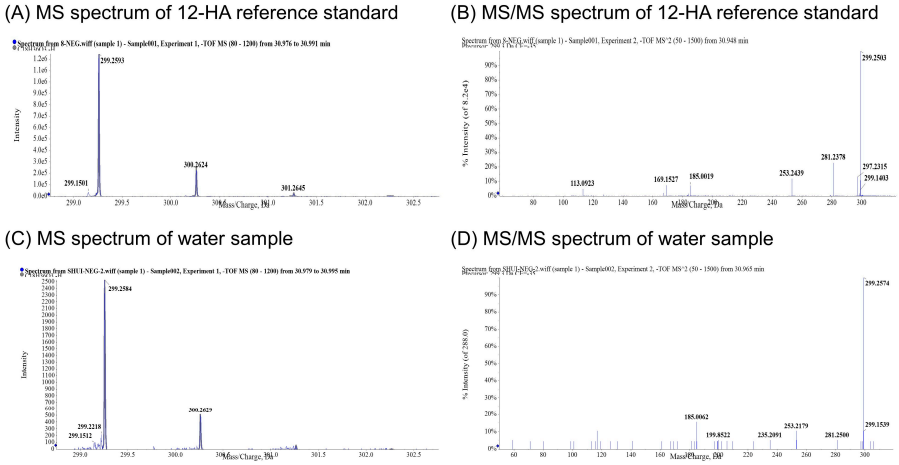

Figure S6 MS and MS/MS spectrum of 12-HA (precursor m/z 299.3) identified in the water sample.

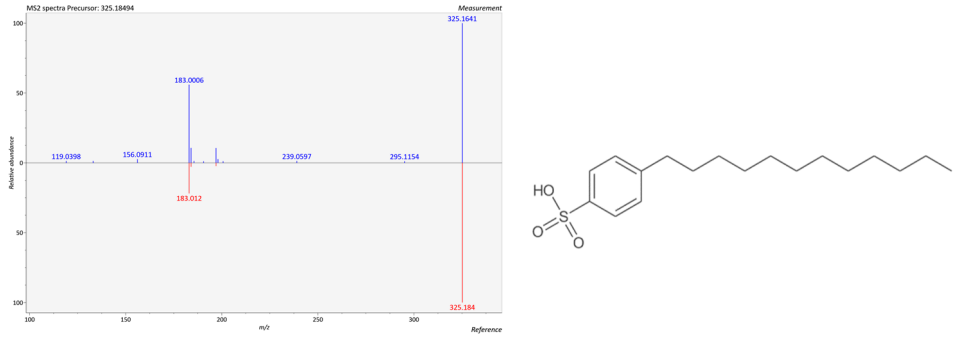

Figure S7 Spectral similarity of *m/z* 325.184 $[M-H]^-$ to MassBank spectrum of DBSA.

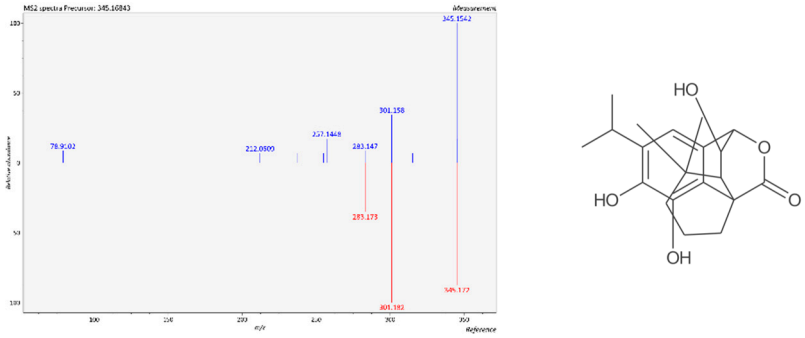

Figure S8 Spectral similarity of *m/z* 345.168 $[M-H]^-$ to MassBank spectrum of ISO.

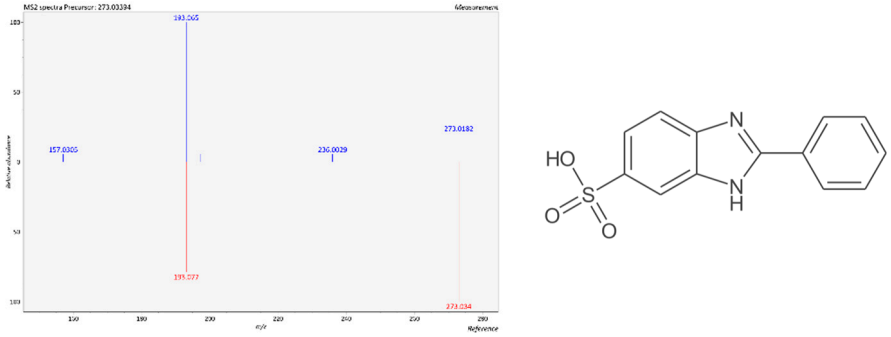

Figure S9 Spectral similarity of *m/z* 273.033 $[M-H]^-$ to MassBank spectrum of PBSA.

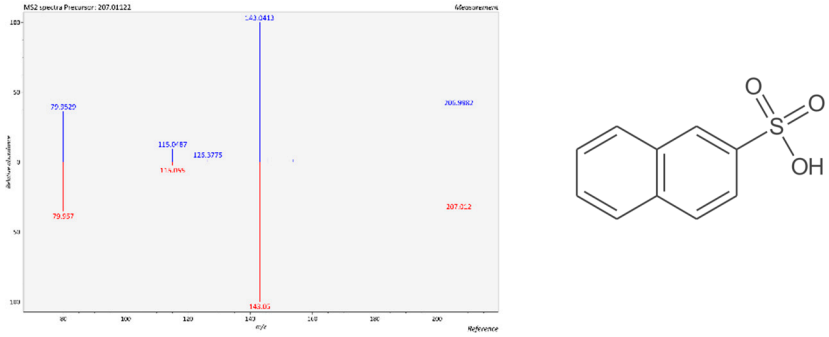

Figure S10 Spectral similarity of *m/z* 207.011 $[M-H]^-$ to MassBank spectrum of 2-NSA.

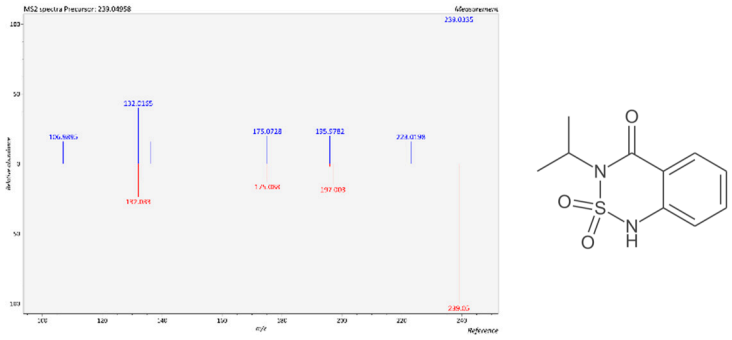

Figure S11 Spectral similarity of *m/z* 239.049 $[M-H]^-$ to MassBank spectrum of BEN.