Supplementary Information

Distribution and Trophodynamics of Substituted Diphenylamine Antioxidants and Benzotriazole UV Stabilizers in a Freshwater Ecosystem and the Adjacent Riparian Environment

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Table S1. National aggregate production volumes of SDPAs and BZT-UVs reported by the USEPA for USA and indication of use in Canada based on listing in the Canadian Domestic Substances List (DSL)

SDPAs			USEPA (tonnes/year (reported year))	Canada DSL
CAS#	Domestic Substances List (DSL) name	Components related to the present study		
184378-08-3	Benzenamine, N-phenyl-, reaction products with isobutylene and 2,4,4- trimethylpentene	C4, C4C4, C8, C4C8, C8C8	<450 (2015)	Not Listed
68411-46-1	Benzenamine, N-phenyl-, reaction products with 2,4,4- trimethylpentene	C4C8, C8,C8C8	4,500-<22,500 (2019)	Listed
68608-79-7	Benzenamine, N-phenyl-, (tripropenyl) derivatives	C9,C9C9	9,000-<45,000 (2015)	Listed
10081-67-1	Benzenamine, 4-(1-methyl-1- phenylethyl)-N-[4-(1-methyl-1- phenylethyl)phenyl]-	diAMS	220-<450 (2019)	Listed
36878-20-3	Benzenamine, ar-nonyl-N-(nonylphenyl)-	C9,C9C9	45,000-<110,000 (2019)	Listed
101-67-7	Benzenamine, 4-octyl-N-(4- octylphenyl)-	C8C8	209 (2019)	Listed
4175-37-5	Benzenamine, 4-octyl-N- phenyl-	C8	22 (2019)	Listed
15721-78-5	Benzenamine, 4-(1,1,3,3-tetramethylbutyl)-N-[4-(1,1,3,3- tetramethylbutyl)phenyl]-	C8C8	<450 (2019)	Listed
24925-59-5	Benzenamine, 4-nonyl-N-(4- nonylphenyl)-	C9C9	not reported	Listed
26603-23-6	Benzenamine, ar-octyl-N- (octylphenyl)-	C8C8	not reported	Listed
27177-41-9	Benzenamine, ar-nonyl-N- phenyl-	C9	not reported	Listed
68921-45-9	Benzenamine, N-phenyl-, reaction products with styrene and 2,4,4-trimethylpentene (BNST)	C8, C8C8	<450 (2019)	Listed
BZT-UVs				
70321-86-7	2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl)phenol (UV234)		450-<9000 (2019)	Not Listed
3896-11-5	2-tert-butyl-6-(5-chloro-2H-benzotriazol-2-yl)-4-methylphenol (UV326)		220-<450 (2019)	Not listed
3864-99-1	2,4-di-*tert*-butyl-6-(5-chloro-2H-benzotriazol-2-yl)phenol (UV327)		<450 (2016); 0 (2019)	Listed
25973-55-1	2-(2H-benzotriazol-2-yl)-4,6-di-tert-pentylphenol (UV328)		450-<4500 (2019)	Listed
3147-75-9	2-(2H-benzotriazol-2-yl)-4-(1,1,3,3-tetramethylbutyl)phenol (UV329)		220-<450 (2019)	Listed
36437-37-3	2-(2H-benzotriazol-2-yl)-4-(tert-butyl)-6-(sec-butyl)phenol (UV350)		not reported	Listed

Data sources:
USEPA - https://chemview.epa.gov/chemview/ (assessed in February 2024)
Canada - https://pollution-waste.canada.ca/substances-search/Substance (assessed in March 2024)

MATERIALS AND METHODS

Chemicals. The monitored SDPA standards including monobutyl-(C4), dibutyl-(C4C4), monooctyl-(C8), monobutyl monooctyl-(C4C8), C8C8 (C4, C4C4, C8, C4C8 and C8C8 are components of the mixture with CAS No. 184378-08-3), mononony1-(C9), dinonyl-(C9C9) (C9 and C9C9 are components of the mixture with CAS No. 6860879-7) and 4,4′-bis (α,α-dimethylbenzyl)-(diAMS) (CAS No. N10081-67-1) DPAs, were purchased from Accustandard (New Haven, CT, USA) or provided by industry. The target BZT-UVs were 2-(2H-benzotriazol-2-yl)-4,6-bis(1-methyl-1-phenylethyl) phenol (UV234; CAS No. 70321–86-7), 2-*tert*-butyl-6-(5-chloro-2H-benzotriazol-2-yl)-4-methylphenol (UV326; CAS No. 3896–11-5), 2,4-di-*tert*-butyl-6-(5-chloro-2H-benzotriazol-2-yl) phenol (UV327; CAS No. 3864–99-1), UV328 (CAS No. 25973–55-1), UV329 (CAS No. 3147-75-9) and 2-(2H-benzotriazol-2-yl)-4-(*tert*-butyl)-6-(*sec*-butyl) phenol (UV350; CAS No. 36437-37-3). BZT-UV analytical standards and surrogate standard 2-allyl-6-benzotriazol-2-yl-4-methyl-phenol (Allyl-BZT; CAS No. 2170-39-0) were purchased from Sigma-Aldrich (Oakville, ON, Canada), with the exception of UV350 which was purchased from BOC Science (Shirley, NY, USA).

Hexane and dichloromethane (Distilled in Glass grade) were purchased from Caledon Laboratory Chemicals (Georgetown, ON, Canada). Solvents (methanol, isopropanol, acetonitrile, methyl tert- butyl ether (MTBE) and water) were HPLC grade from Fisher Scientific (Ottawa, ON, Canada). Bio-Beads S-X3 (200-400 mesh) were purchased from Bio-Rad Laboratories (Hercules, CA, USA). Formic acid (98%) was obtained from Sigma-Aldrich (Oakville, ON, Canada). Anhydrous sodium sulfate (Na_2SO_4) was from VWR (Mississauga, ON, Canada). Na_2SO_4 was heated at 450°C overnight before use. Silica gel (63~200 microns, Caledon Laboratory Chemicals, ON, Canada) was activated at 130°C overnight and deactivated by 5% of water prior to use. OASIS hydrophilic-lipophilic balanced (HLB) solid phase extraction (SPE) cartridges were purchased from Waters (Mississauga, ON, Canada).

Sample Preparation. Water samples were extracted using the OASIS HLB SPE cartridges (200 mg). The cartridges were conditioned by 5 mL of 9:1 MTBE/methanol, followed by 8 mL of isopropanol and 10 mL of HPLC-grade water. The water sample (500 mL) with surrogate standard (Allyl-BZT, 20 μL of 200 ng mL^{-1} standard) was loaded on the SPE cartridges and followed by 5 mL of 5% methanol in HPLC-grade water. The cartridge was dried by vacuum for 30 min and then eluted with 10 mL of 9:1 (*v*:*v*) MTBE/methanol. The eluent was evaporated to dryness using a gentle flow of N_2 and reconstituted in 1 mL of acetonitrile for instrumental analysis. Freeze-dried sediment sample (0.5 g) with surrogate standard (Allyl-BZT, 20 μL of 200 ng mL^{-1} standard) was extracted by ultrasonication with three successions of 5 mL of 9:1 (*v*:*v*) MTBE/methanol. The extract was cleaned using a silica gel packed column. The cleanup column consisted of 5 g of 5% water deactivated silica gel with 1.5 g of Na_2SO_4 on the top. The column was preconditioned by 40 mL of hexane, and then the extracts were loaded and eluted with 30 mL of dichloromethane/hexane (1:1, *v*:*v*) mixture.[1] The eluents were concentrated to dryness using gentle N_2 gas and reconstituted in 1 mL of acetonitrile for instrumental analysis.

Biota sample (0.5 g, wet weight (ww)) was mixed with 2 g of Na_2SO_4 in a glass centrifuge tube. A mixture solvent of 5 mL 1:1 (*v*:*v*) hexane/dichloromethane was used to extract the sample. The sample was treated by 2 min of vortex, followed by 10 min of sonication and 15 min of centrifugation. The extraction was repeated for 3 times and the extracts were combined in a pre-weighted new glass centrifuge tube. The solvent extract was concentrated to dryness under gentle N_2. The lipid content was measured gravimetrically. The extract was then dissolved in 1 mL of 1:1 (*v*:*v*) hexane:dichloromethane and further cleaned by gel permeation chromatography (GPC)

(Express Performance column, 25cm×3.5cm i.d.; packed with 50 g of Bio-Beads S-X3) (J2 scientific; Columbia, MI, USA). The GPC mobile phase was 1:1 hexane: dichloromethane and the flow rate were 5 mL min^{-1}. The fraction corresponding to 7.5 - 22.5 min was collected and concentrated to 1 mL using rotary evaporation. The 1 mL concentrated GPC eluent was further concentrated to dryness using gentle N_2 and reconstituted in 1 mL of acetonitrile for instrumental analysis. [1]

Instrumental Analysis. The details of SDPAs and BZT-UVs analysis were previously published. [1] A Waters Acquity ultra-high performance liquid chromatography coupled with a Sciex 4000 QTRAP tandem mass spectrometer (UPLC-MS/MS) was used for the determination of SDPAs and BZT-UVs. The MS/MS was operated in positive electrospray ionization mode. Analytes were detected using scheduled multiple reaction monitoring (MRM). A 50 mm × 3.0 mm Gemini-NX 3μm C_{18} analytical column (Phenomenex, CA, USA) was used for chromatographic separation. Water and acetonitrile, each containing 0.1% of formic acid, were used as mobile phases. The instrument parameters including LC gradient and MRM transitions are shown in Table S1 and S2. Column temperature was set at 40°C. Injection volume was 10 μL.

Stable Isotope Analysis. Stable isotope analyses of nitrogen (δ^{15}N) and carbon (δ^{13}C) were performed at the University of Waterloo's Environmental Isotope Laboratory (Waterloo, Ontario). Samples (about 1-1.5 mg) were dried at 60 °C for 48 h and ground to a fine powder before analysis. An Isochromatic continuous-flow, stable-isotope mass spectrometer (GVInstruments/Micromass, Manchester, UK) coupled to a Carlo Erba Elemental Analyzer (CHNSeO EA 1108, Milan, Italy) was employed for the analysis. [2] The stable isotopic ratio was reported relative to atmospheric air (N) and the Pee Dee Belemnite (C). For δ^{13}C, lipids in samples were corrected for fish muscle samples with C:N>3.5 using the algorithm of $\delta^{13}C_{corrected}=\delta^{13}C+D\times\left(I+\frac{3.90}{1+287/L}\right)$, where D

(7.018) is the difference in carbon isotopic composition between protein and lipid, I is a constant of 0.048, and L is the percentage of lipid in the sample.[3,4] $\delta^{13}C$ in fish muscle with C:N<3.5 and invertebrates were not corrected as suggested by Skinner et al. (2015) [3] and Kiljunen et al. (2006). [4]

Organic Carbon measurement. Dried and finely ground (<200 mesh) samples are subjected to 6% sulfuric acid treatment to remove inorganic carbonate. Samples were analyzed using a Exeter 440CHNS/O Analyzer via combustion to produce CO_2, measured by thermal conductivity.

1. Z. Lu, A. O. De Silva, T. E. Peart, C. J. Cook, G. R. Tetreault, M. R. Servos and D. C. G. Muir, Distribution, partitioning and bioaccumulation of substituted diphenylamine antioxidants and benzotriazole UV stabilizers in an urban creek in Canada, *Environ. Sci. Technol.*, 2016, **50**, 9089–9097.
2. Z. Lu, A. O. De Silva, W. Zhou, G. R. Tetreault, S. R. de Solla, P. A. Fair, M. Houde, G. Bossart and D. C. G. Muir, Substituted diphenylamine antioxidants and benzotriazole UV stabilizers in blood plasma of fish, turtles, birds and dolphins from North America, *Sci. Total Environ.*, 2019, **647**, 182-190.
3. M. M. Skinner, A. A. Martin and B. C. Moore, Is lipid correction necessary in the stable isotope analysis of fish tissues? *Rapid Commun. Mass Spectrom.*, 2016, **30**, 881–889.
4. M. Kiljunen, J. Grey, T. Sinisalo, C. Harrod, H. Immonen, R. I. Jones, A revised model for lipid-normalizing $\delta^{13}C$ values from aquatic organisms, with implications for isotope mixing models, *J. Appl. Ecol.*, 2006, **43**, 1213–1222.

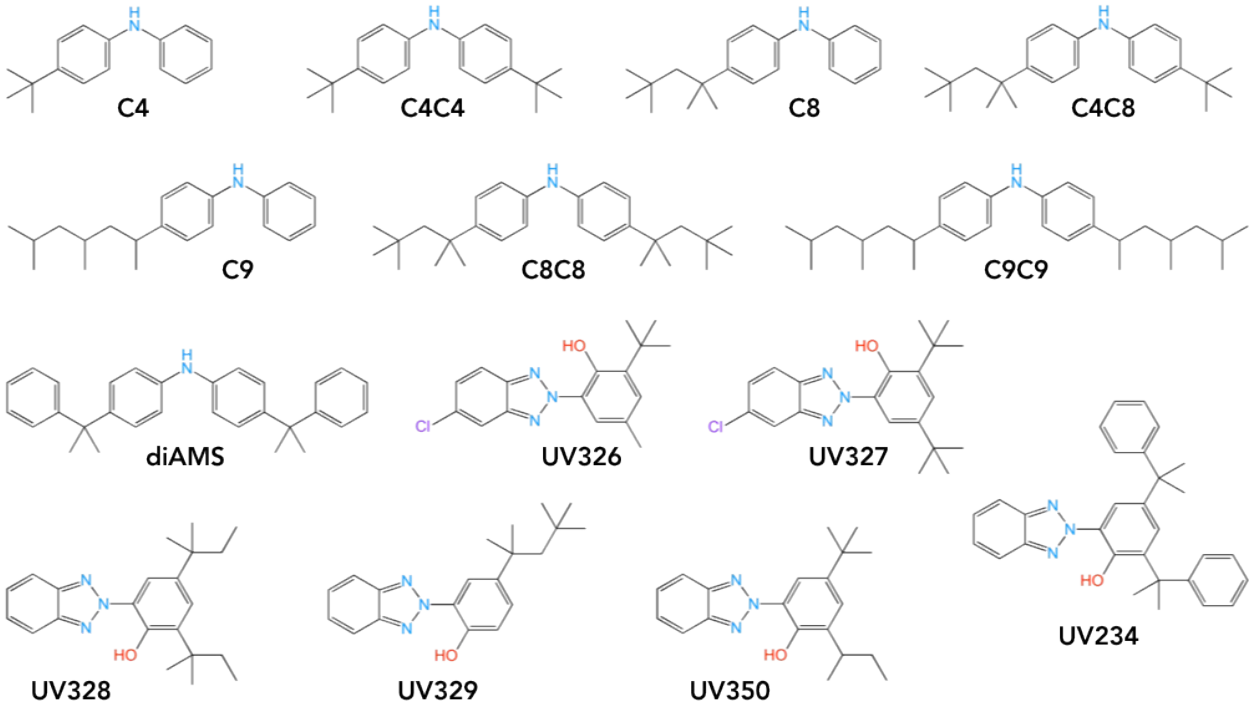

Figure S1. Structures of target SDPAs and BZT-UVs. C9 and C9C9 SDPAs are a mixture of isomers varying in their branched alkyl substituents. The chemical structures of C9 and C9C9 depicted here are most representative and comprise the major proportions within the technical mixture. (Reference: Environment and Climate Change Canada and Health Canada, 2017. Screening assessment for substituted diphenylamines. https://www.canada.ca/en/environment-climate-change/services/evaluating-existing-substances/screening-assessment-substituted-diphenylamines.html; Accessed in March 2020.)

Table S2. LC gradient parameters for SDPAs and BZT-UVs separation on a 50 mm × 3.0 mm Gemini-NX 3μm C_{18} analytical column (Phenomenex, CA, USA). [a]Water containing 0.1% formic acid; [b]Acetonitrile containing 0.1% formic acid.

Time (min)	Flow Rate (mL/min)	%A[a]	%B[b]
0	0.3	40	60
0.5	0.3	40	60
4	0.3	3	97
6	0.3	3	97
6.5	0.5	0.5	99.5
9.5	0.5	0.5	99.5
10	0.3	40	60
12	0.3	40	60
14	0.3	40	60

Table S3. UPLC-MS/MS experimental parameters applied on Sciex 4000 QTRAP tandem mass spectrometer operated in electrospray negative ionization. [a]Declustering potential (V). [b]Collision energy (eV). [c]Collision Cell Exit Potential (V). [d]Surrogate standard. NA: not applicable.

No.	Compound	Precursor ion (*m/z*)	Product ion (*m/z*) for quantification	Product ion (*m/z*) for qualification	DP[a] (V)	CE[b] (eV)	Retention time (min)	Sediment Recovery%	Biota Recovery% (mean±SD)	Water LOD (ng/L)	Sediment LOD (ng/g)	Fish muscle LOD (ng/g)	Mussel LOD (ng/g)	Other biota LOD (ng/g)
1	C4	226	134	106	106	43	4.42	79	70±24	0.02	0.001	0.008	0.001	0.004
2	C4C4	282	134	106	126	49	5.67	61	65±17	0.01	0.004	0.005	0.004	0.004
3	C8	282	134	106	126	49	5.78	80	62±15	0.02	0.002	0.03	0.006	0.05
4	C9	296	134	210	106	47	6.16	56	63±14	0.01	0.01	0.01	0.01	0.005
5	C4C8	338	134	106	131	53	6.55	60	84±30	0.02	0.007	0.02	0.01	0.01
6	C8C8	394	134	106	146	63	7.50	71	72±22	0.02	0.007	0.02	0.02	0.005
7	C9C9	422	134	336	131	61	8.46	74	65±17	0.01	0.033	0.008	0.01	0.01
8	diAMS	406	196	119	156	55	6.02	61	79±20	0.2	0.004	0.04	0.1	0.03
9	UV234	448	370	119	91	31	6.61	44	77±23	0.01	0.03	0.07	0.01	0.1
10	UV326	316	260	107	61	29	6.53	52	77±20	1.0	7.0	2.0	4.0	4.0
11	UV327	358	302	246	46	33	7.10	64	81±16	1.0	3.0	1.0	2.0	2.0
12	UV328	352	282	212	96	33	7.29	63	83±14	0.2	0.3	0.1	2.0	0.7
13	UV329	324	212	253	106	35	6.34	56	69±16	0.03	0.1	1.0	1.0	1.0
14	UV350	324	268	212	86	31	6.61	56	66±11	0.2	0.3	0.1	0.2	0.2
15	Allyl-BZT[d]	266	147	119	71	25	5.29	62	75±28	NA	NA	NA	NA	NA

Table S4. Detection frequency, concentration median and ranges (ng L^{-1} for water; ng g^{-1} for sediment, dry weight; ng g^{-1} for biota, wet weight) of SDPAs and BZT-UVs in Hamilton Harbour.

Matrix	C4			C4C4			C8			C4C8			C9		
	DF	Median	Range	DF	Median	Range	DF	Median	Range	DF	Median	Range	DF	Median	Range
Water	80	0.022	<LOD-0.084	90	0.016	<LOD-0.046	100	0.051	0.028-0.20	90	0.045	<LOD-0.15	100	0.037	0.016-0.13
Sediment	80	0.022	<LOD-0.80	100	0.17	0.098-2.6	100	9.6	8.2-21	100	0.68	0.34-10	100	1.8	0.77-13
Millipede	100	0.005	0.004-0.006	100	0.042	0.037-0.053	67	0.079	<LOD-0.090	100	0.55	0.53-0.60	100	0.15	0.11-0.19
Dragonfly	100	0.022	0.019-0.025	100	0.12	0.069-0.13	100	0.094	0.069-0.099	100	0.23	0.095-0.27	0	NA	<LOD
Large Snail	0	NA	<LOD	50	0.011	<LOD-0.023	0	NA	<LOD	100	0.055	0.025-0.077	100	0.085	0.045-0.15
Chironiomid	0	NA	<LOD	0	NA	<LOD	0	NA	<LOD	100	0.11	0.10-0.16	0	NA	<LOD
Damselfly	0	NA	<LOD	100	0.011	0.007-0.016	0	NA	<LOD	100	0.037	0.030-0.090	0	NA	<LOD
Small Snail	0	NA	<LOD	100	0.016	0.005-0.022	0	NA	<LOD	67	0.035	<LOD-0.066	50	0.061	<LOD-0.11
Whirligig Beetle	0	NA	<LOD	100	0.042	0.037-0.047	0	NA	<LOD	100	0.076	0.069-0.088	0	NA	<LOD
Plankton	100	0.007	0.005-0.014	100	0.03	0.025-0.038	100	0.088	0.080-0.13	100	0.11	0.074-0.14	100	0.06	0.044-0.065
Mussel	100	0.003	0.002-0.003	100	0.061	0.053-0.062	100	0.057	0.055-0.059	100	0.81	0.77-0.81	100	0.091	0.080-0.13
Leech	50	0.004	<LOD-0.006	75	0.026	<LOD-0.094	0	NA	<LOD	88	0.031	<LOD-0.30	100	0.029	0.01-0.30
Dragonfly larva	0	NA	<LOD	100	0.008	0.006-0.009	0	NA	<LOD	67	0.017	<LOD-0.017	100	0.063	0.062-0.080
GZSH Muscle	22	NA	<LOD-0.021	44	0.006	<LOD-0.17	30	0.023	<LOD-0.41	100	0.25	0.016-5.4	78	0.027	<LOD-0.78
CMCR Muscle	80	0.013	<LOD-0.019	90	0.029	<LOD-0.080	30	0.023	<LOD-0.053	90	0.2	<LOD-1.8	70	0.023	<LOD-0.53
BRBH Muscle	10	NA	<LOD-0.015	80	0.006	<LOD-0.12	10	NA	<LOD-0.18	60	0.023	<LOD-0.31	30	0.012	<LOD-0.072
LMBS Muscle	9	NA	<LOD-0.008	91	0.022	<LOD-0.14	18	NA	<LOD-0.19	82	0.032	<LOD-0.090	9	NA	<LOD-0.11
RCBS Muscle	0	NA	<LOD	70	0.007	<LOD-0.014	10	NA	<LOD-0.045	30	0.013	<LOD-0.048	0	NA	<LOD

Matrix	C8C8			C9C9			diAMS			UV234			UV328		
	DF	Median	Range	DF	Median	Range	DF	Median	Range	DF	Median	Range	DF	Median	Range
Water	90	0.13	<LOD-0.25	100	0.071	0.01-0.20	90	0.4	<LOD-1.5	70	0.066	<LOD-0.35	100	0.9	0.3-2.8
Sediment	100	1.02	0.82-9.8	100	4.3	2.7-14	100	0.5	0.22-5.9	100	1.3	0.8-2.8	100	16	8.3-48
Millipede	100	0.26	0.24-0.26	100	0.4	0.32-0.49	100	2.1	1.9-2.1	100	0.16	0.14-0.19	67	1.2	<LOD-1.3
Dragonfly	100	0.14	0.14-0.18	100	0.31	0.28-0.52	100	1.2	1.1-1.5	100	5.8	5.0-6.7	100	19	19-22
Large Snail	100	0.076	0.052-0.12	100	1.0	0.40-1.73	100	0.062	0.042-0.098	75	0.12	<LOD-0.16	100	1.5	0.84-2.2
Chironiomid	100	0.044	0.039-0.045	100	0.54	0.52-0.65	100	0.37	0.33-0.38	100	0.55	0.5-0.81	100	7.7	7.3-10
Damselfly	100	0.069	0.069-0.082	100	0.21	0.20-0.31	100	0.57	0.56-0.66	100	0.17	0.15-0.93	100	1.9	1.3-3.6
Small Snail	100	0.043	0.041-0.045	100	0.24	0.023-0.50	100	0.35	0.33-0.37	67	0.13	<LOD-0.30	100	1.2	0.7-2.0
Whirligig Beetle	100	0.016	0.015-0.021	100	0.034	0.028-0.037	0	NA	<LOD	0	NA	<LOD	0	NA	<LOD
Plankton	100	1.3	0.62-2.3	100	0.088	0.055-0.11	100	0.11	0.094-0.13	100	0.25	0.20-0.43	100	3.7	3.0-4.2
Mussel	100	0.055	0.050-0.059	100	0.067	0.055-0.071	0	NA	<LOD	100	0.07	0.047-0.075	0	NA	<LOD
Leech	75	0.03	<LOD-0.14	75	0.055	<LOD-0.36	25	NA	<LOD-0.27	25	NA	<LOD-0.11	0	NA	<LOD
Dragonfly larva	100	0.01	0.008-0.012	100	0.05	0.045-0.051	100	0.084	0.065-0.10	33	0.05	<LOD-0.11	0	NA	<LOD
GZSH Muscle	30	0.009	<LOD-0.14	22	NA	<LOD-0.039	30	0.014	<LOD-0.14	30	0.084	<LOD-0.44	56	0.32	<LOD-10
CMCR Muscle	80	0.1	<LOD-0.38	90	0.065	<LOD-0.29	10	NA	<LOD-0.085	10	NA	<LOD-0.39	80	0.74	<LOD-5.0
BRBH Muscle	10	NA	<LOD-0.98	0	NA	<LOD	0	NA	<LOD	0	NA	<LOD	0	NA	<LOD
LMBS Muscle	9	NA	<LOD-0.30	36	0.001	<LOD-0.25	0	NA	<LOD	45	0.46	<LOD-2.8	55	0.32	<LOD-0.59
RCBS Muscle	0	NA	<LOD	10	NA	<LOD-0.016	0	NA	<LOD	80	2.2	<LOD-5.3	80	0.34	<LOD-0.65

Note: The target compounds UV326, UV327, UV329, and UV350 were not detected in any samples.
Abbreviation: GZSH- Gizzard Shad; BRBH - Brown Bullhead; RCBS - Rock Bass; LMBS - Largemouth Bass; CMCR - Common Carp; LOD- limit of detection; DF-detection frequency.

Table S5. Trophic shift (mean±SE) for possible predator-prey relationships used for estimation of $\delta^{15}N$ increment in food web samples collected from Hamilton Harbour. (P) indicates that the $\delta^{15}N$ data were obtained from pooled samples.

Consumer	Diet	$\delta^{15}N$ (‰)
Dragonfly Larva (P)	Plankton (P)	-0.3
GZSH	Plankton (P)	-1.4±0.4
CMCR	Plankton (P)	-0.7±0.3
CMCR	Small Snail (P)	1.6±0.3
CMCR	Large Snail	1.4±0.3
BRBH	Small Snail	1.7±0.8
BRBH	Large Snail	1.5±0.8
LMBS	Dragonfly Larva (P)	3.8±0.3
LMBS	Leeches	3.2±0.3
LMBS	GZSH	4.9±0.3
LMBS	BRBH	4.2±0.3
LMBS	Small Snail (P)	5.8±0.3
LMBS	Large Snail	5.6±0.3
RCBS	Dragonfly Larva (P)	4.9±0.3
RCBS	Leeches	4.3±0.3
RCBS	Small Snail (P)	6.8±0.3
RCBS	Large Snail	6.7±0.3

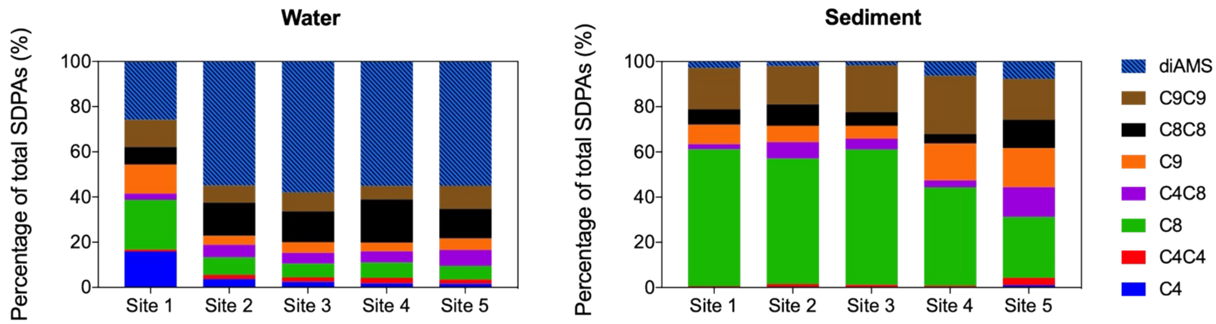

Figure S2. Compositions of SDPAs in the water and sediment of Hamilton Harbour collected in 2016.

Table S6. Pearson correlation coefficients among $\log_{10}$ transformed concentrations of SDPAs and BZT-UVs in water (n=10).

	C4	C4C4	C8	C4C8	C8C8	C9	C9C9	diAMS	UV234
C4	1								
C4C4	0.47	1							
C8	0.78**	0.86**	1						
C4C8	0.36	0.91***	0.81**	1					
C8C8	0.13	0.88***	0.64*	0.86***	1				
C9	0.58	0.87***	0.87***	0.91***	0.69*	1			
C9C9	0.28	0.82**	0.71*	0.95***	0.85**	0.82**	1		
diAMS	0.47	0.97***	0.86***	0.95***	0.91***	0.89***	0.91***	1	
UV234	0.16	0.21	0.18	0.19	0.07	0.38	0.27	0.18	1
UV328	0.55	0.22	0.47	0.11	0.16	0.16	0.07	0.21	-0.19

*p<0.05; **p<0.01; ***p<0.001

Table S7. Pearson correlation coefficients among $\log_{10}$ transformed concentrations of SDPAs and BZT-UVs in sediment (n=5).

	C4	C4C4	C8	C4C8	C8C8	C9	C9C9	diAMS	UV234
C4	1								
C4C4	0.91*	1							
C8	0.89*	0.95*	1						
C4C8	0.95*	0.99***	0.96**	1					
C8C8	0.84	0.97**	0.99**	0.96**	1				
C9	0.81	0.84	0.84	0.81	0.83	1			
C9C9	0.90*	0.91*	0.87	0.89*	0.86	0.98**	1		
diAMS	0.77	0.81	0.80	0.78	0.80	1.00***	0.97**	1	
UV234	0.91*	0.91*	0.77	0.90*	0.79	0.82	0.91*	0.81	1
UV328	0.37	0.16	0.24	0.18	0.15	0.64	0.55	0.65	0.30

*p<0.05; **p<0.01; ***p<0.001

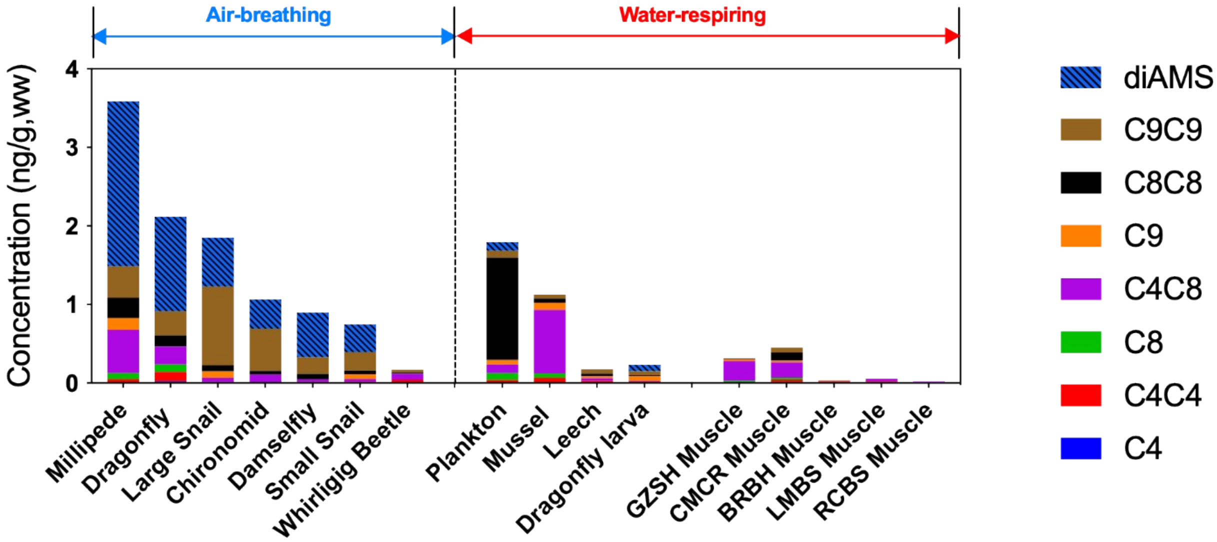

Figure S3. Median concentrations and compositions of SDPAs in biota samples from the Hamilton Harbour collected in 2016.

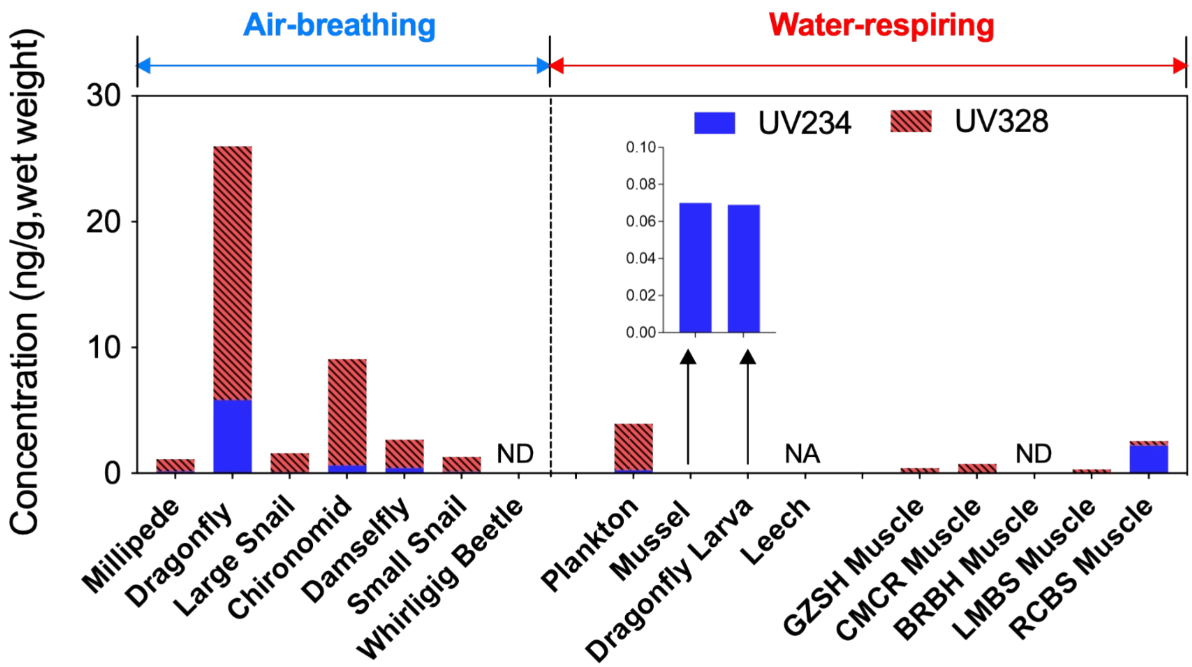

Figure S4. Median concentrations and compositions of UV234 and UV328 in biota samples from the Hamilton Harbour. ND: not detected; NA: Detection frequency <30%.

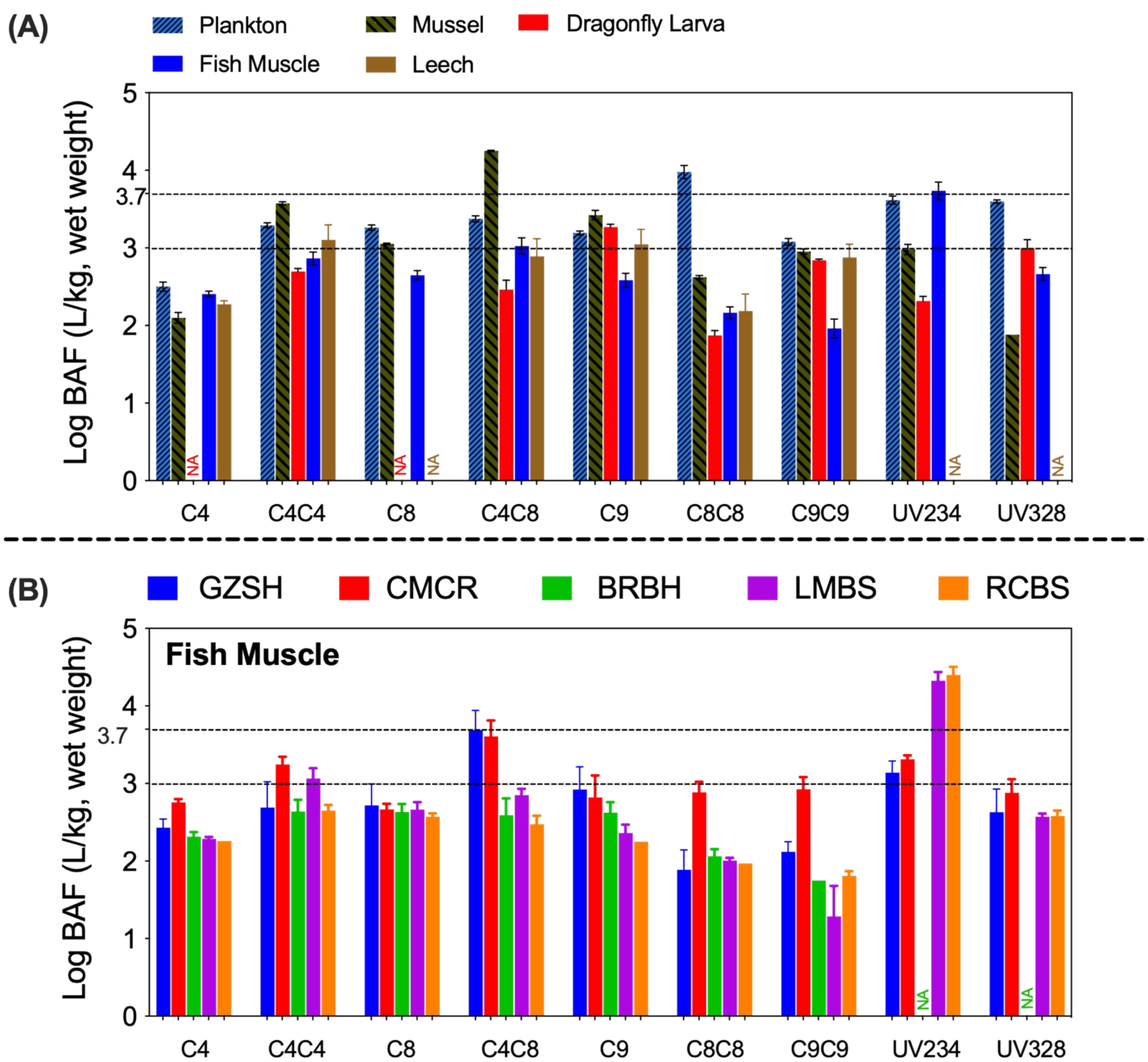

Figure S5. Field based $\log_{10}$ BAF of SDPAs and BZT-UVs (mean ± standard error) in (A) plankton, mussel, leech, dragonfly larva, and fish muscle; and (B) the muscle of different fish species. NA: data is not available because of the concertation in water or biota samples <30% detection. GZSH: Gizzard Shad; BRBH: Brown Bullhead; RCBS: Rock Bass; LMBS: Largemouth Bass; CMCR: Common Carp.

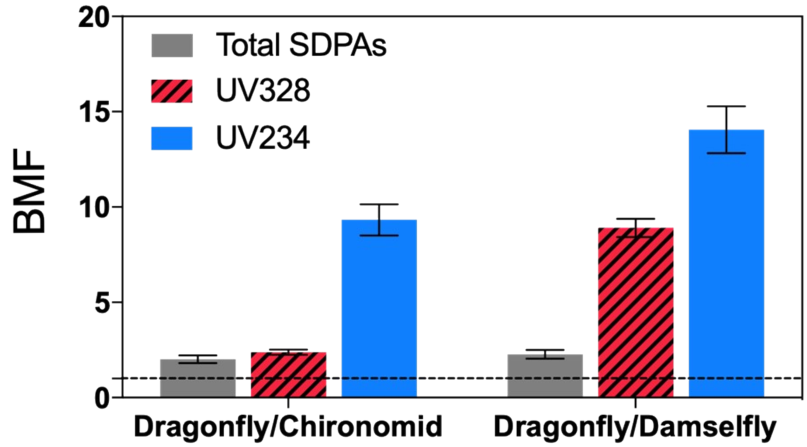

Figure S6. Wet weight based BMFs (mean ± standard error) of SDPAs and BZT-UVs in dragonfly food chain of Hamilton Harbour. The dashed line indicates the BMF equals to 1.