Supporting Information

Occurrence, distribution and fate of organic UV filters in coral communities

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Content in Supporting Information

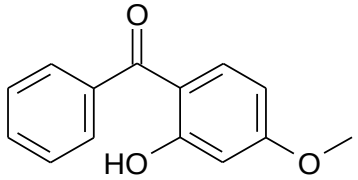
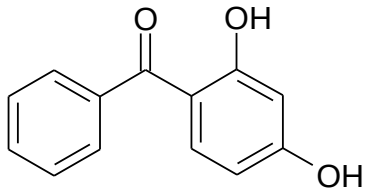
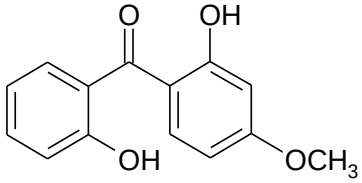
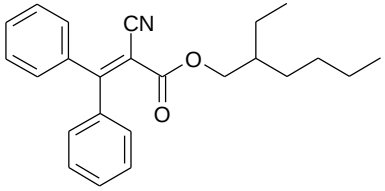
Analytical procedures for ambient water

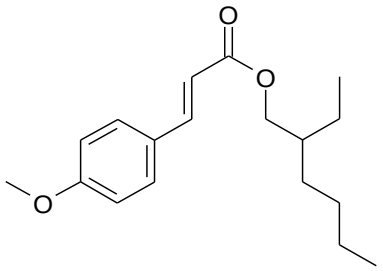
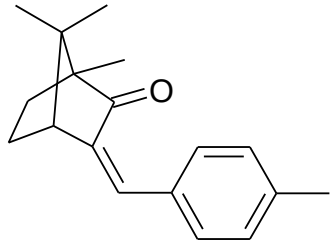
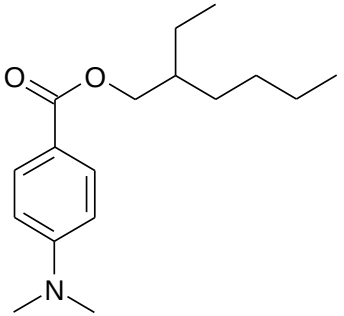
Each cartridge was preconditioned successively with 15 mL of 50:50 v/v methanol: ethyl acetate (MeOH: EA) and 15 mL of Milli-Q water. Isotope-labeled ^{13}C-BP-3 and 3.5 mL of 5% (w/v) Na_2EDTA were added to each sample (350 mL) as a surrogate standard and a chelating agent respectively, before loading to the cartridge at a flow rate of 2 – 3 mL/min. The addition of Na_2EDTA results in better quantification of some UV filters (e.g. prevention of tailing in the chromatogram; reviewed by Salvador and Chisvert, 2005) and method recoveries were found to be improved in this optimized method (Tsui et al., 2014). This improvement could be due to the electron-rich aromatic structures of these compounds that are able to bind with metal ions. Each sample bottle was rinsed with 10 mL Milli-Q water and loaded to the cartridge at the same speed. All eluates were discarded. After loading, the cartridges were washed by 10 mL Milli-Q water and dried under a vacuum for 10 minutes and then subjected to centrifugation at 3000 × *g* for 2 minutes twice for further drying the water inside the cartridges. The target compounds were eluted from the cartridges using 3 × 4 mL of 50:50 v/v MeOH: EA. The volume of extracts was reduced to less than 0.5 mL under a gentle stream of nitrogen and the final volume was adjusted to 0.5 mL with methanol. All sample extracts were subjected to centrifugation at 9000 × *g* for 10 minutes to avoid any suspended particles entering the instrument and then transferred to amber sample vials for standard addition. Finally the extracts were analyzed by an ultra performance liquid chromatography-electrospray ionization-tandem mass spectrometer (UPLC-ESI-MS/MS). Analytical duplication was carried out for each sample.

Instrumental analysis

Separation and quantification of analytes were performed using an Agilent 1290 LC system (Agilent, Palo Alto, CA, USA) interfaced with an AB SCIEX API 3200 triple quadrupole tandem mass spectrometry equipped with a Turbo V ion source (AB SCIEX, Framingham, MA, USA) operated in both negative and positive modes. The mass spectrometer was operated in both negative and positive modes since the negative mode provided higher intensities for some of the benzophenone-group compounds based on our mass tuning results and other literature (Negreira et al., 2009; Kunisue et al., 2010). A 10 μL aliquot of extract was injected onto an XBridge^{TM} C18 column (Waters Corporation, 5 μm, 2.1 mm × i.d. 50 mm length) equipped with a guard column at a flow rate of 0.3 mL min^{-1} using pure Milli-Q water (A) and pure methanol (B) in a gradient elution (0 min, 5% B; 15 min, 100 % B; 20 min, 100% B; 20.1 min, 5% B; 30 min 5% B). Pure methanol and Milli-Q water were found to be the most appropriate mobile phases for separation in this optimized instrumental method in terms of overall intensities and peak shapes for all target compounds. Analytes were determined by ESI-MS/MS either in positive or negative mode by multiple reaction monitoring (MRM). Turbo V ion source and MS/MS parameters were as follows: curtain gas (CUR), 10 psi; collision gas (CAD), high; ion spray voltage, 4500 V (positive mode) or −4500 (negative mode); temperature, 400 °C (positive mode) or 600 °C (negative mode); ion source gas 1 (GS1), 50 psi (positive mode) or 40 psi (negative mode); and ion source gas 2 (GS2), 60 psi (positive mode) or 70 psi (negative mode).

Table S1. Structures and physicochemical properties of the target organic UV filters

Name of UV filter	Structure	Molecular formula	Molecular weight	CAS number	Log K_{ow}	Log BCF
Benzophenone-3 (BP-3)		$C_{14}H_{12}O_3$	228.2	131-57-7	3.52[a] 3.79[b]	1.97[d]
2,4-Dihydroxybenzophenone or benzophenone-1 (BP-1)		$C_{13}H_{10}O_3$	214.22	131-56-6	2.96[c]	N/A
2,2'-Dihydroxy-4-methoxybenzophenone or benzophenone-8 (BP-8)		$C_{14}H_{12}O_4$	244.24	131-53-3	3.82[c]	N/A
Octocrylene (OC)		$C_{24}H_{27}NO_2$	361.5	6197-30-4	6.88[a]	2.13[e]

Ethylhexyl methoxycinnamate (EHMC)		$C_{18}H_{26}O_3$	290.41	5466-77-3	5.8[b]	5.8[f]
4-Methylbenzylidene camphor (4-MBC)		$C_{18}H_{22}O$	254.4	36861-47-9	4.95[a] 5.47[b]	3.51[f]
Octyl dimethyl-p-aminobenzoic acid (ODPABA)		$C_{17}H_{27}NO_2$	277.4	21245-02-3	6.15[a] 5.77[b]	3.74[f]

[a] (Rodil et al., 2008), [b] (Kameda et al., 2011), [c] (Sánchez-Brunete et al., 2011), [d,e] (Blüthgen et al., 2012; 2014), [f] (Giokas et al., 2007).

Table S2. Coral habitat sampling information (n=3 for each sample).

Dry Season (April 2015)	**Wet Season (August 2015)**
Ung Kong	Ung Kong
Platygyra acuta	*Favites abdita*
Porites sp.	*Porites* sp.
Pavona decussata	*Pavona decussata*
Acropora valida[1]	
Wu Pai	Wu Pai
Platygyra acuta	*Favites abdita*
Porites sp.	*Porites* sp.
	Pavona decussata
Sharp Island	Sharp Island
Platygyra acuta	*Favites abdita*
Porites sp.	*Porites* sp.
Pavona decussata	*Pavona decussata*
	Sung Kong
	Favites abdita
	Porites sp.
	Pavona decussata

[1]: n=2 was collected for this sample due to availability in the coral habitat.

Table S3. UPLC-MS/MS analytical parameters for the determination of organic UV filters

MS section	Analyte	RT (min)	Transition[a]	Linearity, R^2	Instrumental DL, Conc. (ng/mL)
ESI+	ODPABA	14.9	278.4 (76) → 151.2 (33)	0.992	0.132
		14.9	278.4 (76) → 166.2 (35)		
	4-MBC	13.9	255.3 (56) → 105.2 (37)	0.991	0.067
		13.9	255.3 (56) → 91.2 (57)		
	EHMC	15.0	291.5 (56) → 161.3 (23)	0.996	0.396
		15.0	291.5 (56) → 179.2 (13)		
	OC	14.6	362.4 (46) → 250.1 (15)	0.991	0.067
		14.6	362.4 (46) → 232.1 (31)		
	BP-3	12.0	229.2 (56) → 151.2 (31)	0.992	0.263
		12.0	229.2 (56) → 105.2 (27)		
ESI-	BP-1	9.71	213.0 (50) → 90.9 (36)	0.990	0.525
		9.71	213.0 (50) → 135.0 (28)		
	BP-8	10.2	242.8 (25) → 93.0 (34)	0.991	0.626
		10.2	242.8 (25) → 122.9 (26)		

[a] m/z precursor ion (declustering potential (V)) and m/z product ion (collision energy (eV)).

Table S4. Method recoveries (± relative standard deviation; n = 9) and method detection limits (MDLs) of the analytical method for the target organic UV filters in coral, water and sediment.

	ODPABA	**4-MBC**	**EHMC**	**OC**	**BP-3**	**BP-1**	**BP-8**
Coral							
(20 ng/g dw spike)							
Recovery (%)	61 ± 7	83 ± 7	64 ± 9	65 ± 4	86 ± 8	86 ± 7	87 ± 7
MDL (ng/g dw)	0.22	0.11	7.06	0.12	0.50	0.85	0.99
Water							
(11 ng/L spike)							
Recovery (%)	73 ± 4	83 ± 4	83 ± 4	76 ± 5	93 ± 8	106 ± 8	100 ± 6
MDL (ng/L)	0.03	0.28	0.41	1.38	0.04	0.11	0.03
Sediment							
(20 ng/g dw spike)							
Recovery (%)	63 ± 4	58 ± 5	76 ± 6	76 ± 3	81 ± 5	81 ± 8	67 ± 7
MDL (ng/g dw)	0.16	0.09	7.55	0.09	0.43	0.98	1.10

Table S5. Concentrations of UV filters detected in coral tissues (ng/g ww), ambient water column (ng/L) and sediment (ng/g dw) in different locations during wet and dry seasons in Hong Kong.

Wet Season									
Location	Sample Matrices	Species	BP-3	BP-8	OC	ODPABA	BP-1	EHMC	4-MBC
Ung Kong	Coral Tissue (ng/g ww)	*FA*	8.0	5.6	1.6	<MDL	<MDL	<MDL	<MDL
			10.5	4.5	1.5	<MDL	<MDL	<MDL	<MDL
			14.3	7.0	2.1	<MDL	<MDL	<MDL	<MDL
		P	22.7	16.7	6.3	17.1	21.1	<MDL	<MDL
			12.8	6.5	2.9	11.0	10.9	<MDL	<MDL
			10.6	8.6	2.9	6.0	8.6	<MDL	<MDL
		PD	2.8	7.6	<MDL	<MDL	<MDL	<MDL	<MDL
			2.3	3.3	<MDL	<MDL	<MDL	<MDL	<MDL
			5.1	3.2	<MDL	<MDL	<MDL	<MDL	<MDL
	Water (ng/L)	-	26.1	<MDL	13.1	15.2	<MDL	<MDL	<MDL
			25.5	<MDL	13.2	15.1	<MDL	<MDL	<MDL
	Sediment (ng/g dw)	-	6.1	<MDL	2.2	3.4	<MDL	<MDL	<MDL
			6.1	<MDL	2.0	3.4	<MDL	<MDL	<MDL
Wu Pai	Coral Tissue (ng/g ww)	*FA*	16.8	17.3	3.2	<MDL	<MDL	<MDL	<MDL
			14.1	17.7	4.3	<MDL	<MDL	<MDL	<MDL
			21.8	15.9	2.0	<MDL	<MDL	<MDL	<MDL
		P	9.4	9.9	<MDL	<MDL	<MDL	<MDL	<MDL
			15.7	13.3	<MDL	<MDL	<MDL	<MDL	<MDL
			10.2	7.7	<MDL	<MDL	<MDL	<MDL	<MDL
		PD	16.7	9.2	<MDL	<MDL	<MDL	<MDL	<MDL
			15.3	12.4	<MDL	<MDL	<MDL	<MDL	<MDL
			9.5	7.0	<MDL	<MDL	<MDL	<MDL	<MDL
	Water (ng/L)	-	14.0	<MDL	11.9	13.2	<MDL	<MDL	<MDL
			13.9	<MDL	11.8	13.2	<MDL	<MDL	<MDL
	Sediment (ng/g dw)	-	9.9	<MDL	2.6	4.3	<MDL	<MDL	<MDL
			9.7	<MDL	2.5	4.5	<MDL	<MDL	<MDL
Sharp Island	Coral Tissue (ng/g ww)	*FA*	16.8	15.4	3.1	3.9	<MDL	<MDL	<MDL
			14.1	8.1	4.8	2.1	<MDL	<MDL	<MDL
			21.8	17.7	4.9	7.3	<MDL	<MDL	<MDL
		P	38.4	12.5	7.0	13.9	<MDL	<MDL	<MDL
			35.0	15.1	6.2	14.8	<MDL	<MDL	<MDL
			22.1	7.4	6.6	8.4	<MDL	<MDL	<MDL
		PD	16.0	6.8	<MDL	<MDL	<MDL	<MDL	<MDL

			26.6	15.3	<MDL	<MDL	<MDL	<MDL	<MDL
			13.9	5.0	<MDL	<MDL	<MDL	<MDL	<MDL
	Water (ng/L)	-	23.2	<MDL	9.8	22.7	<MDL	<MDL	<MDL
			25.6	<MDL	9.6	22.6	<MDL	<MDL	<MDL
	Sediment (ng/g dw)	-	6.6	<MDL	2.7	4.9	<MDL	<MDL	<MDL
			6.5	<MDL	2.7	4.9	<MDL	<MDL	<MDL
Sung Kong	Coral Tissue (ng/g ww)	*FA*	10.7	4.0	2.6	2.6	<MDL	<MDL	<MDL
			11.2	5.2	1.8	2.5	<MDL	<MDL	<MDL
			9.5	2.3	1.9	3.4	<MDL	<MDL	<MDL
		P	24.2	19.9	8.7	8.4	16.5	<MDL	<MDL
			11.3	8.7	6.5	4.4	11.9	<MDL	<MDL
			20.3	19.4	8.5	14.7	22.5	<MDL	<MDL
		PD	10.2	13.3	<MDL	<MDL	<MDL	<MDL	<MDL
			3.9	4.7	<MDL	<MDL	<MDL	<MDL	<MDL
			16.4	14.2	<MDL	<MDL	<MDL	<MDL	<MDL
	Water (ng/L)	-	13.5	<MDL	9.0	14.8	<MDL	<MDL	<MDL
			12.9	<MDL	8.7	14.9	<MDL	<MDL	<MDL
	Sediment (ng/g dw)	-	8.0	<MDL	3.1	8.0	<MDL	<MDL	<MDL
			9.0	<MDL	3.0	8.0	<MDL	<MDL	<MDL

Dry Season

Location	Sample Matrices	Species	BP-3	BP-8	OC	ODPABA	BP-1	EHMC	4-MBC
Ung Kong	Coral Tissue (ng/g ww)	*AV*	9.9	17.2	<MDL	<MDL	<MDL	<MDL	<MDL
			12.3	32.2	<MDL	<MDL	<MDL	<MDL	<MDL
		P	14.7	10.5	<MDL	<MDL	<MDL	<MDL	<MDL
			7.3	13.1	<MDL	<MDL	<MDL	<MDL	<MDL
			5.6	7.8	<MDL	<MDL	<MDL	<MDL	<MDL
		PA	4.2	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			1.0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			5.7	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
		PD	2.1	2.6	<MDL	<MDL	<MDL	<MDL	<MDL
			7.8	4.9	<MDL	<MDL	<MDL	<MDL	<MDL
			5.8	7.9	<MDL	<MDL	<MDL	<MDL	<MDL
	Water (ng/L)	-	28.9	<MDL	14.2	<MDL	<MDL	<MDL	<MDL
			29.2	<MDL	14.1	<MDL	<MDL	<MDL	<MDL

	Sediment (ng/g dw)	-	3.4	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			4.9	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Wu Pai	Coral Tissue (ng/g ww)	*P*	11.1	11.3	<MDL	<MDL	<MDL	<MDL	<MDL
			10.3	13.9	<MDL	<MDL	<MDL	<MDL	<MDL
			11.3	18.9	<MDL	<MDL	<MDL	<MDL	<MDL
		PA	6.1	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			4.8	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			5.3	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
	Water (ng/L)	-	13.7	<MDL	10.8	<MDL	<MDL	<MDL	<MDL
			13.8	<MDL	10.7	<MDL	<MDL	<MDL	<MDL
	Sediment (ng/g dw)	-	16.9	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			17.1	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
Sharp Island	Coral Tissue (ng/g ww)	*P*	14.0	12.9	<MDL	<MDL	<MDL	<MDL	<MDL
			4.7	7.5	<MDL	<MDL	<MDL	<MDL	<MDL
			7.1	4.4	<MDL	<MDL	<MDL	<MDL	<MDL
		PA	2.2	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			6.0	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			4.2	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
		PD	1.7	1.3	<MDL	<MDL	<MDL	<MDL	<MDL
			5.6	4.6	<MDL	<MDL	<MDL	<MDL	<MDL
			1.0	1.4	<MDL	<MDL	<MDL	<MDL	<MDL
	Water (ng/L)	-	31.5	<MDL	13.2	<MDL	<MDL	<MDL	<MDL
			31.9	<MDL	13.2	<MDL	<MDL	<MDL	<MDL
	Sediment (ng/g dw)	-	8.1	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL
			8.1	<MDL	<MDL	<MDL	<MDL	<MDL	<MDL

<MDL: below method detection limit; ww: wet weight; dw: dry weight; *PA*: *Platygyra acuta*; *P*: *Porites sp.*; *PD*: *Pavona decussata*; *AV*: *Acropora valida*; *F*A: *Favites abdita*. Moisture content is 90% for coral samples.

Table S6. Ecotoxicological information of UV filters for coral species used in the environmental risk assessment

Compounds	Test organisms	Species	Toxicity endpoints	Measurement endpoint	Exposure time	Conc. (μg/L)	Reference
BP-3	Coral planula	*Stylophora pistillata*	Mortality	LC50	24 hr	139	Downs et al., 2015
	Coral planula	*Stylophora pistillata*	Deformity	EC50	24 hr	49	Downs et al., 2015
	Hard coral	*Acropora sp.*	Bleaching	Bleaching rate		2376	Danovaro et al., 2008
	Hard coral	*A.pulchra*	Bleaching	Bleaching rate		3600	Danovaro et al., 2008

Table S7. Worst-case and best-case PNECs used in the probabilistic risk assessment

Worst-case scenario	**(Minimum BAF was used for threshold values calculation)**		
Toxicity threshold	Species	Toxicity endpoints	Log_{10}(PNECs) ng/g ww
C_1	*Stylophora pistillata*	Deformity	0.88
C_2	*Stylophora pistillata*	Mortality	1.33
C_3	*Acropora sp.*	Bleaching	2.56
C_4	*A.pulchra*	Bleaching	2.74

Best-case scenario	**(Maximum BAF was used for threshold values calculation)**		
Toxicity threshold	Species	Toxicity endpoints	Log_{10}(PNECs) ng/g ww
C_5	*Stylophora pistillata*	Deformity	1.71
C_6	*Stylophora pistillata*	Mortality	2.16
C_7	*Acropora sp.*	Bleaching	3.40
C_8	*A.pulchra*	Bleaching	3.58

Table S8. Regression coefficients of probabilistic risk assessment of BP-3 in coral tissues samples in Hong Kong dry and wet seasons.

		(y=mx + c)		
		m	**c**	**r^2**
BP-3				
	Hong Kong (Dry season)	1.23	1.69	0.97
	Hong Kong (Wet season)	1.78	1.58	0.89

Figure S1. Map of coral ecosystem sampling locations in Hong Kong.

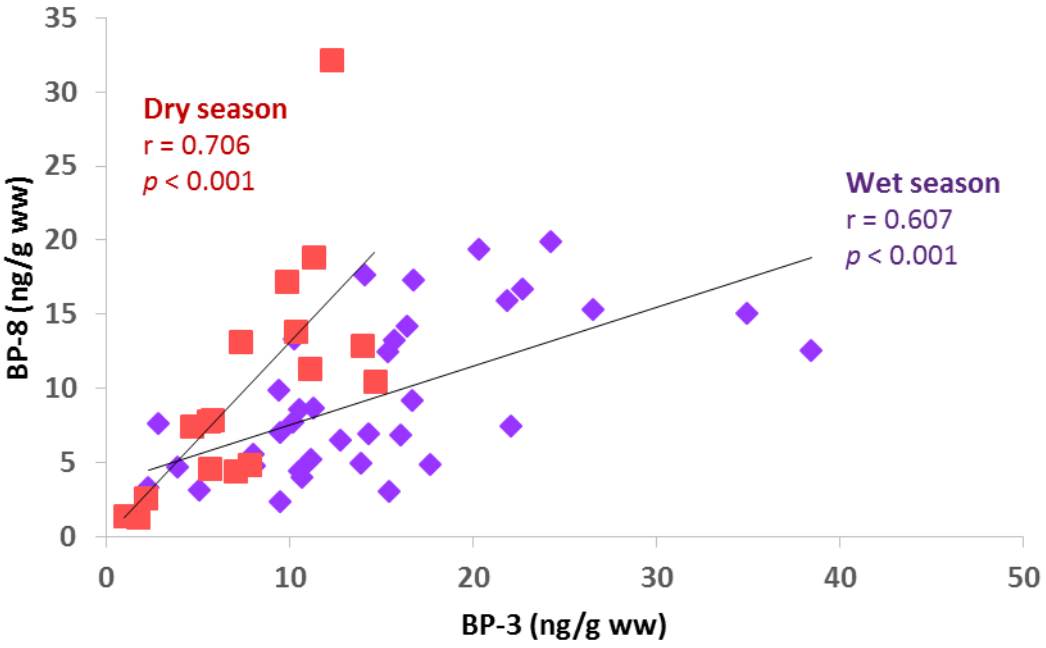


Figure S2. Correlation between coral tissues concentrations of BP-3 and BP-8 in dry and wet seasons.

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