TITLE: Flame retardants and plastic additives in San Francisco Bay: a targeted monitoring of organophosphate esters and bisphenols

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Materials and Methods – Additional Information

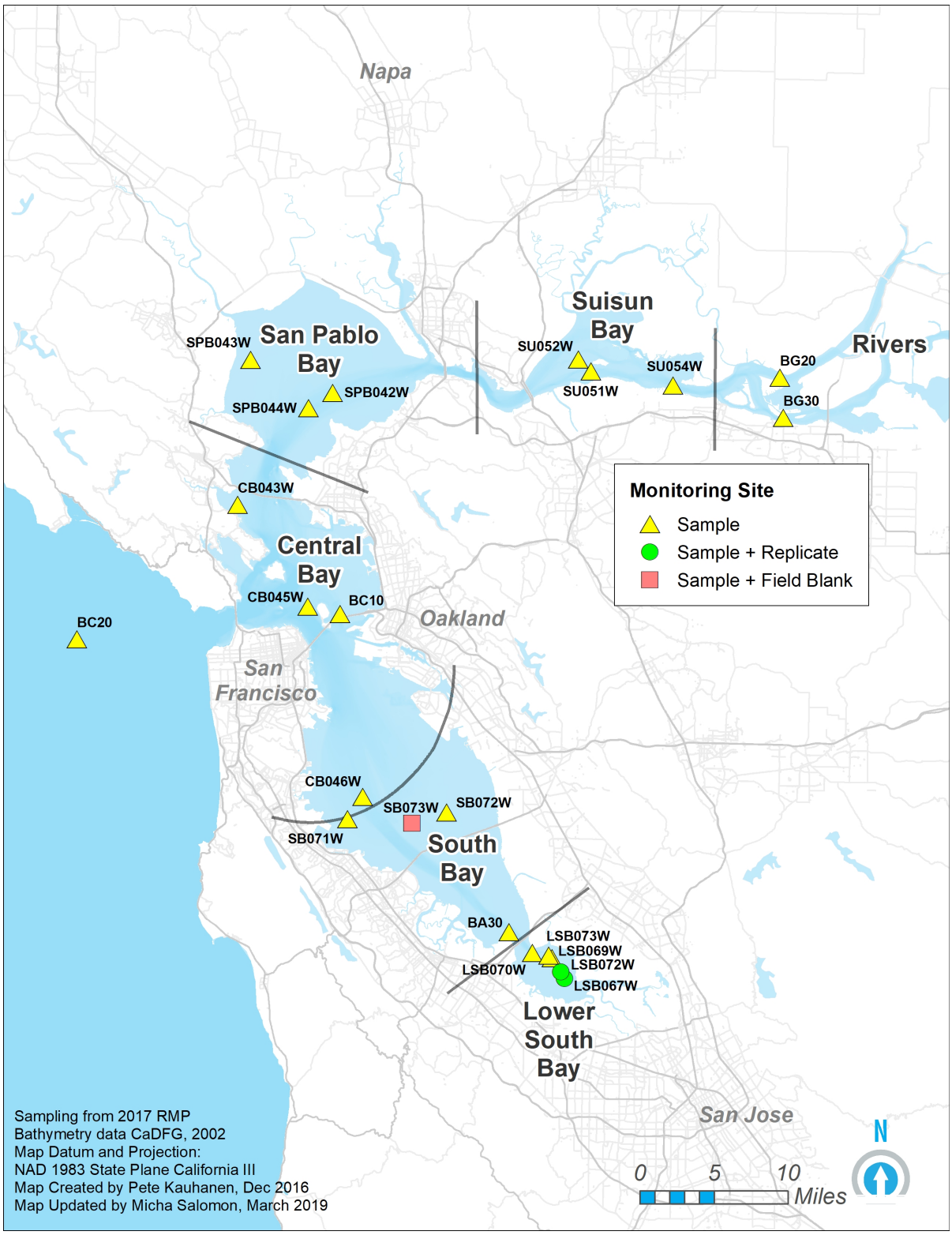

Figure S1. Map of San Francisco Bay water sampling sites.

Table S1. Flame retardant and plastic additive target analytes.

Abbreviation	Compound	CAS No.	Surrogate Standard
Organophosphate Esters			
V6	Tetrakis(2-chloroethyl) dichloroisopentyl diphosphate	38051-10-4	d_{15}-TDCPP
TCEP	Tris(2-chloroethyl) phosphate	115-96-8	d_{12}-TCEP
TCPP	Tris(1-chloro-2-propyl) phosphate	13674-84-5	d_{15}-TDCPP
TDCPP	Tris(1,3-dichloro-2-propyl) phosphate	13674-87-8	d_{15}-TDCPP
TDBPP	Tris(2,3-dibromopropyl) phosphate	126-72-7	d_{15}-TPhP
BPA-BDPP	Bisphenol A bis(diphenyl phosphate)	5945-33-5	d_{15}-TPhP
RBDPP	Resorcinol bis(diphenyl phosphate)	57583-54-7	d_{15}-TPhP
T2iPPP	Tris(2-isopropylphenyl) phosphate	64532-95-2	d_{15}-TPhP
T35DMPP	Tris(3,5-dimethylphenyl) phosphate	25653-16-1	d_{15}-TPhP
BPDPP	Tertbutylphenyl diphenyl phosphate	56803-37-3	d_{15}-TPhP
2iPPDPP	2-isopropylphenyl diphenyl phosphate	64532-94-1	d_{15}-TPhP
CrDPP	Cresyl diphenyl phosphate	5254-12-6	d_{15}-TPhP
TCrP	Tricresyl phosphate	1330-78-5	M_6-TBEP[a]
IDDPP	Isodecyl diphenyl phosphate	29761-21-5	d_{15}-TPhP
EHDPP	2-Ethylhexyl-diphenyl phosphate	1241-94-7	M_6-TBEP[a]
TPhP	Triphenyl phosphate	115-86-6	d_{15}-TPhP
TBEP	Tris(2-butoxyethyl) phosphate	78-51-3	M_6-TBEP[a]
TEHP	Tris(2-ethylhexyl) phosphate	78-42-2	M_6-TBEP[a]
TiBP	Triisobutyl phosphate	126-71-6	d_{27}-TnBP
TPrP	Tripropyl phosphate	513-08-6	d_{15}-TDCPP
TnBP	Tri-n-butyl phosphate	126-73-8	d_{27}-TnBP
TEP	Triethyl phosphate	78-40-0	d_{15}-TEP
Bisphenols			
BPA	Bisphenol A	80-05-7	d_6-BPA
BPAF	Bisphenol AF	1478-61-1	d_6-BPA
BPAP	Bisphenol AP	1571-75-1	d_6-BPA
BPB	Bisphenol B	77-40-7	d_6-BPA
BPBP	Bisphenol BP	1844-01-5	d_6-BPA
BPC	Bisphenol C	79-97-0	d_6-BPA
BPC-dichloride	Bisphenol C-dichloride	14868-03-2	d_6-BPA
BPE	Bisphenol E	2081-08-5	d_6-BPA
BPF	Bisphenol F	620-92-8	d_6-BPA
BPG	Bisphenol G	127-54-8	d_6-BPA
BPM	Bisphenol M	13595-25-0	d_6-BPA
BPP	Bisphenol P	2167-51-3	d_6-BPA
BPPH	Bisphenol PH	24038-68-4	d_6-BPA
BPS	Bisphenol S	80-09-1	d_8-BPS
BP-TMC	Bisphenol TMC	129188-99-4	d_6-BPA
BPZ	Bisphenol Z	843-55-0	d_6-BPA

[a] M6-TBEP: tris(2-butoxy-[$^{13}C_2$]-ethyl) phosphate

Ambient Water Sample Collection – Additional Information
The field blank sample was collected on site at SB073W by pouring 4 L of HPLC gradient grade water (ACROS Organics™) into a 4 L amber glass jug while wearing nitrile gloves.

Standards and Reagents
We screened for 22 organophosphate esters (OPEs) as well as 16 bisphenols. Reference standards for OPEs were purchased from AccuStandard or Wellington Laboratories. Reference standards for bisphenols were purchased from AccuStandard. Surrogate and internal standards (Table S1), including $^{13}C_{18}$-TPhP, d_{15}-TPhP, d_{12}-TCEP, d_{15}-TDCPP, d_{27}-TnBP, tris(2-butoxy-[$^{13}C_2$]-ethyl) phosphate (M_6-TBEP), D_{15}-TEP, d_{16}-BPA, d_6-BPA, and d_8-BPS, were purchased from Wellington or Cambridge Isotope Laboratories (Andover, MA). High performance liquid chromatography (HPLC) grade solvents were purchased from Fisher Scientific (Hanover Park, IL).

Detailed Analytical Methods
Upon receipt at the analytical lab, samples were filtered through a 0.45-µm Whatman filter for analysis of total suspended solids (TSS) and dissolved and particulate-associated phases. Filtered water samples (approximately 1000 mL) were adjusted to approximately pH 3, spiked with surrogate standards (including d_{27}-TnBP, d_{12}-TCEP, d_{15}-TDCPP, d_{15}-TEP, d_{15}-TPhP, M_6-TBEP, d_{16}-BPA, d_8-BPS), and treated via liquid-liquid extraction with dichloromethane (DCM) three times (50, 25, and 25 mL each). The water-DCM mixture was hand shaken for approximately 15 minutes during each extraction. The extracts were combined, concentrated, and divided into two halves. One half was concentrated to near dryness under gentle nitrogen flow, re-constituted with 200 µL methanol, and then spiked with internal standard d_6-BPA prior to instrumental analysis for bisphenol analogues. The other half was cleaned through a solid phase extraction (SPE) cartridge packed with 1 g of ammonium silica (Biotage, Charlotte, NC), which was pre-cleaned with 15 mL each of methanol, DCM, and hexane (HEX) in sequence. After sample loading, the SPE cartridge was cleaned with a 2 mL mixture of HEX:DCM (20:80, v/v), and target analytes were then eluted out with 4 mL of 20:80 (v/v) HEX:DCM and 8 mL of DCM. The final extract (approximately 200 µL) was spiked with an internal standard ($^{13}C_{18}$-TPhP) for the determination of OPEs. The determination of bisphenols and OPEs were conducted based on a highly sensitive liquid chromatography-electrospray ionization-triple quadrupole mass spectrometer (LC-ESI-QQQ-MS/MS).

Dried solid phase portions of the water samples (on the filter) were spiked with surrogate standards and extracted with 5 mL of a mixture of hexane and dichloromethane (1:1, v/v) under ultrasonication for 5 minutes. After centrifugation, the supernatant was transferred to a new glass tube. The extraction was repeated twice and the extracts were combined, concentrated, and then divided into two halves. One half was concentrated to near dryness under gentle nitrogen flow, re-constituted with 200 µL methanol, and spiked with internal standard d_6-BPA. The other half was cleaned through an ammonium silica cartridge, following the same SPE method used for the analysis of OPEs in the aqueous phase.

A total of 38 flame retardants and plastic additives were determined on a Shimadzu HPLC coupled to an AB Sciex Q Trap 5500 MS equipped with a TurboIonSpray® electrospray ionization (ESI) probe. The MRM ion pairs of target analytes, as well as the detailed LC programs, are summarized in Table S2.

Table S2. Liquid chromatography mass spectrometer multiple reaction monitoring (MRM) ions and method limits of detection (MDLs) of individual flame retardants and plastic additives.

Abbreviation	Full Name	MRM Pairs (m/z)	MDL (aq.)	MDL (solid)
			ng/L	ng/g dw
Organophosphate Esters (OPEs)				
V6	Tetrakis(2-chloroethyl)dichloroisopentyl diphosphate	582.9 → 99.1 582.9 → 65.1	1.2	2.2
TCEP	Tris(2-chloroethyl)phosphate	288.2 → 73.0 288.2 → 242	0.4	0.5
TCPP	Tris(1-chloro-2-propyl)phosphate	331 → 99 331 → 279	0.4	0.6
TDCPP	Tris(1,3-dichloro-2-propyl) phosphate	430 → 73 430 → 341.9	0.4	0.8
TDBPP	Tris(2,3-dibromopropyl) phosphate	697.4 → 360.3 697.4 → 466.9	0.8	2
BPA-BDPP	Bisphenol A bis(diphenyl phosphate)	693 → 367.2 693 → 178.2	0.5	1
RBDPP	Resorcinol bis(diphenyl phosphate)	575 → 152.2 575 → 77.1	0.6	1.2
T2iPPP	Tris(2-isopropylphenyl)phosphate	451 → 73.1 451 → 229.1	0.4	0.8
T35DMPP	Tris(3,5-dimethylphenyl)phosphate	411.1 → 179.1 411.1 → 76.9	0.4	0.7
BPDPP	Tertbutylphenyl diphenyl phosphate	382.9 → 321.1 382.9 → 77.1	0.6	1.1
2iPPDPP	2-isopropylphenyl diphenyl phosphate	391 → 251.1 391 → 77.1	0.4	0.8
CrDPP	Cresyl diphenyl phosphate	340.9 → 151.9 340.9 → 91.1	0.5	0.9
TCrP	Tricresyl Phosphate	371 → 185 371 → 239	0.4	1.2
IDDPP	Isodecyl diphenyl phosphate	363.2 → 250.9 363.2 → 76.9	0.5	0.9

EHDPP	2-Ethylhexyl-diphenyl phosphate	363.2 → 250.9	0.4	1.1
		363.2 → 76.9		
TPhP	Triphenyl phosphate	327 → 77	0.4	0.8
		327 → 215		
TBEP	Tris(2-butoxyethyl)phosphate	399.1 → 199	0.5	0.9
		399.1 → 299.1		
TEHP	Tris(2-ethylhexyl) phosphate	436.9 → 207	0.4	0.8
		436.9 → 215.1		
TiBP	Triisobutyl Phosphate	267.1 → 81	0.2	0.5
		267.1 → 99		
TPrP	Tripropyl Phosphate	225 → 81	0.4	0.6
		225 → 99		
TnBP	Tri-n-butyl phosphate	267.1 → 81	0.2	0.5
		267.1 → 99		
TEP	Triethyl Phosphate	183.1 → 81	0.2	0.4
		183.1 → 98.9		
Bisphenols				
BPA	Bisphenol A	227.0 → 133.0	0.7	1.1
BPAF	Bisphenol AF	334.9 → 265.1	0.8	1.5
BPAP	Bisphenol AP	289.0 → 194.9	0.7	1.5
BPB	Bisphenol B	241.0 → 211.1	0.8	1.4
BPBP	Bisphenol BP	351.0 → 273.0	0.8	1.5
BPC	Bisphenol C	255.0 → 147.1	0.7	1.1
BPC-dichloride	Bisphenol C-dichloride	278.9 → 70.9	0.9	1.6
BPE	Bisphenol E	213.0 → 119.0	0.8	1.2
BPF	Bisphenol F	199.0 → 93.0	0.8	1.2
BPG	Bisphenol G	311.0 → 175.3	1	1.8
BPM	Bisphenol M	345.1 → 133.0	0.9	1.6
BPP	Bisphenol P	345.2 → 133.3	1	2
BPPH	Bisphenol PH	378.9 → 208.9	0.7	1.3
BPS	Bisphenol S	248.9 → 108.1	1	1.8
BP-TMC	Bisphenol TMC	309.2 → 215.2	1.1	2
BPZ	Bisphenol Z	267.1 → 172.8	1.4	2.7

Table S3. Average relative standard deviations for field replicate grab sample recoveries for semi-quantitative analytes. Two field duplicates were collected for each analyte.

Fraction	Analyte	Average RSD
Dissolved	Triisobutyl phosphate	141%
Dissolved	Triphenyl phosphate	103%
Dissolved	Tris(1,3-dichloro-2-propyl) phosphate	141%
Dissolved	Tris(1-chloro-2-propyl) phosphate	109%
Dissolved	Tris(2-butoxyethyl) phosphate	135%
Particulate	Tris(2-butoxyethyl) phosphate	141%
Dissolved	Tris(2-chloroethyl) phosphate	127%
Dissolved	Bisphenol F	121%
Dissolved	Bisphenol S	124%

Results and Discussion – Additional Information

Table S4. Ambient Bay dissolved water flame retardant and plastic additive concentrations by site (ng/L).

Site ID	Field Blank	LSB067W[d]	LSB069W	LSB070W	LSB072W[d]	LSB073W	BA30	SB071W	SB072W	SB073W	BC10	BC20	CB043W	CB045W	CB046W	SPB042W	SPB043W	SPB044W	SU051W	SU052W	SU054W	BG20	BG30
Embayment		LSB	LSB	LSB	LSB	LSB	SB	SB	SB	SB	CB	CB	CB	CB	CB	SPB	SPB	SPB	SU	SU	SU	RIV	RIV
TSS (mg/L)	0	61	115	56	108	50	46	54	47	46	45	62	76	65	51	52	132	41	52	30	25	9	12
Organophosphate esters																							
V6	nd	2.0	1.9	2.1	1.0	1.9	2.0	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2
TCEP	nd	17	18	15	19	16	18	4.3	5.3	3.8	3.0	7.8	3.7	4.1	5.5	3.8	5.0	3.5	5.7	6.1	4.0	4.3	4.0
TCPP	0.7	150	140	130	120	140	130	48	66	69	30	11	15	26	74	18	20	26	38	26	24	19	23
TDCPP	nd	22[a]	18[a]	19[a]	15[a]	21	20[a]	5.2	6.0	5.0	3.7	8.8	4.0[a]	4.0	6.4	2.8[a]	4.0[a]	4.2	10	10	11	6.0[a]	9.4[a]
TDBPP	nd	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPA-BDPP	nd	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5
RBDPP	nd	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6
T2iPPP	nd	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
T35DMPP	nd	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
BPDPP	nd	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	0.7	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6
2iPPDPP	nd	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
CrDPP	nd	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5
TCrP	nd	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
IDDPP	nd	<0.5	<0.5	<0.5	<0.5	1.7	1.2	0.9	1.6	0.9	0.8	4.8	<0.5	1.2	1.3	<0.5	<0.5	<0.5	2.3	<0.5	<0.5	<0.5	0.8
EHDPP	nd	<0.4	<0.4	<0.4	<0.4	0.6	5.6	0.8	0.8	1.3	<0.4	0.5	<0.4	<0.4	0.5	<0.4	<0.4	<0.4	0.7	<0.4	<0.4	<0.4	0.7
TPhP	nd	8.8[b]	<0.4[a]	<0.4[a]	8.3[a,b]	18[b]	15[b]	4.9[b]	2.2[a]	4.0[b]	5.8[b]	52[b]	<0.4[a]	12[b]	3.6[b]	0.7[a]	<0.4[a]	4.6[b]	10[b]	3.9[b]	3.0[b]	2.1[a]	7.4[b]
TBEP	nd	61	1.9	0.9	62	2.0	1.6	<0.5	1.1	<0.5	0.6	21	1.8	<0.5	<0.5	0.7	1.0	0.9	2.8	5.4	10	18	8.0
TEHP	nd	<0.4	<0.4	<0.4	<0.4	1.0	0.5	0.9	0.6	0.9	0.5	<0.4	<0.4	0.6	0.6	<0.4	<0.4	<0.4	0.7	<0.4	<0.4	<0.4	<0.4
TiBP	nd	1.1	1.7	1.5	1.1	1.8	2.4	2.0	1.7	1.6	1.0	0.7	0.7	0.8	2.1	0.8	0.8	0.8	0.9	0.8	0.6	0.7	0.7
TPrP	nd	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
TnBP	nd	13	8.5	9.9	14	9.1	13	4.8	7.6	6.6	11	1.1	4.8	3.8	8.1	2.3	2.8	2.1	3.0	4.9	4.9	8.9	2.5
TEP	nd	20	19	18	21	16	17	4.5	5.8	5.3	3.8	2.1	6.5	3.7	5.8	5.7	6.9	4.1	6.5	6.6	6.3	5.6	3.6
ΣOPEs		290	210	190	260	230	220	76	98	99	60	110	37	56	110	34	41	46	81	63	64	65	60

Bisphenols																							
BPA	2.7	0.7	<0.7	<0.7	2.8	4.1	<0.7	<0.7	2.9	3.0	8.8	3.5	2.1	1.9	1.5	<0.7	0.8	2.0	2.8	1.2	1.9	1.8	3.6
BPAF	nd	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPAP	nd	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
BPB	nd	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPBP	nd	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPC	nd	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
BPC-dichloride	nd	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9
BPE	nd	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPF[c]	89	4.7	<0.8	85	26	41	<0.8	81	<0.8	<0.8	19	14	24	6.9	<0.8	9.5	41	2.9	150	1.0	29	12	18
BPG	nd	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
BPM	nd	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9
BPP	nd	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
BPPH	nd	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
BPS	nd	4.9	<1	<1	30	14	<1	<1	<1	8.9	<1	<1	<1	<1	<1	120	5.6	4.9	<1	<1	2.9	<1	<1
BP-TMC	nd	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1
BPZ	nd	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4
ΣBisphenols		10	0	85	59	59	0	81	3	12	28	17	26	9	1	130	48	10	150	2	33	14	22

[a] Data qualified - analyte detected in lab-generated blank, flagged by quality-assurance officer.
[b] Data rejected - analyte detected in lab-generated blank at levels higher than 3x the standard deviation of averaged lab-blank contamination levels.
[c] All data censored due to field blank contamination
[d] Data are averaged across field sample and field replicate

Table S5. Ambient Bay particulate water flame retardant and plastic additive concentrations by site (ng/g dw).

Site ID	**Field Blank**	**LSB067W[a]**	**LSB069W**	**LSB070W**	**LSB072W[a]**	**LSB073W**	**BA30**	**SB071W**	**SB072W**	**SB073W**	**BC10**	**BC20**	**CB043W**	**CB045W**	**CB046W**	**SPB042W**	**SPB043W**	**SPB044W**	**SU051W**	**SU052W**	**SU054W**	**BG20**	**BG30**
Embayment		LSB	LSB	LSB	LSB	LSB	SB	SB	SB	SB	CB	CB	CB	CB	CB	SPB	SPB	SPB	SU	SU	SU	RIV	RIV
TSS (mg/L)	0	61	115	56	108	50	46	54	47	46	45	62	76	65	51	52	132	41	52	30	25	9	12
Organophosphate esters																							
V6	nd	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2	<2.2
TCEP	nd	<0.5	<0.5	<0.5	<0.5	<0.5	19	<0.5	<0.5	<0.5	45	20	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	120	34
TCPP	nd	17	11	<0.6	16	210	160	110	18	300	260	230	<0.6	140	87	1.7	<0.6	220	95	<0.6	<0.6	48	170
TDCPP	nd	5.0	<0.8	<0.8	9.0	42	14	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
TDBPP	nd	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2
BPA-BDPP	nd	<1	<1	<1	<1	<1	6.2	<1	<1	8.1	14.9	<1	<1	<1	2.1	<1	<1	11	<1	<1	<1	8.9	<1
RBDPP	nd	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2
T2iPPP	nd	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
T35DMPP	nd	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
BPDPP	nd	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1
2iPPDPP	nd	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	6.1	<0.8	<0.8	<0.8	<0.8	1.1	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
CrDPP	nd	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9
TCrP	nd	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2
IDDPP	nd	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9
EHDPP	nd	<1.1	<1.1	<1.1	<1.1	9.0	<1.1	<1.1	25.5	<1.1	<1.1	<1.1	<1.1	<1.1	100	<1.1	<1.1	<1.1	140	<1.1	<1.1	<1.1	<1.1
TPhP	nd	0.4	<0.8	<0.8	<0.8	150	100	44	51	160	170	170	<0.8	91	100	2.1	<0.8	110	140	<0.8	<0.8	1.7	180
TBEP	nd	11	6.3	<0.9	12	280	630	21	5.9	82	250	210	<0.9	330	8.6	7.2	2.3	440	78	11	27	99	36
TEHP	nd	4.8	1.1	1.1	4.4	150	90	45	50	130	150	110	1.9	60	52	2.3	1.3	130	120	6.9	14	28	96
TiBP	nd	2.3	1.6	2.9	2.9	1.8	2.5	1.9	2.4	<0.5	<0.5	<0.5	1.4	2.7	2.0	1.9	<0.5	5.2	<0.5	4.3	5.5	<0.5	<0.5
TPrP	nd	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6
TnBP	nd	9.1	7.6	17	14	29	25	18	13	43	26	30	4.2	16	14	7.2	<0.5	28	8.4	16	15	39	29
TEP	nd	3.0	3.1	1.3	1.7	38	25	15	12	46	55	36	1.5	28	22	2.1	<0.4	48	28	7.3	5.8	34	46
ΣOPEs		53	31	22	60	900	1100	260	180	770	960	800	9	670	390	25	4	990	610	45	67	380	590

Bisphenols																							
BPA	nd	180	51	340	150	630	<1.1	<1.1	<1.1	63	<1.1	<1.1	320	<1.1	<1.1	270	100	<1.1	39	600	560	2300	2100
BPAF	nd	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5
BPAP	nd	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5
BPB	nd	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4
BPBP	nd	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5	<1.5
BPC	nd	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1
BPC-dichloride	nd	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6
BPE	nd	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2
BPF[a]	nd	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	120	23	<1.2	<1.2	<1.2	<1.2	<1.2	140	190	<1.2	230	<1.2	<1.2
BPG	nd	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8
BPM	nd	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6	<1.6
BPP	nd	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2
BPPH	nd	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3	<1.3
BPS	nd	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	<1.8	38	13	<1.8	<1.8
BP-TMC	nd	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2	<2
BPZ	nd	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7	<2.7
ΣBisphenols		180	51	340	150	630	0	0	0	63	120	23	320	0	0	270	100	140	220	640	800	2300	2100

[a] Data are averaged across field sample and field replicate

Table S6. Ambient Bay total water flame retardant and plastic additive concentrations by site (ng/L). Concentrations include both dissolved and solid-phase contributions.

Site ID	**LSB067W[b]**	**LSB069W**	**LSB070W**	**LSB072W[b]**	**LSB073W**	**BA30**	**SB071W**	**SB072W**	**SB073W**	**BC10**	**BC20**	**CB043W**	**CB045W**	**CB046W**	**SPB042W**	**SPB043W**	**SPB044W**	**SU051W**	**SU052W**	**SU054W**	**BG20**	**BG30**
Embayment	LSB	LSB	LSB	LSB	LSB	SB	SB	SB	SB	CB	CB	CB	CB	CB	SPB	SPB	SPB	SU	SU	SU	RIV	RIV
TSS (mg/L)	0	61	115	56	108	50	46	54	47	46	45	62	76	65	51	52	132	41	52	30	25	9
Organophosphate Esters																						
V6	2.0	1.9	2.1	1.0	1.9	2.0	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2	<1.2
TCEP	17	18	15	19	16	19	4.3	5.3	3.8	5.0	9.0	3.7	4.1	5.5	3.8	5.0	3.5	5.7	6.1	4.0	5.3	4.5
TCPP	150	140	130	120	150	140	54	67	83	41	26	15	35	79	18	20	35	43	26	24	19	25
TDCPP	22	18	19	16	23	20	5.2	6.0	5.0	3.7	8.8	4.0	4.0	6.4	2.8	4.0	4.2	10	10	11	6.0	9.4
TDBPP	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPA-BDPP	<0.5	<0.5	<0.5	<0.5	<0.5	0.3	<0.5	<0.5	0.4	0.7	<0.5	<0.5	<0.5	0.1	<0.5	<0.5	0.5	<0.5	<0.5	<0.5	0.1	<0.5
RBDPP	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6
T2iPPP	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
T35DMPP	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
BPDPP	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	0.7	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6	<0.6
2iPPDPP	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	0.3	<0.4	<0.4	<0.4	<0.4	0.1	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
CrDPP	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5	<0.5
TCrP	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
IDDPP	<0.5	<0.5	<0.5	<0.5	1.7	1.2	0.9	1.6	0.9	0.8	4.8	<0.5	1.2	1.3	<0.5	<0.5	<0.5	2.3	<0.5	<0.5	<0.5	0.8
EHDPP	<0.4	<0.4	<0.4	<0.4	1.0	5.6	0.8	2.0	1.3	<0.4	0.5	<0.4	<0.4	5.7	<0.4	<0.4	<0.4	8.1	<0.4	<0.4	<0.4	0.7
TPhP	8.9	<0.4	<0.4	8.3	25	19	7.2	2.4	11	13	63	<0.4	18	8.7	0.1	<0.4	9.3	17	3.9	3.0	0.0	9.5
TBEP	62	2.6	0.9	63	16	30	1.1	1.4	3.7	12	34	1.8	22	0.4	1.1	1.3	19	6.8	5.8	11	19	8.5
TEHP	0.3	0.1	0.1	0.5	8.3	4.7	3.3	2.9	6.7	7.2	6.7	0.1	4.5	3.2	0.1	0.2	5.2	6.8	0.2	0.4	0.2	1.2
TiBP	1.2	1.9	1.6	1.4	1.9	2.5	2.1	1.8	1.6	1.0	0.7	0.8	1.0	2.2	0.9	0.8	1.0	0.9	0.9	0.8	0.7	0.7
TPrP	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4	<0.4
TnBP	13	9.4	11	15	11	14	5.8	8.2	8.5	12	3.0	5.1	4.8	8.9	2.7	2.8	3.3	3.4	5.4	5.2	9.2	2.9
TEP	21	19	18	21	18	18	5.3	6.3	7.4	6.3	4.3	6.6	5.5	6.9	5.8	6.9	6.1	8.0	6.8	6.4	5.9	4.2
ΣOPEs	300	210	200	270	270	270	90	110	130	100	160	38	99	130	35	41	87	110	65	65	66	67

Bisphenols																						
BPA	11	5.9	19	19	35	<0.7	<0.7	2.9	5.9	8.8	3.5	27	1.9	1.5	14	14	2.0	4.8	19	16	22	29
BPAF	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPAP	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
BPB	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPBP	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPC	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
BPC-dichloride	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9
BPE	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8	<0.8
BPF[a]	4.7	<0.8	85	26	41	<0.8	81	<0.8	<0.8	25	15	24	6.9	<0.8	9.5	41	8.5	160	1.0	34	12	17
BPG	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
BPM	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9	<0.9
BPP	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1	<1
BPPH	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7	<0.7
BPS	4.9	<1	<1	30	14	<1	<1	<1	8.9	<1	<1	<1	<1	<1	120	5.6	4.9	<1	1.1	3.2	<1	<1
BP-TMC	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1	<1.1
BPZ	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4	<1.4
ΣBisphenols	21	6	100	75	90	0	81	3	15	33	19	50	9	1	140	61	15	160	21	54	34	47

[a] All data censored due to field blank contamination
[b] Data are averaged across field sample and field replicate

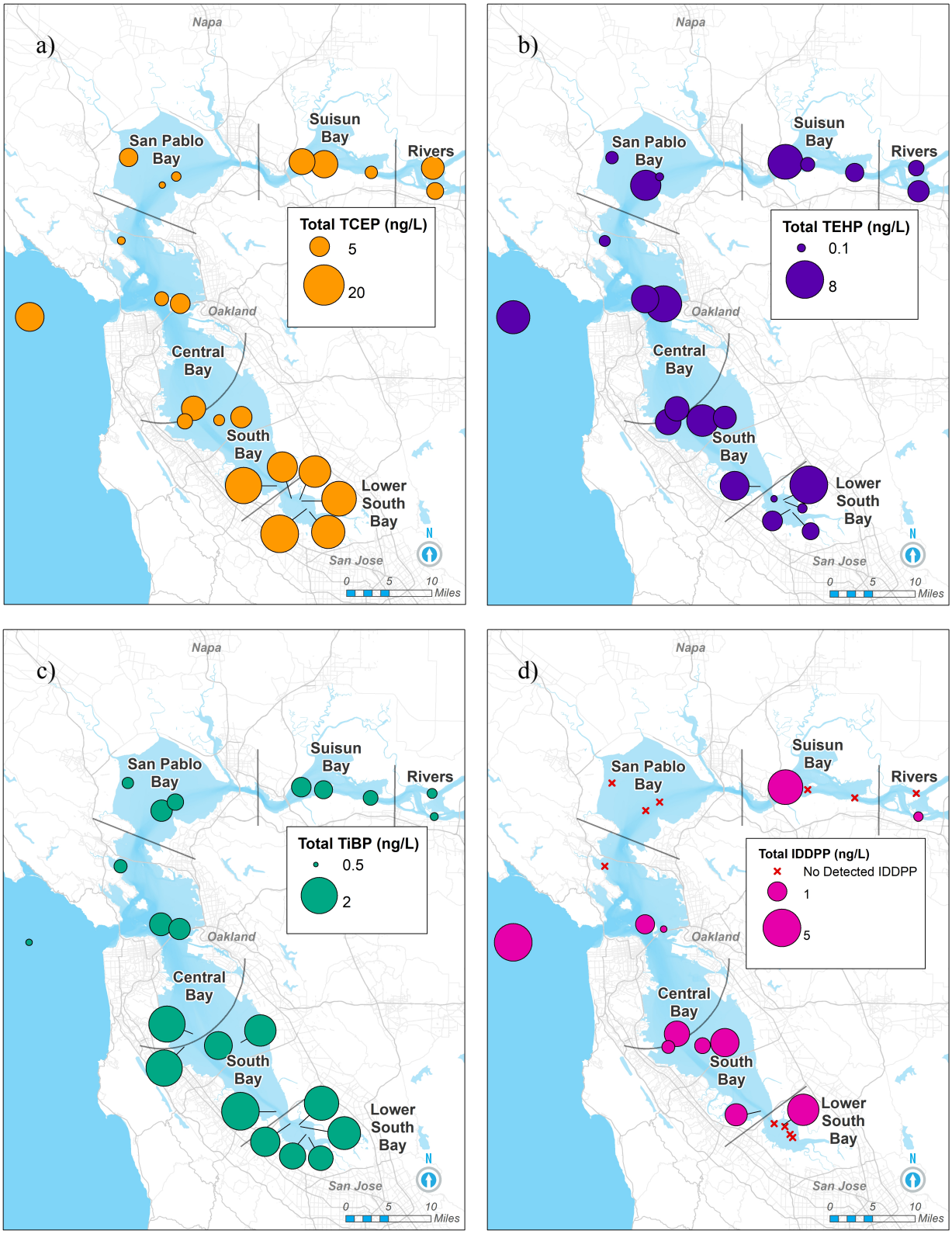

Figure S2. Concentrations of four remaining OPEs detected in at least 50% of Bay samples: TCEP (a), TEHP (b), TiBP (c), and IDDPP (d). The maximum concentration of each compound, and therefore the maximum size of the circle represented in each map, varies between figure.