OCCURRENCE OF PLASTICIZERS, BISPHENOLS, AND FLAME RETARDANTS IN POTABLE WATER IN CANADA AND SOUTH AFRICA

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Supplemental Information

Table S1- Concentrations of PBDEs in drinking water published prior to October 15, 2021. TW: Tap water, BW: Bottled water, DF: Detection frequency, NS: Not specified, <LOD(): Limit of detection, "-" compound not included in study.

Location (year published)	Water Type	Total # of samples	BDE-28		BDE-47		BDE-99		BDE-100		BDE-153		BDE-154		BDE-183		BDE-209	
			DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]
Argentina[1] (2009)	TW	1	-	-	0	<LOD (1.2)	0	<LOD (1.5)	0	<LOD (1.0)	0	<LOD (2.0)	-	-	-	-	-	-
U.S.A[2] (2015)	TW	27	33	0.5	81	0.84	81	0.81	81	0.33	33	0.05	52	0.11	15	0.36	0	<LOD (1.0)
Pakistan[3] (2016)	PW	39	41	<LOD (0.00003) – 0.00028	64	<LOD (0.00002) – 0.00059	56	<LOD (0.000017) – 0.0006	31	<LOD (0.00003) – 0.000082	44	<LOD (0.00003) – 0.00025	26	<LOD (0.00003) – 0.00058	51	<LOD (0.00003) – 0.0007	51	<LOD (0.000024) – 0.0007
China[4] (2019)	BW	NS	0	<LOD (0.0075)	0	<LOD (0.0058)	0	<LOD (0.0063)	0	<LOD (0.0099)	-	-	0	<LOD (0.0022)	-	-	-	-

Table S2 – Concentrations of Dechloranes in drinking water prior to October 15, 2021. TW: Tap water, DF: Detection frequency, <LOD(): Limit of detection.

Location (year published)	Water Type	Total # of samples	a-DP		s-DP	
			DF [%]	Conc. [pg/L]	DF [%]	Conc. [pg/L]
Pakistan[3] (2016)	PW	41	36	<LOD (0.031) – 0.29	31	<LOD (0.03) – 0.1

Table S3 – Concentrations of OPEs in drinking water prior to October 15, 2021. TW: Tap water, DW: Drinking water, DF: Detection frequency, <LOD(): Limit of detection, "-" compound not included in study.

Location (year published)	Water Type	Total # of samples	TBOEP		TCEP		TCIPP		TDCIPP		TEHP		TPHP		DPHP	
			DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]
U.S. A[5] (2004)	DW	12	83	350	100	99	-	-	100	250	-	-	0	<LOD (500)	-	-
Germany[6] (2006)	DW	5	0	<LOD (3)	100	99	-	-	100	2	-	-	-	-	-	-
Italy[7] (2007)	TW	6	NS		0	<LOD (1.5)	0	<LOD (1)	0	<LOD (0.7)	-	-	-	-	-	-
U.S. A[8] (2009)	DW	15	-	-	40	150	40	220	-	-	-	-	-	-	-	-
Spain[9] (2012)	TW	28	-	-	71	7	92	50	0	<LOD (NS)	-	-	0	<LOD (NS)	0	<LOD (NS)
China[10] (2014)	TW	39	NS	70.1	NS	12.5	NS	33.4	0	<LOD (1)	0	<LOD (0.5)	NS	40	-	-
	BW	8	100	19.5 – 81.7	25	<LOD (1) – 48.8	100	1.33– 16.2	0	<LOD (1)	0	<LOD (0.5)	100	2.57 – 14.8	-	-
Spain[11] (2014)	TW	6	50	<LOD (0.002) – 33.5	67	<LOD (0.034 – 165.4	50	<LOD (0.002) – 37.1	-	-	-	-	-	-	-	-
China[12] (2015)	BW	23	91	0.3	100	0.5	96	0.6	87	0.6	-	-	100	0.8	-	-
	TW	21	100	3.7	100	48.5	100	43	100	5.8	-	-	100	1.4	-	-
South Korea[13] (2016)	Various	127	59	26.1	75	38.8	82	67	9	4.46	2	0.94	26	2.12	-	-
Pakistan[3] (2016)	PW	39	-	-	69	<LOD (0.03) – 29.7	74	<LOD (0.03) – 86	64	<LOD (0.03) – 21.4	44	<LOD (0.03) – 8.14	34	<LOD (0.03) – 7.86	-	-
U.S.A.[14] (2018)	TW	58	90	10	9	0.45	91	11.6	38	4.75	21	0.12	53	3.72	-	-
South Korea[15] (2018)	TW	44	100	43.9	100	39.5	100	49.5	18	2	0	<LOD (0.31)	98	23	-	-
China[16] (2019)	TW	18	-	-	100	15.1 – 160	100	7.4 – 132	11	<LOD (6.2) – 16	11	<LOD (1.4) – 17.9	17	<LOD (7.8) – 45.6	-	-
China[17] (2019)	TW	79	36	<LOD (0.42) – 20.6	100	0.78 – 89	100	2.39 – 101	85	<LOD (1.4) – 22.3	71	<LOD (1.32) – 59	70	<LOD (1.28) – 37.6	-	-

South Korea[18] (2020)	DW	6	NS	5.66 – 13.0	NS	13.5 – 21.8	NS	15.0 – 35.9	NS	2.17 – 3.23	NS	3.05 – 3.07	NS	305 – 7.47	-	-
South Korea[19] (2021)	DW	36	100	8.32	100	17.3	100	17.9	11	0.15	53	0.27	67	1.73	-	-
China[20] (2021)	TW	1	-	-	100	0.31	100	8.99	-	-	-	-	100	7.47	-	-

Table S4 - Concentrations of plasticizers in drinking water prior to October 15, 2021. TW: Tap water, BW: Bottled water, DW: Drinking water, DWF: drinking water fountain DF: Detection frequency, <LOD(): Limit of detection, <LOQ(): Limit of quantification, "-" compound not included in study.

Location (year published)	Water Type	Total # of samples	DBP		DEHP		DEP		DEHA		DINP		MEHP	
			DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]
Germany[21] (2001)	TW	1	100	380	100	50	100	200	-	-	-	-	-	-
Poland[21] (2001)	TW	1	100	640	100	60	100	160	-	-	-	-	-	-
Portugal[22] (2006)	TW	NS	NS	520	NS	60	NS	190	NS	90	-	-	-	-
	BW	NS	NS	350	NS	170	NS	40	NS	150	-	-	-	-
Canada[23] (2006)	DW	NS	NS	50	NS	188	-	-	-	-	-	-	-	-
	DW	NS	NS	46	NS	103	-	-	-	-	-	-	-	-
Canada[24] (2008)	BW	1	100	1720	100	223	100	67	0	<LOD (17)	-	-	-	-
	BW	6	100	138	100	118	100	80	0	<LOD (17)	-	-	-	-
Italy[25] (2008)	BW	142	NS	210	NS	20	NS	170	-	-	-	-	-	-
Greece[26] (2011)	BW	6	NS	44	NS	350	NS	33	-	-	-	-	-	-
Portugal[27] (2013)	TW	4	0	<LOD (10)	50	<LOD (10) – 130	-	-	-	-	-	-	-	-
	BW	1	100	1890	100	20	-	-	-	-	-	-	-	-
	BW	5	100	100-1420	100	80-180	-	-	-	-	-	-	-	-
Hungary[28] (2013)	BW	3	NS	<LOQ (6.6) – 800	NS	<LOQ (16) – 1700	NS	<LOQ (22.2)	-	-	-	-	-	-
France[29] (2013)	BW	2	0	<LOQ (20)	0	<LOQ (10)	0	<LOQ (30)	-	-	-	-	-	-
China[30] (2013)	DW	8	100	68 – 200	100	10 – 61	100	5.6 – 54	-	-	-	-	-	-
Spain[31] (2014)	BW	362	0	736	8	985 – 5510	4	920 – 9340	3	182 – 2040	-	-	-	-
International[32] (2014)	BW	77	5	100	0	<LOD (66)	-	-	-	-	91	<LOD (1) – 447	-	-
Taiwan[33] (2014)	TW	23	92	<LOD (1) – 103	100	131 – 239	54	<LOD (1) – 7	-	-	85	<LOD (1) – 316	-	-
	DWF	20	100	12 – 47	100	34 – 283	45	<LOD (1) – 3	-	-	-	-	-	-
Spain[34] (2014)	TW	7	100	633	0	<LOD (460)	14	<LOD (330) – 381	-	-	-	-	-	-
China[35] (2015)	DW	225	100	350	94	770	88	35	-	-	-	-	-	-

Iran[36] (2015)	BW	12	NS	135	NS	217	-	-	-	-	NS	<LOD (420)	-	-
Taiwan[37] (2016)	DW	109	NS	<LOQ (610 –840	NS	<LOQ (930) – 2880	-	-	-	-	NS	<LOD (NS)	-	-
China[38] (2017)	DW	NS	NS	17	NS	150	NS	<LOQ (NS)	-	-	-	-	-	-
South Africa[39] (2017)	DW	20	100	176 – 629	100	60 – 3415	-	-	100	1.97 – 4.07	100	8.34-350	-	-
South Africa[40] (2018)	BW	10	0	<LOD (5.7)	0	<LOD (4.4)	-	-	0	<LOD (8.7)	-	-	-	-
Iran[41] (2018)	TW	66	21	<LOD (0.01) – 67	67	<LOD (0.06) – 606	29	<LOD (0.14) – 113	-	-	-	-	-	-
Egypt[42] (2018)	BW	12	58	82	50	104	0	<LOD (12)	-	-	-	-	-	-
Iran[43] (2019)	DW	40	NS	90	NS	150	NS	50	-	-	-	-	-	-
	BW	10	NS	70	NS	100	NS	180	-	-	-	-	-	-
China[44] (2019)	DW	146	86	596	77	178	65	5.9	-	-	-	-	37	9.86
China[45] (2019)	BW	60	NS	200	NS	18	NS	23	-	-	NS	20	-	-
France[46] (2020)	DW	89	100	951	0	<LOD (500)	100	255	0	<LOD (500)	-	-	-	-
China[47] (2021)	DW	NS	NS	153	NS	645	NS	8.69	-	-	-	-	-	-
China[48] (2021)	TW	6	100	340 – 670	100	1097 – 1505	0	<LOD (21)	-	-	-	-	-	-
China[48] (2021)	BW	6	100	465 - 517	100	880 – 1257	0	<LOD(21)	-	-	-	-	-	-
Hong Kong[49] (2021)	TW	12	83	346	25	85.3	100	102	-	-	-	-	-	-
Hong Kong[49] (2021)	BW	3	100	95	0	<LOD(0.8)	100	38.7		-	-	-	-	-

Table S5 - Concentrations of Bisphenols in drinking water between 2012 – October 2021. TW: Tap water, DW: Drinking water, BW: Bottled water, DF: Detection frequency, <LOD(): Limit of detection, <LOQ(): Limit of quantification, "-" compound not included in study

Location (year published)	Water Type	Total # of samples	BPA		BPAF		BPF		BPS	
			DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]	DF [%]	Conc. [ng/L]
Italy[50] (2012)	DW	35	29	<LOD(0.73) – 102	-	-	-	-	-	-
	BW	5	40	<LOD(0.73) – 1.13	-	-	-	-	-	-
Malaysia[51] (2012)	TW	30	100	14.1	-	-	-	-	-	-
Taiwan[52] (2013)	DW	NS	NS	<LOQ (4.3) - 38	-	-	-	-	-	-
France[53] (2014)	TW	291	4	<LOD(25) – 1430	-	-	0	<LOD(25)	-	-
Spain[31] (2014)	BW	362	10	<LOD(NS) – 24200	-	-	-	-	-	-
Lebanon[54] (2014)	BW	22	59	169	-	-	-	-	-	-
Korea[55] (2014)	DW	25	40	<LOD (1.99) - 324	-	-	-	-	-	-
India[56] (2015)	TW	1	100	11.83	-	-	-	-	-	-
Cape Town[39] (2017)	DW	40	93	1.45	-	-	-	-	-	-
Pretoria[39] (2017)	DW	40	90	1.33	-	-	-	-	-	-
South Africa[40] (2018)	BW	10	90	2.78	-	-	-	-	-	-
China[57] (2018)	DW	2	0	<LOD (0.3)	-	-	-	-	-	-
Egypt[58] (2019)	DW	446	15	36.1	-	-	-	-	-	-
Canada[59] (2019)	TW	11	0	<LOQ(1.5)	-	-	-	-	-	-
China[60] (2019)	DW	20	40	1.6	30	0.4	5	0.04	25	0.1
China[61] (2020)	BW	21	100	675	33	<LOD(1.56) – 4.9	0	<LOD(0.91)	10	<LOD(2.3) – 10.6
China[62] (2020)	DW	52	67	<LOD (7) – 898.7	-	-	-	-	-	-
Italy[63] (2021)	DW	12	100	<LOQ (0.99) – 6.27	-	-	-	-	-	-
Hong Kong[49] (2021)	TW	12	-	-	83.7	0.96	83	1.51	33	2.95
Hong Kong[49] (2021)	BW	3	-	-	100	0.96	67	1.52	0	<LOD(0.5)

Table S6 - List of target analytes with CAS number and supplier of native standards

Family	Analyte acronym	Target analyte	CAS number	Supplier
Plasticizer	DEHP	Bis(2-ethylhexyl) phthalate	117-81-7	Sigma Aldrich
Plasticizer	DEP	Diethyl phthalate	84-66-2	Sigma Aldrich
Plasticizer	DBP	Dibutyl phthalate	84-74-2	Sigma Aldrich
Plasticizer	DEHA	Bis(2-ethylhexyl) adipate	103-23-1	Toronto Research Chemicals
Plasticizer	DINCH	Bis(7-methyloctyl) Cyclohexane-1,2-dicarboxylate	166412-78-8	Toronto Research Chemicals
Plasticizer	DIDA	Diisodecyl adipate	27178-16-1	Sigma Aldrich
Plasticizer	DINP	Diisononyl phthalate	68515-48-0	Sigma Aldrich
Plasticizer	MEHP	Mono(ethylhexyl) phthalate	4376-20-9	Toronto Research Chemicals
OPEs	TBOEP	Tris(2-butoxyethyl) phosphate	78-51-3	Sigma Aldrich
OPEs	TCEP	Tris(2-chloroethyl) phosphate	115-96-8	Sigma Aldrich
OPEs	TCIPP	Tris(1-chloro-2-propyl) phosphate	13674-84-5	Cambridge Isotope Lab. Inc
OPEs	TDCIPP	Tris(1,3-dichloro-2-propyl) phosphate	13674-87-8	Toronto Research Chemicals Inc.
OPEs	TEHP	Tris(2-ethylhexyl) phosphate	78-42-2	Wellington Laboratories
OPEs	TPHP	Triphenyl phosphate	115-86-6	Supelco Analytical
OPEs – metabolite	DPHP	Diphenyl phosphate	838-85-7	Sigma Aldrich
OPEs – metabolite	Ip-PPP	4-Isopropylphenyl phenyl phosphate	69415-02-7	Toronto Research Chemicals
OPEs – metabolite	BCIPP	Bis(1-chloro-2-propyl) phosphate	789440-10-4	Toronto Research Chemicals
OPEs – metabolite	BCEP	Bis(2-chloroethyl) phosphate	3040-56-0	Toronto Research Chemicals
OPEs – metabolite	BBOEP	Bis(2-butoxyethyl) phosphate	14260-97-0	Toronto Research Chemicals
OPEs – metabolite	BDCIPP	Bis(1,3-dichloro-2-propyl) phosphate	72236-72-7	Wellington Laboratories
OPEs – metabolite	BEHP	Bis(2-ethylhexyl) phosphate	298-07-7	Toronto Research Chemicals
OPEs – metabolite	BTBOEP	Bis(2-butohexylethyl) 2-Hydroxyethyl Phosphate Triester	1477494-86-2	Toronto Research Chemicals
OPEs – metabolite	DCP	Di-cresyl phosphate	36400-46-1	Toronto Research Chemicals
PBDE	BDE 28	2,4,4'-Tribromodiphenyl ether	41318-75-6	Wellington Laboratory
PBDE	BDE 47	2,2',4,4'-Tetrabromodiphenyl ether	5436-43-1	Wellington Laboratory
PBDE	BDE 99	2,2',4,4',5-Pentabromodiphenyl ether	60348-60-9	Wellington Laboratory
PBDE	BDE 100	2,2',4,4',6-Pentabromodiphenyl ether	189084-64-8	Wellington Laboratory
PBDE	BDE 153	2,2',4,4',5,5'-Hexabromodiphenyl ether	68631-49-2	Wellington Laboratory
PBDE	BDE 154	2,2',4,4',5,6'-Hexabromodiphenyl ether	207122-15-4	Wellington Laboratory
PBDE	BDE 183	2,2',3,4,4',5',6-Heptabromodiphenyl ether	207122-16-5	Wellington Laboratory
PBDE	BDE 209	Decabromodiphenyl ether	1163-19-5	Wellington Laboratory
Dechlorane	DEC-602	Dechlorane 602	31107-44-5	Toronto Research Chemicals
Dechlorane	DEC-603	Dechlorane 603	13560-92-4	Toronto Research Chemicals
Dechlorane	a-DP	Anti-dechlorane plus	13560-89-9	Toronto Research Chemicals
Dechlorane	s-DP	Syn-dechlorane plus	135821-03-3	Cambridge Isotope Lab. Inc.
Bisphenol	BPA	Bisphenol A	80-05-7	Toronto Research Chemicals
Bisphenol	BPAF	Bisphenol AF	1478-61-1	Sigma Aldrich
Bisphenol	BPF	Bisphenol F	620-92-8	Toronto Research Chemicals
Bisphenol	BPS	Bisphenol S	80-09-1	Sigma Aldrich

Table S6.1 – Organophosphate ester parent compounds and metabolites.

Parent OPEs			OPE Metabolite	
CASRN	**Full Name**	**Acronym**	**Full name**	**Acronym**
78-51-3	Tris(2-butoxyethyl) phosphate	TBOEP	Bis (2-butoxyethyl) phosphate	BBOEP
			Bis (2-butoxyethyl) 2-Hydroxyethyl-phosphate	BTBOEP
78-42-2	Tris(2-ethylhexyl) phosphate	TEHP	Bis (2-ethylhexyl) phosphate	BEHP
115-86-6	Triphenyl phosphate	TPHP	Diphenyl phosphate	DPHP
115-96-8	Tris(chloroethyl) phosphate	TCEP	Bis (2-chloroethyl) hydrogen phosphate	BCEP
13674-84-5	Tris(2-chloroisopropyl) phosphate	TCIPP	Bis (1-chloro-2-propyl) phosphate	BCIPP
13674-87-8	Tris(1,3-dichloro-2-propyl) phosphate	TDCIPP	Bis (1,3-dichloro-2-propyl) phosphate	BDCIPP
78-30-8 563-04-2 78-32-0	Tri-o-cresyl phosphate Tri-m-cresyl phosphate Tri-p-cresyl phosphate	TMPP*	Di-cresyl phosphate	DCPs
64532-94-1 69515-46-4 55864-04-5	Mono-substituted o-isopropyl triphenyl phosphate Mono-substituted m-isopropyl triphenyl phosphate Mono-substituted p-isopropyl triphenyl phosphate	IPPP*	Diphenyl phosphate	DPHP
			Isopropylphenyl phenyl phosphate	Ip-PPPs

(*) Mixture of isomers (Ortho, meta and para position), not included in the study

Table S7 – Labelled surrogates used for recovery and matrix effect in each sample with CAS numbers and suppliers

Family	**Analyte acronym**	**Target analyte**	**CAS number**	**Supplier**
Plasticizer	DEHP-d4	Bis(2-ethylhexyl) phthalate-d4	117-81-7	Toronto Research Chemicals
Plasticizer	DEP-d4	Diethyl phthalate-d4	84-66-2	Toronto Research Chemicals
Plasticizer	DBP-d4	Dibutyl phthalate-d4	84-74-2	Toronto Research Chemicals
Plasticizer	DEHA-d4	Bis(2-ethylhexyl) adipate-d4	103-23-1	Toronto Research Chemicals
Plasticizer	DINP-d4	Diisononyl phthalate-d4	68515-48-0	Toronto Research Chemicals
Plasticizer	DINCH-13C4	Bis(7-methyloctyl) Cyclohexane-1,2-dicarboxylate-13C4	166412-78-8	Toronto Research Chemicals
Plasticizer	MEHP-d4	Mono(ethylhexyl) phthalate-d4	4376-20-9	Toronto Research Chemicals
OPEs	TEHP-d51	Tris(2-ethylhexyl) phosphate-d51	1259188-37-8	Toronto Research Chemicals
OPEs	TCEP-d12	Tris(2-chloroethyl) phosphate-d12	115-96-8	Wellington Laboratories
OPEs	TDCIPP-d15	Tris(1,3-dichloro-2-propyl) phosphate-d15	1447569-77-8	Wellington Laboratories
OPEs	TPHP-d15	Triphenyl phosphate	1173020-30-8	Wellington Laboratories
OPEs – metabolite	DPHP-d10	Diphenyl phosphate-d10	1477494-97-5	Toronto Research Chemicals Inc.
OPEs – metabolite	Ip-PPP-d7	4-Isopropylphenyl phenyl phosphate-d7	69415-02-7	Toronto Research Chemicals Inc.
OPEs – metabolite	BCIPP-d12	Bis(1-chloro-2-propyl) phosphate-d12	789440-10-4	Toronto Research Chemicals Inc.
OPEs – metabolite	BBOEP-d8	Bis(2-butoxyethyl) phosphate-d8	14260-97-0	Toronto Research Chemicals Inc.
OPEs – metabolite	BEHP-d34	Bis(2-ethylhexyl) phosphate-d34	1773493-20-1	Toronto Research Chemicals Inc.
OPEs – metabolite	DCP—d14	Di-cresyl phosphate-d14	36400-46-1	Toronto Research Chemicals Inc.
PBDE	BDE 28-13C12	2,4,4'-Tribromodiphenyl ether-13C12	41318-75-6	Wellington Laboratory
PBDE	BDE 47-13C12	2,2',4,4'-Tetrabromodiphenyl ether-C13C12	5436-43-1	Wellington Laboratory
PBDE	BDE 99-13C12	2,2',4,4',5-Pentabromodiphenyl ether-13C12	60348-60-9	Wellington Laboratory
PBDE	BDE 100-13C12	2,2',4,4',6-Pentabromodiphenyl ether-13C12	189084-64-8	Wellington Laboratory
PBDE	BDE 153-13C12	2,2',4,4',5,5'-Hexabromodiphenyl ether-13C12	68631-49-2	Wellington Laboratory
PBDE	BDE 154-13C12	2,2',4,4',5,6'-Hexabromodiphenyl ether-13C12	207122-15-4	Wellington Laboratory
PBDE	BDE 183-13C12	2,2',3,4,4',5',6-Heptabromodiphenyl ether-13C12	207122-16-5	Wellington Laboratory
PBDE	BDE 209-13C12	Decabromodiphenyl ether-13C12	1163-19-5	Wellington Laboratory
Dechlorane	DEC-602-13C10	Dechlorane 602-13C10	31107-44-5	Cambridge Isotope Lab. Inc.
Dechlorane	a-DP-13C10	Anti-dechlorane plus-13C10	135821-74-8	Cambridge Isotope Lab. Inc.
Dechlorane	s-DP-13C10	Syn-dechlorane plus-13C10	135821-03-3	Cambridge Isotope Lab. Inc.
Bisphenol	BPA-C13	Bisphenol A-C13	80-09-1	Toronto Research Chemicals Inc.
Bisphenol	BPAF-d4	Bisphenol AF-d4	263261-65-0	Toronto Research Chemicals Inc.
Bisphenol	BPF-C13	Bisphenol F-C13	1410794-06-7	Toronto Research Chemicals Inc.
Bisphenol	BPS-C13	Bisphenol S-C13	80-09-1	Toronto Research Chemicals Inc.

Table S8 – Analysis parameters and instrument detection limits for PBDEs used in Montreal campaign 1

Compound	Analyte		Internal standard		Retention time [min]	Recovery [%]	IDL [ng/L]
	SIM-Q (m/z)	SIM-C (m/z)	SIM-Q (m/z)	SIM-C (m/z)			
BDE-28	405.8	407.8	6.42	417.8	419.8	77.9	0.12
BDE-47	483.7	485.7	7.27	497.8	499.7	75.3	0.52
BDE-99	563.6	565.6	8.16	575.6	577.7	75.0	0.41
BDE-100	641.5	643.5	7.94	653.6	655.6	72.9	0.28
BDE-153	721.4	723.4	9.27	733.5	735.5	64.8	1.09
BDE-154	799.4	801.3	8.87	811.4	813.4	66.5	0.80
BDE-183	879.3	881.3	10.61	891.3	893.3	70.1	0.58
BDE-209	957.2	959.2	16.93	971.2	973.2	377.9	9.61

Table S9 - SRM transition and instrument detection limits for PBDEs used in all campaigns except Montreal campaign 1 (Montreal campaigns 2-3 and South Africa campaigns 1-2)

Compound	Transition ions monitored		IDL [ng/L]
	Congener	Internal standard	
BDE-28	407.8 → 247.9	419.8 → 260.0	0.02
BDE-47	485.7 → 325.9	497.8 → 337.8	0.02
BDE-99	403.8 → 137.0	415.8 → 148.0	0.01
BDE-100	403.8 → 137.0	415.8 → 148.0	0.01
BDE-153	643.5 → 483.7	655.6 → 495.7	0.01
BDE-154	643.5 → 483.7	655.6 → 495.7	0.04
BDE-183	723.4 → 563.6	733.5 → 573.6	0.01

Table S10 – Analysis parameters and instrument detection limits for dechloranes in Montreal campaign 1

Compound	Analyte		Internal standard		Recovery [%]	IDL [ng/L]	Retention time [min]
	SIM-Q (m/z)	SIM-C (m/z)	SIM-Q (m/z)	SIM-C (m/z)			
DEC 602	271.8	273.8	276.9	278.8	36.9	0.10	8.13
DEC 603	260.8	262.8	-	-	35.9	0.27	10.18
a-DP	271.8	273.8	276.9	278.8	158.3	0.16	12.45
s-DP	271.8	273.8	-	-	46.7	0.04	11.94

Table S11 – Analysis parameters and instrument detection limits for all campaigns except Montreal campaign 1 (Montreal campaigns 2-3 and South Africa campaigns 1-2). SIM-Q is quantification and SIM-C is confirmation.

Compound	Retention time [min]	SIM-Q (m/z)	SIM-C (m/z)	Internal standard (m/z)	IDL [ng/L]
Dechlorane 602	29.69	614	612	624	1.0
Dechlorane 603	34.89	638	636	624	2.4
s-DP	35.99	654	652	664	1.7
a-DP	36.19	654	652	664	0.9

Table S12 – Analysis parameters and instrument detection limits for OPEs

	Analyte		Internal standard				
Compound	MRM transition [Collision energy, eV]	Cone Voltage (V)	MRM transition [Collision energy, eV]	Cone Voltage (V)	**Ionisation mode**	**Recovery [%]**	**IDL [ng/L]**
TBOEP	399.37 → 45.04 [22]	38	426.42 → 208.09 [16]	36	ESI+	60.7	0.34
TCEP	287.10 → 99.01 [24]	36	299.17 → 67.10 [26]	40	ESI+	78.1	0.48
TCIPP	329.18 → 99.01 [20]	32	342.19 → 81.82 [40]	64	ESI+	83.1	0.70
TDCIPP	431.04 → 99.01 [22]	36	446.14 → 102.00 [26]	40	ESI+	112.1	0.18
TEHP	435.53 → 99.00 [16]	18	486.85 → 102.19 [22]	28	ESI+	419.4	0.03
TPHP	327.18 → 77.13 [38]	56	342.19 → 81.82 [40]	64	ESI+	118.7	0.11
BDCIPP	318.64 → 34.42 [8]	18	328.71 → 34.74 [8]	8	ESI-	159.9	0.55
DPHP	249.03 → 93.03 [24]	56	259.15 → 98.04 [26]	54	ESI-	115.3	0.24
BCIPP	253.00 → 98.81 [20]	25	264.98 → 100.88 [14]	26	ESI+	140.0	0.17
BCEP	222.93 → 98.86 [18]	32	230.9 → 100.9 [18]	36	ESI+	84.3	0.23
DCPs	279.21 → 91.13 [30]	46	293.30 → 97.25 [30]	56	ESI+	85.6	0.24
ip-PPPs	293.24 → 77.08 [36]	46	293.30 → 97.25 [30]	56	ESI+	81.8	0.21
BTBOEP	343.15 → 44.88 [18]	22	347.14 → 44.95 [18]	32	ESI+	75.8	0.28
BBOEP	299.28 → 45.04 [18]	34	307.33 → 49.01 [18]	32	ESI+	99.7	0.26
BEHP	321.01 → 78.88 [32]	58	355.41 → 227.26 [24]	60	ESI-	187.4	0.25

Table S13 - Analysis parameters and instrument detection limits for bisphenols

	Analyte		**Internal standard**				
Compound	**Retention time [min]**	**m/z**	**Retention time [min]**	**m/z**	**Linearity**	**Recovery [%]**	**IDL [ng/L]**
BPA	14.9	227.10	14.9	239.15	0.99	140	0.32
BPAF	15.5	335.05	15.5	339.08	0.99	108	0.1
BPF	13.9	199.08	13.9	211.12	0.99	126	0.71
BPS	12.2	249.02	12.2	261.06	0.98	57.0	0.82

Table S14 - Analysis parameters and method detection limits for plasticizers. SIM-Q is used for quantification and SIM-C is used for confirmation. MS^2 was used for confirmation with the exception of MEHP which used MS^3.

Compound	Retention time [min]	SIM-Q m/z	SIM-C m/z	Linearity	Recovery [%]	IDL [ng/L]
DEHP	8.54	391.28	278.9	0.99	82.8	1.35
MEHP	6.95	279.16	167.0	0.99	77.5	1.32
DEP	6.60	223.10	163.0	0.99	83.4	1.29
DBP	6.80	279.16	205.1	0.99	77.7	1.70
DEHA	8.60	371.32	129.0	0.99	85.7	1.54
DINCH	9.80	425.36	155.9	0.99	76.0	1.93
DINP	9.20	419.32	129.2	0.99	87.9	1.68
DIDA	9.50	427.38	269.1	0.99	82.4	1.68

Table S15 - Concentration of target analytes in Montreal bottled water. ND represents samples which had non-detect, <LOQ represents samples which were detected but below the limit of quantification. Compounds not detected in any samples: BDE-154, BDE-183, BDE-209, DEC 602, DEC 603, a-DP, s-DP, and ip-PPP, BPA, BPAF, BPF, BPS

Comp-ound	**BW #1**			**BW #2**			**BW #3**			**BW #4**			**BW #5**		
	Camp. 1	**Camp. 2**	**Camp. 3**	**Camp. 1**	**Camp. 2**	**Camp. 3**	**Camp. 1**	**Camp. 2**	**Camp. 3**	**Camp. 1**	**Camp. 2**	**Camp. 3**	**Camp. 1**	**Camp. 2**	**Camp. 3**
Flame retardants															
BDE-28	ND	<LOQ	ND	<LOQ	ND	<LOQ	<LOQ	ND	ND	ND	<LOQ	ND	ND	ND	ND
BDE-47	ND	<LOQ	0.06	ND	<LOQ	0.07	ND	ND	0.13	ND	ND	<LOQ	ND	<LOQ	<LOQ
BDE-99	ND	<LOQ	ND	ND	ND	ND	ND	ND	ND	ND	0.03	ND	ND	ND	ND
BDE-100	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	0.02	ND	ND	ND	ND
BDE-153	ND	ND	ND	ND	ND	ND	ND	ND	0.02	ND	ND	ND	ND	ND	ND
TBOEP	0.57	3.40	ND	8.11	26.33	3.14	5.00	ND	ND	2.11	ND	ND	15.40	ND	3.13
TCEP	ND	33.54	10.41	ND	51.45	11.53	ND	4.71	6.47	ND	46.31	4.23	ND	32.09	6.44
TCIPP	ND	8.24	0.52	ND	11.17	0.37	ND	1.02	1.61	ND	0.69	0.95	ND	2.45	0.56
TDCIPP	5.12	2.08	0.97	ND	21.24	2.92	4.81	1.16	1.54	ND	24.59	0.23	ND	9.89	3.86
TEHP	ND	ND	0.06	ND	ND	0.21	ND	ND	6.28	ND	ND	1.22	ND	ND	2.01
TPHP	1.01	1.19	0.62	0.46	1.92	0.80	0.87	0.79	0.85	0.61	2.20	1.09	0.22	0.99	0.67
BDCIPP	0.66	3.72	ND	0.39	8.32	ND	0.51	ND	ND	ND	ND	ND	0.73	7.14	ND
DPHP	2.68	5.11	3.05	ND	5.11	2.29	0.16	16.91	5.77	6.54	4.23	3.30	7.30	6.77	0.72
BCIPP	ND	ND	<LOQ	ND	ND	0.43	ND	ND	0.44	ND	ND	0.53	ND	ND	0.27
BCEP	1.37	ND	0.26	1.58	ND	0.68	1.12	ND	ND	0.37	ND	0.68	1.17	ND	ND
DCPs	0.86	<LOQ	0.31	ND	<LOQ	<LOQ	ND	0.68	<LOQ	ND	<LOQ	<LOQ	ND	<LOQ	<LOQ
BTBOEP	0.55	1.15	0.13	1.17	3.72	0.23	0.76	0.74	0.83	0.39	2.45	ND	0.45	0.38	0.53
BBOEP	0.27	0.92	ND	0.86	4.08	0.51	0.94	0.17	1.10	ND	1.81	ND	ND	ND	ND
BEHP	ND	66.78	27.87	ND	53.54	30.33	ND	66.73	42.98	ND	81.45	28.92	ND	70.71	25.80
Plasticizers															
DEHP	128.73	137.38	116.50	39.32	34.09	59.97	45.78	55.21	71..89	247.12	339.86	378.83	247.12	340.86	274.43
MEHP	ND	ND	13.08	ND	ND	<LOQ	ND	ND	<LOQ	ND	ND	15.98	ND	ND	10.02
DEP	30.94	15.50	27.98	10.98	7.82	17.50	8.10	12.05	6.08	18.26	18.24	30.11	11.25	22.73	22.61
DBP	10.17	13.74	10.41	137.69	23.93	202.94	24.36	24.15	29.07	73.05	56.39	96.11	54.32	54.60	32.40
DEHA	67.95	63.92	82.49	ND	ND	<LOQ	33.94	33.65	20.26	40.53	51.53	31.41	13.16	14.53	17.95
DINCH	112.63	125.22	154.53	175.35	158.54	142.40	195.89	193.96	183.35	136.96	104.92	192.43	147.16	140.06	185.42
DINP	168.03	146.43	79.64	162.19	156.59	237.11	257.79	241.16	368.64	84.77	94.79	121.22	146.87	151.31	216.05
DIDA	36.34	9.09	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND

Table S16 - Concentration of target analytes in Montreal drinking water. ND represents samples which had non-detect, <LOQ represents samples which were detected but below the limit of quantification. Compounds not detected in any samples: BDE-99, BDE-153, BDE-183, BDE-209, DEC 602, DEC 603, a-DP, s-DP, BPA, BPAF, BPF, BPS

Compound	DWTP #1			DWTP #2			DWTP #3		
	Camp. 1	Camp. 2	Camp. 3	Camp. 1	Camp. 2	Camp. 3	Camp. 1	Camp. 2	Camp. 3
Flame retardants									
BDE-28	ND	<LOQ	ND	ND	ND	<LOQ	ND	0.05	ND
BDE-47	ND	ND	ND	ND	<LOQ	ND	ND	0.08	ND
BDE-100	ND	ND	ND	ND	ND	0.03	ND	ND	ND
BDE-154	ND	0.06	ND	ND	ND	ND	ND	ND	ND
TBOEP	11.14	39.13	4.64	26.82	8.16	0.47	21.76	16.41	9.02
TCEP	107.87	159.05	15.92	182.78	91.90	2.94	86.96	92.57	21.35
TCIPP	13.56	24.11	14.39	26.36	16.14	8.73	19.88	10.82	9.08
TDCIPP	55.79	76.34	11.34	149.76	32.24	10.33	16.38	42.97	24.09
TEHP	0.23	ND	0.06	0.62	ND	0.23	ND	ND	9.50
TPHP	10.17	10.39	3.25	39.18	10.92	1.75	3.86	18.30	2.13
BDCIPP	3.70	3.49	ND	11.13	4.51	ND	8.25	ND	ND
DPHP	36.49	49.80	2.65	50.69	19.59	1.04	31.64	50.94	1.42
BCIPP	204.90	287.46	1.47	303.34	154.15	1.53	223.04	293.47	1.10
BCEP	ND	ND	0.53	ND	ND	0.84	ND	ND	0.69
DCPs	ND	1.11	<LOQ	ND	<LOQ	<LOQ	<LOQ	<LOQ	ND
BTBOEP	6.81	15.38	1.27	12.91	3.63	0.58	12.76	10.69	3.83
BBOEP	2.50	9.08	ND	6.95	0.35	ND	3.56	3.19	1.76
BEHP	59.94	49.21	26.32	40.85	58.69	22.73	50.96	49.61	30.15
Ip-PPP	0.60	ND	ND	ND	ND	ND	ND	0.41	ND
Plasticizers									
DEHP	204.28	185.17	105.37	225.39	168.30	249.01	13.47	22.26	27.71
MEHP	ND	ND	15.75	ND	ND	15.34	ND	ND	20.47
DEP	35.83	48.83	47.84	5.6	4.83	8.94	<LOQ	ND	<LOQ
DBP	26.49	57.50	36.68	84.10	62.60	90.83	98.96	86.03	59.19
DEHA	20.69	14.39	22.11	85.63	71.96	52.98	5.08	<LOQ	5.83
DINCH	96.70	108.37	60.07	65.34	55.20	51.53	426.09	339.31	372.74
DINP	64.72	49.62	79.89	36.30	37.38	26.73	199.48	218.41	234.47
DIDA	ND	ND	10.59	9.26	14.57	14.46	ND	ND	18.43

Table S17 - Concentration of target analytes in South Africa water. ND represents samples which had non-detect, <LOQ represents samples which were detected but below the limit of quantification. Compounds not detected in any samples: BDE-153, BDE-183, DEC 602, DEC 603, a-DP, BDCIPP, BPA, BPAF, BPF, BPS

Compound	Vhembe		Vhembe – small containers		Vhembe – large containers		Pretoria	
	Camp. 1	Camp. 2	Camp. 1	Camp. 2	Camp. 1	Camp. 2	Camp. 1	Camp. 2
				Flame retardants				
BDE-28	0.09	ND	<LOQ	ND	ND	ND	<LOQ	<LOQ
BDE-47	0.12	ND	1.18	ND	0.05	ND	0.53	<LOQ
BDE-99	0.06	ND	0.26	ND	0.03	ND	0.05	ND
BDE-100	0.06	0.24	0.08	ND	0.02	ND	0.16	ND
BDE-154	<LOQ	ND	<LOQ	ND	ND	ND	ND	ND
a-DP	ND	ND	ND	ND	ND	ND	ND	1.09
TBOEP	ND	3.37	ND	0.37	ND	1.17	ND	9.28
TCEP	9.97	6.94	97.55	14.06	86.0	9.03	100.37	47.69
TCIPP	1.40	7.55	21.58	7.16	9.70	4.61	204.49	148.39
TDCIPP	36.86	12.93	119.19	1.21	108.40	ND	100.77	33.09
TEHP	ND	0.74	ND	0.13	ND	ND	ND	0.33
TPHP	2.03	3.51	3.49	3.37	3.39	3.11	3.93	4.90
DPHP	29.52	0.77	28.81	0.36	12.82	0.82	172.58	128.13
BCIPP	138.63	0.83	184.31	0.34	73.81	0.08	215.35	14.13
BCEP	ND	ND	5.58	ND	ND	ND	ND	0.29
DCPs	0.42	<LOQ	<LOQ	<LOQ	ND	<LOQ	0.53	ND
BTBOEP	ND	0.77	ND	0.65	ND	0.94	11.98	14.55
BBOEP	ND	ND	ND	ND	2.85	0.44	11.14	1.97
BEHP	42.98	26.87	34.96	34.35	29.85	21.22	44.17	26.32
Ip-PPP	ND	ND	ND	<LOQ	ND	ND	0.512	<LOQ
				Plasticizers				
DEHP	4.79	4.27	4.99	5.04	15.71	14.03	9.71	4.07
MEHP	10.56	<LOQ	ND	<LOQ	<LOQ	<LOQ	10.73	<LOQ
DEP	17.44	31.05	37.55	55.83	16.76	74.48	23.55	42.42
DBP	10.22	18.36	54.51	37.82	7.99	34.67	8.72	24.02
DEHA	12.35	26.70	4.32	96.66	66.16	62.32	8.98	56.68
DINCH	94.78	8.35	2.42	9.95	6.70	7.89	71.85	ND
DINP	<LOQ	ND	<LOQ	<LOQ	<LOQ	<LOQ	<LOQ	ND
DIDA	ND	31.05	37.55	55.83	16.76	74.48	ND	42.42

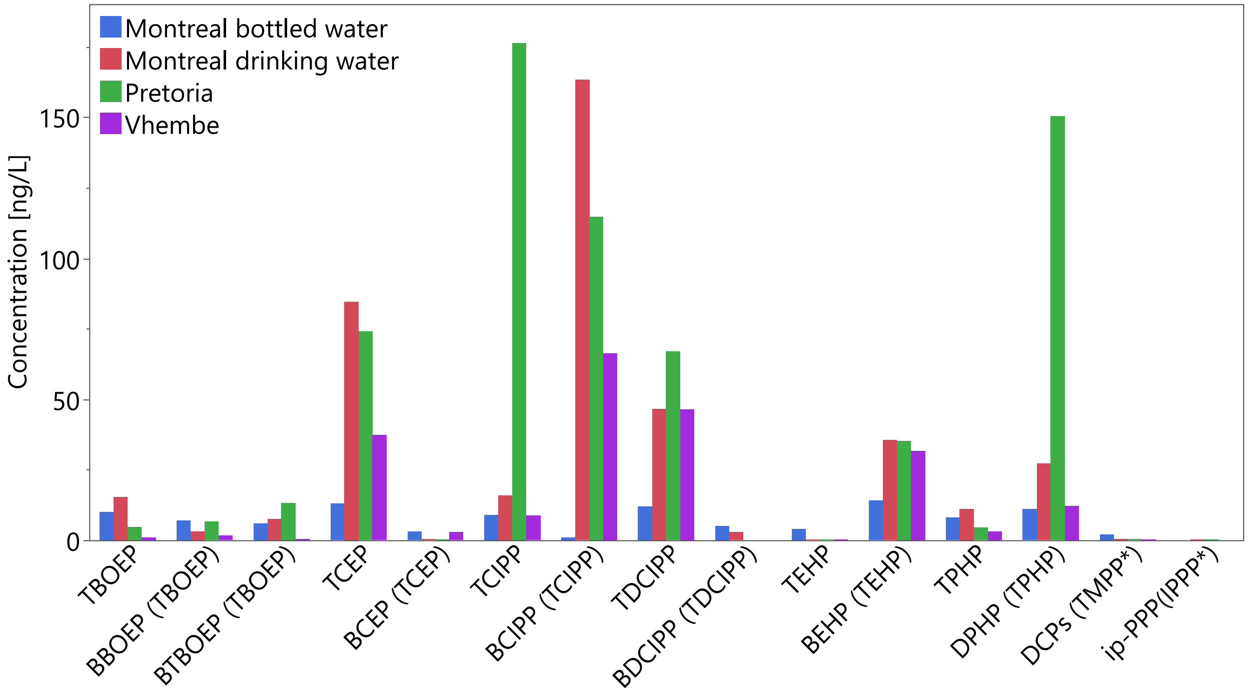

Figure S1 - Comparison of concentrations of OPE parent compounds and their metabolites. For the metabolites, their parent compound is specified in brackets. *Denotes parent compounds which were not included in the present study.

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