Supplemental Information

Estimating Dietary Exposure to Polycyclic Aromatic Compounds from Food Grade Plastics

Kara B. Loudon[1*] and Thane M.Z. Tomy[1]; Erin C. Liebzeit[1]; Thor Halldorson[1]; Zhe Xia[1]; Sara Sambanthan[1]; Duc Luong Hoang[1]; Nipuni Vitharana[1] and Gregg T. Tomy[1*]

1. Department of Chemistry, University of Manitoba, Winnipeg, Manitoba R3T 2N2 Canada

*To whom correspondence may be addressed: loudonk@myumanitoba.ca; gregg.tomy@myumanitoba.ca

Table SI-1. Arithmetic mean recoveries and relative standard deviations (RSD) of replicate measurements of deuterated polycyclic aromatic compounds in 1 g of oil from our refrigeration studies.

Plastic type	PE					PETG					PC					PP				
Recoveries (%)	t0		t10		*p* value[1]	t0		t10		*p* value[1]	t0		t10		*p* value[1]	t0		t10		*p* value[1]
	Avg	RSD (%)	Avg	RSD (%)		Avg	RSD (%)	Avg	RSD (%)		Avg	RSD (%)	Avg	RSD (%)		Avg	RSD (%)	Avg	RSD (%)	
d_{10}-Acenapthene	65.0	3.1	65.3	6.2	0.958	66.7	7.0	65.5	5.9	0.657	65.9	2.1	61.0	6.9	0.165	68.9	4.6	62.8	5.3	0.003
d_8-Acenapthylene	62.0	2.0	62.5	6.6	0.904	63.9	6.3	62.7	6.6	0.517	63.6	2.9	58.8	7.4	0.200	65.9	5.7	61.4	6.2	0.003
d_{12}-Benz[*a*]anthracene	62.8	2.3	67.7	5.0	0.107	66.0	2.6	83.0	8.0	0.063	66.7	3.9	76.1	11.0	0.335	66.6	7.6	84.8	3.4	0.013
d_{12}-Benzo[*a*]pyrene	71.0	0.9	83.7	3.8	0.041	70.0	4.0	102.2	11.7	0.082	72.7	4.5	99.5	10.8	0.087	67.8	8.0	110.7	4.2	0.001
d_{12}-Benzo[*b*]fluoranthene	64.5	0.5	67.6	6.1	0.412	61.5	4.8	83.8	9.6	0.089	65.0	5.3	82.8	11.5	0.175	63.1	12.9	90.4	5.3	0.007
d_{14}-Benzo[*g,h,i*]perylene	63.9	0.7	77.1	1.6	0.002	63.2	2.3	89.2	8.1	0.036	69.0	2.7	83.5	8.1	0.135	67.6	5.9	91.6	2.9	0.013
d_{12}-Benzo[*k*]fluoranthene	62.2	3.2	68.5	5.8	0.186	62.8	9.7	79.2	7.9	0.160	60.7	3.6	83.3	11.6	0.073	59.1	4.7	91.6	5.9	0.007
d_{12}-Chrysene	63.6	4.0	64.9	3.9	0.295	65.9	3.6	75.2	7.3	0.140	64.8	2.7	69.1	6.7	0.298	65.2	5.5	77.4	5.4	0.002
d_{14}-Dibenzo[*a,h*]anthracene	61.3	3.5	83.2	2.5	0.000	64.3	3.0	99.0	11.8	0.052	69.0	2.0	92.2	11.1	0.099	66.6	5.3	98.2	2.8	0.005
d_{10}-Fluoranthene	64.5	4.6	64.0	2.2	0.718	64.9	6.5	70.7	7.4	0.173	65.7	2.5	66.1	8.1	0.945	66.4	6.2	70.2	4.2	0.050
d_{10}-Fluorene	63.9	2.9	64.9	4.9	0.797	66.8	5.9	66.4	6.5	0.753	64.8	2.5	61.7	8.1	0.426	67.1	4.0	64.2	4.1	0.015
d_{12}-Indeno[1,2,3-*c,d*]pyrene	64.4	1.2	82.1	1.8	0.001	66.3	5.9	97.8	8.4	0.031	69.6	3.6	90.8	11.0	0.116	66.3	5.3	97.6	2.7	0.004
d_8-Naphthalene	61.9	3.1	58.4	8.4	0.548	60.7	8.7	58.2	7.7	0.288	62.5	2.1	51.4	8.1	0.060	66.3	3.2	58.1	6.6	0.021
d_{10}-Phenanthrene	64.5	3.7	64.4	1.3	0.968	66.6	4.3	67.8	8.1	0.696	65.6	1.1	63.1	7.9	0.570	66.3	4.0	65.9	4.4	0.338
d_{10}-Pyrene	67.7	2.4	67.9	2.6	0.890	68.6	6.7	76.5	7.1	0.094	68.3	3.6	70.4	8.5	0.545	69.5	6.0	75.7	5.2	0.040

[1]double tail, paired student t-test

Table SI-2. Arithmetic mean amounts (pg) and standard deviations (SDs) of replicate measurements of polycyclic aromatic hydrocarbons in procedural blanks (*n=5*) from our microwave migration study. Recoveries are the arithmetic mean ± SD of corresponding mass-labeled internal standard in all samples (*n=80*).

Compound	**pg**	**Mean + 3 × SD**[1]	**Recovery**
Acenaphthene	7.0 ± 1.3	10.9	82.2±15.6
Acenaphthylene	22.8 ± 3.2	32.5	69.8±14.9
Anthracene	8.5 ± 1.6	13.5	-[2]
Benz(*a*)anthracene	2.0 ± 0.4	3.2	86.2±13.2
Benzo(*a*)pyrene	0.5 ± 0.1	0.9	90.6±16.3
Benzo(*b*)fluoranthene	1.3 ± 0.2	2.0	87.7±13.1
Benzo(*g*,*h*,*i*)perylene	0.7 ± 0.1	1.1	80.5±11.0
Benzo(*k*)fluoranthene	1.9 ± 0.4	3.0	84.4±13.9
Chrysene	9.4 ± 1.8	14.8	84.3±13.6
Dibenzo(*a*,*h*)anthracene	0.3 ± 0.1	0.7	71.8±15.2
Fluoranthene	28.9 ± 5.6	45.6	90.9±12.1
Fluorene	15.6 ± 3.1	24.9	84.4±8.9
Indeno(1,2,3-*c*,*d*)pyrene	1.4 ± 0.2	2.1	81.6±11.5
Naphthalene	78.4 ± 11.5	112.9	61.9±20.2
Phenanthrene	140.4 ± 21.6	205.1	89.2±8.6
Pyrene	29.0 ± 3.7	40.0	90.9±12.7

[1]If our analytes in samples were smaller than their respective mean + 3 × SD amounts then it was considered a non-detect. [2]Mass labeled anthracene was purposely not added as a recovery internal standard because it was used as an instrument performance standard.

Table SI-3. Arithmetic mean amounts (pg) and standard deviations of replicate measurements of alkylated polycyclic aromatic compounds in procedural blanks from our refrigeration (*n=30*) and microwave (*n=5*) migration studies[1].

Compound	Mean amount ± SD (pg)[2]	Mean + 3 × SD (pg)[3]
1,7-Dimethylphenanthrene	9.3±1.6; 5.5±1.0	14.1; 8.5
1,8-Dimethylphenanthrene	1.3±0.3; 1.3±0.9	2.2; 4.0
1-Methylnaphthalene	8.6±1.9; 14.8±2.2	14.2; 21.3
1-Methylphenanthrene	16.6±3.8; 10.9±2.2	27.8; 17.5
2,6-Dimethylphenanthrene	4.8±0.9; 3.1±0.6	7.6; 4.9
2-Methylnaphthalene	13.1±2.5; 23.7±3.2	20.7; 33.3
2-Methylphenanthrene	22.2±5.4; 13.5±2.4	38.5; 20.6
3,6-Dimethylphenanthrene	8.6±1.8; 6.0±0.8	14.1; 8.5
3-Methylphenanthrene	18.1±4.2; 14.4±2.7	30.8; 22.4
9/4-Methylphenanthrene	13.9±3.4; 9.1±1.7	24.3; 14.4
C2-Naphthalene	26.1±3.8; 43.9±5.2	37.4; 59.5
C3-Naphthalene	28.1±6.3; 58.5±10.6	47.1; 90.3
C4-Naphthalene	25.6±5.6; 30.4±5.3	42.6; 46.3
C2-Phenanthrene	42.3±7.4; 32.9±6.3	64.6; 51.7
C3-Phenanthrene	58.7±14.0; 27.9±7.9	100.7; 51.7
C4-Phenanthrene	14.6±3.3; 8.6±2.1	24.6; 15.0
C1-Chrysene	6.8±1.6; 3.8±0.5	11.6; 5.3
C2-Chrysene	29.6±5.6; 24.4±4.7	46.5; 38.4
C3-Chrysene	4.0±0.7; 4.3±1.0	6.2; 7.4
C4-Chrysene	4.2±0.9; 4.1±0.9	7.0; 7.0
Retene	11.0±2.6; 5.9±1.2	18.9; 9.5
C1-Benzo(*a*)pyrene	6.8±1.4; 1.4±0.3	11.0; 2.3
C2-Benzo(*a*)pyrene	19.0±4.6; 16.8±3.4	32.9; 27.1
Dibenzothiophene	20.8±3.7; 14.5±1.9	32.0; 20.1
C1-Dibenzothiophene	69.9±10.2; 54.3±8.2	100.5; 78.8
C2-Dibenzothiophene	129.1±23.1; 106.1±19.7	198.3; 165.3
C3-Dibenzothiophene	57.8±5.4; 26.7±5.2	74.0; 42.3
C4-Dibenzothiophene	23.4±3.3; 18.2±3.4	33.5; 28.4
C1-Fluorene	58.9±11.0; 30.1±6.2	92.0; 48.4
C2-Fluorene	52.5±9.3; 12.1±2.4	80.4; 19.3
C3-Fluorene	54.0±11.1; 48.2±9.2	87.3; 75.9
C4-Fluorene	56.5±10.7; 39.1±6.9	88.8; 59.5
C1-Pyrene	27.6±3.0; 20.5±3.7	36.6; 31.5
C2-Pyrene	12.8±1.9; 9.2±1.8	18.4; 14.6
C3-Pyrene	26.5±6.7; 21.2±4.1	46.6; 33.4
C4-Pyrene	22.6±5.0; 14.6±2.7	37.6; 22.7

[1] If analyte amounts in samples were smaller than their respective mean + 3 × SD then it was considered a non-detect; [2]First and second mean ± SD values are refrigeration and microwave, respectively; [3]First and second mean ± 3 × SD values are refrigeration and microwave, respectively.

Table SI-4. Amount of PAHs and alkylated polycyclic aromatic compounds (pg) in 1 g of oil incubated under microwave conditions[1].

Analyte	PE	PP	PETG	PC
Acenaphthene	58.0(67.3)[2] 35.9(31.3)[3] 75[4]	nd	nd	116.6(37.7) 116.6(26.7) 50
Acenaphthylene	nd	nd	nd	138.8(152.2) 138.8(107.7) 50
Benz(*a*)anthracene	nd	nd	nd	52.3(35.4) 52.30(25.0) 50
Benzo(*a*)pyrene	nd	nd	289.7(215.9) 172.4(74.7) 100	nd
Benzo(*b*)fluoranthene	15.3(10.9) 16.3(9.3) 75	nd	nd	nd
Benzo(*g*,*h*,*i*)perylene	10.6(5.5) 12.0(2.9) 100	nd	nd	nd
Chrysene	nd	nd	nd	144.8(68.0) 144.8(48.1) 50
Dibenzo(*a*,*h*)anthracene	nd	nd	82.1(63.0) 76.8(51.9) 100	nd
Fluoranthene	nd	nd	2802.7(162.1) 2710.1(23.4) 75	283.2(58.2) 283.2(41.6) 50
Fluorene	nd	nd	683.4(22.6) 710.8(146.8) 75	538.1(106.8) 283.2(41.6) 50
Naphthalene	nd	nd	5183.1(806.2) 5124.4(799.8) 75	1056.8(1178.1) 1056.8(833.0) 50
Phenanthrene	nd	nd	4960.6(749.9) 4582.2(364.8) 75	545.1(123.8) 545.1(87.5) 50
Pyrene	nd	nd	2703.5(1110.8) 2763.2(1105.9) 75	nd
Anthracene	nd	nd	516.7(189.8) 445.1(143.7)	253.7(246.0) 253.7(173.9)

			75	50
Low molecular weight PACs				
1-Methylnaphthalene	nd	435.1(263.8) 435.1(186.5) 50	nd	nd
2-Methylnaphthalene	1041.0(1166.2) 1041.0(824.6) 50	686.7(366.8) 686.7(259.4) 50	nd	739.6(639.6) 531.9(201.7) 100
C2-Naphthalene	1395.0(1265.5) 858.8(235.5) 100	1176.7(330.9) 1176.7(234.0) 50	nd	nd
C3-Naphthalene	2677.7(1269.9) 2063.9(43.6) 100	3869.8(67.9) 3869.8(48.0) 50	nd	1823.2(98.9) 1823.2(70.0) 50
C4-Naphthalene	1287.5(680.1) 1226.9(497.0) 100	1939.7(373.2) 1939.7(263.9) 50	1097.2(885.2) 1133.9(829.4) 75	1242.5(1174.4) 1111.2(840.8) 100
2-Methylphenanthrene	nd	456.7(193.8) 456.7(137.0) 50	41.6(38.0) 40.6(36.5) 75	nd
3-Methylphenanthrene	nd	475.3(182.0) 475.3(128.7)	193.4(208.2) 163.9(162.3) 75	nd
1,7-Dimethylphenanthrene	73.1(64.4) 73.1(45.5) 50	nd	199.0(174.3) 164.0(104.2) 100	296.8(395.8) 296.8(279.9) 50
1,8-Dimethylphenanthrene	nd	nd	169.8(73.1) 200.4(22.2) 75	188.2(114.7) 170.6(68.7) 100
1-Methylphenanthrene	nd	294.0(202.8) 294.0(143.4) 50	142.1(49.2) 159.6(20.6) 75	nd
2,6-Dimethylphenanthrene	144.8(150.1) 144.8(106.2) 50	163.8(3.6) 163.8(2.5) 50	1238.0(242.6) 1313.9(75.9) 100	nd
3,6-Dimethylphenanthrene	nd	170.7(71.9) 170.7(50.8) 50	222.0(145.2) 274.1(59.9) 75	nd
9/4-Methylphenanthrene	nd	260.9(68.8) 260.9(48.6) 50	94.2(86.9) 94.2(61.3) 50	nd
C2-Phenanthrene	538.2(64.4) 538.2(45.5) 50	nd	571.3(627.5) 465.0(461.3) 75	1436.1(428.9) 1417.9(305.6) 100

C3-Phenanthrene	6243.1(4231.1) 5125.4(1445.3) 100	809.4(88.2) 809.4(62.4) 50	739.7(127.7) 739.7(90.3) 75	nd
C4-Phenanthrene	992.1(544.9) 895.3(294.3) 100	216.4(163.1) 216.4(115.3) 50	nd	nd
C1-Fluorene	1170.3(731.7) 1170.3(517.4) 50	nd	2351.2(22.62.9) 1277.8(87.2) 100	nd
C2-Fluorene	791.5(183.9) 791.5 (130.1) 50	833.0(186.2) 833.0(131.7) 50	1944.3(249.1) 1975.5(140.3) 100	nd
C3-Fluorene	2913.8(205.2) 2913.8(145.1) 50	1960.9(189.6) 1960.9(134.1) 50	5544.4(1847.8) 5397.0(1405.4) 100	nd
C4-Fluorene	2296.3(1049.2) 2296.3(741.9) 50	1561.7(973.0) 1561.7(688.0) 50	4303.9(879.7) 4488.5(459.4) 100	nd
Dibenzothiophene	68.5(40.1) 68.5(28.4) 50	63.9(40.1) 63.9(28.3) 50	983.3(123.8) 1009.9(64.4) 100	nd
C1-Dibenzothiophene	1348.2(397.2) 1348.2(280.9) 50	nd	3600.2(464.9) 3762.3(145.5) 100	nd
C2-Dibenzothiophene	4121.0(339.1) 4121.0(239.9) 50	1866.7(309.0) 1866.7(218.5) 50	5924.6(1334.9) 5813.8(899.5) 100	nd
C3-Dibenzothiophene	888.3 (678.4) 888.3 (479.7) 50	574.0(644.7) 574.0(455.9) 50	2428.3(625.2) 5397.0(1405.4) 100	nd
C4-Dibenzothiophene	1505.3(1554.1) 1505.3 (1098.9) 50	1250.2(1476.9) 1250.2(1044.3) 50	2746.9(1043.0) 2756.0(848.6) 100	nd
Retene	1518.4(210.2) 1433.2(40.9) 100	130.1(129.4) 130.1(91.5) 50	560.1(287.2) 666.9(111.7) 75	nd
High molecular weight PACs				
C1-Chrysene	556.5(272.1) 405.2(11.6) 75	nd	nd	1059.3(328.8) 1240.2(17.7) 75
C2-Chrysene	766.5(841.2) 430.7(285.6) 75	nd	nd	4709.3(3582.4) 4717.6(3569.9) 75
C3-Chrysene	324.2(169.6)	nd	2489.2(2371.3)	nd

	319.7(163.2) 75		2489.2(1676.7) 50	
C4-Chrysene	nd	nd	1797.6(1986.0) 1260.4(754.7) 100	1129.4(927.2) 607.3(26.4) 75
C1-Benzo(*a*)pyrene	129.6(21.0) 129.6(14.8) 50	37.2(16.3) 37.2(11.5) 50	499.5(301.5) 429.8(134.9) 100	100.5(37.0) 100.5(26.2) 50
C2-Benzo(*a*)pyrene	nd	nd	2175.7(1439.8) 2391.1(927.7) 100	nd
C1-Pyrene	1427.7(999.6) 1427.7 (706.9) 50	nd	2048.4(470.6) 2092.4(332.2) 100	nd
C2-Pyrene	807.7(14.7) 807.7 (10.4) 50	459.3(12.7) 459.3(9.0) 50	1667.9(1102.8) 1310.0(352.3) 100	nd
C3-Pyrene	3473.2(2868.9) 3473.2(2028.6) 50	1757.3(2230.2) 1757.3(1577.0) 50	3476.3(1241.0) 3560.9(813.9) 100	nd
C4-Pyrene	2627.5(1941.8) 2627.5(1373.1) 50	1322.8(1484.8) 1322.8(1049.9) 50	3145.6(1064.8) 3259.1(709.8) 100	nd

[1]Total surface area of plastic used in each incubation was 19.36 mm^2 (2×9.68 mm^2). [2]Arithmetic mean and standard deviation (shown in brackets); [3]Median and median absolute error (shown in brackets); [4]The frequency of detection.

Table SI-5. Estimated incremental lifetime cancer risk (ILCR) from exposure to PACs migrating from PE, PE, PETG and PP under refrigeration and microwave conditions.

Compound	**TEF**[1]	**PE**	**PC**	**PETG**	**PP**
		Refrigeration conditions			
Acenapthene	0.001	8.7×10^{-9}			
Acenaphthylene	0.001		4.9×10^{-11}		
C4-naphthalene	0.001	6.9×10^{-8}	5.6×10^{-10}	3.3×10^{-9}	1.6×10^{-8}
C4-phenanthrene	0.001			1.7×10^{-9}	
C4-fluorene	0.001			1.6×10^{-9}	
C4-pyrene	0.001			1.1×10^{-9}	
C2-dibenzothiophene	0.001	3.2×10^{-8}			
∑ILCR[2]		1.1×10^{-7}	6.1×10^{-10}	7.8×10^{-9}	1.6×10^{-8}
		Microwave conditions			
Naphthalene	0.001			1.5×10^{-9}	
Phenanthrene	0.001			1.4×10^{-9}	
Fluorene	0.001			2.0×10^{-10}	
Dibenzoanthracene	1			2.9×10^{-7}	
Dibenzothiophene	0.001			2.9×10^{-10}	
2,6-dimethylphenanthrene	0.001			3.6×10^{-10}	
C1-pyrene	0.001			6.0×10^{-10}	
C2-fluorene	0.001			5.7×10^{-9}	
C2-dibenzothiophene	0.001			1.7×10^{-9}	
C4-fluorene	0.001			1.3×10^{-9}	
C2-phenanthrene	0.001		1.3×10^{-10}		
Retene	0.001	1.0×10^{-8}			
∑ILCR		1.0×10^{-8}	1.3×10^{-10}	3.0×10^{-7}	

[1]Toxic equivalence factors obtained from Nisbet and LaGoy (1992) and Samburova *et al*. (2017). [2]Total ILCR (∑) determined by summing ILCR values for individual PACs detected.

Figure SI-1. Arithmetic mean ± standard deviation percent of mass labeled polycyclic aromatic hydrocarbons measured in oil on days 0.08, 1, 4, 6, 8 and 10.