Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supplementary Material

Table S1: Limit of Detection (LOD)

PAHs	Abbreviation	Number of Rings	m/z ratio	LOD (μg ml^{-1})
Napthalene	Nap	2	128	0.84
Acenapthylene	Acy	3	152	1.85
Acenapthene	Ace	3	154	0.05
Fluorene	Fluo	3	166	0.51
Phenanthrene	Phen	3	178	0.78
Anthracene	Anth	3	178	0.02
Fluoranthene	Fla	4	202	0.01
Pyrene	Pyr	4	202	0.01
Benzo(a)anthracene	BaA	4	228	0.15
Chrysene	Chy	4	228	0.02
Benzo(b)fluoranthene	BbF	5	252	0.18
Benzo(k)fluoranthene	BkF	5	252	0.18
Benzo(a)pyrene	BaP	5	252	1.42
Indeno[*1*,*2*,*3-cd*]pyrene	IP	5	276	0.12
Dibenz[a,h]anthracene	DbA	5	278	0.11
Benzo[g,h,j]perylene	BghiP	6	276	0.06
3-Nitrofluoranthene	3-Nfla	4	247	0.01
1-Nitropyrene	1-Npyr	4	247	1.19

Table S2: Concentration of PAHs

PAHs	Rural Site		Traffic Site		Gas + Particulate(ng m^{-3})		
	Gas phase (ng m^{-3})	Particulate phase (ng m^{-3})	Gas phase (ng m^{-3})	Particulate phase (ng m^{-3})	Rural Site	Traffic Site	Traffic / Rural
Nap	6 ± 4.8	1.4 ± 1.8	7.8 ± 6	11.5 ± 1	7.5	19.4	2.5
Acy	5.8 ± 3.2	5.8 ± 3.5	9.8 ± 8.7	8.4 ± 3	11.6	18.2	1.5
Ace	17.6 ± 15.8	30.4 ± 25	26.7 ± 25	101.2 ± 56.4	48	127.9	2.6
Fluo	20.9 ± 18.9	25.6 ± 24.2	33.7 ± 18.4	119.4 ± 74	46.6	153.2	3.2
Phen	80.2 ± 47.6	9.5 ± 9.5	167.5 ± 118.3	91.1 ± 54.5	89.7	258.6	2.8
Anth	29.9 ± 32.8	2.9 ± 2.2	56.6 ± 37.9	42.3 ± 17	32.8	98.9	3
Fla	11.2 ± 9.9	1.6 ± 1.7	30.4 ± 27.9	31 ± 23	12.8	61.5	4.7
Pyr	56.5 ± 62	17.3 ± 22.8	58.7 ± 30.6	89.7 ± 69.4	73.8	148.4	2
BaA	10.8 ± 12.6	18.5 ± 14.5	29.4 ± 28.2	265.6 ± 210	29.3	295	10
Chy	35.5 ± 32.8	34.9 ± 26.1	48.3 ± 23.6	375.7 ± 194.4	70.4	424.1	6
BbF	1.6 ± 2.9	40.1 ± 43.3	4.1 ± 2.4	499.8 ± 262	41.7	503.9	12
BkF	0.6 ± 1.3	52.6 ± 28.8	4.1 ± 2.7	520.8 ± 302.3	53.2	524.9	9.8
BaP	9.7 ± 2.7	36.5 ± 23.9	15 ± 3.2	400.9 ± 241.2	46.2	416	9
IP	1.2 ± 1.3	34.1 ± 22.6	5.2 ± 4	370.3 ± 229	35.4	375.5	10.5
DbA	0.9 ± 0.5	9.4 ± 7.1	4.2 ± 3	111.3 ± 78.7	10.3	115.5	11.1
BghiP	0.7 ± 1.7	13.1 ± 14.1	4.6 ± 4	468.8 ± 286.2	13.9	473.4	34
∑ of PAHs	289.8 ± 22.6	334.2 ± 15.7	506.8 ± 40.9	3508.3 ± 189.2	624	4015.2	6.4
3-Nfla	3.7 ± 4.2	3.9 ± 2.0	4.5 ± 2.3	14.7 ± 6.5	7.6	19.3	2.5
1-Npyr	12.1 ± 4.4	9.2 ± 12.4	13.2 ± 5.1	18.9 ± 9	21.4	32.2	1.5
∑ of Nitro-PAHs	15.8 ± 5.9	13.2 ± 3.7	17.8 ± 6.1	33.7 ± 2.9	29	51.5	1.7

Table S3: Mean, minimum and maximum of log *Kp*

PAHs	log *Kp*					
	Traffic site			Rural site		
	Mean	Min	Max	Mean	Min	Max
Nap	-2.66	-3.58	-1.69	-3.15	-3.98	-1.46
Acy	-2.68	-3.53	-2.05	-2.44	-2.83	-2.16
Ace	-1.92	-2.81	0.44	-2.02	-2.50	-0.54
Fluo	-2.17	-2.62	-1.51	-2.34	-2.96	-1.47
Phen	-2.80	-3.65	0.93	-3.51	-4.66	-2.34
Anth	-2.55	-3.54	1.16	-2.51	-4.95	0.53
Fla	-2.39	-3.46	1.20	-2.97	-3.75	-0.10
Pyr	-2.28	-2.94	1.83	-1.78	-3.50	1.02
BaA	-1.48	-2.83	0.36	-2.01	-3.09	-1.01
Chy	-1.83	-2.55	-1.31	-2.04	-3.39	0.84
BbF	-0.58	-1.67	1.30	-0.45	-1.98	0.76
BkF	-0.57	-2.75	1.12	-0.09	-1.33	0.48
BaP	-1.37	-2.03	-0.85	-1.97	-2.57	-1.46
IP	-0.83	-1.99	0.05	-1.04	-1.69	-0.33
DaA	-1.26	-2.22	-0.54	-1.51	-1.85	-1.21
BghiP	-0.42	-1.19	1.77	-0.42	-2.30	0.63
3-Nfla	-2.27	-2.88	-1.61	-2.05	-2.78	0.47
1-Npyr	-2.60	-3.12	-2.25	-2.69	-3.06	-1.82

Table S4: Regression Statistics of log *Kp* vs log P^o_l

PAHs	Rural Site			Traffic Site		
	m	b	r^2	M	b	r^2
Ace	-0.08	-0.24	0.69	-0.04	-0.15	0.95
Fluo	-0.19	-0.29	0.78	-0.13	-0.19	0.76
Phen	-0.27	-0.47	0.75	-0.21	-0.31	0.92
Anth	-0.06	0.28	0.88	-0.21	-0.22	0.72
Fla	-0.17	0.46	0.92	-0.74	-1.41	0.58
Pyr	-0.15	0.66	0.93	-2.83	-6.68	0.75
BaA	-0.84	-0.30	0.81	-0.06	1.95	0.82
Chy	-0.33	1.20	0.98	-1.87	-1.06	0.74
BbF	-0.56	2.59	0.71	-0.59	2.54	0.84
BkF	-0.81	2.29	0.80	-0.71	2.31	0.85
BaP	-3.15	-3.61	0.80	-2.78	-1.64	0.87

Table S5: Regression parameters for temperature dependence of log *Kp*and ln P

PAHs	log *Kp Vs 1/T*						ln P Vs 1/T					
	Traffic site			Rural site			Traffic site			Rural site		
	m	b	r^2	m	b	r^2	m	b	r^2	m	b	r^2
Nap	26932	-95.29	0.95	4585	-19.09	0.13	-11070	10.3	0.21	-16494	29.5	0.47
Acy	8540	-31.93	0.54	3244	-13.45	0.60	-20926	44.5	0.46	-7336.4	-3.1	0.64
Ace	15112	-54.38	0.66	4930	-19.13	0.59	-22846	52.2	0.23	-37296	101.3	0.49
Fluo	10972	-39.97	0.71	11892	-43.01	0.56	-15474	27.1	0.36	-29137	73.4	0.51
Phen	14559	-53.29	0.77	7953	-30.63	0.68	-27043	68.8	0.91	-17375	34.7	0.81
Anth	11500	-42.34	0.47	23404	-83.94	0.28	-20076	43.4	0.21	-21141	46.7	0.31
Fla	20569	-73.35	0.55	2979.9	-13.66	0.47	-38918	107.5	0.37	-20256	42.3	0.48
Pyr	12903	-47.08	0.23	33717	-118.01	0.48	-27231	68.2	0.65	-25038	60.8	0.49
BaA	33777	-117.77	0.79	16877	-60.04	0.92	-52883	115.4	0.53	-20594	43.1	0.34
Chy	5704.7	-21.21	0.44	11768	-42.89	0.79	-25600	61.7	0.34	-24671	58.4	0.53
BbF	16986	-59.04	0.50	18706	-64.96	0.77	-9848.6	5.1	0.09	-1179.5	-28.3	0.08
BkF	51299	-177.35	0.76	8561	-29.44	0.67	-8642.1	0.9	0.02	-979.6	-29	0.07
BaP	3061	-11.84	0.32	2367	-9.78	0.17	-2689.5	-18	0.07	-4246.5	-13	0.08
IP	85736	-296.90	0.68	8230	-29.58	0.72	-8132.2	-0.9	0.03	-1373	-26	0.06
DbA	10789	-38.09	0.47	12801	-45.78	0.64	-937.5	-25.3	0.008	-860.15	-26.7	0.01
BghiP	17472	-61.36	0.24	16133	-56.10	0.62	-1287	-23.9	0.003	-9681.2	0.3	0.05
3-Nfla	14539	-52.34	0.64	12350	-44.94	0.27	-32021	81.8	0.65	-22008	46.8	0.46
1-Npyr	7871	-29.62	0.27	6078	-23.55	0.78	-23346	52.6	0.43	-16672	30	0.40

m = slope
b = intercept
r^2 = coefficient of determination

Table S6: Toxic Equivalence Factors for PAHs

PAHs	TEF*	Rural site				Traffic site			
		Gas phase		Particulate phase		Gas phase		Particulate phase	
		Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.
BaA TEQ	0.1	1.09	1.26	1.85	1.45	2.95	2.82	26.56	21.00
Chy TEQ	0.01	0.36	0.33	0.35	0.26	0.48	0.24	3.76	1.94
BbF TEQ	0.1	0.16	0.29	4.01	4.34	0.42	0.24	49.98	26.20
BkF TEQ	0.1	0.07	0.13	5.26	2.88	0.41	0.28	52.08	30.23
BaP TEQ	1	9.74	2.76	36.50	23.92	15.08	3.20	400.96	241.20
IP TEQ	0.1	0.13	0.14	3.42	2.26	0.52	0.41	37.03	22.91
DbA TEQ	5	4.59	2.60	47.24	35.55	21.06	15.18	556.62	393.88
BghiP TEQ	0.01	0.01	0.02	0.13	0.14	0.05	0.04	4.69	2.86
∑8 PAHs	NA	16.15	3.48	98.76	18.53	40.97	8.20	1131.68	213.08
3-NFla	0.0026	0.01	0.01	0.01	0.01	0.01	0.01	0.04	0.02
1-NPyr	0.1	1.21	0.45	0.93	1.24	0.45	0.23	1.90	0.91
∑2 N-PAHs	NA	1.22	0.85	0.94	0.65	0.47	0.31	1.94	1.31

*TEF: toxic equivalency factors for cancer potency relative to BaP (Nisbet and LaGoy, 1992) for priority PAH and for nitro-PAHs (Wei *et al*., 2014)

BaP-TEQ: Carcinogenic equivalents calculated from the cancer potency relative to BaP (TEF) multiplied by the concentration of PAH in a sample.

Σ8 PAH includes Benz(a)Anthracene (BaA), Chrysene (Chy), Benzo(b)Fluoranthene (BbF), Benzo(k)Fluoranthene (BkF), Benzo (a) Pyrene (BaP), Indeno (1,2,3-c,d) Pyrene (IP), Dibenz (a,h) Anthracene (DbA), and Benzo (ghi) Perylene (BghiP).

Σ2 N-PAHs includes: 3- NitroFluoranthene (3-NFla) and 1-NitroPyrene (1-NPyr)

Table S7: Mutagenic Equivalence Factors for PAHs

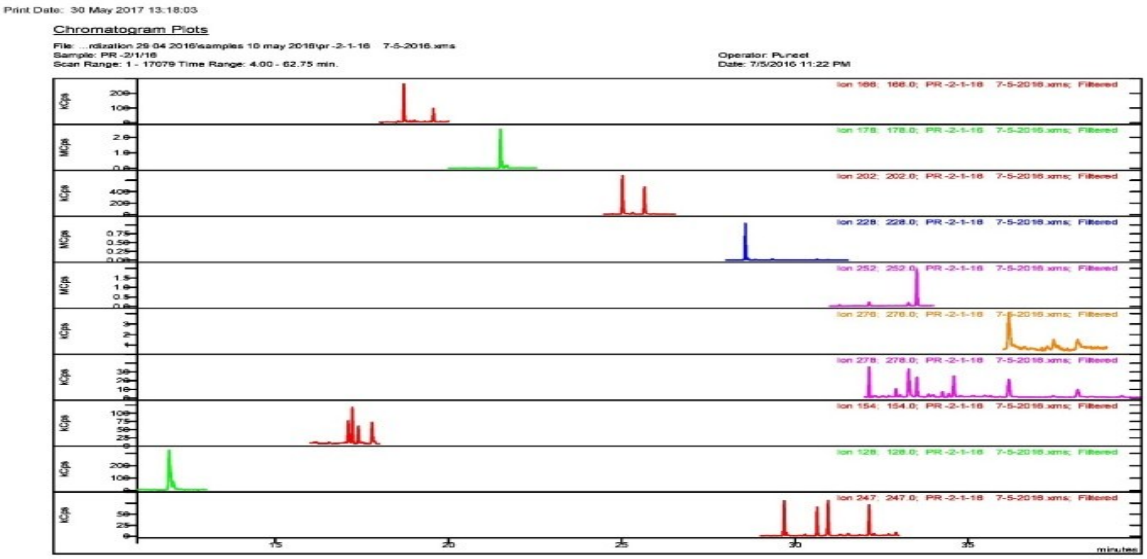
PAHs	MEF*	Rural site				Traffic site			
		Gas phase		Particulate phase		Gas phase		Particulate phase	
		Mean	S.D.	Mean	S.D.	Mean	S.D.	Mean	S.D.
BaA MEQ	0.082	0.89	1.04	1.52	1.19	2.42	2.32	21.78	17.22
Chy MEQ	0.017	0.60	0.56	0.59	0.45	0.82	0.40	6.39	3.31
BbF MEQ	0.25	0.40	0.73	10.03	10.84	1.04	0.60	124.95	65.51
BkF MEQ	0.11	0.07	0.14	5.79	3.17	0.45	0.31	57.29	33.25
BaP MEQ	1	9.74	2.76	36.50	23.92	15.08	3.20	400.96	241.20
IP MEQ	0.31	0.40	0.42	10.59	7.01	1.62	1.26	114.80	71.02
DbA MEQ	0.29	0.27	0.15	2.74	2.06	1.22	0.88	32.28	22.84
BghiP MEQ	0.19	0.01	0.03	0.25	0.27	0.09	0.08	8.91	5.44
∑8 PAHs	NA	12.38	3.32	68.01	12.01	22.74	5.00	767.36	131.41

*MEF: mutagenic potency factor relative to BaP (Durant *et al*., 1996 and 1999)

BaP-MEQ: Mutagenic equivalents calculated from the mutagenic potency relative to BaP (MEF) multiplied by the concentration of PAH in a sample.

Σ8PAH includes Benz(a)Anthracene (BaA), Chrysene (Chy), Benzo(b)Fluoranthene (BbF), Benzo(k)Fluoranthene (BkF), Benzo (a) Pyrene (BaP), Indeno (1,2,3-c,d) Pyrene (IP), Dibenz (a,h) Anthracene (DbA), and Benzo (ghi) Perylene (BghiP).

Figure S1: Chromatogram of Samples in Selected Ion Monitoring (SIM) Mode (a) Gas phase- Rural site (b) Particulate phase – Rural site (c) Gas phase - Traffic site (d) Particulate phase - Traffic Site



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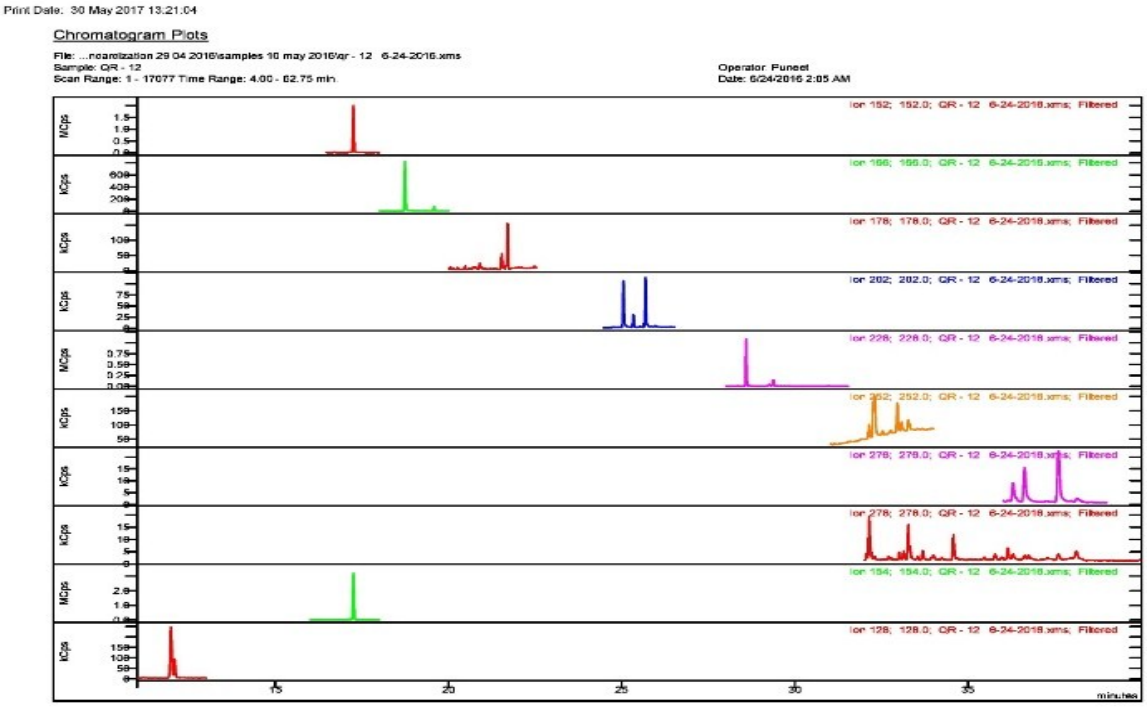

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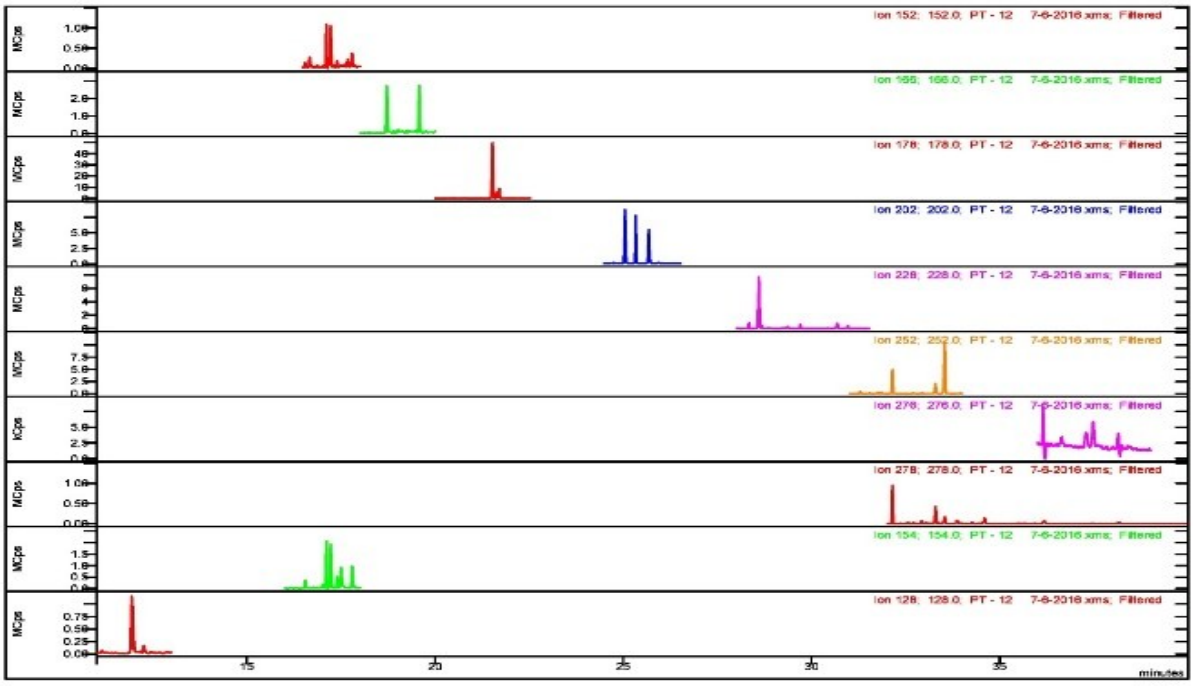

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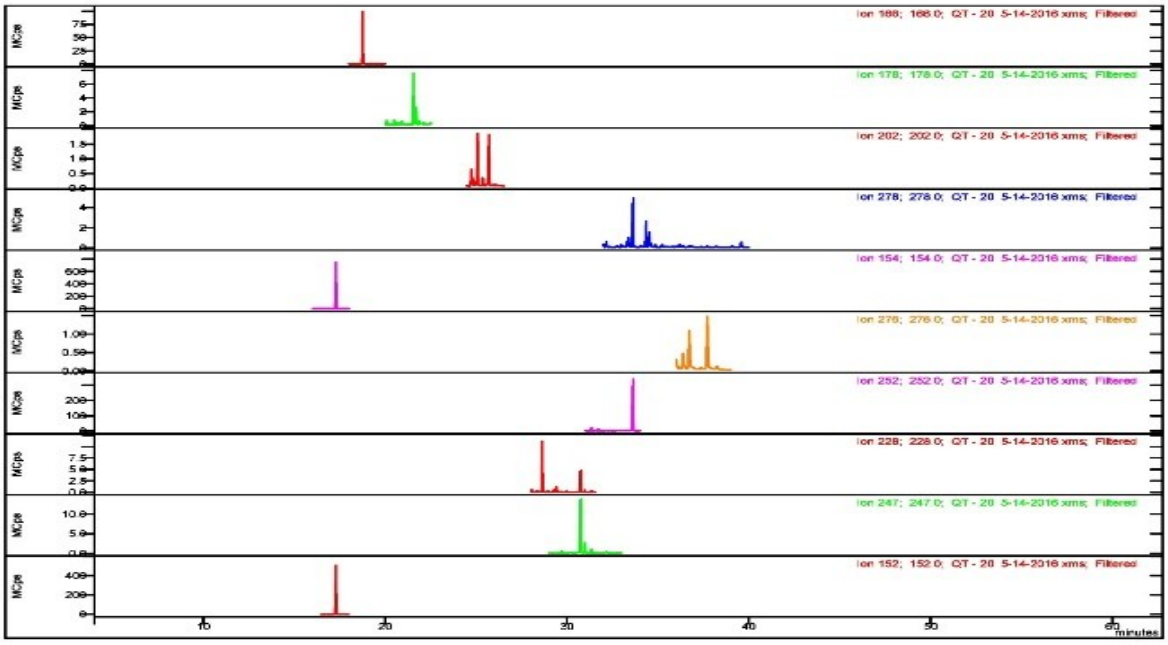

(d)