Supplementary Material (ESI) for Journal of Environmental Monitoring

Electronic supplementary information

Evaluation of PAH Diagnostic Ratios as Source Apportionment Tools for Inhalable Air Particulate Collected in an Urban-industrial Environment

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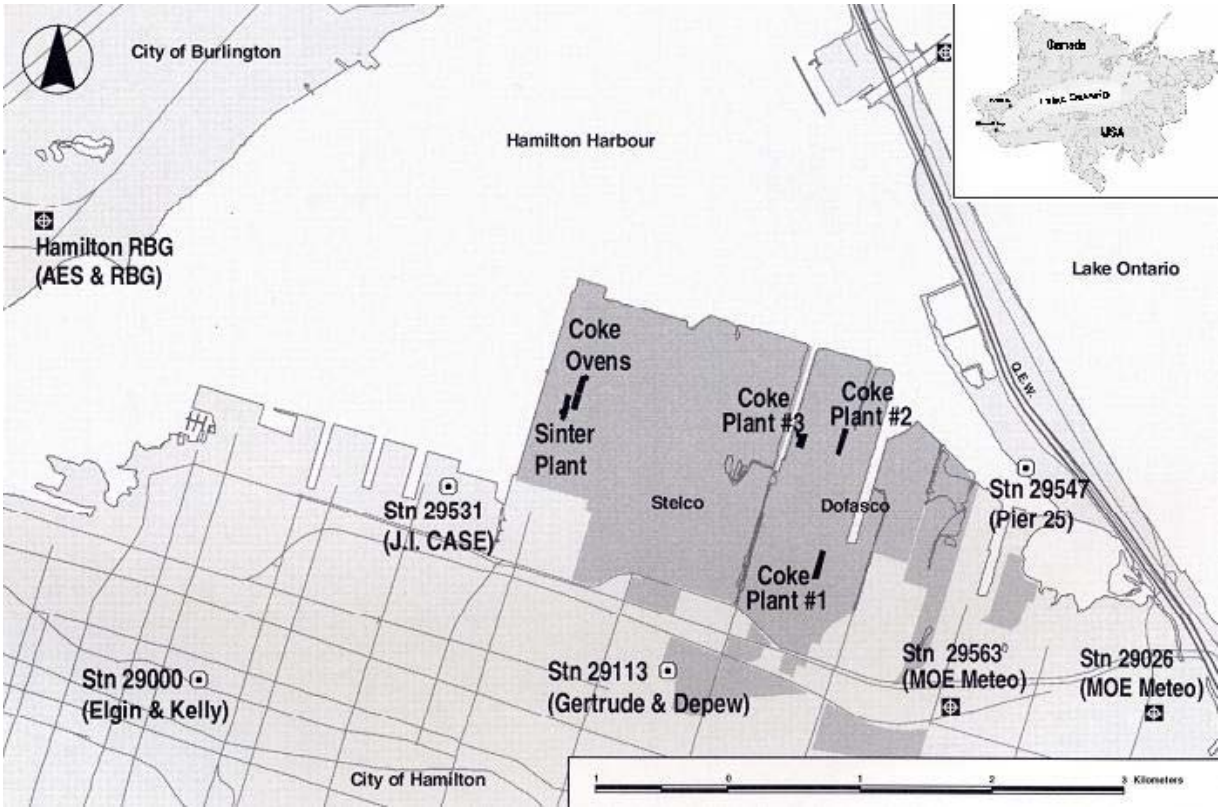

Figure S1: Map of Hamilton showing locations of air particulate sampling and meteorological stations of study in relation to the steel industries shaded dark grey. (Inset map courtesy Great Lakes Website: http://www.epa.gov/glnpo/lakeont/2002highlight/index.html).

Table S1: GC/MS SIM program and instrumental conditions used for current work

Group #	Start Time (min)	Ions Monitored
1	10	128,129,139,141,142,151,152,153,154,165,166, 178,179,184,188,189,191,192,197,198
2	35	152,180,191,192,197,198,202,203,205,206,208, 211,212,219,220,225,226,229.230
3	43	163,191,202,203,205,206,208,212,213,215,216, 219,220,221,222,225,226,229,230,231
4	50	117,189,202,215,216,221,222,226,227,228,229, 230,234,235,236,243,244
5	56	117,189,202,226,227,228,229,230,234,235,236, 239,240,241,242,243,244,247,248,255,256
6	59	117,189,201,202,217,230,234,239,240,241,242, 243,244,247,248,255,256,261,262,275,276
7	61	201,217,230,239,240,241,242,247,248,253,254, 255,256,258,261,262,269,270,275,276
8	63	201,217,230,239,240,241,242,247,253,254,255, 256,258,261,262,267,268,269,270,275,276
9	65	213,252,253,254,255,256,258,261,262,265,266, 267,268,269,270,271,272,275,276
10	69	213,252,253,254,258,260,264,265,266,267,268. 269,270,271,272,275,276,285,286,280
11	70	213,252,253,258,260,264,265,266,268,269,270, 271,272,275,276,279,280,285,286,299,300
12	72	239,252,265,266,268,269,270,271,272,275,276, 278,279,280,284,285,286,293,294,299,300
13	76	239,271,272,276,277,278,279,280,284,285,286, 288,289,290,292,293,294,299,300,303,304
14	79	239,271,272,276,277,278,279,280,284,285,286, 289,290,292,293,294,299,300,303,304,306
15	81	150,239,276,277,278,284,285,286,289,290,292, 293,294,299,300,302,303,304,306,317,318

Property	**Conditions**
Stationary Phase	DB-17ht
Column Length (m)	30
Column I.D. (mm)	0.25
Film Thickness (μm)	0.15
Injector Type	Cool on-column
Detector Temp. (^{o}C)	300
Carrier Gas	He
Flow Rate (mL/min)	1.0
Oven Temperature Program	
Initial Temp. (^{o}C)	90
Rate (^{o}C /min)	2.5
Final Temp. (^{o}C)	300
Final Time (min)	20

Table S2: PAH diagnostic ratios measured in air particulate samples used in current work and their TPAH concentrations. 178-228 MeanRatio is defined as 0.5(BaA/∑228 + An/∑178). (SRM 1649a = NIST urban dust standard; SRM 1650b = NIST diesel particulate standard; SRM 1597a = NIST coal tar standard; Gert = GERTRUDE; P25P10 = Pier 25 PM_{10})

Site-Date	1,7/1,7+ 2,6 DMP	Phen/(Phen+∑MePher	IP/(BghiP+IF	BaA/∑228	Fl/Fl+Py	An/∑178	178-228 MeanRa	TPAH (ng m-3
GERT-Jul 20	0.42	0.68	0.483	0.297	0.539	0.172	0.235	1.16
GERT-Jul 23	0.47	0.63	0.499	0.330	0.551	0.110	0.220	0.74
GERT-Jul 29	0.50	0.44	0.413	0.298	0.522	0.139	0.219	1.79
GERT-Aug 01	0.39	0.66	0.657	0.313	0.545	0.172	0.242	2.62
GERT-Aug 04	0.51	0.66	0.511	0.388	0.529	0.148	0.268	9.58
GERT-Aug 05	0.56	0.37	0.470	0.333	0.532	0.150	0.242	0.88
GERT-Aug 06	0.57	0.54	0.536	0.401	0.523	0.111	0.256	3.23
GERT-Aug 07	0.55	0.29	0.484	0.424	0.515	0.148	0.286	6.55
GERT-Aug 08	0.56	0.70	0.551	0.423	0.545	0.200	0.312	14.92
GERT-Aug 09	0.00	0.65	0.685	0.388	0.531	0.218	0.303	6.00
GERT-Aug 10	0.44	0.66	0.649	0.357	0.522	0.172	0.265	5.02
GERT-Aug 11	0.50	0.64	0.407	0.344	0.555	0.114	0.229	1.16
GERT-Aug 12	0.52	0.67	0.445	0.422	0.477	0.204	0.313	7.60
GERT-Aug 13	0.46	0.69	0.538	0.392	0.511	0.187	0.289	13.29
GERT-Aug 14	0.52	0.53	0.544	0.428	0.503	0.220	0.324	51.89
GERT-Aug 15	0.00	0.67	0.634	0.394	0.541	0.173	0.283	3.10
GERT-Aug 16	0.50	0.67	0.478	0.390	0.538	0.203	0.297	12.54
GERT-Aug 18	0.00	0.58	0.579	0.404	0.518	0.264	0.334	16.65
GERT-Aug 19	0.54	0.48	0.554	0.255	0.528	0.000	0.128	20.04
GERT-Aug 20	0.45	0.62	0.709	0.336	0.527	0.103	0.220	17.82
JICASE-Jul 20	0.45	0.72	0.605	0.375	0.527	0.152	0.263	2.94
JICASE-Jul 23	0.52	0.62	0.536	0.359	0.552	0.125	0.242	0.80
JICASE-Jul 27	0.44	0.62	0.604	0.426	0.518	0.227	0.327	42.56
JICASE-Jul 28	0.49	0.58	0.537	0.438	0.524	0.168	0.303	19.50
JICASE-Jul 29	0.50	0.55	0.231	0.309	0.432	0.130	0.220	1.43
JICASE-Aug 01	0.63	0.65	0.717	0.400	0.511	0.167	0.283	9.85
JICASE-Aug 02	0.00	0.63	0.354	0.455	0.492	0.275	0.365	*101*
JICASE-Aug 04	0.47	0.61	0.510	0.402	0.516	0.213	0.307	18.64
JICASE-Aug 05	0.53	0.10	0.485	0.251	0.543	0.000	0.125	0.34
JICASE-Aug 06	0.40	0.47	0.505	0.448	0.491	0.218	0.333	48.37
JICASE-Aug 07	0.47	0.56	0.449	0.451	0.501	0.243	0.347	172.68
JICASE-Aug 08	0.45	0.58	0.479	0.441	0.504	0.205	0.323	102.60
JICASE-Aug 09	0.46	0.60	0.656	0.409	0.468	0.225	0.317	29.50
JICASE-Aug 10	0.41	0.60	0.694	0.384	0.512	0.164	0.274	13.11
JICASE-Aug 11	0.51	0.63	0.177	0.272	0.569	0.098	0.185	1.67
JICASE-Aug 12	0.50	0.66	0.496	0.368	0.534	0.170	0.269	1.04
JICASE-Aug 13	0.45	0.57	0.555	0.437	0.503	0.261	0.349	33.70
JICASE-Aug 14	0.48	0.60	0.574	0.427	0.486	0.213	0.320	76.99
JICASE-Aug 15	0.44	0.57	0.554	0.319	0.528	0.165	0.242	10.32
JICASE-Aug 16	0.00	0.55	0.679	0.444	0.491	0.223	0.333	47.23
JICASE-Aug 18	0.47	0.55	0.532	0.417	0.485	0.224	0.321	64.39
JICASE-Aug 19	0.52	0.51	0.457	0.405	0.498	0.178	0.292	92.68
JICASE-Aug 20	0.51	0.55	0.562	0.356	0.530	0.105	0.230	10.91

Site-Date	1,7/1,7+ 2,6 DMI	Phen/(Phen+∑MePhe	IP/(BghiP+IF	BaA/∑228	Fl/Fl+Py	An/∑178	178-228	MeanR	TPAH (ng m-3)
KELLY-Jul 20	0.48	0.66	0.280	0.352	0.512	0.117	0.235		1.26
KELLY-Jul 23	0.51	0.65	0.364	0.428	0.505	0.120	0.274		4.45
KELLY-Aug 02	0.50	0.66	0.347	0.460	0.516	0.218	0.339		13.51
KELLY-Aug 06	0.58	0.51	0.394	0.441	0.514	0.174	0.308		11.53
KELLY-Aug 07	0.52	0.64	0.351	0.450	0.510	0.212	0.331		22.03
KELLY-Aug 08	0.45	0.55	0.378	0.424	0.481	0.211	0.318		15.87
KELLY-Aug 09	0.46	0.58	0.385	0.409	0.492	0.199	0.304		16.58
KELLY-Aug 11	0.52	0.50	0.303	0.293	0.549	0.078	0.185		0.98
KELLY-Aug 12	0.00	0.67	0.256	0.361	0.554	0.098	0.230		1.05
KELLY-Aug 15	0.49	0.64	0.195	0.273	0.518	0.096	0.185		1.18
P25P10-Jul 20	0.45	0.62	0.559	0.449	0.504	0.286	0.368		37.72
P25P10-Jul 23	0.47	0.58	0.573	0.454	0.507	0.252	0.353		54.86
P25P10-Jul 27	0.49	0.62	0.555	0.299	0.544	0.108	0.203		3.99
P25P10-Jul 28	0.47	0.65	0.513	0.405	0.524	0.224	0.314		18.18
P25P10-Jul 29	0.48	0.54	0.499	0.445	0.504	0.220	0.332		67.34
P25P10-Aug 01	0.40	0.52	0.646	0.429	0.518	0.240	0.334		30.92
P25P10-Aug 02	0.45	0.59	0.364	0.308	0.514	0.167	0.237		2.16
P25P10-Aug 04	0.46	0.55	0.520	0.379	0.539	0.213	0.296		18.56
P25P10-Aug 05	0.61	0.53	0.553	0.385	0.495	0.048	0.217		4.22
P25P10-Aug 06	0.65	0.26	0.489	0.288	0.504	0.000	0.144		0.23
P25P10-Aug 07	0.65	0.14	0.424	0.275	0.488	0.000	0.138		0.73
P25P10-Aug 08	0.45	0.64	0.643	0.286	0.513	0.157	0.222		2.20
P25P10-Aug 09	0.44	0.64	0.672	0.319	0.527	0.161	0.240		1.28
P25P10-Aug 10	0.45	0.57	0.703	0.390	0.513	0.199	0.295		4.58
P25P10-Aug 11	0.55	0.57	0.508	0.438	0.481	0.246	0.342		40.73
P25P10-Aug 12	0.49	0.56	0.589	0.439	0.515	0.158	0.299		8.18
P25P10-Aug 13	0.46	0.61	0.497	0.252	0.531	0.129	0.191		1.04
P25P10-Aug 14	0.47	0.58	0.525	0.411	0.521	0.188	0.299		28.15
P25P10-Aug 15	0.41	0.53	0.699	0.434	0.497	0.223	0.328		16.14
P25P10-Aug 16	0.49	0.60	0.474	0.332	0.531	0.177	0.254		6.09
P25P10-Aug 18	0.45	0.59	0.551	0.307	0.538	0.190	0.248		1.97
P25P10-Aug 19	0.50	0.53	0.530	0.212	0.545	0.109	0.161		1.00
P25P10-Aug 20	0.52	0.23	0.533	0.206	0.530	0.132	0.169		15.19
SRM 1650b	0.40	0.27	0.43	0.22	0.52	0.10	0.158		
SRM 1649a	0.52	0.92	0.44	0.33	0.55	0.09	0.214		
SRM 1597a	0.58	0.70	0.52	0.56	0.58	0.19	0.373		

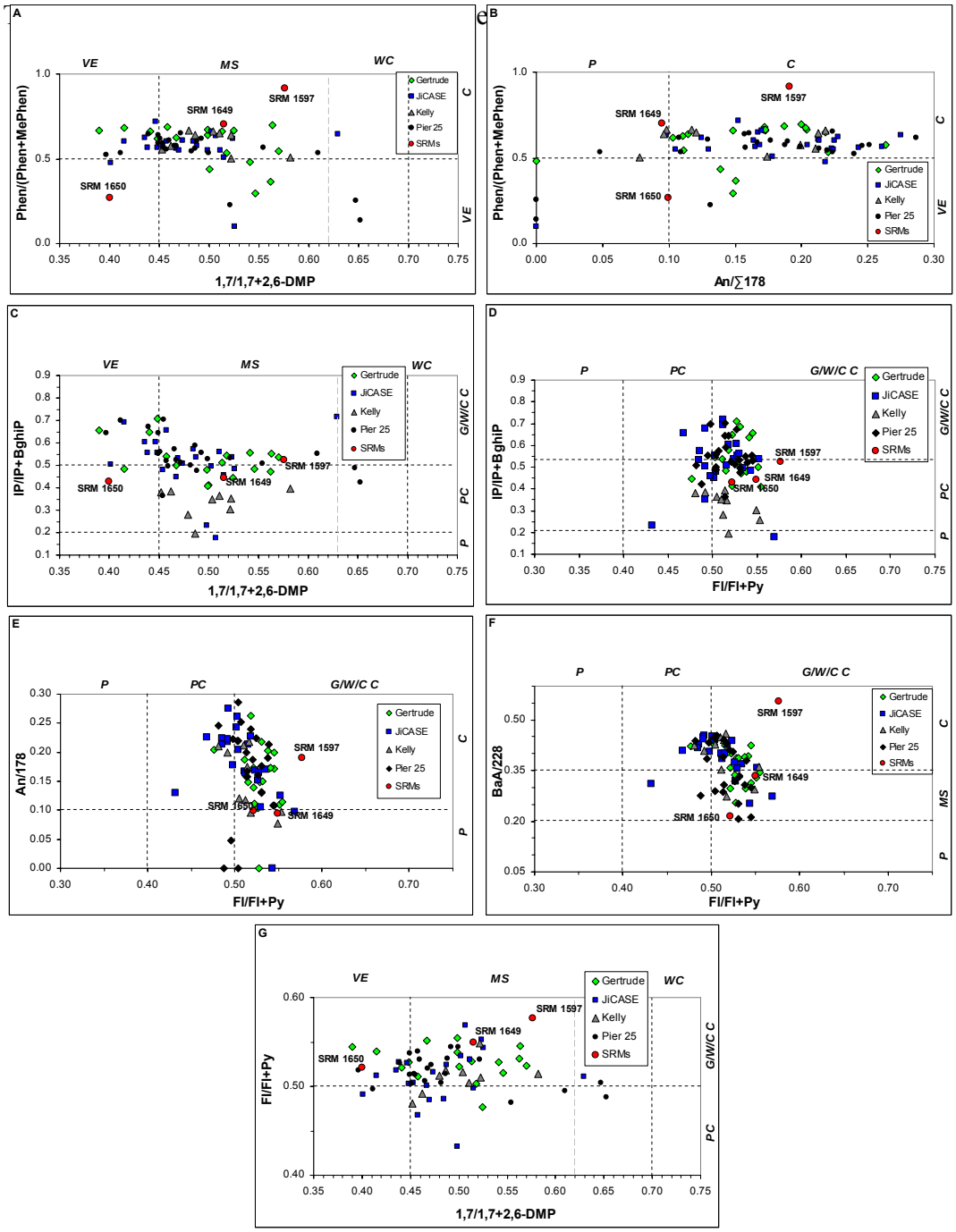

Figure S2: Bi-variate plots of PAH diagnostic ratios for Hamilton air particulates; A: Phen/(Phen+∑MePhen) vs. 1, 7/1, 7 + 2, 6 DMP; B: Phen/(Phen+∑MePhen) vs. An/∑178; C: IP/IP+BghiP vs. 1, 7/1, 7 + 2, 6 DMP; D: IP/IP+BghiP vs. Fl/Fl+Py; E: An/∑178 vs. Fl/Fl+Py; F: BaA/∑228 vs. Fl/Fl+Py; G:Fl/Fl+Py vs. 1, 7/1, 7 + 2, 6 DMP;G: An/∑178 vs. BaA/∑228. Thresholds are taken from Yunker et al (11). P = Petroleum; PC = Petroleum combustion; C = Combustion; WC = Wood combustion; G/W/C C = Grass; wood & coal combustion; MS = Mixed sources; VE = Vehicular emissions. Faint broken line represents brown coal combustion (11) on 1, 7/1, 7 + 2, 6 DMP -axis.

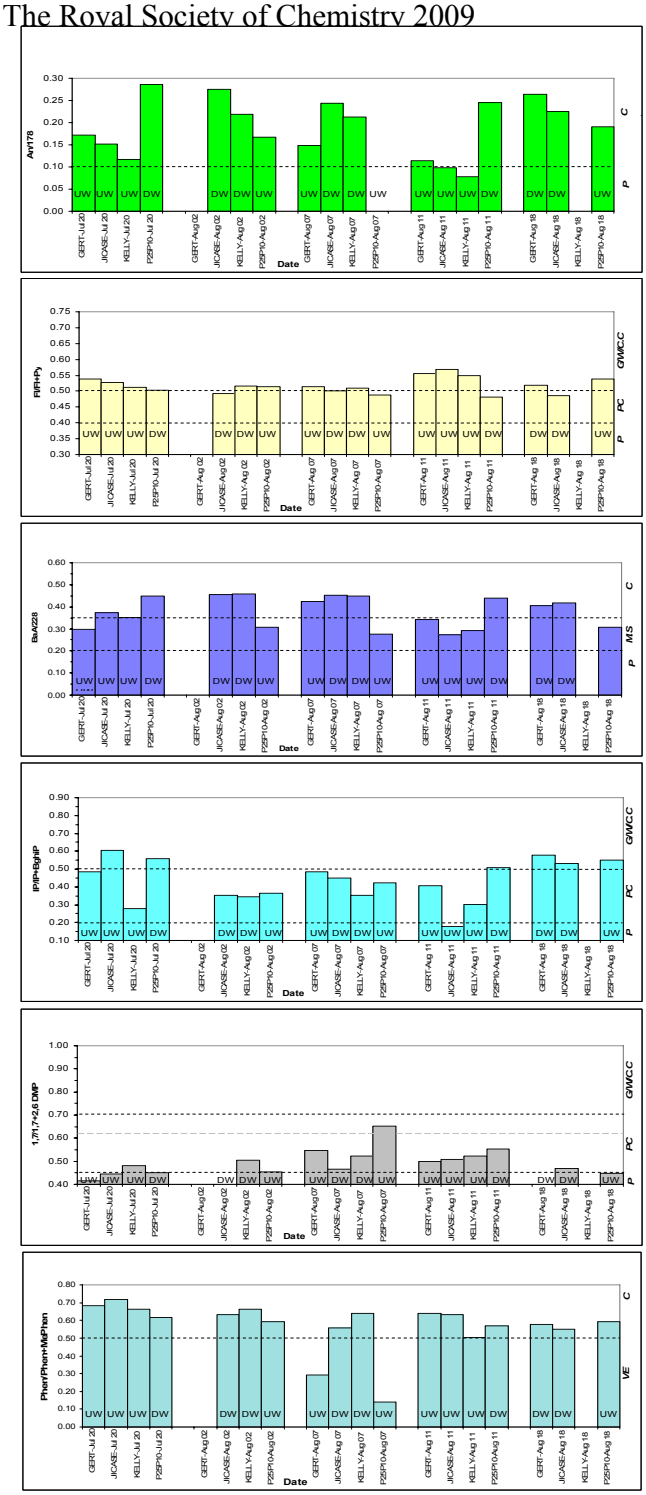

Figure S3: Variations of PAH diagnostic ratios in upwind/downwind classified sample subset. Ratio thresholds are taken from Yunker et al (11) and Gogou et al. (9). P = Petroleum; PC = Petroleum combustion; C = Combustion; W.C = Wood combustion; G/W/C. C = Grass; wood & coal combustion; M.S = Mixed sources; V.E = Vehicular emissions; UW = Upwind of industrial area; DW = Downwind of industrial area. Broken grey line in 1,7/1,7 + 2, 6 DMP plot represents brown coal combustion (11).

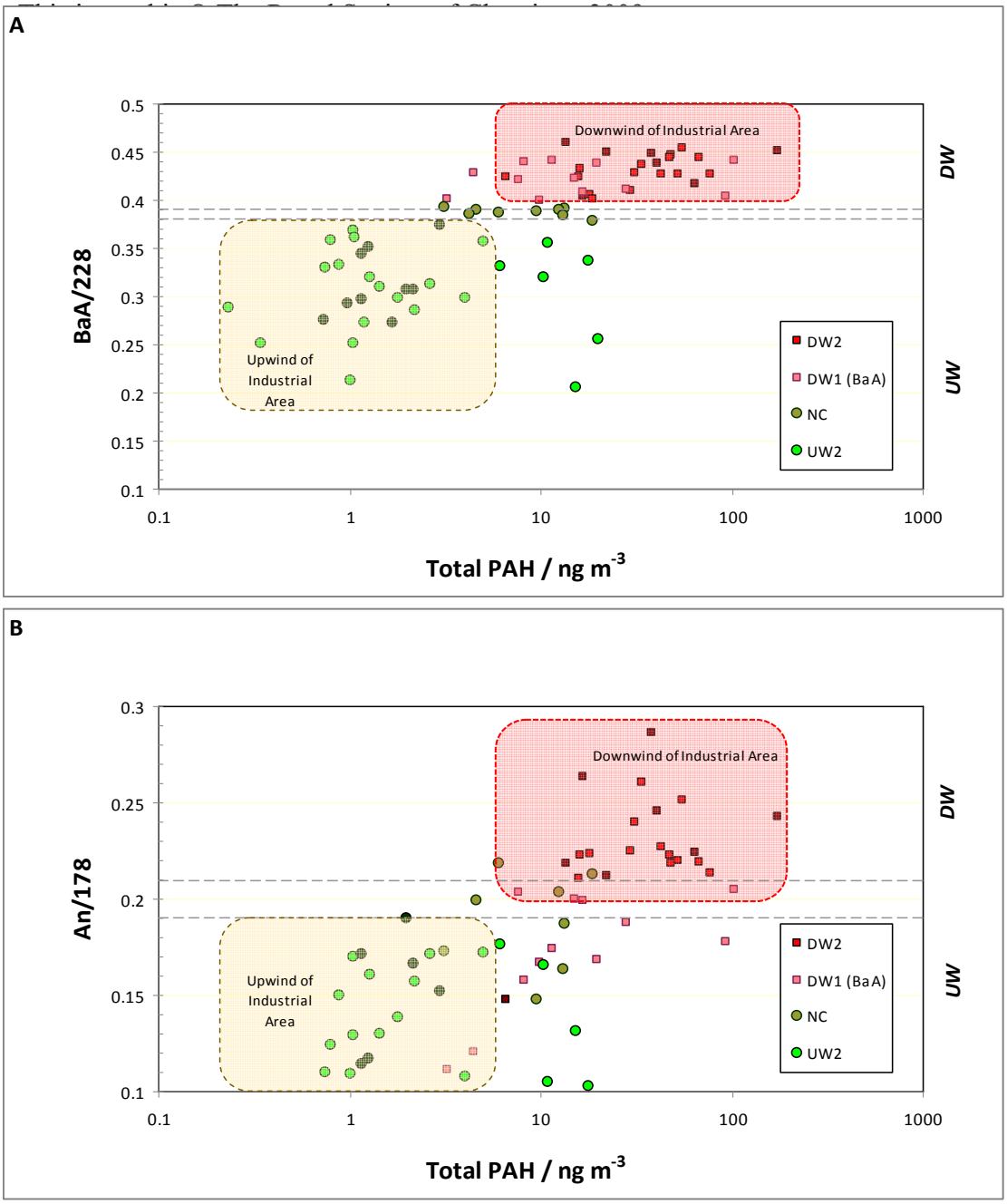

Figure S4: Plot of A: BaA/∑228 and B: An/∑178 Ratios variations with total PAH (TPAH). Boxes represent locations of most samples 'upwind or downwind of industrial area'. UW = Upwind; DW = Downwind. DW2 = Downwind by both ratios; NC = non-classifiable; UW1 = Upwind by the BaA/∑228 ratio; UW2 = Upwind by both ratios. See text for ratio boundaries. Darkened points represent the 18 members of the originally classified sub-set (Table 2).

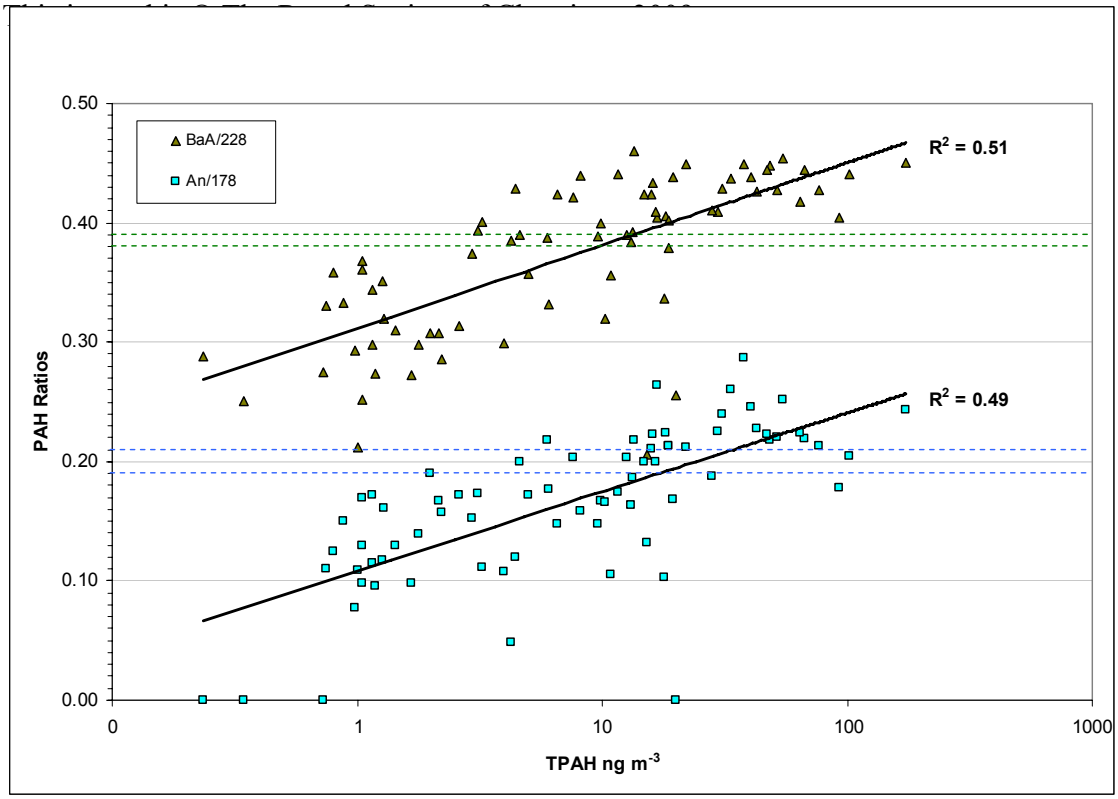

Figure S5: Correlation of BaA/∑228 and An/∑178 ratios with total PAH (TPAH) for all the samples in the data set. Dashed lines represent thresholds for discrimination between samples 'upwind and downwind of industrial area' based on the 18 members of the originally classified sub-set (Table 2).