Electronic supplementary information

A Comparative Study of Two Factor Analytic Models Applied to PAH Data from Inhalable Air Particulate Collected in an Urban-industrial Environment

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Figure S8: A: Percentage PMF Factor 3 contribution (%G_3) to TPAH; B: Absolute PMF Factor 3 contribution to the TPAH; C: Percentage PMF Factor 2 contribution (%G_2) to TPAH; D: Absolute PMF Factor 2 contribution to the TPAH; E: Percentage PMF Factor 1 contribution (%G_1) to the TPAH; F: Absolute PMF Factor 1contribution to the TPAH for entire data set. PMF Factor 1 = Urban dust; PMF Factor 2 = Diesel emissions; PMF Factor 3 = Coke oven impacts. TPAH and absolute amounts are in ng m^{-3}

<div align="right">S10</div>

Figure S9: Comparisons of coke oven impact profiles reported by Bzdusek et al (Reference #14) with F_3 profile from the PMF analysis on Hamilton air particulates.

<div align="right">S12</div>

Figure S10: Left column: Variation of 178-228 MeanRatio defined as $0.5(BaA/\sum228 + An/\sum178)$ with percentage PMF Factor contributions for the entire sample data set: %G_1 (A), %G_2 (C), %G_3 (E; shaded intermediate region and colour codes explained in main text). Right column: The corresponding variations of 178-228 MeanRatio values with TPAH / ng m^{-3} sectioned in quartiles according to increasing percentage PMF factor contributions %G_1 (B), %G_2 (D), %G_3 (F; shaded 'upwind' and 'downwind' regions indicate sample positions relative to the wind direction from the industrial area) for the entire sample data set.

<div align="right">S13</div>

Figure S11: Left column: Loadings (A) and scores (B) plots for PC1 and PC2 when three principal components are extracted and Varimax rotated. Right column is included to show the invariant nearly nature of loadings (C) of PC1 and PC2 when the most concentrated sample is removed from the data set prior to PCA which extracted and rotated only two components.

<div align="right">S14</div>
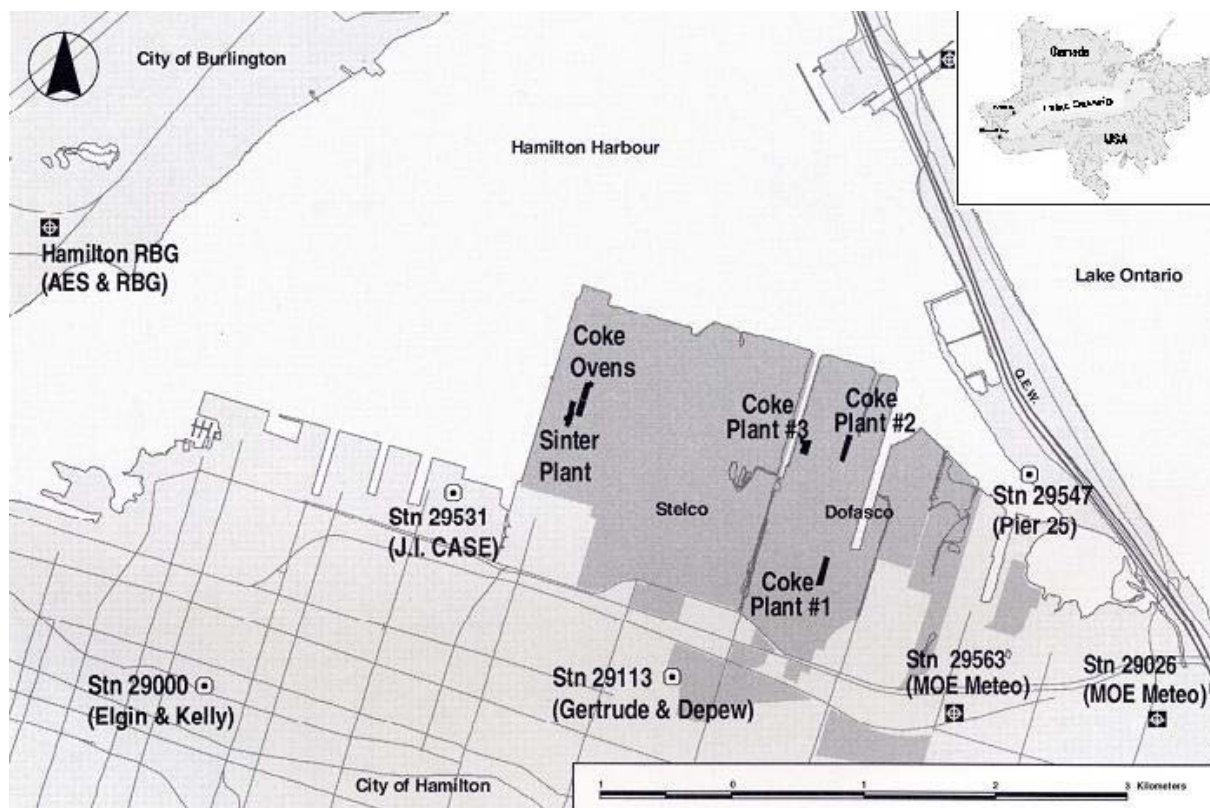
Figure S1: Map of Hamilton showing locations of air particulate sampling and meteorological stations of study in relation to the steel industries shaded dark grey. (Inset map courtesy Great Lakes Website: http://www.epa.gov/glnpo/lakeont/2002highlight/index.html).
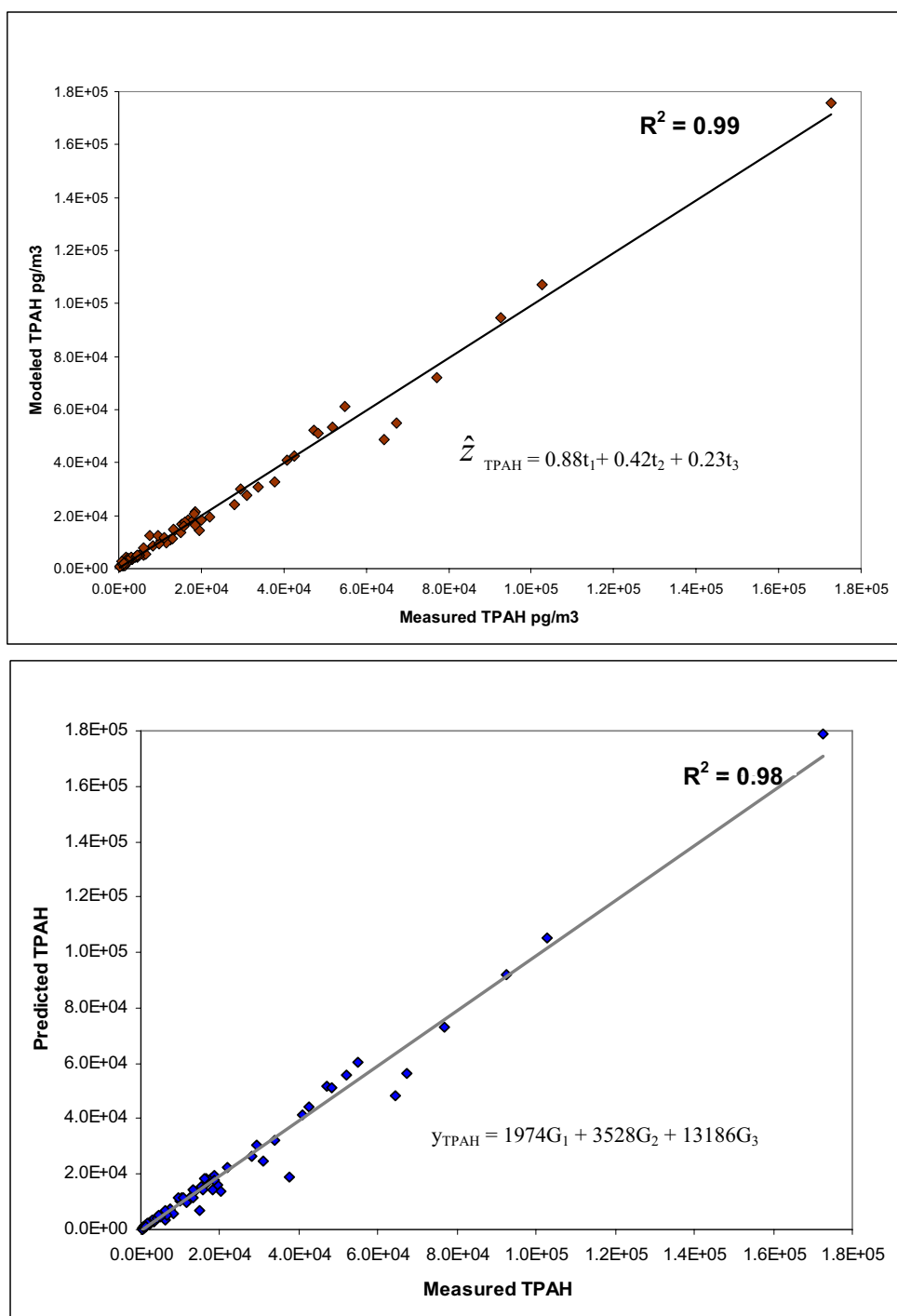
Figure S2: (a) PCA-MLR regression plot for total PAH (TPAH pg m^{-3}) measured in air particulate samples at all four sampling sites of study. (b) PMF regression plot for total PAH (TPAH pg m^{-3}) measured in air particulate samples at all four sampling sites of study.
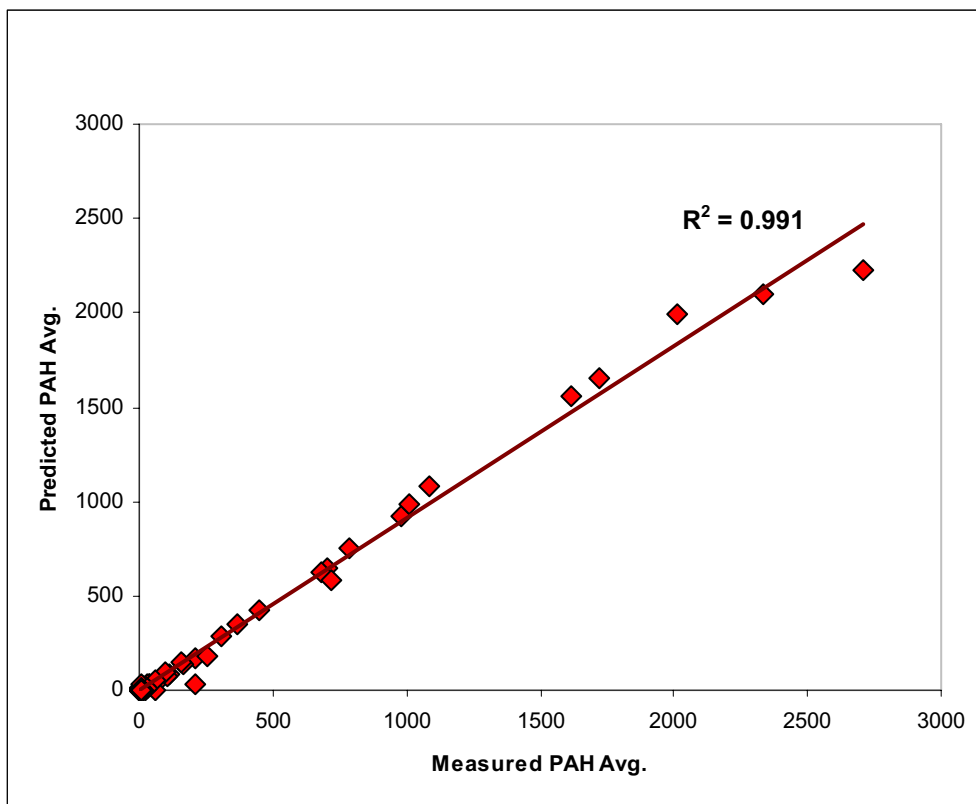
Figure S3: PMF modeled PAH average concentrations (pg m^{-3}) for 48+ polycyclic aromatic compounds
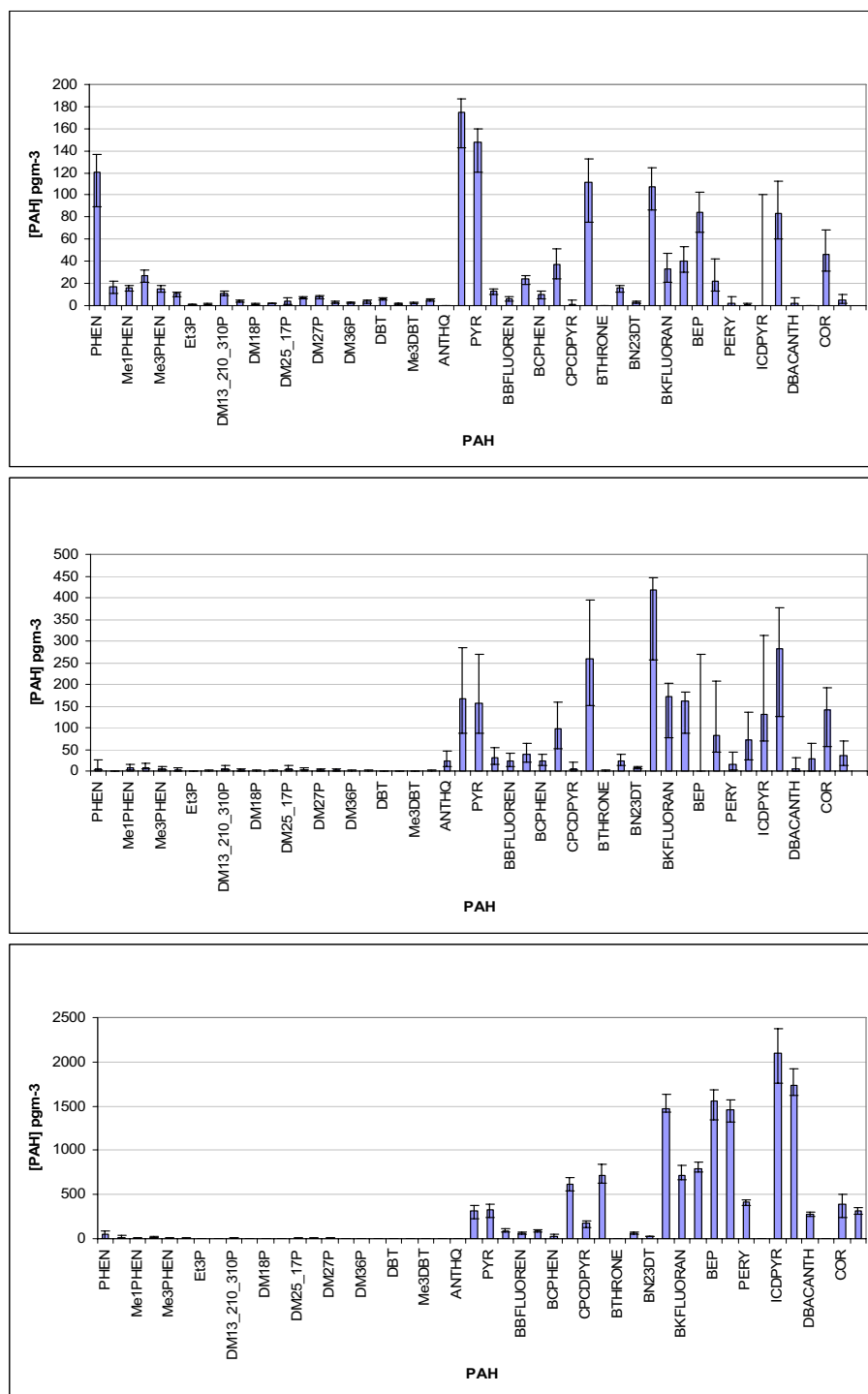
Figure S4: PMF factor profiles from 100 bootstrap runs showing the 5th to the 95th percentiles as minimum and maximum limits of error bars. Profile 1: F_1 (urban dust); Profile 2: F_2 (diesel emissions); Profile 3: F_3 (coke oven impacts). See Table S2 and Table 2 for complete order and names of PAH respectively.
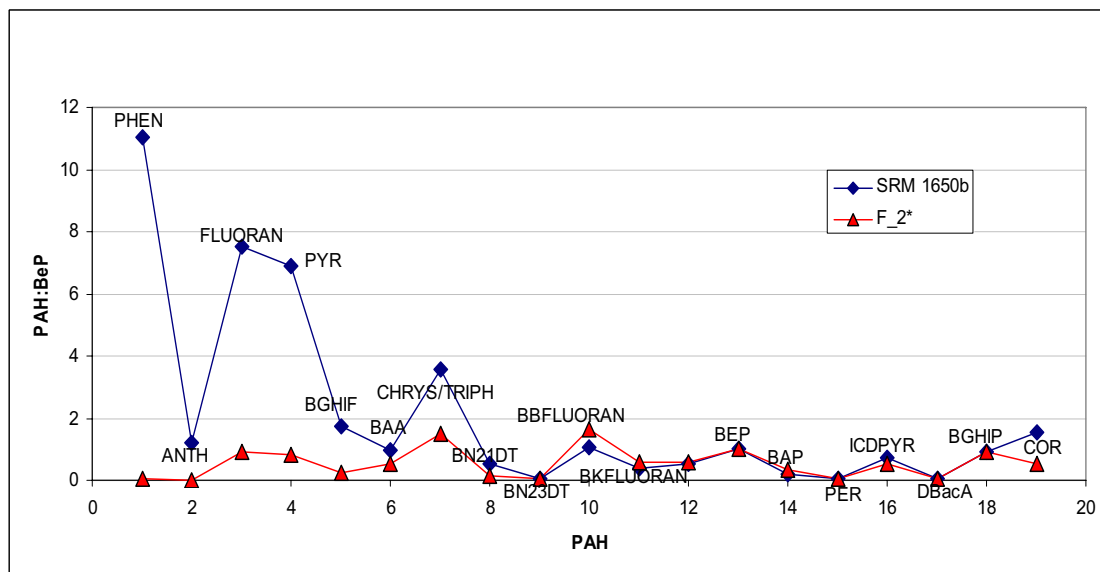
Figure S5: Factor profile comparisons of 'Diesel Emissions' (from a similar Q solution with positive a BeP value) and NIST SRM 1650b. The lower molecular mass PAH seem depleted while the heavier PAH are in good agreement with the standard reference material.
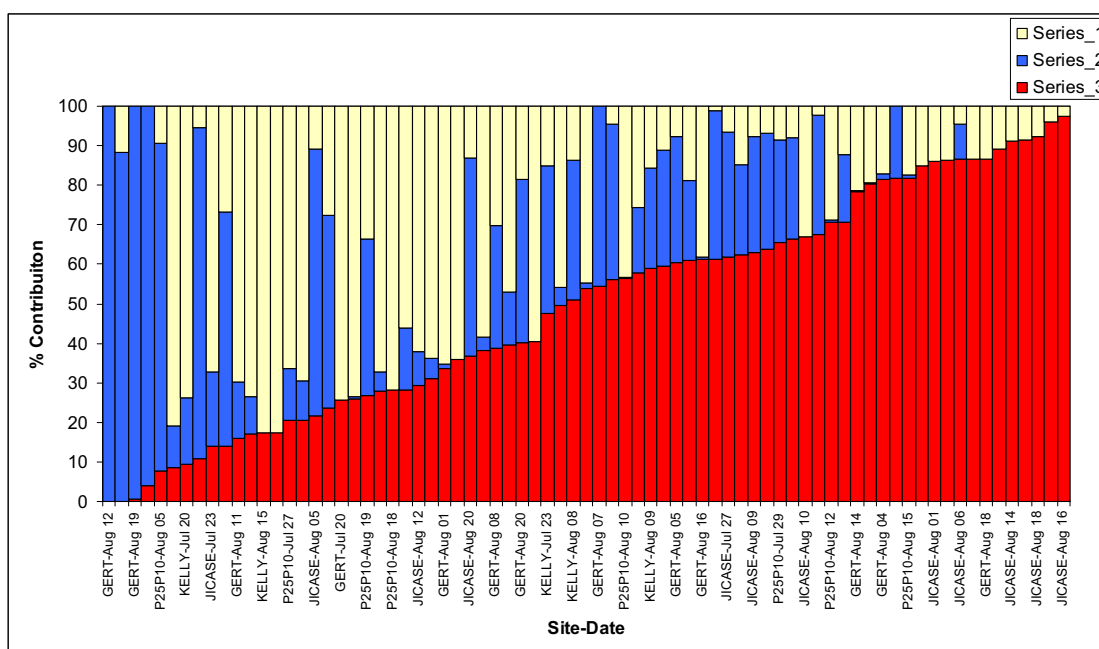
Figure S6: All air particulate samples from current work sorted as a function of increasing percentage contribution of Series_3 (coke oven impacts)
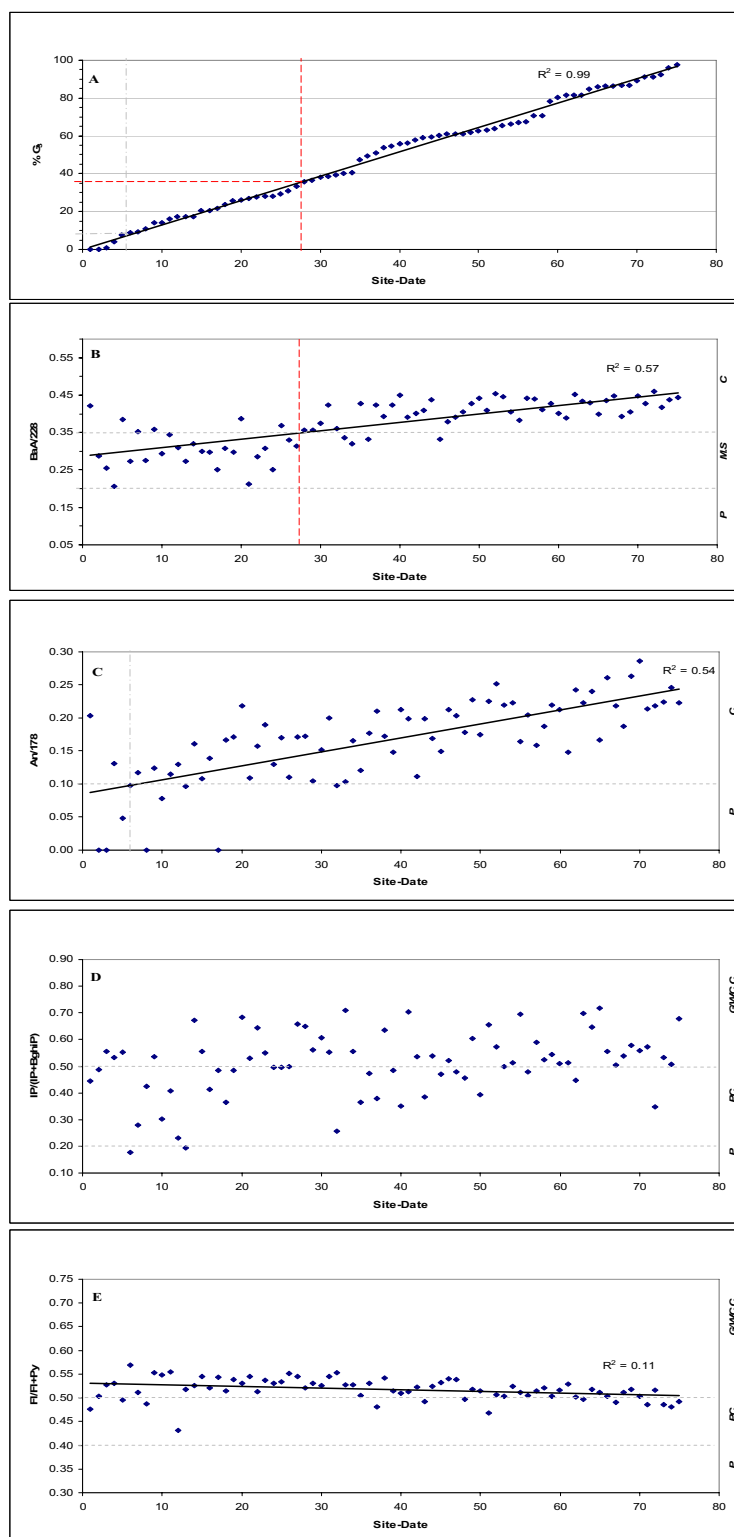
Figure S7: Hamilton air particulate data sorted by increasing percent contribution of PMF Factor 3 (coke oven emissions, G_3); A: PMF Factor 3; B-E: diagnostic PAH ratios: B: BaA/$\sum$228 ratio; C: An/$\sum$178 ratio; D: IP/IP+BghiP ratio; E: Fl/Fl+Py ratio. Horizontal dashed lines indicate threshold values as defined by Yunker et al. (Reference #6). Vertical dashed lines indicate cross-over points on B and C.

Table S1: Factor percentage contributions to the TPAH measured in all air particulate samples at the sampling sites of study by both models. Note: There is no correspondence in chronological order of factors in the two models.

PMF	F_1 (%)	F_2 (%)	F_3 (%)
Station 29113 (Gertrude)	35.5 ± 27.5	20.0 ± 31.0	44.4 ± 26.5
Station 29531 (JICASE)	25.4 ± 27.3	16.1 ± 18.9	58.5± 28.3
Station 29000 (Kelly)	30.3 ± 27.9	24.9 ± 18.5	44.8 ± 25.5
Station 29547 (Pier 25)	28.4 ± 25.1	25.9± 32.1	45.7 ± 29.9

PCA	PC_1 (%)	PC_2 (%)	PC_3 (%)
Station 29113 (Gertrude)	64.0 ± 209.4	36.6± 169.1	-0.7 ± 47.0
Station 29531 (JICASE)	114.8 ± 235.9	-11.7± 177.3	-3.1 ± 61.7
Station 29000 (Kelly)	92.7 ± 200.9	5.4 ± 168.7	1.9 ± 40.6
Station 29547 (Pier 25)	109.6 ± 221.3	-6.7 ± 176.8	-2.9 ± 50.8
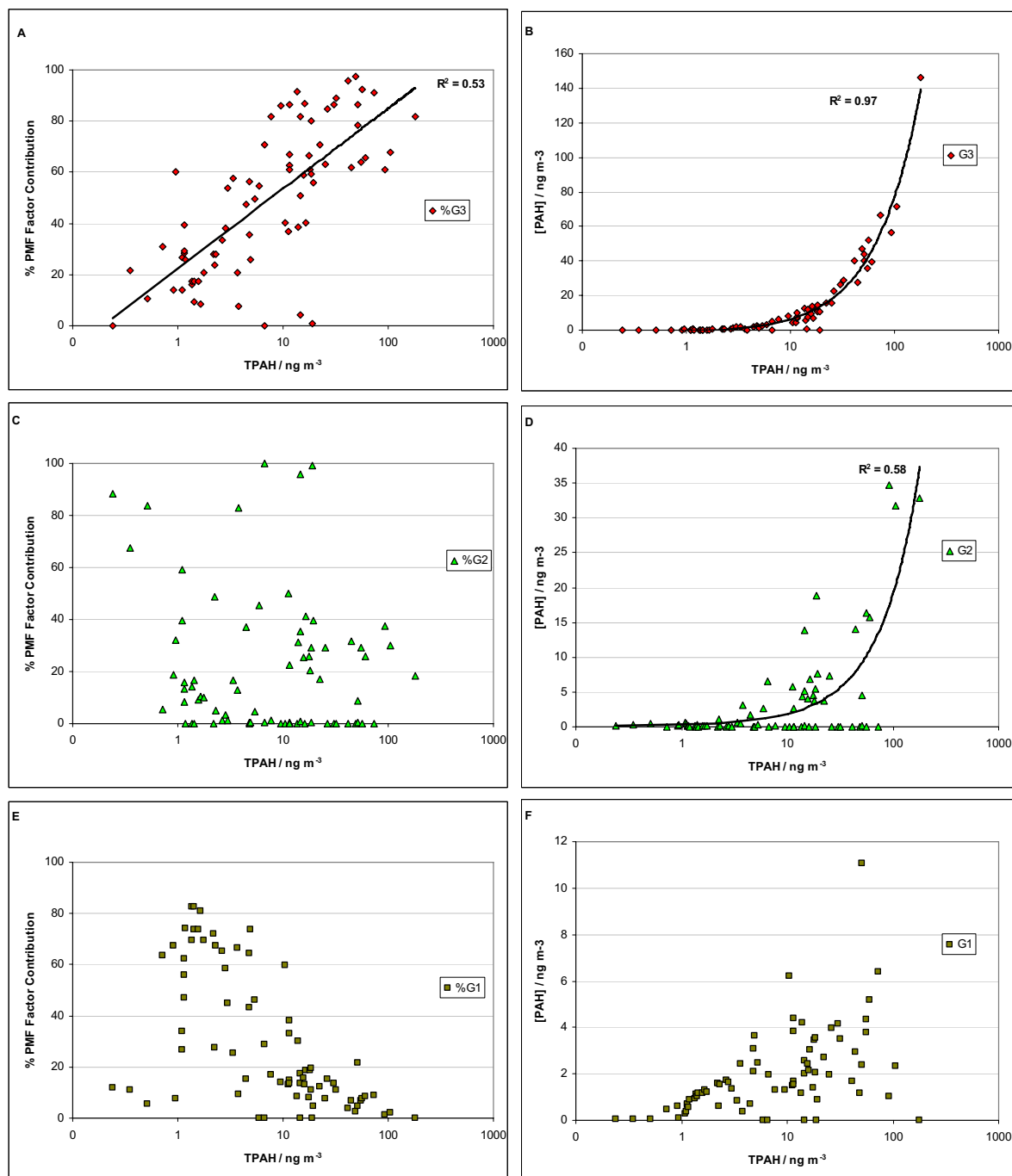
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Table S2: PMF factor profiles (pg m^{-3}) and their 5th and 95th percentiles from 100 bootstrap runs. Profile 1: F_1 (urban dust); Profile 2: F_2 (diesel emissions); Profile 3: F_3 (coke oven impacts). See Table 2 for names of PAH (ANTHQ= anthraquinone, BTHRONE = benzanthrone, PIC = picene).

Species	F_1			F_2			F_3		
	X	5th	95th	X	5th	95th	X	5th	95th
PHEN	120.59	89.92	136.49	5.82	2.14	26.02	47.07	0.00	26.02
ANTH	17.33	11.29	22.19	0.00	0.00	0.43	16.17	1.02	0.43
Me1PHEN	16.38	12.79	18.53	6.85	3.42	15.41	10.91	4.27	15.41
Me2PHEN	27.49	21.55	32.23	7.93	4.42	18.23	18.52	7.87	18.23
Me3PHEN	15.33	11.85	17.62	4.79	2.71	10.53	8.80	2.96	10.53
Me9PHEN	10.75	8.30	12.30	3.00	0.57	8.39	6.21	2.61	8.39
Et3P	1.27	0.83	1.44	0.24	0.02	0.60	0.00	0.00	0.60
DM12P	1.48	1.07	1.78	0.76	0.39	1.78	1.29	0.74	1.78
DM13_210_310P	11.09	8.80	12.66	5.08	2.57	12.38	11.09	6.31	12.38
DM16P	4.32	3.43	4.95	1.69	0.96	3.97	2.80	0.77	3.97
DM18P	1.19	0.73	1.54	0.61	0.14	1.73	1.13	0.18	1.73
DM19P	2.12	1.55	2.49	1.04	0.55	2.57	1.83	0.83	2.57
DM25_17P	4.13	0.62	7.31	4.93	2.33	12.47	0.00	0.00	12.47
DM26P	7.38	5.62	8.53	2.88	1.57	6.77	4.79	2.48	6.77
DM27P	8.04	6.22	9.27	2.48	1.28	5.79	7.04	4.02	5.79
DM29P	3.10	2.27	3.74	1.82	1.09	4.03	2.39	1.14	4.03
DM36P	2.70	2.04	3.16	1.21	0.64	2.69	2.30	1.39	2.69
DM39P	3.97	2.12	4.90	0.57	0.00	3.66	0.00	0.00	3.66
DBT	6.19	4.71	7.07	0.13	0.00	1.04	1.98	0.00	1.04
Me2DBT	1.63	1.26	1.84	0.26	0.10	0.78	0.37	0.00	0.78
Me3DBT	2.22	1.67	2.54	0.37	0.15	1.00	0.32	0.00	1.00
Me4DBT	5.05	3.86	5.87	0.66	0.27	2.27	1.02	0.00	2.27
ANTHQ	0.00	0.00	0.04	24.08	9.15	46.71	0.00	0.00	46.71
FLUORAN	174.50	142.66	187.34	166.55	87.22	284.78	308.47	232.15	284.78
PYR	147.99	120.97	159.72	156.67	87.57	270.21	320.66	239.24	270.21
BAFLUOREN	12.94	9.92	15.42	30.73	15.94	53.86	92.35	78.67	53.86
BBFLUOREN	6.00	4.08	7.82	22.95	10.89	39.94	60.05	50.47	39.94
BGHIF	24.42	19.26	26.78	38.48	21.54	65.00	88.12	75.35	65.00
BCPHEN	9.85	6.19	12.70	24.15	11.70	39.69	26.37	0.11	39.69
BAA	37.44	24.11	51.32	96.93	52.10	160.23	615.77	539.81	160.23
CPCDPYR	1.19	0.00	4.68	5.04	1.88	21.55	175.01	127.00	21.55
CHRYS/TRIPH	111.65	74.98	132.53	259.94	151.84	393.83	714.08	634.21	393.83
BTHRONE	0.15	0.00	0.37	0.07	0.00	2.17	0.00	0.00	2.17
BN21DT	15.78	12.04	18.34	23.85	13.13	39.14	59.41	50.74	39.14
BN23DT	2.94	2.13	3.69	7.60	4.89	9.00	24.86	21.91	9.00
BBFLUORAN	107.18	86.63	125.09	417.28	255.17	447.03	1472.40	1433.76	447.03
BKFLUORAN	33.37	20.83	46.77	171.16	77.38	201.77	716.71	666.27	201.77
BJFLUORAN	40.68	30.63	52.85	160.67	87.20	183.13	786.92	755.25	183.13
BEP	84.65	66.27	102.69	0.00	0.00	267.96	1563.90	1338.61	267.96
BAP	22.39	13.16	42.48	82.66	42.32	208.88	1451.20	1325.17	208.88
PERY	1.61	0.00	8.53	15.58	2.43	43.96	410.39	373.02	43.96
BAA712DIO	0.66	0.14	1.66	71.71	26.52	135.39	0.00	0.00	135.39

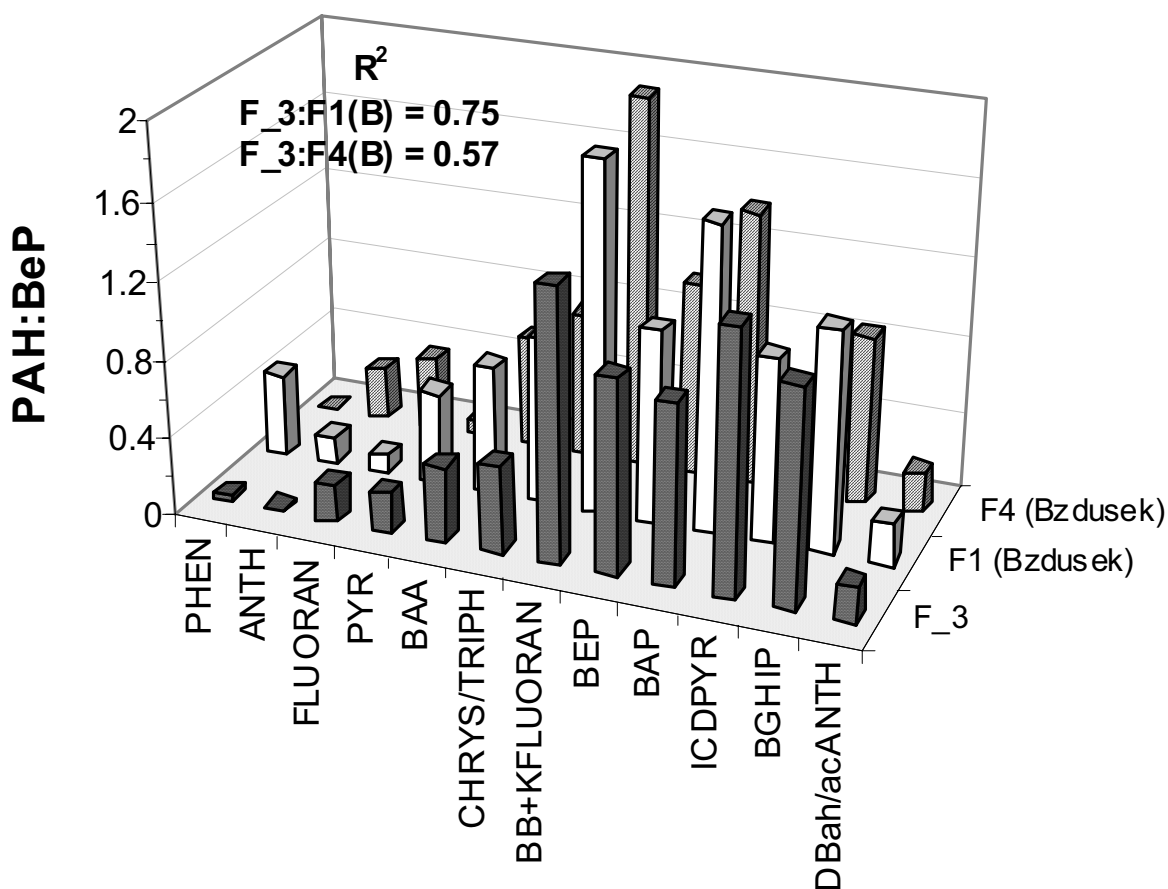| Species	F_1			F_2			F_3		
	X	5th	95th	X	5th	95th	X	5th	95th
ICDPYR	0.00	0.00	100.05	131.77	69.03	311.58	2096.90	1752.53	311.58
BGHIP	82.95	60.47	112.67	282.08	125.51	377.44	1736.50	1621.79	377.44
DBACANTH	2.19	0.01	7.26	4.11	0.00	31.13	280.95	250.96	31.13
PIC	0.00	0.00	0.12	29.02	1.23	64.10	0.01	0.00	64.10
COR	45.82	31.49	68.11	142.30	55.50	193.45	392.08	244.24	193.45
DBAEPYR	5.16	2.00	9.91	36.30	13.57	68.69	311.67	279.17	68.69

Figure S9: Comparisons of coke oven impact profiles reported by Bzdusek et al (Reference #14) with F_3 profile from the PMF analysis on Hamilton air particulates.
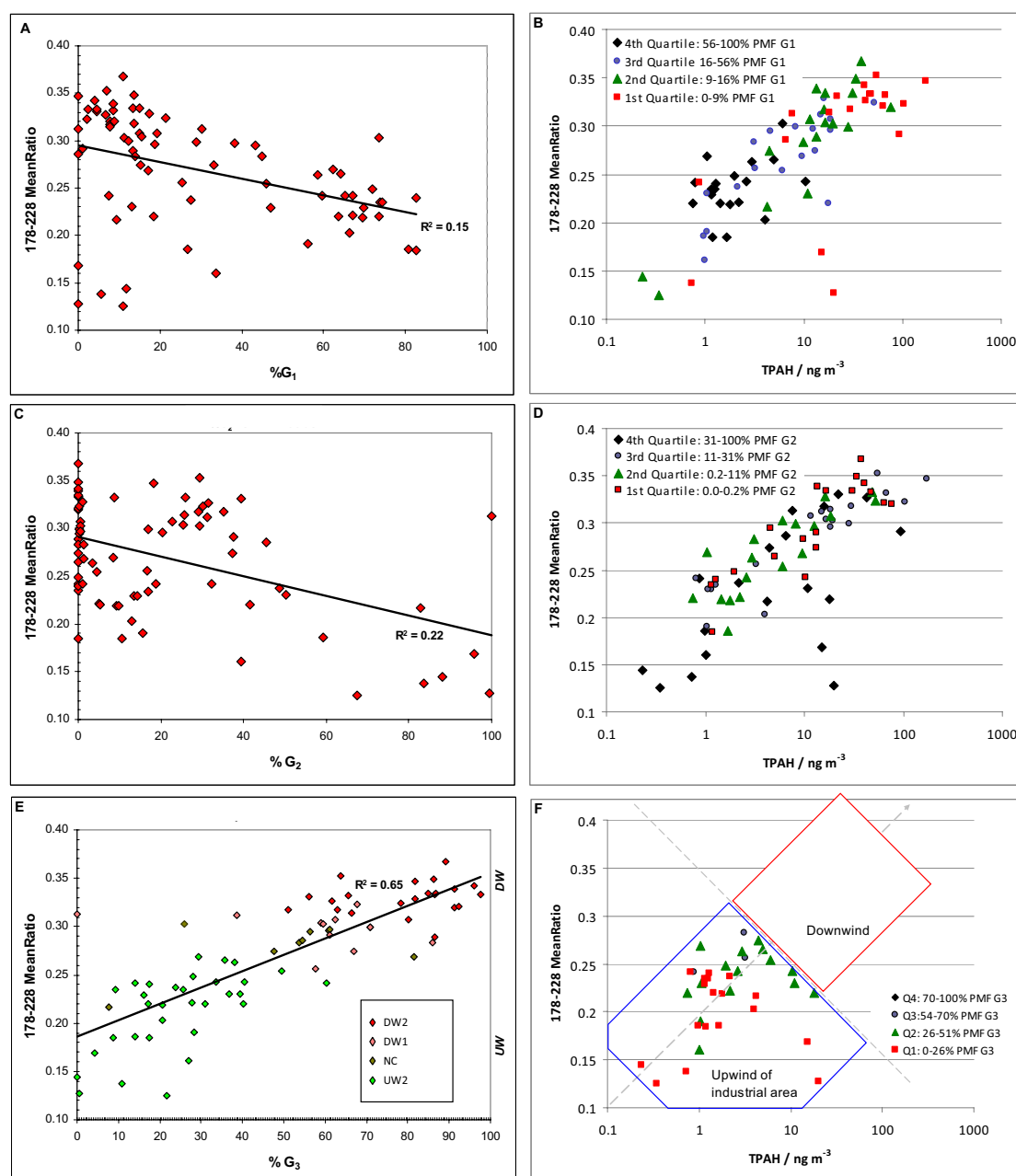
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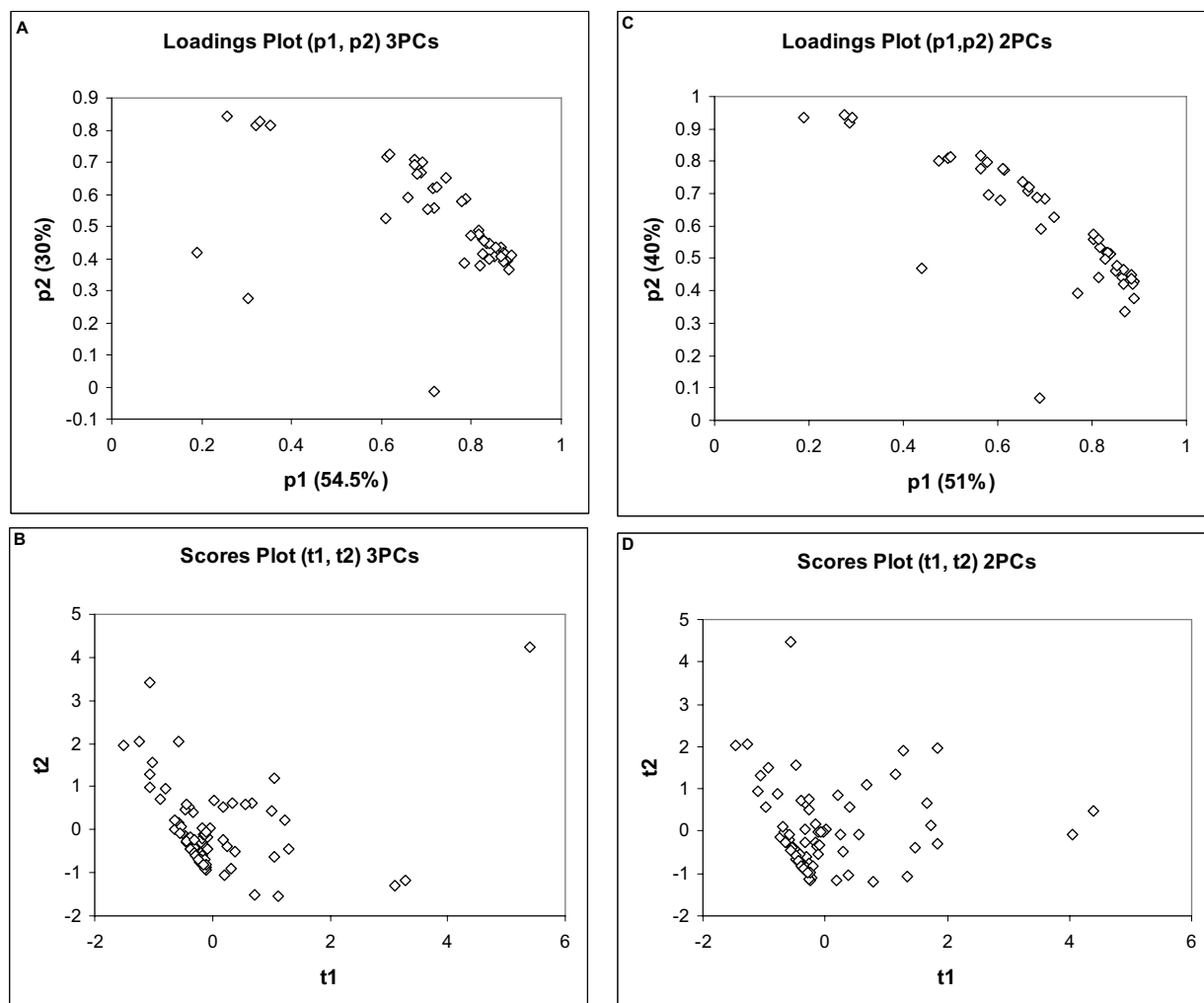
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