Supporting Information

Benzo[a]pyrene and Phenanthrene Hemoglobin Adducts as Biomarkers of Longer-Term Air Pollution Exposure

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List of Figure and Table in Support Information

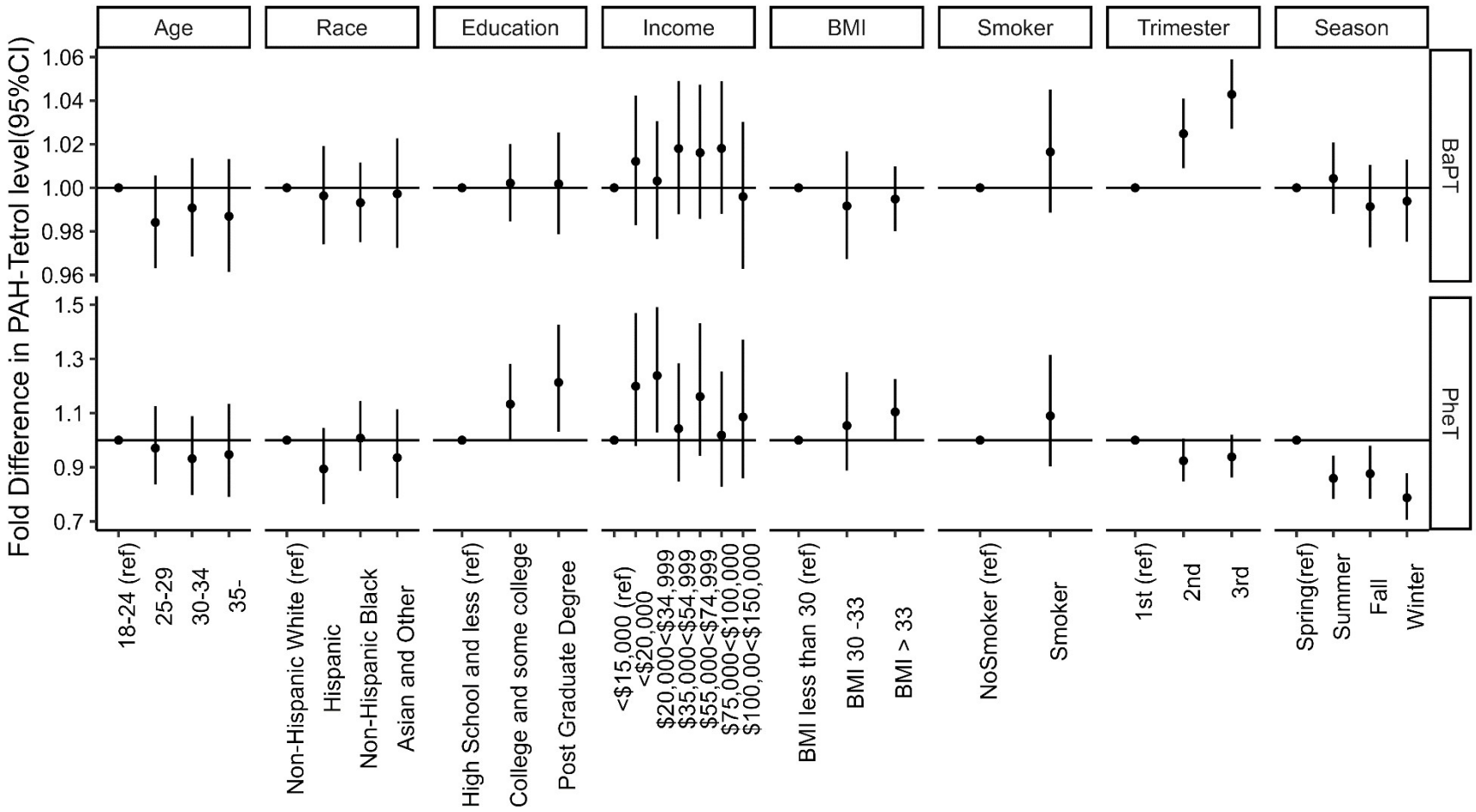
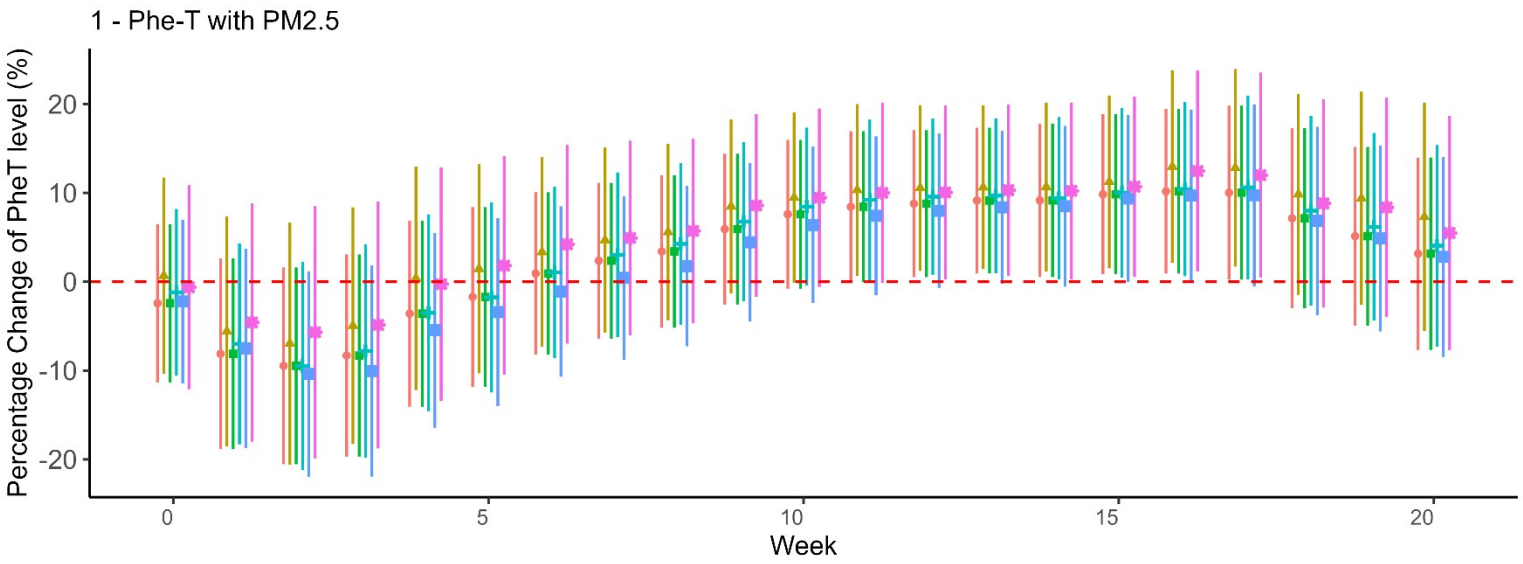


Figure S1. **Fold difference in PAH-tetrols (PHET and BaPT) levels in association with age, race/ethnicity, education, household income, pre-pregnancy BMI, smoker, gestational age, and season of sample collection.** Differences were tested by linear mixed-effects models with random intercepts of study participants.


1 - Phe-T with PM2.5
Percentage Change of PheT level (%)
20
10
0
-10
-20
0
5
10
15
20
Week

60

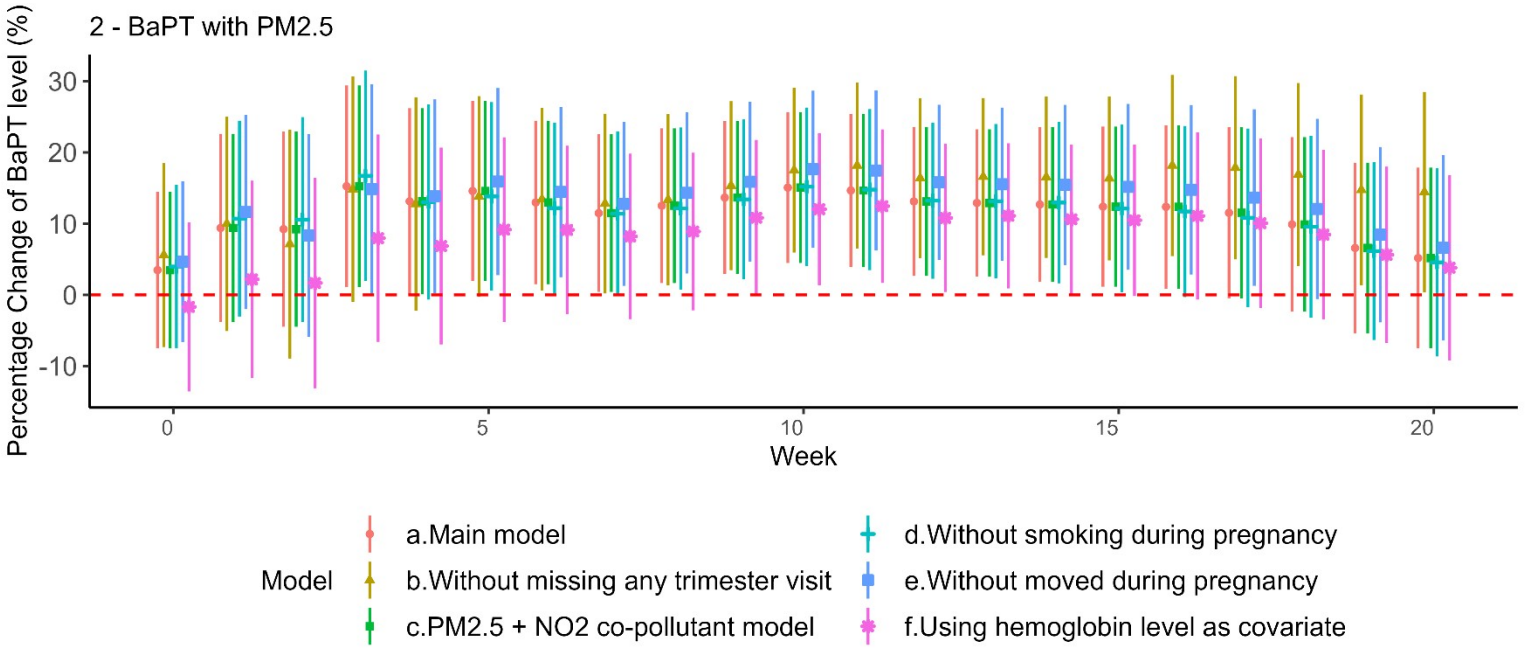


Figure S2. **Sensitive analysis: Difference of 1-Phenanthrene-Tetrols (PHET) and 2-Benzo(a)Pyrene-Tetrols (BaPT) concentrations association with one interquartile increase in Weekly cumulative $PM_{2.5}$**: a. main model, b. excluded participants who were missing one or two urine collections, c. included a co-pollutant $PM_{2.5}$ + NO_2 as covariates in the model, d. excluded participants who were smoking during pregnancy, e. excluded participants who moved to another address during pregnancy, f. using hemoglobin level as a covariate instead of normalization. Generated using mixed-effects models with random intercepts of study participants and controlling for age, gestation age, pre-pregnancy body mass index (BMI), income groups, education groups, and season.

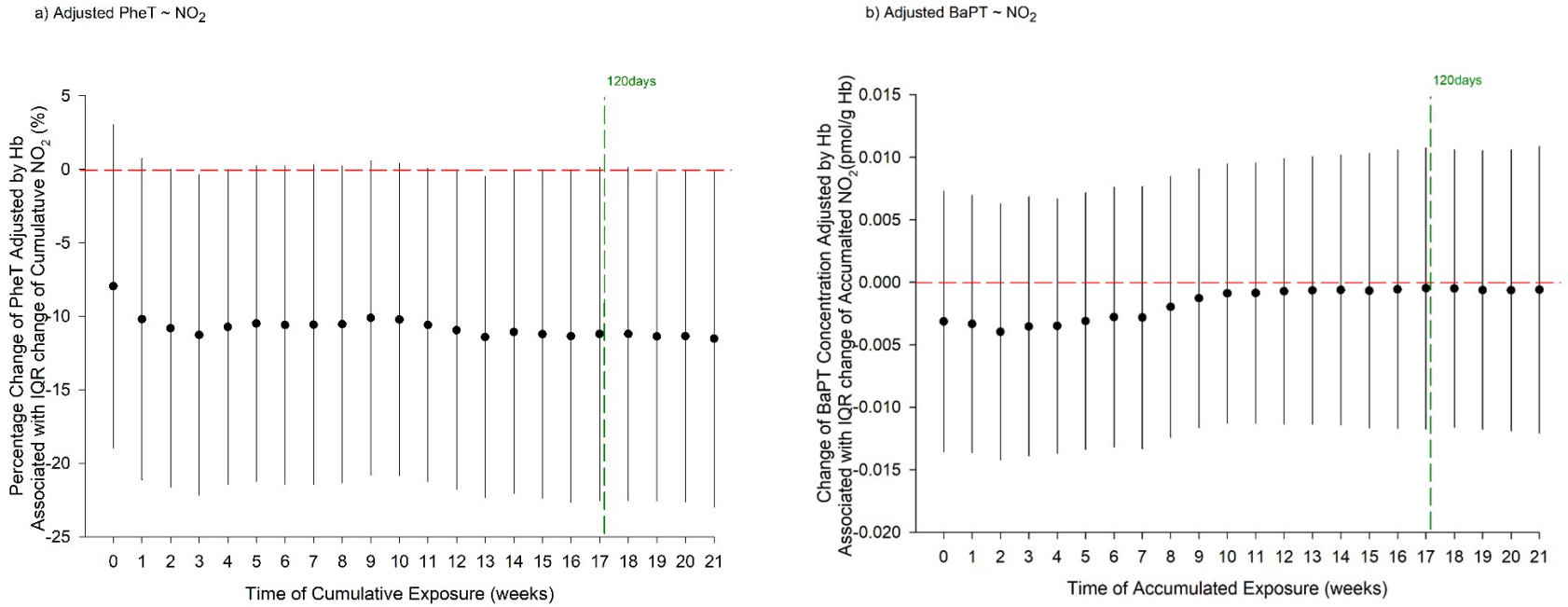
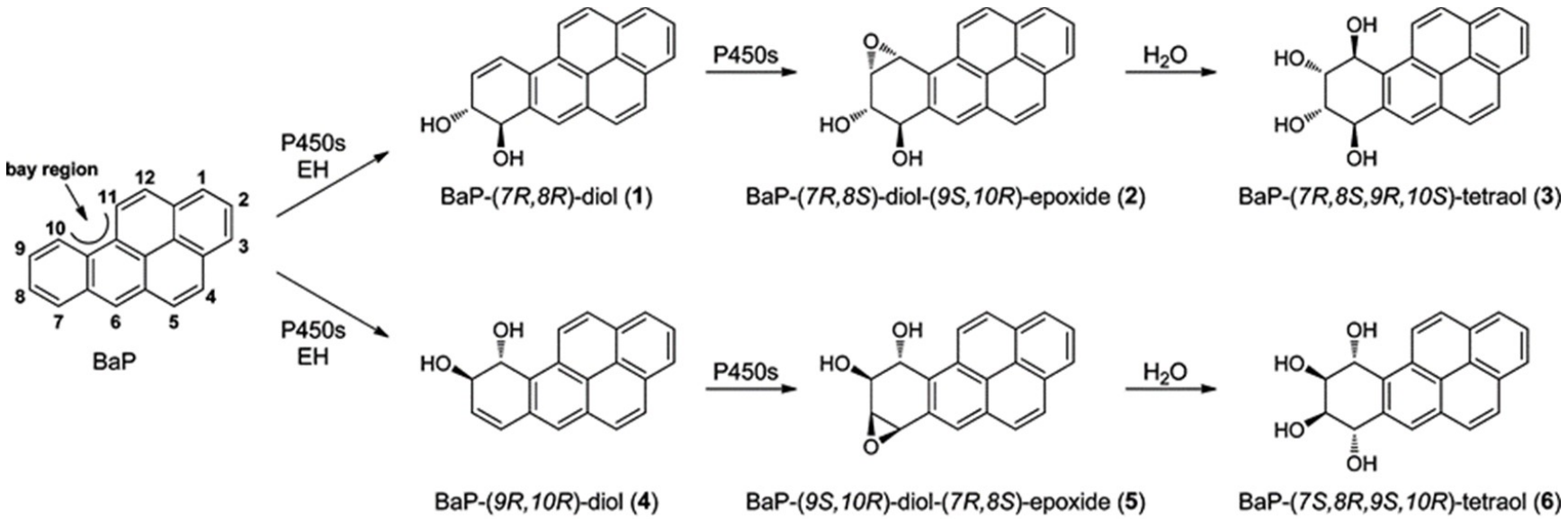


Figure S3. The Change of PAH-Tetrols Concentration with an IQR Change of Weekly Cumulative NO_2 Exposure: (a) Phenanthrene-Tetrols (PHET) Adjusted by Hemoglobin Levels; (b) Benzo(a)Pyrene-Tetrols (BaPT) Adjusted by Hemoglobin Levels. Generated using mixed-effects models with random intercepts of study participants and controlling for age, gestation age, pre-pregnancy body mass index (BMI), income groups, education groups.



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78 **Figure S4. Metabolic Activation of Benzo(a)pyrene: Formation of Diols, Di-Epoxides, and Tetrols.**

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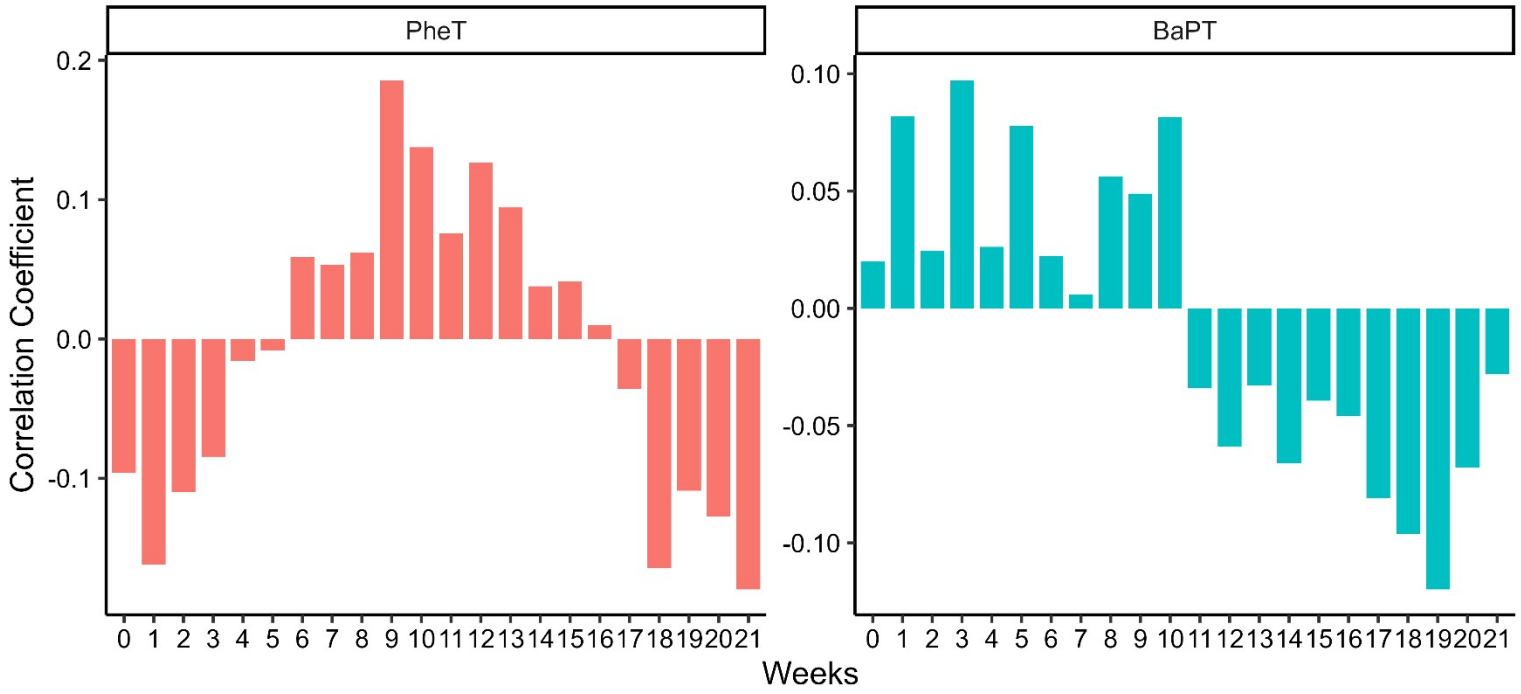

Figure S5. Pearson correlation coefficient between PAH tetrols with weekly cumulative PM2.5 concentration. PheT-Phenanthrene-Tetrols; BaPT- Benzo(a)Pyrene-Tetrols

Table S1-1. HPLC mobile phase gradient program

Time(min)	A%	B%	flow rate (μl/min)
0	90	10	400
2	90	10	400
4	40	60	400
6	40	60	400
12	20	80	400
14	0	100	400
16	0	100	400
18	40	60	400
20	90	10	400
22	90	10	400

Mobile phase : A: 0.01% formic acid in water; B: 0.01% formic acid in methanol

Table S1-2. Parameters used for the HPLC-MS/MS analysis

	PHET	BaPT
Ion Source Type	APCI	APCI
Polarity	Positive	Positive
Vaporizer Temperature	300	400
Sheath Gas Pressure	20	30
Aux Gas Pressure	5	5
Capillary Temperature	200	200
Capillary Offset	35	35

Table S2. Estimated percentage change of PAH-tetrols concentration associated with each interquartile range (IQR) change in cumulative $PM_{2.5}$ weekly concentrations.

1) PheT ~ PM2.5

Weeks	Percentage Change	95% CI Lower	95% CI Upper	p-value	IQR(μg/m³)
0	-2.36	-11.52	6.65	0.603	2.821
1	-8.27	-19.20	2.66	0.139	2.543
2	-9.75	-20.97	1.62	0.092	2.460
3	-8.71	-20.24	2.95	0.145	2.398
4	-3.84	-14.62	6.94	0.486	2.201
5	-1.92	-11.96	8.27	0.718	2.120
6	0.74	-8.42	9.90	0.874	1.906
7	2.22	-6.65	10.93	0.626	1.848
8	3.25	-5.47	11.82	0.465	1.773
9	5.76	-2.81	14.33	0.186	1.717
10	7.53	-1.03	16.10	0.084	1.644
11	8.27	-0.30	16.84	0.058	1.555
12	8.71	0.30	17.13	**0.042**	1.448
13	9.01	0.74	17.28	**0.033**	1.306
14	9.01	0.30	17.73	**0.042**	1.261
15	9.60	0.59	18.61	**0.036**	1.188
16	10.19	0.74	19.65	**0.035**	1.118
17	9.90	0.00	19.79	**0.050**	1.049
18	7.09	-3.25	17.28	0.180	0.972
19	5.02	-5.17	15.21	0.338	0.868
20	2.95	-7.98	13.88	0.591	0.855

2) BaPT ~ PM2.5

Weeks	Percentage Change	95% CI Lower	95% CI Upper	p-value	IQR(μg/m³)
0	3.48	-7.52	14.48	0.536	2.77
1	9.40	-3.81	22.61	0.164	2.52
2	9.23	-4.48	22.94	0.188	2.44
3	15.26	1.11	29.41	**0.035**	2.37
4	13.14	0.07	26.21	**0.049**	2.16
5	14.59	1.94	27.23	**0.024**	2.14
6	12.97	1.50	24.45	**0.027**	1.93
7	11.48	0.41	22.54	**0.043**	1.86
8	12.52	1.66	23.38	**0.024**	1.79
9	13.67	2.94	24.40	**0.013**	1.71
10	15.06	4.47	25.65	**0.006**	1.63

11	14.66	3.90	25.43	**0.008**	1.56
12	13.12	2.66	23.58	**0.014**	1.44
13	12.91	2.56	23.25	**0.015**	1.31
14	12.69	1.85	23.53	**0.022**	1.27
15	12.39	1.14	23.63	**0.031**	1.20
16	12.36	0.88	23.84	**0.035**	1.11
17	11.53	-0.47	23.53	0.060	1.05
18	9.90	-2.36	22.15	0.114	0.97
19	6.59	-5.38	18.55	0.281	0.86
20	5.17	-7.52	17.87	0.425	0.85

Table S3. Percentage changes of PAH-tetrols concentrations with one interquartile range (IQR) increase in proximity to a source traffic variable, with 95% confidence intervals and p-values.

Variable	Unit	Change (%)	CI Lower	CI Upper	P Value
a. PHET					
Distance to Airport	Km	1.13	-5.54	7.80	0.74
Distance to Railway Yard	Km	3.45	-0.82	7.73	0.11
AADT_300_RD	vehicles per year	1.07	-1.48	3.61	0.41
TruckAADT_300_RD	vehicles per year	1.10	-0.86	3.07	0.27
FastFoodWithin1000mBuffer	count	0.00	0.00	0.00	0.39
CrossingWithin1000mBuffer	count	0.41	-2.57	3.39	0.79
GasStationWithin1000mBuffer	count	0.00	0.00	0.00	0.27
RailwayWithin1000mBuffer	count	-0.89	-2.48	0.70	0.28
b. BaPT					
Distance to Airport	Km	-0.91	-1.88	0.07	0.07
Distance to Railway Yard	Km	-0.14	-0.77	0.48	0.65
AADT_300_RD	vehicles per year	0.24	-0.13	0.61	0.20
TruckAADT_300_RD	vehicles per year	0.17	-0.12	0.46	0.24
FastFoodWithin1000mBuffer	count	0.00	0.00	0.00	0.24
CrossingWithin1000mBuffer	count	0.24	-0.19	0.67	0.28
GasStationWithin1000mBuffer	count	0.00	0.00	0.00	0.42
RailwayWithin1000mBuffer	count	-0.22	-0.45	0.00	0.06

All models were adjusted for maternal age, gestation age, pre-pregnancy body mass index(BMI), income groups, education groups, sample collected season.

Abbreviations: AADT: annual average daily traffic.