

Supplementary data for:

Spatiotemporal Variation, Source Analysis and Health

Risk Assessment of Particle-bound PAHs in Urumqi, China

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Table S1 General situation of the sampling points

Sampling sites	Functional area	Site description	No.*
Santunbei (STB)	Traffic area	STB is the largest passenger station in Urumqi and located in the northern part.	10 samples
Dabazha (DBZ)	Commercial/residential area	DBA is the largest bazaar in the world, which integrates commerce, entertainment, and catering.	11 samples
Shuimogou (SMG)	Residential area	SMG is located in the northeast of the city, belonging to the low mountain and hilly area, Strong winds in spring and Autumn	11 samples
Youhao (YH)	Commercial area	YH is one of the largest commercial areas, there are shopping malls and restaurants around the site.	13 samples
Nongda (ND)	Educational area	ND is a typical educational area, there are teaching buildings, office buildings, cafeteria and apartments around the site. No typical source of pollution.	12 samples
Xiaoxigou (XXG)	Traffic area	XXG site is located in the intersection of the main traffic lines of Urumqi, such as Beijing Road, Suzhou Road, outer ring road and Hetan expressway, it is the center of the city.	14 samples
Midong (MD)	Industrial area	MD site is close to the industrial park, there are a lot of houses use the coal as heating and cooking sources, located in the northern part of the city.	14 samples
Airport (AP)	Traffic area	There is an international airport within 800 m of the site and the traffic volume is larger.	14 samples
Bagang (BG)	Residential/industrial area	Within 700 m of the site, there are West Railway Station and traffic roads, a large number of delivery trucks, Bayi Iron and Steel Group and other enterprises.	11 samples

* Number of samples indicates only the number of valid samples which were successfully completed all procedures of collecting, transporting, storing and analyzing.

Table S2 Gradient elution procedure

Time/min	Flow rate/(mL/min)	Water (%)	Acetonitrile (%)
0	1.00	35	65
12	1.00	35	65
15	1.00	11	89
32	1.00	11	89
40	1.00	0	100
65	1.00	0	100

Table S3 Characteristic ratio of PAHs

Site	Season	CPAHs/ $\Sigma_{16}\text{PAH}$	BaP/BghiP	Flur/(Flur +Pyr)	BaA/(BaA+ Chr)	Flur/Pyr	Pyr/BaP
STB	HS	0.78	0.68	0.39	0.47	0.65	1.84
	NHS	0.86	0.57	0.46	0.47	0.85	1.33
DBZ	HS	0.76	0.91	0.43	0.52	0.75	1.50
	NHS	0.82	1.08	0.37	0.54	0.59	0.77
SMG	HS	0.77	0.84	0.43	0.54	0.74	2.08
	NHS	0.89	0.45	0.28	0.43	0.38	1.28
YH	HS	0.77	0.84	0.43	0.50	0.75	1.77
	NHS	0.81	0.60	0.31	0.50	0.48	1.38
ND	HS	0.76	0.90	0.45	0.43	0.83	1.23
	NHS	0.76	0.95	0.33	0.21	0.48	1.19
XXG	HS	0.76	0.58	0.40	0.48	0.66	2.04
	NHS	0.83	0.43	0.46	0.51	0.85	1.77
MD	HS	0.83	1.02	0.53	0.48	1.13	1.79
	NHS	0.85	1.33	0.55	0.53	1.22	0.89
AP	HS	0.78	0.75	0.43	0.53	0.75	1.85
	NHS	0.85	0.63	0.37	0.49	0.58	1.26
BG	HS	0.81	0.76	0.55	0.47	1.23	1.55
	NHS	0.84	1.03	0.53	0.37	1.11	1.12
Non-traffic emission	Biomass and Coal	0.87 ^a	<0.6 ^c	>0.5 ^d	0.2~0.35 ^f	1.0~1.4 ^a	<1.0 ^g
Traffic emission	Diesel	0.78 ^b	>0.6 ^c	0.40 ^e	0.35~0.64 ^e	<1.0 ^a	1.0~6.0 ^g
	Gasoline	0.73 ^b	>0.6 ^c	<0.5 ^d	0.22~0.55 ^e	<1.0 ^a	1.0~6.0 ^g

HS: Heating season; NHS: Non-heating season

CPAH: Flur+Pyr+BaA+Chry+Bbf+BFs+Bkf+BaP+BghiP+InP

^a Shi et al. (2010)

^b Mantis et al. (2005)

^c Katsoyiannis et al. (2007)

^d Yunker et al. (2002)

^e Manoli et al. (2004)

^f Park et al. (2011)

^g Teixeira et al. (2012)

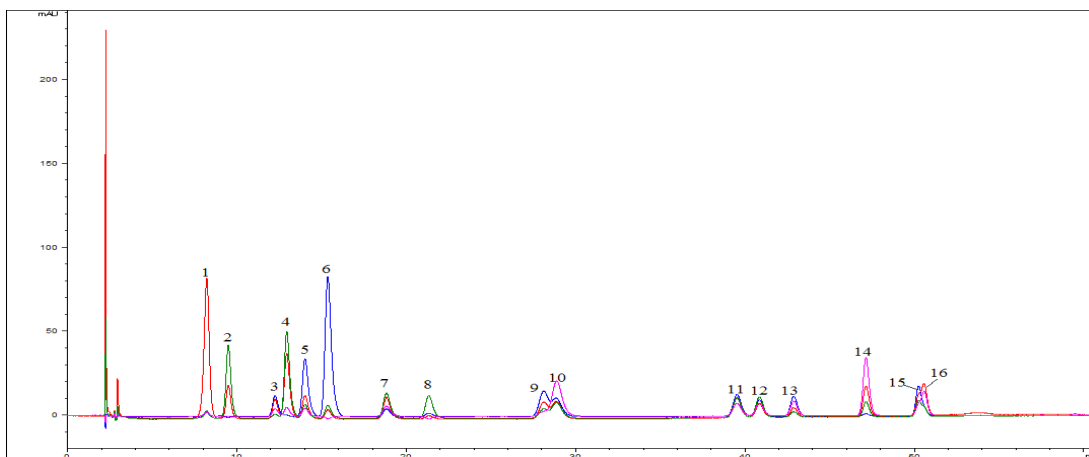


Fig. S1 UV spectrogram of 16 kinds of PAHs

1.Naphthalene (Nap); 2.Acenaphthylene (Acy); 3.Flourene (Flu); 4.Acenaphthene (Ace); 5.Phenanthrene (Phe); 6.Anthracene (Ant); 7.Flouanthene (Flur); 8.Pyrene (Pyr); 9.Chrysene (Chry); 10.Benzo[a]anthracene (BaA); 11.Benzo[b]fluoranthene (BbF); 12.Benzo[k]fluoranthene (BkF); 13.Benzo[a]pyrene (BaP); 14.Dibenzo[ah]anthracene (DbA); 15.Benzo[ghi]perylene (BghiP); 16.Indeno[1,2,3-cd]pyrene (Ind).

Reference:

- Shi, J., Peng, Y., Li, W., Qiu, W., Bai, Z., Kong, S., Jin, T., 2010. Characterization and Source Identification of PM₁₀-bound Polycyclic Aromatic Hydrocarbons in Urban Air of Tianjin, China. *Aerosol & Air Quality Research*. 10, 507-518.
- Mantis, J., Chaloulakou, A., & Samara, C. (2005). PM₁₀-bound polycyclic aromatic hydrocarbons (PAHs) in the greater area of Athens, Greece. *Chemosphere*, 59(5), 593-604.
- Katsoyiannis, A., Terzi, E., Cai, Q. Y., 2007. On the use of PAH molecular diagnostic ratios in sewage sludge for the understanding of the PAH sources. is this use appropriate?. *Chemosphere*, 69(8), 1337-1339.
- Yunker, M.B., Macdonald, R.W., Vingarzan, R., Mitchell, R.H., Goyette, D., Sylvestre, S., 2002. PAHs in the Fraser River basin: a critical appraisal of PAH ratios as indicators of PAH source and composition. *Organic Geochemistry*. 33, 489-515.
- Manoli, E., Kouras, A., Samara, C., 2004. Profile analysis of ambient and source emitted

particle-bound polycyclic aromatic hydrocarbons from three sites in northern Greece. *Chemosphere*, 56(9), 867-78.

Park, S.U., Kim, J.G., Jeong, M.J., Song, B.J., 2011. Source identification of atmospheric polycyclic aromatic hydrocarbons in industrial complex using diagnostic ratios and multivariate factor analysis. *Archives of Environmental Contamination & Toxicology*. 60, 576-589.

Teixeira, E.C., Agudelo-Castañeda, D.M., Fachel, J.M.G., Leal, K.A., Garcia, K.D.O., Wiegand, F., 2012. Source identification and seasonal variation of polycyclic aromatic hydrocarbons associated with atmospheric fine and coarse particles in the Metropolitan Area of Porto Alegre, RS, Brazil. *Atmospheric Research*. 118(3), 390-403.