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Characterization of organic aerosols from a Chinese megacity during winter: predominance of fossil fuel combustion

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Table S1. Concentrations of identified organic compounds (ng m^{-3}) in the atmospheric aerosol samples ($PM_{2.5}$) from Nanjing, China.

Compounds	Daytime				Nighttime			
	Mean	Min[a]	Max[b]	SD[c]	Mean	Min[a]	Max[b]	SD[c]
				n-Alkanes				
C_{13}	1.91	1.59	3.27	0.29	1.93	1.58	3.50	0.39
C_{14}	1.24	0.89	2.16	0.27	1.17	0.93	1.79	0.22
C_{15}	1.26	0.82	1.97	0.25	1.11	0.77	1.60	0.23
C_{16}	0.35	0.00	0.88	0.27	0.32	0.00	0.96	0.28
C_{17}	1.04	0.37	2.41	0.45	0.99	0.39	1.99	0.34
C_{18}	1.11	0.32	2.66	0.48	1.22	0.58	2.78	0.48
C_{19}	2.50	1.17	5.69	1.11	2.65	1.05	7.30	1.42
C_{20}	3.79	1.09	7.99	1.60	4.64	1.01	15.5	2.76
C_{21}	6.28	3.30	12.9	2.26	8.31	2.50	25.7	4.75
C_{22}	10.1	5.02	27.5	4.31	14.0	2.77	33.7	7.53
C_{23}	13.0	6.10	38.5	6.08	17.1	3.22	44.6	8.86
C_{24}	12.6	6.59	36.0	6.03	16.9	2.94	46.1	8.27
C_{25}	12.7	5.57	36.4	6.39	16.4	2.60	44.6	8.21
C_{26}	11.3	4.97	28.9	5.77	15.3	3.43	34.9	6.62
C_{27}	12.3	5.25	33.7	6.19	15.6	2.97	32.9	6.65
C_{28}	9.19	4.80	29.3	5.01	11.9	3.14	24.2	4.74
C_{29}	14.0	5.76	44.9	8.00	17.9	3.05	43.5	8.27
C_{30}	8.03	4.36	25.9	4.51	10.8	3.20	21.8	4.06
C_{31}	10.9	4.80	35.9	6.06	13.7	4.01	35.6	6.15
C_{32}	5.56	3.09	14.9	2.28	6.87	4.18	13.1	1.98
C_{33}	6.48	4.01	18.5	2.79	7.55	3.55	18.5	2.87
C_{34}	4.80	3.57	9.94	1.36	5.56	4.04	10.2	1.40
C_{35}	4.73	3.61	9.29	1.20	5.06	3.80	9.37	1.15
C_{36}	4.77	4.10	8.02	0.91	4.61	3.95	6.78	0.57
C_{37}	5.00	4.35	8.80	0.80	4.76	4.35	5.97	0.35
C_{38}	5.35	4.67	9.46	0.85	5.01	4.75	5.53	0.20
C_{39}	6.71	5.89	11.6	1.04	6.41	5.64	7.79	0.53
Subtotal	177	96.1	467	76.6	218	74.4	500	89.3
CPI (C_{20}–C_{39})	1.28	1.18	1.32	1.32	1.24	1.10	1.37	1.35
				Plant Wax Alkanes				
C_{23}	1.64	0.30	6.72	1.19	1.80	0.00	4.98	1.56
C_{25}	0.81	0.00	3.93	0.82	0.76	0.00	4.13	1.07
C_{27}	2.02	0.00	5.28	1.18	2.00	0.00	5.69	1.65
C_{29}	5.42	0.47	17.4	3.58	6.55	0.00	20.5	4.47
C_{31}	4.08	0.25	15.5	2.87	4.82	0.00	18.2	3.54
C_{33}	1.30	0.10	6.05	1.15	1.36	0.00	6.85	1.38
C_{35}	0.16	0.00	0.86	0.26	0.22	0.00	1.04	0.33
C_{37}	0.10	0.00	0.53	0.17	0.10	0.00	0.74	0.19
Subtotal	15.5	1.12	56.2	11.2	17.6	0	62.1	14.2

Table 1. (Continued)

Compounds	Daytime				Nighttime			
	Mean	Min[a]	Max[b]	SD[c]	Mean	Min[a]	Max[b]	SD[c]
				Fatty acids				
$C_{12:0}$	0.54	0.12	2.04	0.44	0.60	0.19	1.57	0.31
$C_{13:0}$	0.55	0.11	2.08	0.40	0.74	0.03	2.38	0.57
$C_{14:0}$	0.81	0.27	2.48	0.39	1.05	0.21	1.87	0.40
$C_{15:0}$	0.61	0.19	1.88	0.34	0.69	0.05	1.50	0.29
$C_{16:0}$	18.9	5.12	56.8	11.2	30.5	3.87	89.2	20.9
$C_{17:0}$	0.60	0.18	1.99	0.37	0.77	0.11	1.80	0.36
$C_{18:0}$	7.46	1.88	23.4	4.11	12.2	1.48	28.9	7.16
$C_{19:0}$	0.36	0.08	1.07	0.23	0.48	0.02	1.41	0.30
$C_{20:0}$	1.40	0.38	5.06	0.92	1.78	0.18	4.19	0.92
$C_{21:0}$	0.81	0.14	2.87	0.57	0.96	0.03	2.32	0.55
$C_{22:0}$	2.70	0.57	10.4	1.90	3.16	0.17	7.51	1.85
$C_{23:0}$	1.94	0.43	8.47	1.55	2.38	0.10	5.41	1.34
$C_{24:0}$	16.8	3.28	73.8	13.5	19.4	1.51	50.9	11.7
$C_{25:0}$	1.11	0.16	4.34	0.82	1.37	0.00	3.45	0.85
$C_{26:0}$	2.75	0.37	10.6	2.08	3.22	0.10	9.07	2.09
$C_{27:0}$	0.62	0.09	1.94	0.46	0.74	0.00	2.07	0.54
$C_{28:0}$	2.27	0.38	10.3	1.95	2.86	0.23	6.88	1.81
$C_{29:0}$	0.63	0.09	2.88	0.56	0.79	0.00	2.10	0.49
$C_{30:0}$	2.35	0.34	12.6	2.32	2.99	0.17	9.40	2.14
$C_{31:0}$	0.26	0.00	1.38	0.25	0.35	0.05	1.17	0.28
$C_{32:0}$	1.13	0.00	7.48	1.44	1.55	0.07	6.04	1.35
$C_{18:1}$	0.36	0.04	1.62	0.33	0.39	0.00	1.66	0.37
$C_{18:2}$	1.81	0.10	8.18	1.80	2.31	0.00	10.9	2.58
Subtotal	66.8	14.3	254	47.9	91.3	8.57	252	59.2
CPI ($C_{20:0}$-$C_{32:0}$)	5.41	4.24	6.50	0.54	5.52	4.29	13.2	1.51
				Fatty alcohols				
C_{12}	1.74	0.26	5.76	1.12	1.99	0.16	7.33	1.38
C_{14}	3.58	0.70	23.9	4.11	4.13	0.10	11.6	2.60
C_{15}	0.60	0.22	1.81	0.39	0.66	0.05	1.33	0.38
C_{16}	0.66	0.16	1.60	0.34	0.71	0.05	2.32	0.45
C_{17}	0.42	0.10	1.30	0.26	0.46	0.13	1.98	0.34
C_{18}	0.91	0.19	2.33	0.57	1.43	0.13	6.35	1.25
C_{19}	0.54	0.15	2.09	0.35	0.56	0.15	1.34	0.30
C_{20}	1.08	0.18	2.71	0.66	1.11	0.27	3.06	0.63
C_{21}	0.74	0.15	2.98	0.56	0.75	0.12	2.12	0.45
C_{22}	1.76	0.47	6.37	1.26	2.11	0.13	6.92	1.44
C_{23}	0.68	0.14	1.97	0.43	0.92	0.23	2.92	0.60
C_{24}	1.22	0.19	7.86	1.31	1.28	0.16	3.50	0.77
C_{25}	0.64	0.21	1.94	0.35	0.55	0.11	1.26	0.27
C_{26}	2.99	0.18	10.7	2.03	3.34	0.68	7.77	1.93
C_{27}	0.83	0.19	2.27	0.48	0.87	0.00	3.74	0.70
C_{28}	5.72	1.17	19.3	3.69	6.44	1.09	18.7	3.62

Table 1. (continued)

Compounds	Daytime				Nighttime			
	Mean	Min[a]	Max[b]	SD[c]	Mean	Min[a]	Max[b]	SD[c]
C_{29}	0.97	0.16	5.20	0.90	0.94	0.00	2.38	0.55
C_{30}	8.73	1.87	51.7	8.66	11.6	0.87	32.6	6.36
C_{31}	0.67	0.00	2.46	0.47	0.78	0.00	2.86	0.51
C_{32}	2.39	0.61	10.4	1.91	3.14	0.18	9.29	2.15
Subtotal	36.9	7.30	165	29.9	43.8	4.61	129	26.7
CPI (C_{20}-C_{32})	5.22	2.56	10.3	1.67	6.32	3.06	15.5	2.45
			Anhydro-sugars					
Galactosan	2.26	0.65	7.47	1.36	3.13	0.48	7.75	2.07
Mannosan	1.62	0.36	4.30	0.93	2.06	0.27	5.73	1.36
Levoglucosan	38.4	4.79	179	38.6	66.0	4.96	354	76.7
Subtotal	42.3	5.8	191	40.9	71.2	5.71	367	80.1
			Sugars					
Erythritol	0.24	0.04	0.64	0.13	0.27	0.02	0.58	0.15
Mannitol	0.30	0.09	0.91	0.17	0.30	0.07	0.70	0.14
Inositol	0.18	0.05	0.40	0.07	0.20	0.05	0.43	0.10
Arabitol	0.43	0.08	1.20	0.21	0.50	0.04	1.10	0.26
Fructose	0.69	0.15	1.45	0.36	0.60	0.11	1.50	0.32
Glucose	1.14	0.27	2.77	0.51	1.16	0.20	2.86	0.58
Sucrose	0.25	0.05	0.71	0.15	0.23	0.06	0.87	0.17
Trehalose	0.21	0.05	0.81	0.15	0.17	0.04	0.45	0.09
Subtotal	3.44	0.78	8.89	1.75	3.43	0.59	8.49	1.81
			Phthalate esters					
Diethyl (DEP)	0.14	0.03	0.57	0.12	0.15	0.03	0.50	0.11
Diisobutyl (DiBP)	2.56	0.59	8.54	2.03	2.72	0.63	7.19	1.67
Di-n-butyl (DnBP)	8.18	1.30	20.0	5.52	8.12	2.08	22.8	5.04
Di-(2-ethylhexyl) (DEHP)	3.00	0.74	10.9	2.38	5.32	1.06	21.3	4.24
Subtotal	13.9	2.66	40.0	10.1	16.3	3.80	51.8	11.1
			Glycerol and Polyacids					
Glycerol	2.67	0.66	5.99	1.63	3.50	0.73	8.72	2.36
Glyceric acid	1.59	0.28	8.34	1.58	1.68	0.34	4.30	1.09
Malic acid	1.09	0.07	4.66	1.12	1.19	0.36	3.35	0.81
Tartaric acid	1.93	0.51	8.57	1.44	2.57	1.02	5.74	1.31
Citric acid	0.50	0.07	2.15	0.40	0.36	0.09	0.98	0.22
Subtotal	7.78	1.59	29.7	6.17	9.30	2.54	23.1	5.79
			Aromatic acids					
Benzoic acid	0.45	0.17	0.95	0.18	0.54	0.24	1.22	0.21
Phthalic acid	0.68	0.24	1.24	0.30	0.65	0.28	1.80	0.37
Isophthalic acid	0.13	0.03	0.33	0.08	0.14	0.05	0.40	0.10
Terephthalic acid	5.44	1.09	20.6	4.13	7.04	1.42	15.0	4.15
Subtotal	6.70	1.53	23.1	4.69	8.37	1.99	18.4	4.83

42 **Table 1. (Continued)**

Compounds	Daytime				Nighttime			
	Mean	Min[a]	Max[b]	SD[c]	Mean	Min[a]	Max[b]	SD[c]
Lignin and Resin products								
4-Hydroxybenzoic acid	1.80	0.65	4.31	0.79	2.01	0.62	4.96	1.02
Vanillic acid	0.25	0.04	0.92	0.15	0.25	0.08	0.66	0.12
Syringic acid	0.17	0.04	0.57	0.09	0.20	0.05	0.43	0.09
Dehydroabietic acid	0.46	0.11	1.16	0.26	0.93	0.00	8.29	1.47
Subtotal	2.68	0.84	6.96	1.29	3.39	0.75	14.3	2.70
PAHs								
Napthalene (Nap)	0.52	0.45	0.80	0.07	0.51	0.41	0.60	0.05
Acenaphthylene (Acnl)	2.01	1.80	3.47	0.28	1.95	1.66	2.17	0.10
Acenapthene (Ace)	0.64	0.56	1.22	0.11	0.61	0.55	0.69	0.04
Fluorene (Flu)	1.00	0.83	1.70	0.14	0.94	0.85	1.05	0.05
Phenanthrene (Phe)	1.95	0.68	4.52	0.96	2.03	0.33	4.62	1.17
Anthracene (Ant)	1.38	1.11	4.21	0.56	1.30	1.00	2.02	0.23
Fluoranthene (Flut)	7.21	3.01	18.2	3.19	9.34	2.14	27.6	5.33
Pyrene (Pyr)	5.33	2.15	11.4	2.15	7.59	1.32	26.8	4.78
Benzo[a]anthracene (BaA)	3.98	2.37	6.44	1.07	6.14	1.87	14.8	3.54
Chrysene (Chry)	5.31	2.50	9.11	1.78	7.70	1.24	17.0	4.11
Benzo[b]fluoranthene (BbF)	4.88	2.42	8.40	1.52	6.88	1.51	14.4	3.57
Benzo[k]fluoranthene (BkF)	2.47	0.94	4.28	0.80	3.39	0.84	7.19	1.56
Benzo[e]pyrene (BeP)	3.08	1.39	6.01	1.18	4.71	0.68	11.6	2.84
Benzo[a]pyrene (BaP)	3.46	1.86	6.35	1.08	5.23	1.31	13.1	2.88
Indeno[1,2,3-cd]pyrene (IP)	4.52	2.85	8.01	1.24	6.50	2.11	24.5	4.21
Benzo[ghi]perylene (BghiP)	3.66	1.91	6.93	1.22	5.85	1.40	26.1	4.64
Dibenzo[a,h]anthracene (DahA)	3.08	2.70	5.19	0.46	4.11	2.49	28.7	4.68
Subtotal	54.5	29.5	106	17.8	74.8	21.7	223	43.8
Hopanes								
17 α(H)-22,29,30-Trisnorhopane	0.23	0.00	1.51	0.28	0.43	0.03	1.46	0.35
17 α(H)-21 β(H)-30-Norhopane	0.53	0.03	2.65	0.50	0.64	0.03	3.39	0.65
17 α(H)-21 β(H)-Hopane	1.18	0.02	8.91	1.54	1.71	0.07	8.88	1.73
17 β(H)-21 α(H)-Hopane	0.22	0.01	1.12	0.25	0.26	0.00	0.93	0.27
17 α(H)-21 β(H)-22S-Homohopane	0.58	0.00	2.07	0.53	0.90	0.00	3.94	0.95
17 α(H)-21 β(H)-22R-Homohopane	1.05	0.01	4.58	1.05	0.70	0.00	7.52	1.36
Subtotal	3.79	0.07	20.8	4.15	4.64	0.13	26.1	5.31
Steranes								
ααα 20S-Cholestane	0.41	0.19	1.64	0.31	0.42	0.18	1.42	0.25
αββ 20R-Cholestane	0.36	0.18	1.74	0.27	0.40	0.17	1.43	0.25
ααα 20R-Cholestane	0.38	0.18	1.98	0.33	0.42	0.18	2.01	0.35
αββ 20R, 24S-Methylcholestane	0.35	0.19	1.13	0.19	0.36	0.16	1.25	0.22
αββ 20R, 24R-Ethylcholestane	0.44	0.22	1.06	0.19	0.55	0.23	2.34	0.38
ααα 20R, 24R-Ethylcholestane	0.35	0.17	1.60	0.27	0.50	0.16	2.65	0.47
Subtotal	2.29	1.13	9.15	1.56	2.65	1.08	11.1	1.92

[a]Minimum, [b]Maximum, [c]Standard deviation

CPI: carbon preference index: $(C_{21}+C_{23}+C_{25}+C_{27}+C_{29}+C_{31}+C_{33}+C_{35}+C_{37}+C_{39})/(C_{20}+C_{22}+C_{24}+C_{26}+C_{28}+C_{30}+C_{32}+C_{34}+C_{36}+C_{38})$ for n-alkanes; $(C_{20}+C_{22}+C_{24}+C_{26}+C_{28}+C_{30}+C_{32})/(C_{21}+C_{23}+C_{25}+C_{27}+C_{29}+C_{31})$ for fatty acids; $(C_{20}+C_{22}+C_{24}+C_{26}+C_{28}+C_{30}+C_{32})/(C_{21}+C_23+C_{25}+C_{27}+C_{29}+C_{31})$ for fatty alcohols.

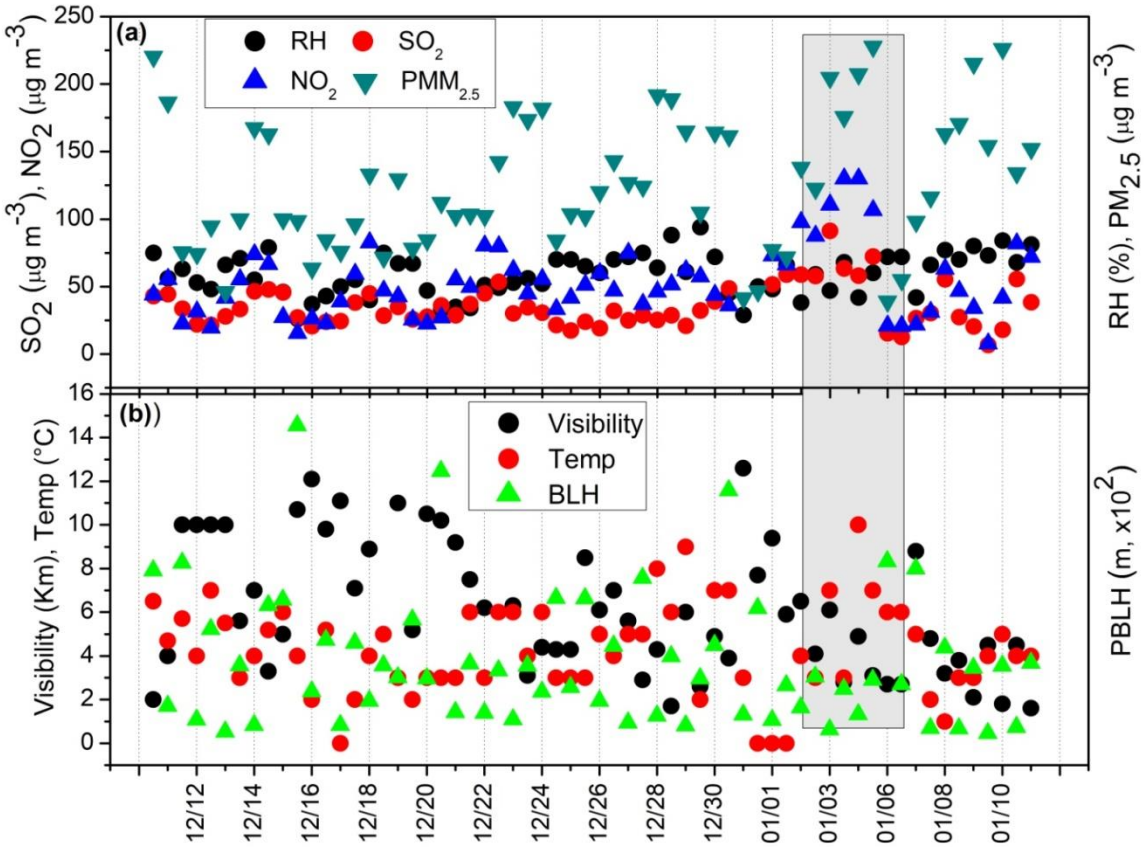
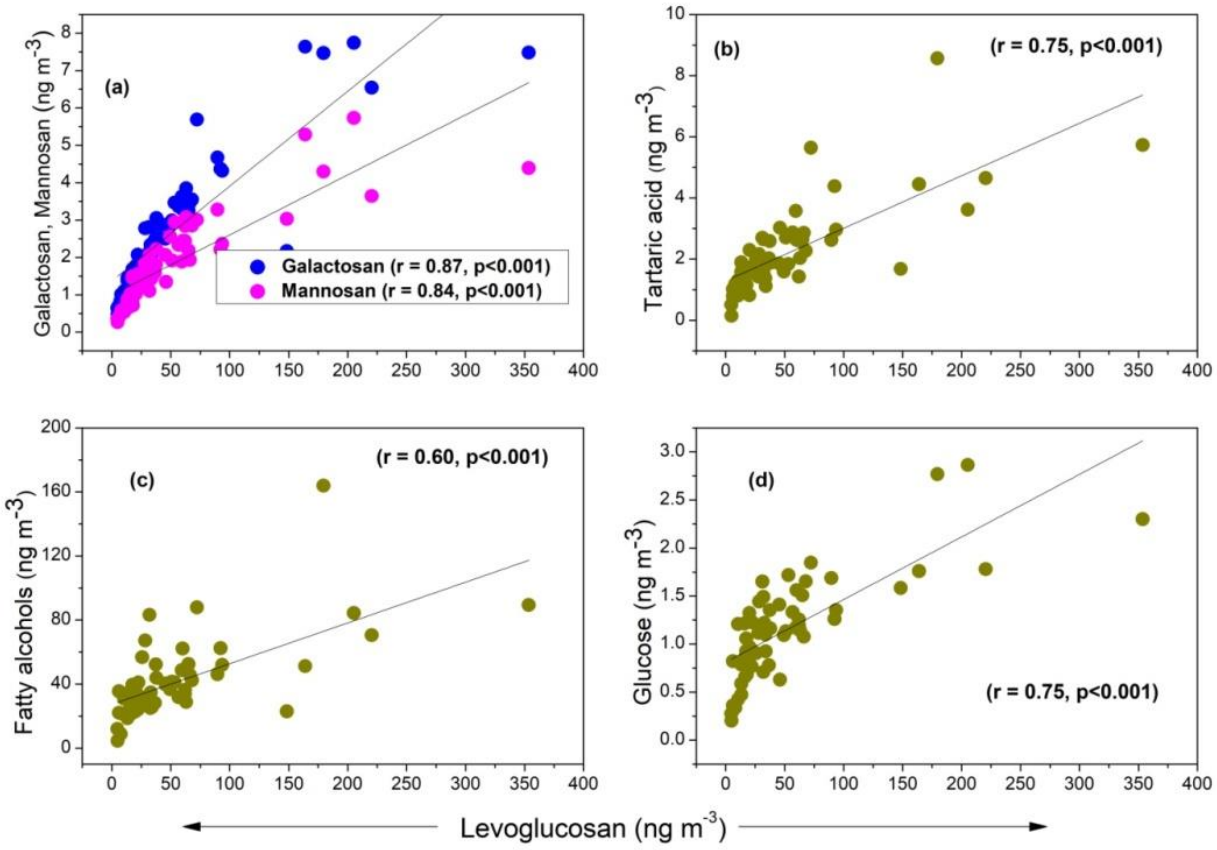


Figure S1. Diurnal variations of (a) SO_2, NO_2, Relative Humidity (RH), and $PM_{2.5}$ (b) Visibility, Temperature (Temp) and Planetary Boundary Layer Height (PBLH) in Nanjing aerosols during study period.



54

55 **Figure S2.** Correlation coefficients of levoglucosan with galactosan, mannosan, glucose, tartaric acid
56 and fatty alcohols in urban aerosols in Nanjing.

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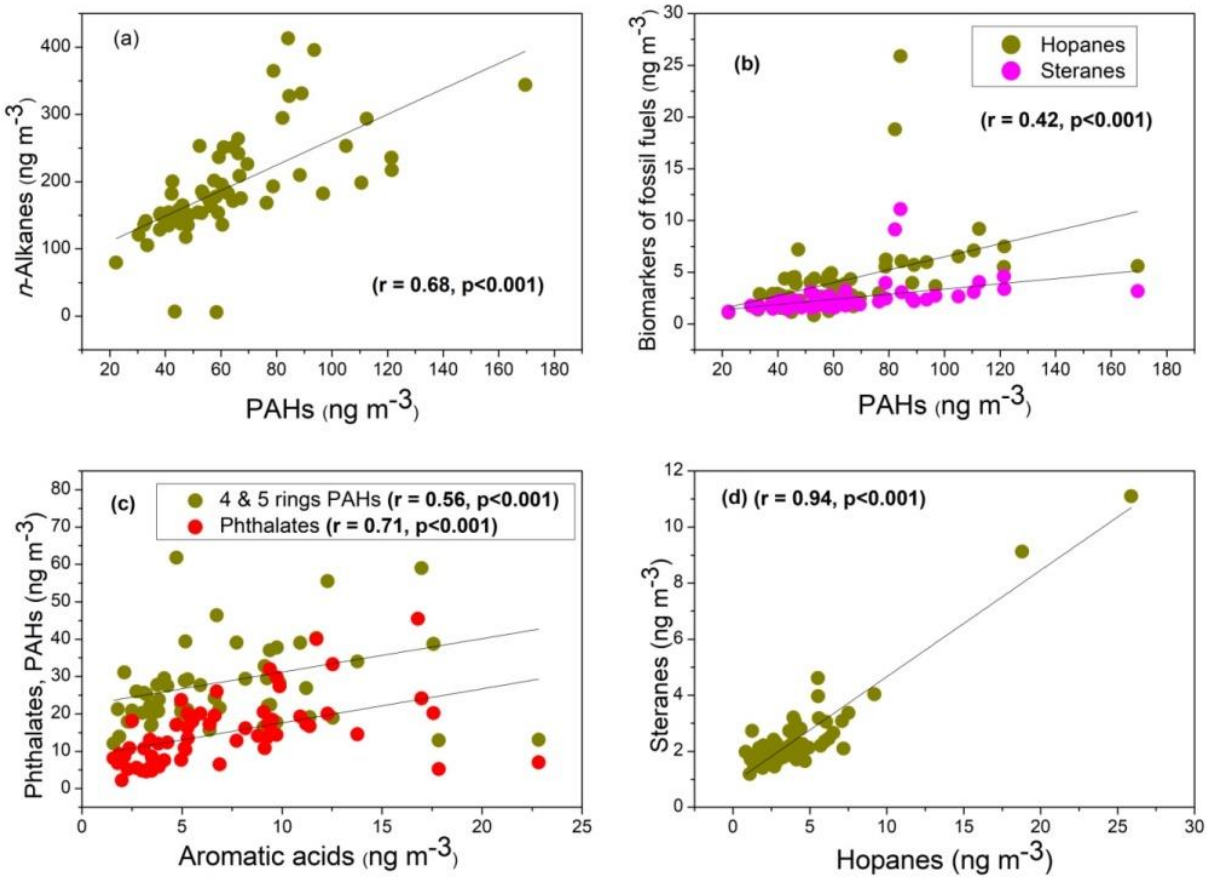
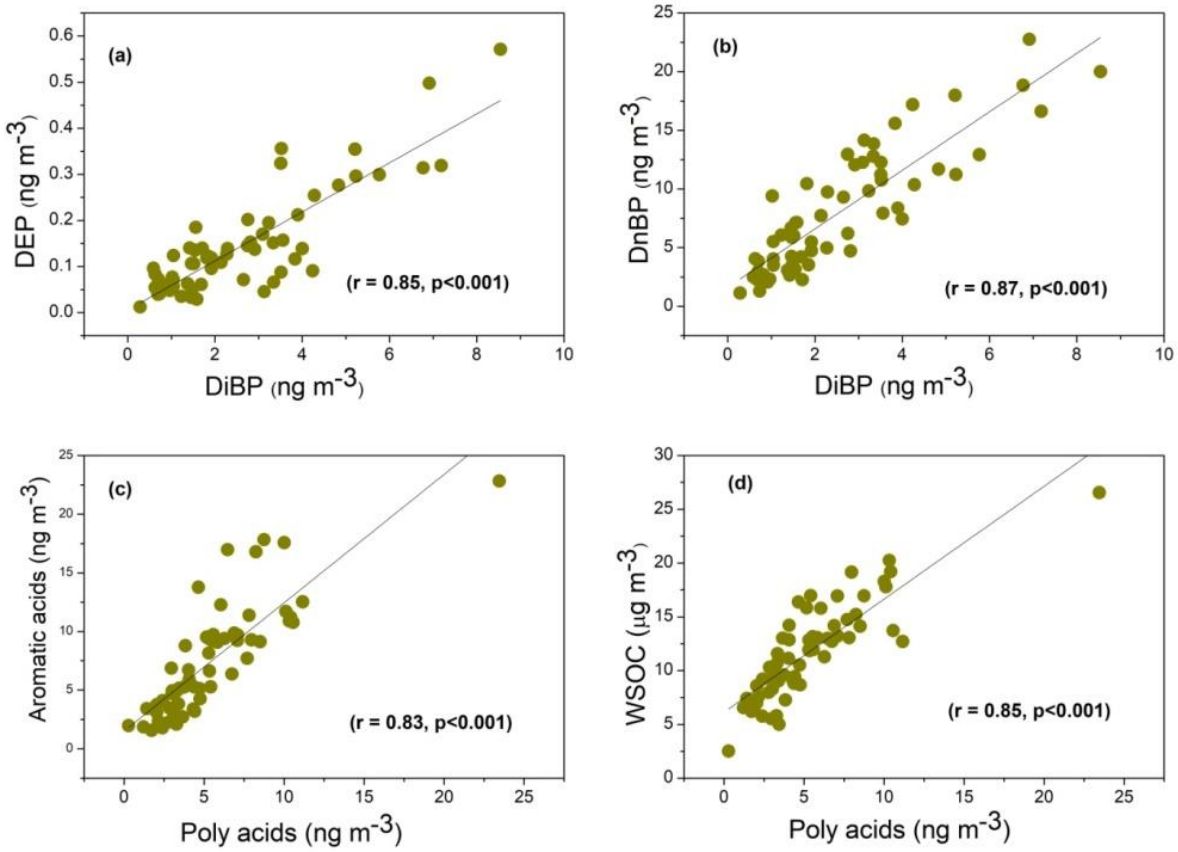


58

59 **Figure S3.** Correlations between the concentrations of **(a)** PAHs and *n*-alkanes **(b)** PAHs and
60 hopanes/steranes **(c)** aromatic acids and phthalates/PAHs **(d)** hopanes and steranes.

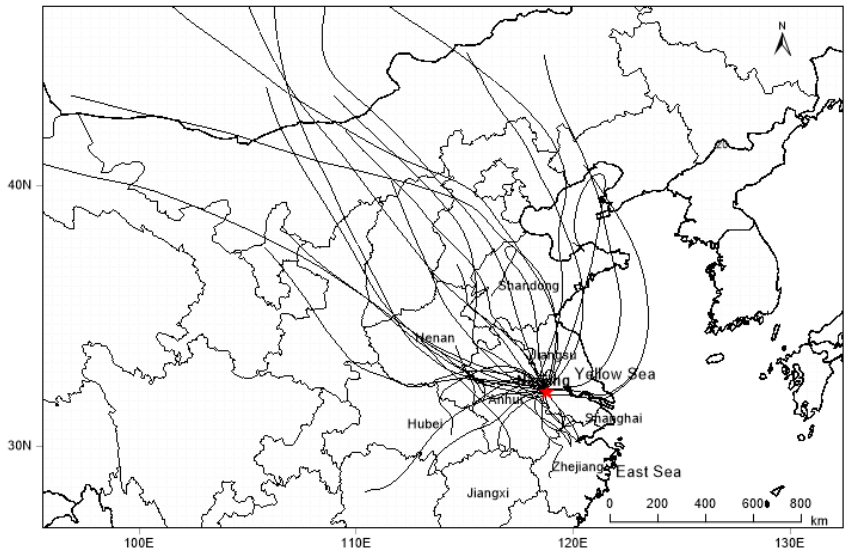
61



62

63 **Figure S4.** Relationships between the concentrations of **(a)** DiBP (di-iso-butyl phthalate) and DEP
64 (diethyl phthalate) **(b)** DiBP (di-iso-butyl phthalate) and DnBP (di-n-butyl phthalate) **(c)** poly acids
65 and aromatic acids **(d)** poly acids and WSOC.

66



67

68 **Figure S5.** 48 hrs backward air mass trajectories arriving at 500 m above the ground level to Nanjing,
69 China during 11 Dec 2014–11 Jan 2015.