

1 Supporting information for

2 **Characterization of organic aerosols from a Chinese Mega-City during winter:**
3 **predominance of fossil fuel combustion**

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33 **Table S1.** Concentrations of identified organic compounds (ng m⁻³) in the atmospheric aerosol
 34 samples (PM_{2.5}) from Nanjing, China.
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Compounds	Daytime				Nighttime			
	Mean	Min ^a	Max ^b	SD ^c	Mean	Min ^a	Max ^b	SD ^c
<i>n</i> -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

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38 **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

40 **Table 1. (continued)**

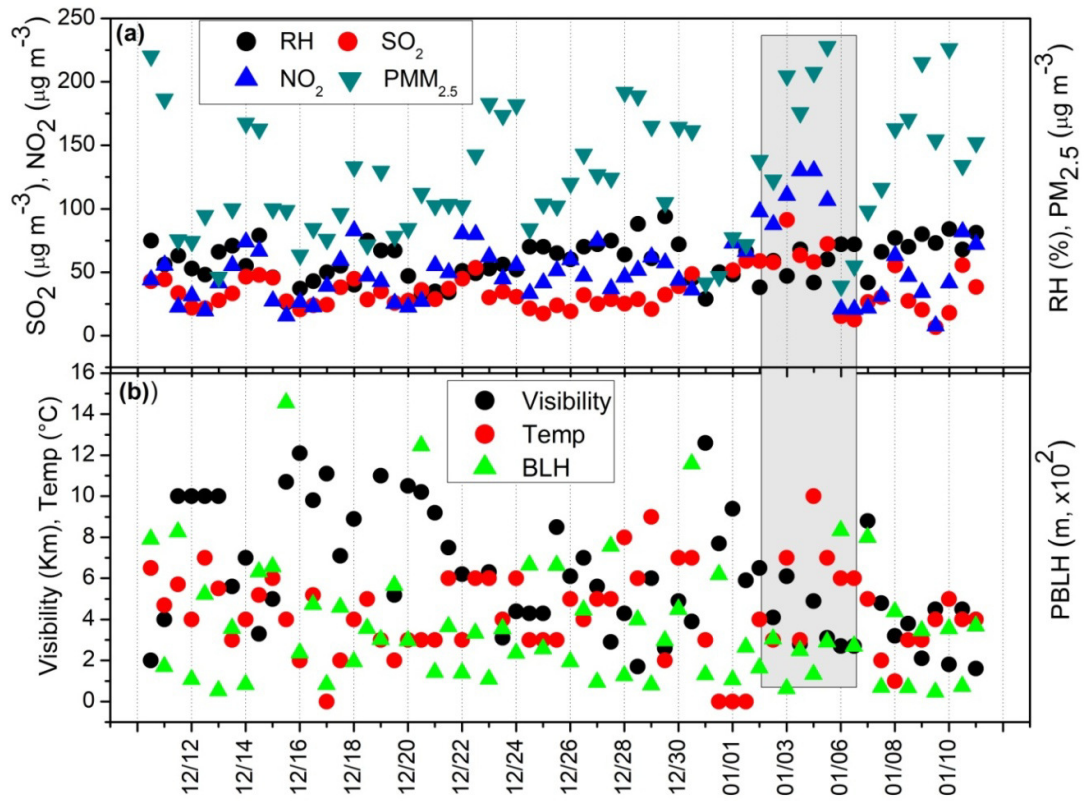
Compounds	Daytime				Nighttime			
	Mean	Min ^a	Max ^b	SD ^c	Mean	Min ^a	Max ^b	SD ^c
C ₂₉	0.97	0.16	5.20	0.90	0.94	0.00	2.38	0.55
C ₃₀	8.73	1.87	51.7	8.66	11.6	0.87	32.6	6.36
C ₃₁	0.67	0.00	2.46	0.47	0.78	0.00	2.86	0.51
C ₃₂	2.39	0.61	10.4	1.91	3.14	0.18	9.29	2.15
Subtotal	36.9	7.30	165	29.9	43.8	4.61	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
Levoglucoosan	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
Acenaphthene (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								
$\alpha\alpha\alpha$ 20S-Cholestane	0.41	0.19	1.64	0.31	0.42	0.18	1.42	0.25
$\alpha\beta\beta$ 20R-Cholestane	0.36	0.18	1.74	0.27	0.40	0.17	1.43	0.25
$\alpha\alpha\alpha$ 20R-Cholestane	0.38	0.18	1.98	0.33	0.42	0.18	2.01	0.35
$\alpha\beta\beta$ 20R, 24S-Methylcholestane	0.35	0.19	1.13	0.19	0.36	0.16	1.25	0.22
$\alpha\beta\beta$ 20R, 24R-Ethylcholestane	0.44	0.22	1.06	0.19	0.55	0.23	2.34	0.38
$\alpha\alpha\alpha$ 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

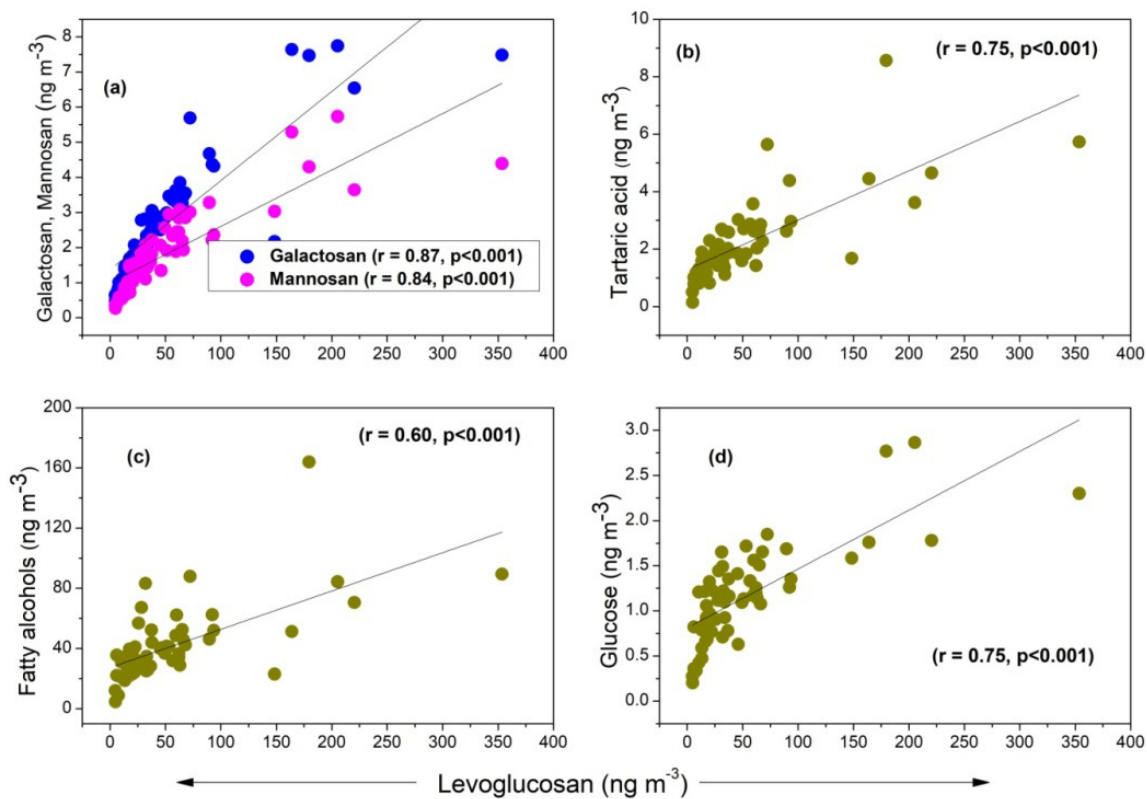
^aMinimum, ^bMaximum, ^cStandard deviation

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.



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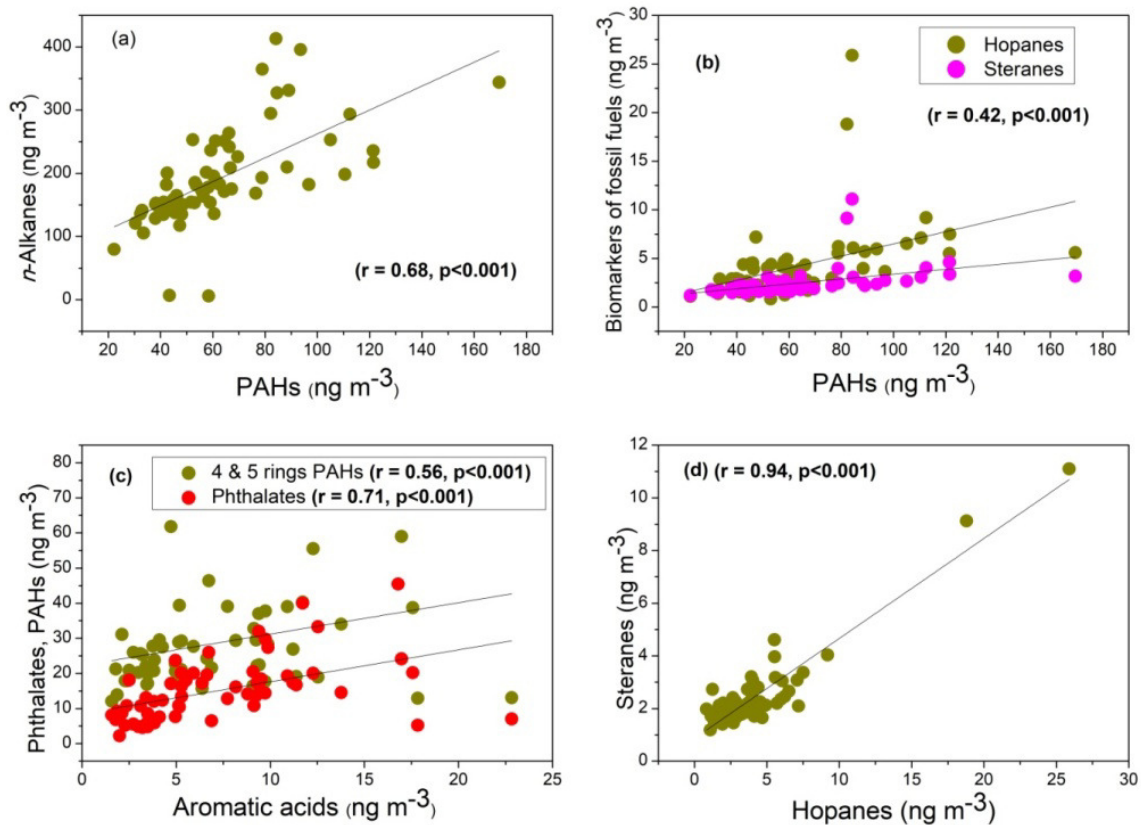
45 **Figure S1.** Diurnal variations of (a) SO₂, NO₂, Relative Humidity (RH), and PM_{2.5} (b)
 46 Visibility, Temperature (Temp) and Planetary Boundary Layer Height (PBLH) in Nanjing
 47 aerosols during study period.
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55 **Figure S2.** Correlation coefficients of levoglucosan with galactosan, mannosan, glucose, tartaric acid
 56 and fatty alcohols in urban aerosols in Nanjing.

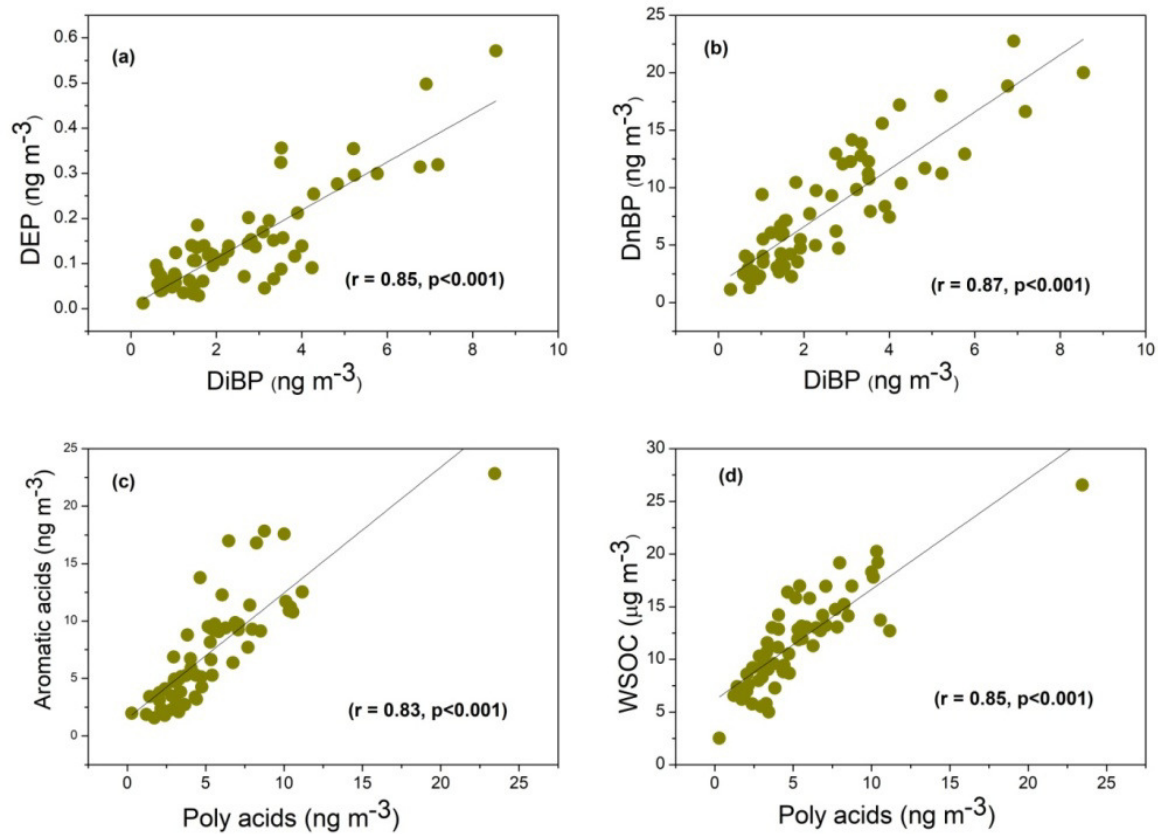
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59 **Figure S3.** Correlations between the concentrations of (a) PAHs and n -alkanes (b) PAHs and
 60 hopanes/steranes (c) aromatic acids and phthalates/PAHs (d) hopanes and steranes.

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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.

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