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Measurement report: Vertical distribution of biogenic and anthropogenic secondary organic aerosols in the urban boundary layer over Beijing during late summer

Hong Ren et al.

Correspondence to: Pingqing Fu (fupingqing@tju.edu.cn)

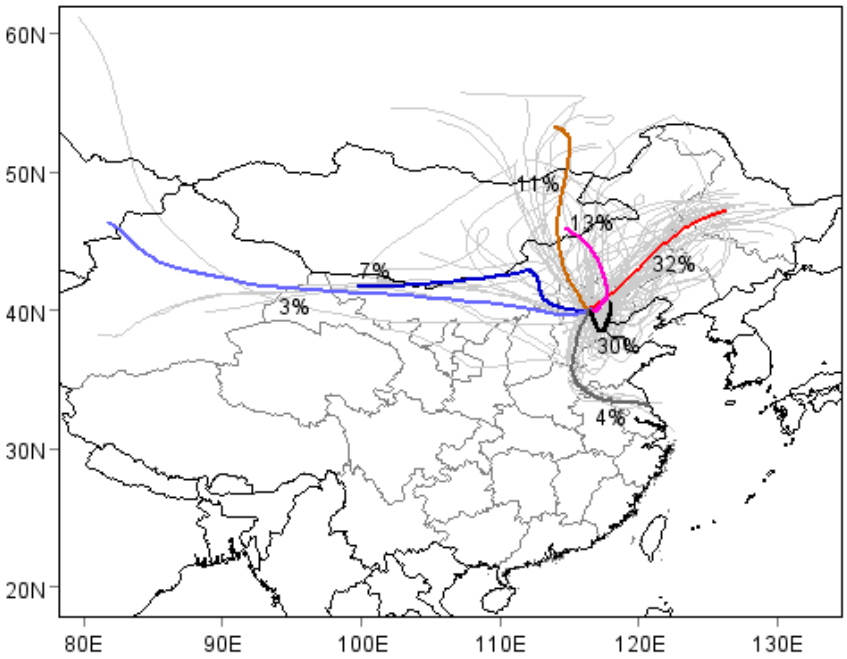

Figure S1. Three-day back trajectories of air mass during August 15th to September 10th at 300 m (a.g.l) by using MeteoInfo Software with the meteorological date from the NOAA website (https://ready.arl.noaa.gov/archives.php). The trajectories are calculated every 6 hours. Total seven air mass clusters are calculated, the numbers in the figure indicate the percentages of air mass with each cluster and marked with different colors. The origins of air masses were mainly from southeast and northeast.

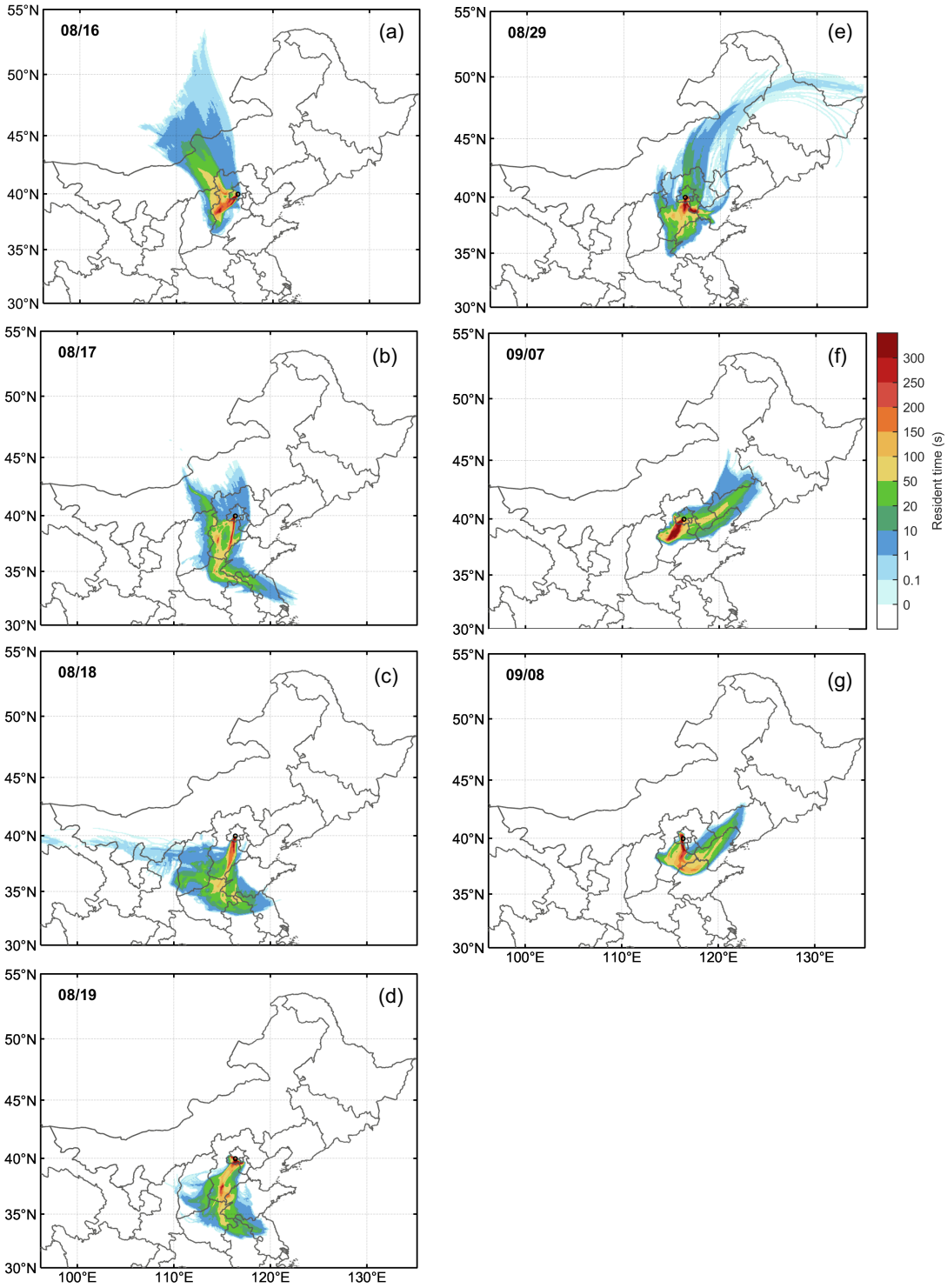

Figure S2. Retroplumes of air masses at 300 m (a.g.l) at the sampling site (marked as black dot) using the FLEXPART model. The color scales indicate the residence times (s) of air masses in the grid cell. The longer residence time in the region, the greater impact from that region.

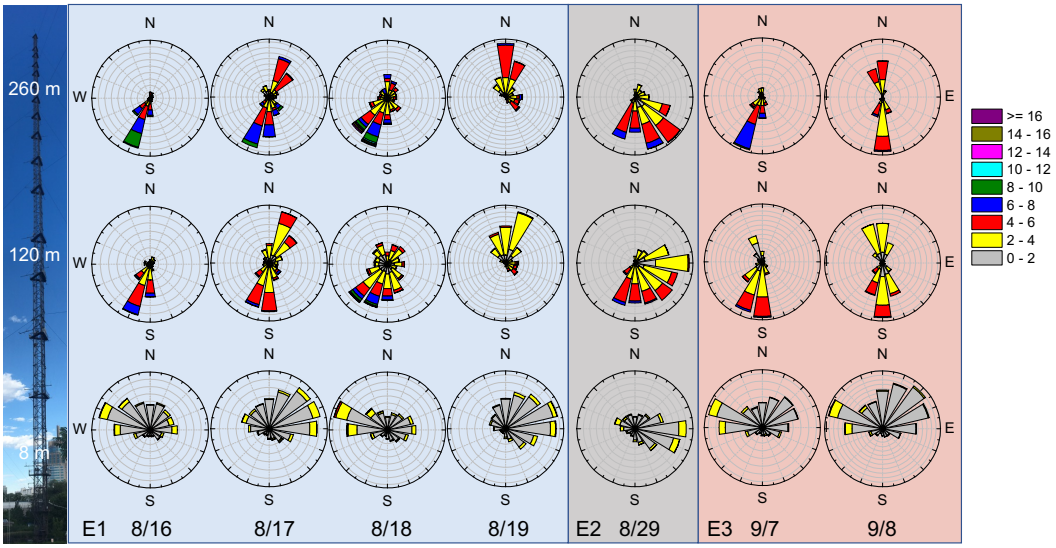

Figure S3. Wind roses of each day at 8 m, 120 m, and 260 m during the E1, E2, and E3 periods. E1 (left) is in light blue shadow, E2 (middle) is in grey shadow, and E3 (right) is in pink shadow.

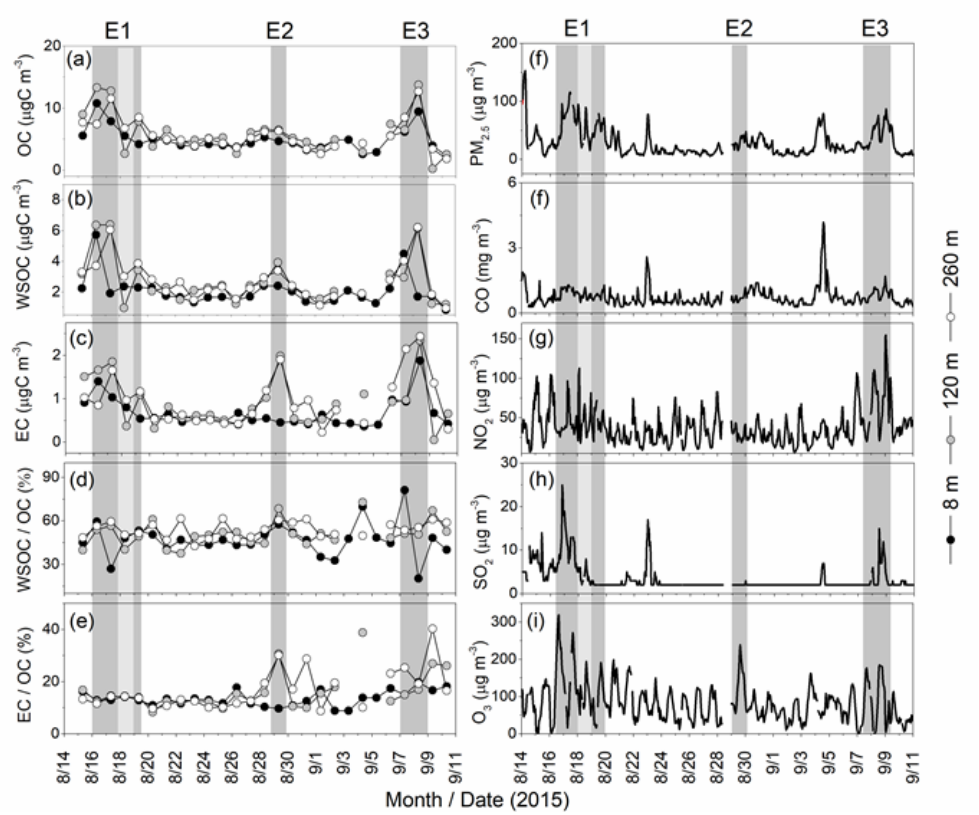

Figure S4. Time variations in (a) OC, (b) WSOC, (c) EC, (d) WSOC/OC, (e) EC/OC, and (f) to (i) are the levels of $PM_{2.5}$, CO, NO_2, SO_2 and O_3 from the monitor station of the Olympic center near the sampling site, respectively.

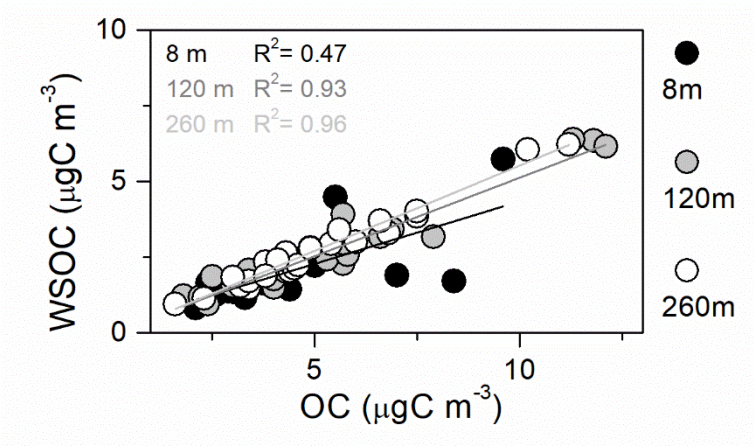

Figure S5. Correlations between WSOC and OC at 8 m, 120 m, and 260 m in $PM_{2.5}$ of Beijing.

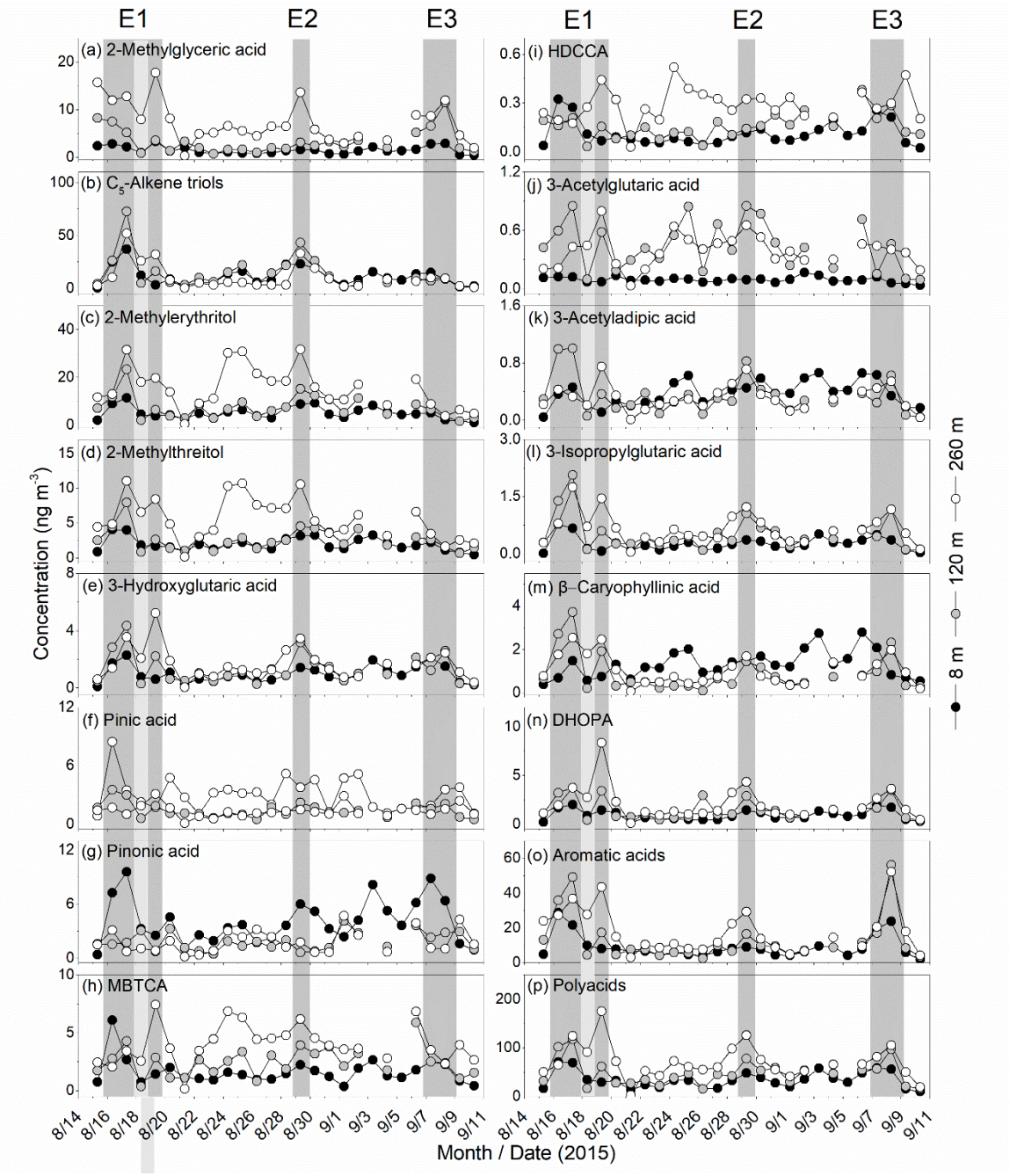

Figure S6. Time variations in SOA tracer from (a–d) isoprene, (e–l) monoterpene, (m) β-caryophyllinic acid, (n) dihydroxy-4-oxopentanoic acid (DHOPA), (o) aromatic acid, and (p) polyacids at three heights in $PM_{2.5}$ of Beijing.

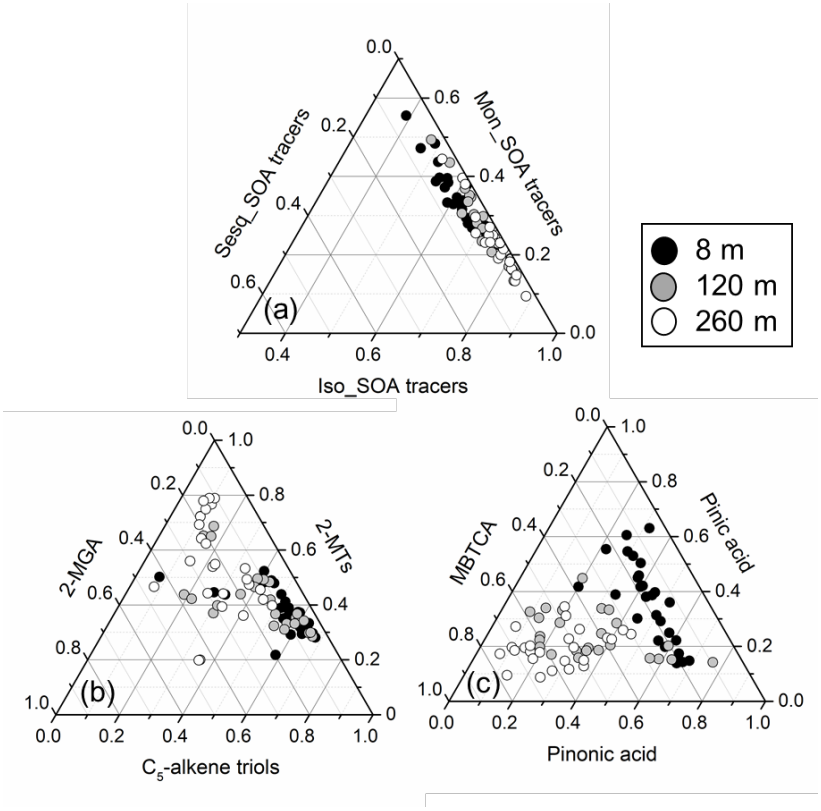

Figure S7. Compositions of BSOA tracers from (a) isoprene (Iso_SOA tracers), monoterpene (Mon_SOA tracers), and sesquiterpene (Sesq_SOA tracers), (b) isoprene derived products, and (c) monoterpene derived products at three heights.

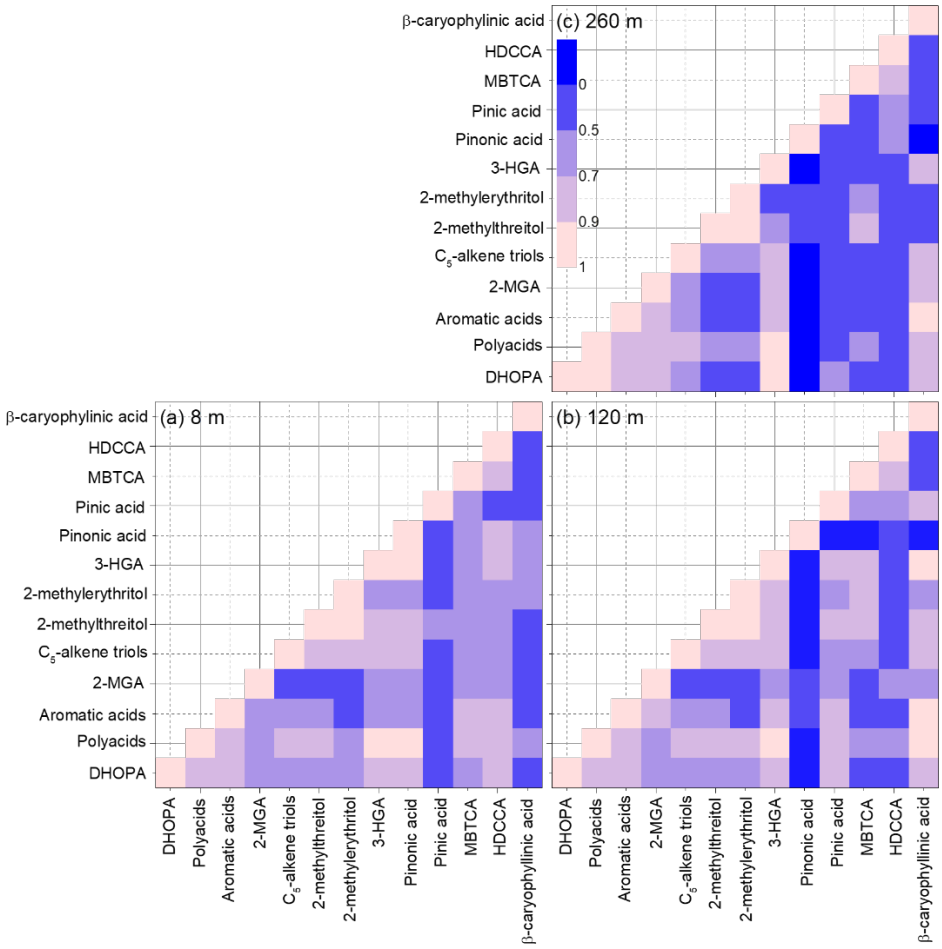

Figure S8. Correlations in SOA tracers (DHOPA, sum of polyacids, sum of aromatic acids, BSOA tracers) at 8 m, 120 m, and 260 m in $PM_{2.5}$ of Beijing. The color bar (blue to pinky) is represented the magnitude of Pearson's coefficient values (R).

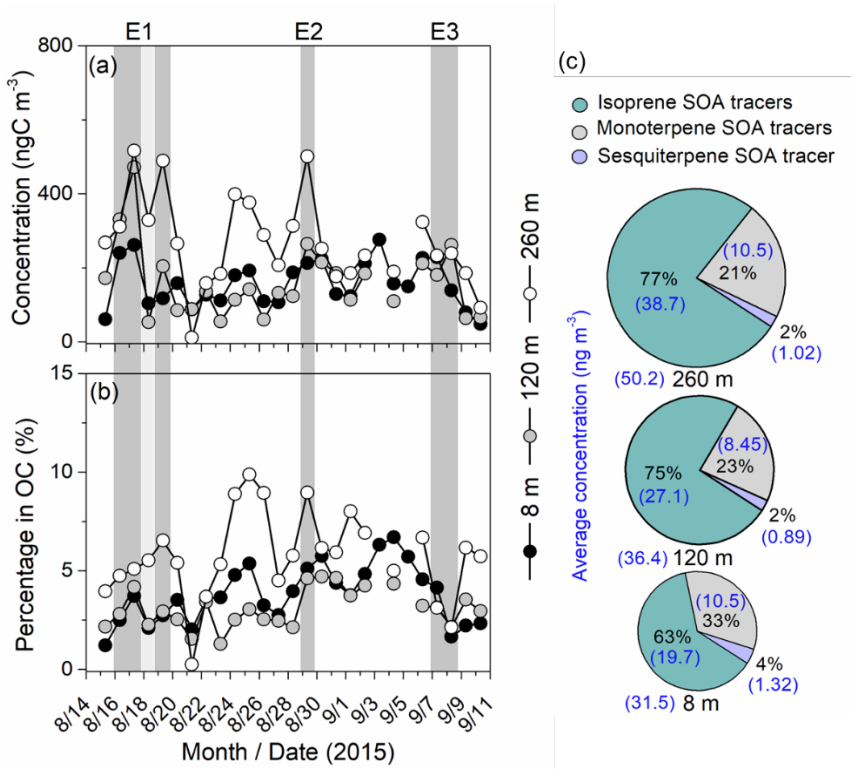

Figure S9. Temporal variations in (a) the estimated BSOC concentrations, (b) the percentage of estimated BSOC in OC and (c) relative mass contributions of estimated BSOC.

Table S1. Summary of the average meteorological parameters, concentrations of secondary organic tracers (SOA), OC and WSOC and their ratios in $PM_{2.5}$ collected at the surface layer (8 m, a two-story building) and 120 m and 260 m (platform of the 325 m a.g.l. meteorological tower) in urban of Beijing during the whole sampling period (Aug. 15th Aug to Sep. 10th).

	8 m				120 m				260 m			
Compound	Min	Max	Mean	Std	Min	Max	Mean	Std	Min	Max	Mean	Std
Meteorological parameters												
Tem [a]	14.2	35.2	25.2	3.99	13.0	34.3	24.3	3.96	11.8	33.0	23.2	3.74
RH [a]	20.0	100	60.6	17.5	21.0	100	61.9	18.5	23.0	100	65.5	20.4
WS [a]	0.30	7.90	1.23	0.68	0.30	17.3	3.02	1.39	0.30	15.8	3.47	1.66
Isoprene SOA tracers (ng m^{-3})												
2-Methylglyceric acid	0.43	3.36	1.53	0.81	0.71	11.5	3.35	2.66	0.32	17.8	7.37	4.39
C5-alkene triols	0.43	36.8	11.3	8.47	1.13	72.7	13.8	15.9	0.39	51.81	10.6	12.6
2-Methylthreitol	0.43	4.02	1.95	0.95	0.65	7.91	2.61	1.60	0.15	11.1	5.56	3.02
2-Methylerythritol	0.98	11.3	4.99	2.58	1.54	23.2	7.32	4.87	0.42	31.6	15.4	8.80
Subtotal	***4.02***	***54.3***	***19.7***	***12.0***	***5.20***	***109***	***27.1***	***22.4***	***1.27***	***107***	***38.7***	***24.1***
Monoterpene SOA tracers (ng m^{-3})												
3-Hydroxyglutaric acid	0.10	2.27	0.96	0.58	0.26	4.33	1.30	1.05	0.05	5.23	1.67	1.14
Pinonic acid	0.40	9.55	4.06	2.46	0.47	4.10	1.84	1.01	0.15	4.69	1.81	1.27
Pinic acid	0.83	8.46	3.01	1.74	0.48	3.49	1.40	0.76	0.09	3.10	1.35	0.67
MBTCA [b]	0.38	6.08	1.61	1.10	0.38	5.88	2.46	1.24	0.15	7.43	4.01	1.71
HDCCA [c]	0.02	0.32	0.11	0.08	0.03	0.38	0.16	0.08	0.03	0.52	0.29	0.10
3-Acetylglutaric acid	0.03	0.17	0.09	0.03	0.09	0.85	0.43	0.25	0.03	0.80	0.39	0.17
3-Acetyladipic acid	0.04	0.66	0.38	0.17	0.04	1.00	0.34	0.26	0.01	0.75	0.31	0.18
3-Isopropylglutaric acid	0.01	0.77	0.26	0.19	0.09	2.07	0.52	0.46	0.04	1.74	0.65	0.41
Subtotal	***2.28***	***25.1***	***10.5***	***5.18***	***3.62***	***17.4***	***8.45***	***3.68***	***0.56***	***20.0***	***10.5***	***3.86***
Sesquiterpene SOA tracer (ng m^{-3})												
β-Caryophyllinic acid	0.39	2.78	1.32	0.63	0.11	3.72	0.89	0.89	0.06	2.54	1.02	0.69
Total BSOA tracers	***7.46***	***75.2***	***31.5***	***16.8***	***10.8***	***130.2***	***36.4***	***26.1***	***1.90***	***121***	***50.2***	***27.0***

Table S1. Continued.

	8 m				120 m				260 m			
Compound	Min	Max	Mean	Std	Min	Max	Mean	Std	Min	Max	Mean	Std
Toluene SOA tracer (ng m^{-3})												
DHOPA [d]	0.13	1.98	0.90	0.53	0.35	3.74	1.50	1.09	0.09	8.35	2.03	1.69
Poly acids (ng m^{-3})												
Glycolic acid	4.42	33.2	12.6	6.66	5.55	43.7	15.3	8.64	1.33	44.4	18.0	9.49
Salicylic acid	0.01	0.45	0.16	0.11	0.05	0.93	0.26	0.22	0.02	0.95	0.34	0.21
Glyceric acid	0.60	5.43	2.33	1.42	0.61	10.4	3.63	2.76	0.15	15.9	5.59	3.63
Malic acid	2.27	28.1	13.8	7.37	4.96	50.0	20.2	12.2	0.99	78.7	29.6	15.9
Tartaric acid	0.51	8.18	2.80	2.04	0.80	10.0	4.59	2.99	0.15	23.7	10.5	5.22
Citric acid	0.03	1.14	0.38	0.24	0.08	2.26	0.69	0.61	0.02	3.47	1.65	0.83
Tricarballylic acid	0.47	5.74	2.13	1.31	0.61	11.6	2.98	2.42	0.14	10.9	4.64	2.54
Subtotal	***9.76***	***70.7***	***34.2***	***17.1***	***15.8***	***117.5***	***47.7***	***27.1***	***2.79***	***175***	***70.4***	***35.6***
Aromatic acids (ng m^{-3})												
Benzoic acid	0.11	2.19	0.64	0.46	0.35	3.62	1.01	0.78	0.52	4.62	1.74	1.15
o-Toluic acid	0.04	0.25	0.10	0.05	0.05	0.32	0.12	0.07	0.04	0.34	0.13	0.07
m-Toluic acid	0.08	1.10	0.19	0.19	0.10	4.52	0.39	0.87	0.13	5.42	0.49	1.03
p-Toluic acid	0.06	0.25	0.11	0.05	0.05	0.49	0.13	0.09	0.05	0.46	0.17	0.10
Phthalic	0.53	5.71	2.66	1.27	0.65	9.97	3.59	2.54	1.00	14.7	5.17	2.89
Isophthalic	0.11	0.60	0.26	0.15	0.07	1.64	0.39	0.35	0.13	1.35	0.58	0.36
Terephthalic	0.81	20.8	4.90	4.85	1.21	37.5	7.44	9.73	1.10	33.5	9.23	8.42
Subtotal	***1.78***	***28.7***	***8.86***	***6.58***	***2.51***	***56.1***	***13.06***	***13.8***	***2.98***	***52.2***	***17.5***	***12.8***
Concentrations (μgC/m^{-3})												
WSOC [e]	0.83	5.73	2.03	0.99	0.95	6.36	2.69	1.55	0.94	6.21	2.73	1.31
OC [e]	2.06	9.63	4.37	1.69	1.82	12.15	5.32	2.88	1.60	11.2	5.03	2.28
EC [e]	0.32	1.66	0.60	0.30	0.28	2.06	0.82	0.48	0.20	2.16	0.84	0.52
Percentage in OC (%)												
WSOC / OC	20.2	81.2	46.9	11.9	37.6	72.9	51.1	8.88	42.7	61.6	54.0	5.63
EC / OC	8.89	19.8	13.6	2.92	8.37	38.8	16.2	7.13	8.79	40.3	16.7	7.69

[a] Tem: temperature, RH: relative humidity and WS: wind speed;

[b] MBTCA: 3-methyl-1,2,3-butanetricarboxylic acid;
[c] HDCCA: 3-(2-hydroxyethyl)-2,2-dimethyl-cyclobutane carboxylic acid;
[d] DHOPA: 2,3-dihydroxy-4-oxopentanoic acid;
[e] Water soluble organic carbon (WSOC), organic carbon (OC) detected in aerosols (μgC/m^{-3})

Table S2. Results of single-factor analysis to test the significantly different of these average concentrations at tree heights.

Component (ng m^{-3})[a]	8 m	120 m	260 m
Isoprene SOA tracers	19.7±12.0 **b**[b]	27.1±22.4 **b**	38.7±24.1 **a**
Monoterpene SOA tracers	10.5±5.18 **a**	8.45±3.68 **a**	10.5±3.86 **a**
β-Caryophyllinic acid	1.32±0.63 **a**	0.89±0.89 **b**	1.02±0.69 **ab**
DHOPA	0.90±0.53 **b**	1.50±1.09 **ab**	2.03±1.69 **a**
Phthalic	2.66±1.27 **b**	3.59±2.54 **a**	5.17±2.89 **a**
WSOC	2.03±0.99 **a**	2.69±1.55 **a**	2.73±1.31 **a**
OC	4.37±1.69 **a**	5.32±2.88 **a**	5.03±2.28 **a**
WSOC / OC (%)	46.9±11.9 **b**	51.1±8.88 **a**	54.0±5.63 **a**
2-MTs / 2-MGA	5.20 ± 2.24 **a**	3.80 ± 1.95 **b**	3.15 ± 1.83 **b**
2-MTs / C5-alkene triols	0.97±1.17 **b**	1.33±1.24 **b**	3.97±3.08 **a**
MBTCA / (PAN+PN)	0.24±0.10 **b**	0.84±0.44 **b**	1.49±0.77 **a**

[a] The concentrations of these components are expressed as mean ± STD;
[b] Different lowercase letters in bold indicate significant differences at $P < 0.05$ of the mean concentrations of these compounds in aerosols collected at three heights. The same lowercase letters in bold indicate no significant differences.

Table S3. Concentrations and mass contributions of estimated SOC (including ASOC and BSOC) at three heights in $PM_{2.5}$ in Beijing during the 2015 China Parade (Aug. 15th Aug to Sep. 10th).

	8 m				120 m				260 m			
Component	Min	Max	Mean	Std	Min	Max	Mean	Std	Min	Max	Mean	Std
Concentration (ngC / m^{-3})												
Toluene SOC	16.1	251	114	67.5	43.9	474	189	137	12.0	1057	257	214
Naphthalene SOC	13.9	149	69.2	33.2	16.8	260	93.4	66.0	26.0	382	135	75.4
ASOC [a]	***45.1***	***400***	***184***	***98.2***	***68.9***	***734***	***283***	***195***	***38.0***	***1438***	***391***	***285***
Iso_SOC	11.9	113	54.6	24.7	23.8	235	85.7	48.9	5.71	360	183	90.9
Mon_SOC	9.88	109	45.4	22.4	15.7	75.5	36.6	15.9	2.43	86.7	45.4	16.7
Sesq_SOC	17.0	121	57.4	27.5	4.57	162	38.7	38.8	2.81	110	44.4	29.8
BSOC [b]	***48.1***	***276***	***157***	***62.5***	***53.2***	***472***	***161***	***97.4***	***11.0***	***517***	***272***	***121***
Total SOC	***93.3***	***661***	***341***	***150***	***135***	***1205***	***444***	***283***	***49.0***	***1928***	***664***	***380***
Percentage in OC (%)												
Toluene SOC	0.67	5.01	1.62	0.81	0.72	4.45	1.74	0.81	0.60	5.20	2.74	1.09
Naphthalene SOC	0.67	5.01	1.62	0.81	0.72	4.45	1.74	0.81	0.60	5.20	2.74	1.09
ASOC	***1.27***	***10.8***	***4.25***	***1.98***	***2.07***	***16.5***	***5.52***	***3.17***	***0.87***	***19.2***	***7.63***	***3.51***
Iso_SOC [c]	0.47	2.43	1.29	0.53	0.67	2.83	1.67	0.62	0.13	7.97	3.91	1.79
Mon_SOC [c]	0.20	1.82	1.05	0.37	0.36	1.28	0.76	0.25	0.06	2.44	1.05	0.52
Sesq_SOC [c]	0.31	2.73	1.45	0.73	0.19	1.43	0.66	0.35	0.06	1.60	0.84	0.36
BSOC	***1.22***	***6.70***	***3.80***	***1.46***	***1.29***	***4.71***	***3.09***	***0.97***	***0.25***	***9.87***	***5.80***	***2.20***
Total SOC	***2.48***	***17.5***	***8.05***	***3.17***	***3.36***	***19.0***	***8.60***	***3.66***	***1.12***	***25.7***	***13.4***	***4.81***

[a] Anthropogenic secondary organic carbon (ASOC) : the sum of toluene SOC and naphthalene SOC;
[b] Biogenic secondary organic carbons (BSOC): the sum of Iso_SOC, Mon_SOC and Sesq_SOC;
[c] Iso_SOC: isoprene tracers estimated SOC, Mon_SOC: monoterpene tracers estimated SOC and Sesq_SOC: sesquiterpene tracer estimated SOC