



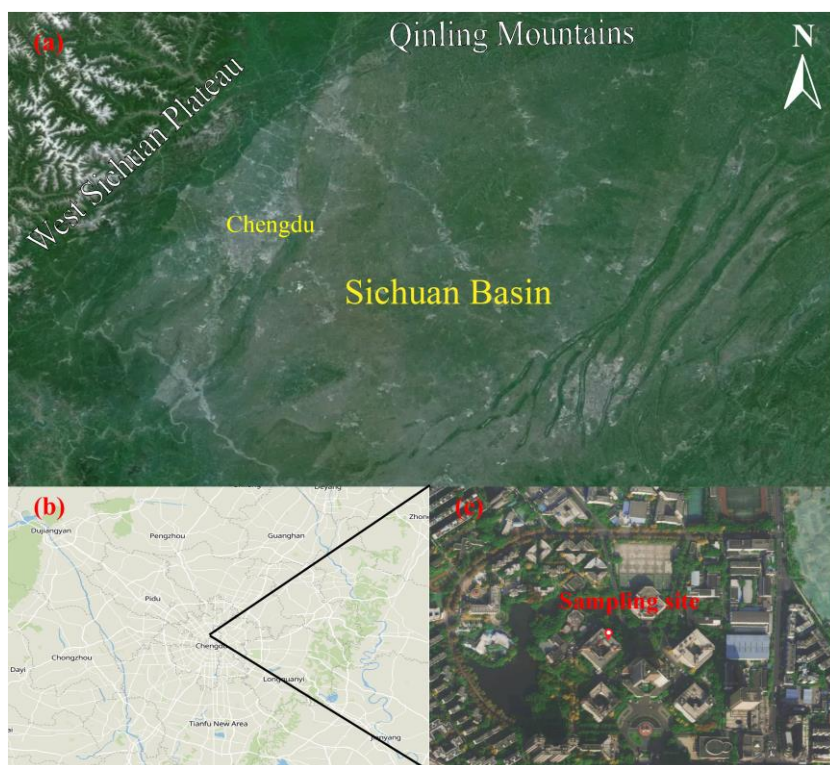
*Supplement of*

## **Measurement report: Molecular composition, sources, and evolution of atmospheric organic aerosols in a basin city in China**

**Junke Zhang et al.**

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**Figure S1: Topography of the Sichuan Basin and sampling site (all graphs are from Baidu Maps: <https://map.baidu.com/>).**

### S1 Sample extraction, derivatization, and determination

One fourth ( $\text{PM}_{2.5} \leq 100 \mu\text{g m}^{-3}$ ) or one eighth ( $\text{PM}_{2.5} > 100 \mu\text{g m}^{-3}$ ) of the sample/blank filter was cut into pieces and extracted with a mixture of dichloromethane and methanol (2:1, v/v) under ultrasonication (10 min each, repeated three times). The extracts were filtered through quartz fiber wool packed within a Pasteur pipette, concentrated using a rotary evaporator under vacuum conditions and then dried using pure nitrogen. After reaction with a mixture of N,O-bis-(trimethylsilyl) trifluoroacetamide (BSTFA) and pyridine (5:1, v/v) at 70°C for 3 h, the derivatives were diluted using an internal standard (*n*-alkane  $\text{C}_{13}$ ) at a concentration of 3.024 ng  $\mu\text{L}^{-1}$ . The derivatives were determined using gas chromatography–mass spectrometry (GC/MS) as described below.

GC/MS analysis of the derivatized fraction was performed using an Agilent 7890B GC coupled with an Agilent 5977B MSD (Agilent Company, USA). The GC separation was carried out using a HP-5MS fused silica capillary column with the GC oven temperature programmed from 50°C (2 min) to 120°C at 15°C  $\text{min}^{-1}$  and then to 300°C at 5°C  $\text{min}^{-1}$  with a final isothermal hold at 300°C for 16 min. The sample was injected in a splitless mode at an injector temperature of 280°C, and scanned from 50 to 650 Daltons using electron impact (EI) mode at 70 eV. Data were acquired and processed with the Chem-Station software. All the detected compounds were quantified using the peak area of the individual characteristic ion. In addition, GC/MS response factors of 3-MeTHF-3,4-diols (*cis*- and *trans*-3-methyltetrahydrofuran-3,4-diol), C5-alkene triols (*cis*-2-methyl-1,3,4-trihydroxy-1-butene, 3-methyl-2,3,4-trihydroxy-1-butene, and *trans*-2-methyl-1,3,4-trihydroxy-1-butene), and 2-methyltetrols (2-methylthreitol and 2-methylerythritol) were replaced by that of erythritol, and response factors of 2-methylglyceric acid, 3-hydroxyglutaric acid, 3-methyl-1,2,3-butanetricarboxylic acid, and  $\beta$ -Caryophyllinic acid were replaced by those of glyceric acid, tartaric acid, suberic acid, and *cis*-pinic acid, respectively, because the authentic standards are not commercially available. No significant contamination (< 10% of those in the samples) was found in the blanks. Average recoveries of the target compounds were better than 70%. Compounds used in a recovery experiment are usually pure agents

while those in real samples are a mixture with other organic and inorganic components, which means that the recovery experiment could not entirely reflect the conditions of target compounds in the atmosphere. Thus, data presented here were corrected for the field blanks but not corrected for the recoveries (Wang et al., 2006; Li et al., 2013).

## 35 S2 PMF analysis

Positive matrix factorization (PMF) is a bilinear factor analysis method, which is widely used to identify pollution sources and quantify their contributions to the ambient air pollutants at receptor sites, with an assumption of mass conservation between emission sources and receptors. The method is described in detailed by Paatero and Tapper (1994) and Paatero and Hopke (2003). Briefly, PMF decomposes the sample data matrix  $x_{ij}$  into two matrices—a factor profile matrix  $f_{kj}$ , and a factor contribution matrix  $g_{ik}$  (Eq. S1).

$$x_{ij} = \sum_{k=1}^p f_{kj} g_{ik} + e_{ij} \quad (S1)$$

Where  $x_{ij}$  is the measured ambient concentration of the target pollutants,  $f_{kj}$  is the factor profile of the  $j$ th species in the  $k$ th factor,  $g_{ik}$  is the source contribution of the  $k$ th factor to the  $i$ th sample, and  $e_{ij}$  is the residual concentration for each data point. PMF seeks a solution that minimizes an object function  $Q$  (Eq. S2), with the uncertainties in each observation ( $u_{ij}$ ).

$$Q = \sum_{i=1}^n \sum_{j=1}^m (e_{ij}/u_{ij})^2 \quad (S2)$$

In this study, the OC source profiles were identified and quantified by United States Environmental Protection Agency (USEPA) PMF version 5.0. The chemical species selected as input to the PMF model include 2 carbon fractions (OC and EC), 8 inorganic species ( $\text{NO}_3^-$ ,  $\text{SO}_4^{2-}$ ,  $\text{NH}_4^+$ ,  $\text{K}^+$ ,  $\text{Ca}^{2+}$ ,  $\text{Na}^+$ ,  $\text{Mg}^{2+}$ , and  $\text{Cl}^-$ ), and selected representative molecular markers. “Missing” data and data below method detection limit (MDL) were replaced by the geometric means of concentrations ( $C_{\text{gm}}$ ) and half of the MDL, respectively.

The uncertainty ( $u_{ij}$ ) for each species was calculated according to previous studies (Polissar et al., 1998; Norris G. and R., 2014):

(1) If the concentration is missing,  $C_{\text{gm}}$  was used for the uncertainty (Eq. S3):

$$u_{ij} = 4 * C_{\text{gm}} \quad (S3)$$

(2) If the concentration is less than or equal to the MDL, the uncertainty was calculated using a fixed fraction of the MDL (Eq. S4):

$$u_{ij} = \text{MDL} * 5/6 \quad (S4)$$

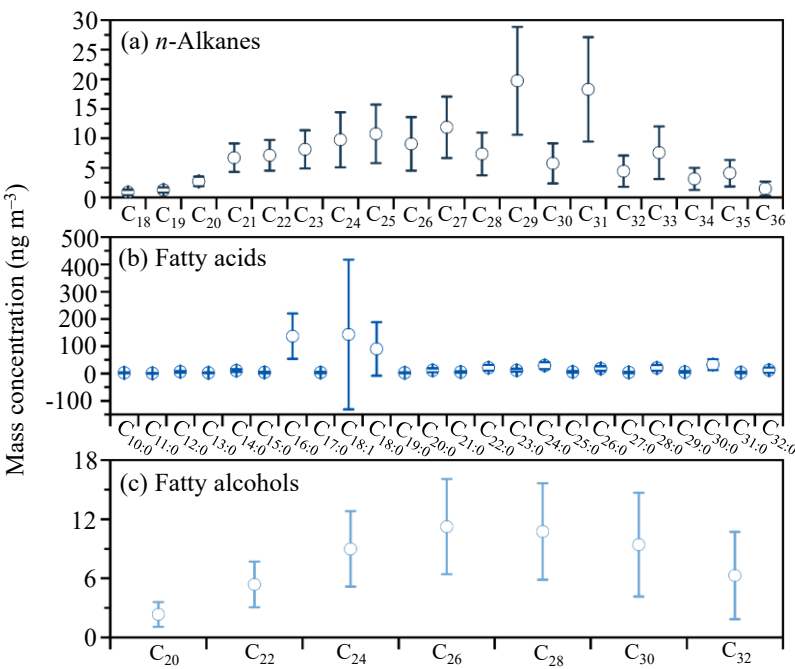
(3) If the concentration is greater than the MDL, the calculation was based on the concentration and MDL (Eq. S5):

$$u_{ij} = \sqrt{(\text{error fraction} * \text{concentration})^2 + (0.5 * \text{MDL})^2} \quad (S5)$$

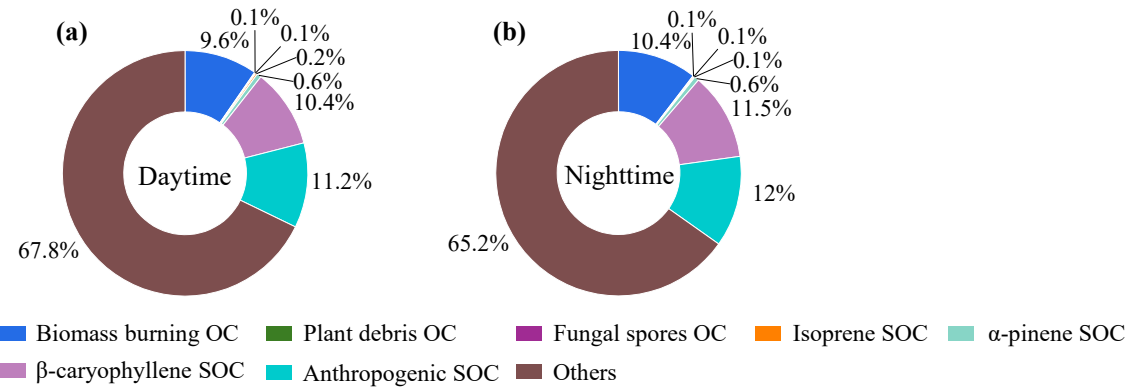
Bootstrapping (BS), displacement (DISP), and bootstrapping with displacement (BS-DISP) were employed to exam the solutions. In BS, data matrices are randomly resampled for mapping the BS solutions with base functions. This could express

the reproducibility of factors under random error. In DISP, elements  $f_{ij}$  in resolved profiles are displaced for testing the rotational ambiguity of solution. BS-DISP is the combination of BS and DISP by providing resampled matrices with displayed elements  $f_{ij}$  in factor profiles to simultaneously examine both random error and rotational ambiguity (Paatero et al., 2014; Chow et al., 2022).

The optimal number of factors is a compromise between identifying factors with the best physical explanations and achieving a sufficiently good fit for all species. In PMF solutions of too few factors, different sources are combined and unresolved, and the resolved sources cannot fully explain the individual species. On the other hand, in PMF solutions of too many factors, one source may be split into multiple uninterpretable factors. In this study, based on given understanding of OC sources, five to nine factors with random seeds were examined, and seven factors were determined. A detailed discussion on the PMF results can be found in S3 of this file and Sect. 3.3.2 of the main text.



**Figure S2: Molecular distributions of (a) n-alkanes, (b) fatty acids, and (c) fatty alcohols in PM<sub>2.5</sub> samples.**



**Figure S3: The OC sources in (a) daytime and (b) nighttime in winter in Chengdu.**

### S3 PMF source identification

80 Figure S4 demonstrated the factor profiles and the percentages of the various species contributed by each factor. Factor 1 was heavily weighted by PAHs species, such as BaA (46.9%), BbF (42.5%), BkF (42.6%), BaP (49.9%), Per (50.4%), and DBA (57.5%). Meanwhile, this factor contained abundant  $\text{Cl}^-$  (55.4%), which is often used as an important tracer for coal combustion (Zhang et al., 2012). Thus this source was defined as the coal combustion. Factor 2 was characterized by the dominance of two hopane species, i.e., C29 $\alpha\beta$  (53.8 %) and C30 $\alpha\beta$  (45.2 %). As discussed above, the hopanes in winter in Chengdu mainly  
85 came from motor vehicles. Meanwhile, this factor contained abundant phthalate esters, such as DEHP (37.8%), which may be related to plastic emissions during motor vehicle operation, such as brake wear (Ge et al., 2024). So this factor was indentified as vehicular emissions. Factor 3 was dominated by the  $\text{K}^+$  (61.3%) and anhydrosugars, i.e., levoglucosan (55.1%), mannosan (59.8%), and galactosan (63.8%). It was well documented that all of these tracers are mainly derived from biomass burning (Huang et al., 2017; Simoneit, 1999). Thus, this factor could be interpreted as biomass burning. Factor 4 exhibited the highest  
90 loading of trehalose (67.1%), followed by sucrose (55.0%), mannitol (51.9%), and arabitol (41.2%). They are usually originate from some primary biogenic emissions, such as soil dust, microbial, pollen, and fungal spores (Wang et al., 2021; Verma et al., 2021). Therefore, this factor can be treated as an primary biogenic emissions. Factor 5 was characterized by high loadings of  $\text{Ca}^{2+}$  (75.5%),  $\text{Mg}^{2+}$  (60.9%), and  $\text{Na}^+$  (39.3%), which are considered typical tracers of dust sources (Sun et al., 2022; Huang et al., 2021). Factor 6 was characterized by abundant DiBP (62.2%) and DnBP (55.3%), which are closely related to plastic  
95 emissions (Wang et al., 2006). Therefore, this source has been identified as plastic related sources. Factor 7 illustrated high loadings of secondary inorganic and organic species, such as  $\text{NO}_3^-$  (51.2%),  $\text{SO}_4^{2-}$  (47.4%),  $\text{NH}_4^+$  (50.0%), phthalic acids (such as o-isomers (64.4%), m-isomers (50.6%), and p-isomers (53.2%)), and biogenic SOA tracers (such as 2-MT (96.6%), 2-ME (73.1%), pinic acid (39.7%), MBTCA (71.8%), 3-HGA (39.0%), and  $\beta$ -Caryophyllinic acid (51.4%)). Therefore, this source is closely related to the secondary aging of primary emissions from anthropogenic (such as  $\text{SO}_2$ ,  $\text{NO}_x$ , and PAHs) and  
100 biological sources (Fine et al., 2004), and can be defined as secondary formation.

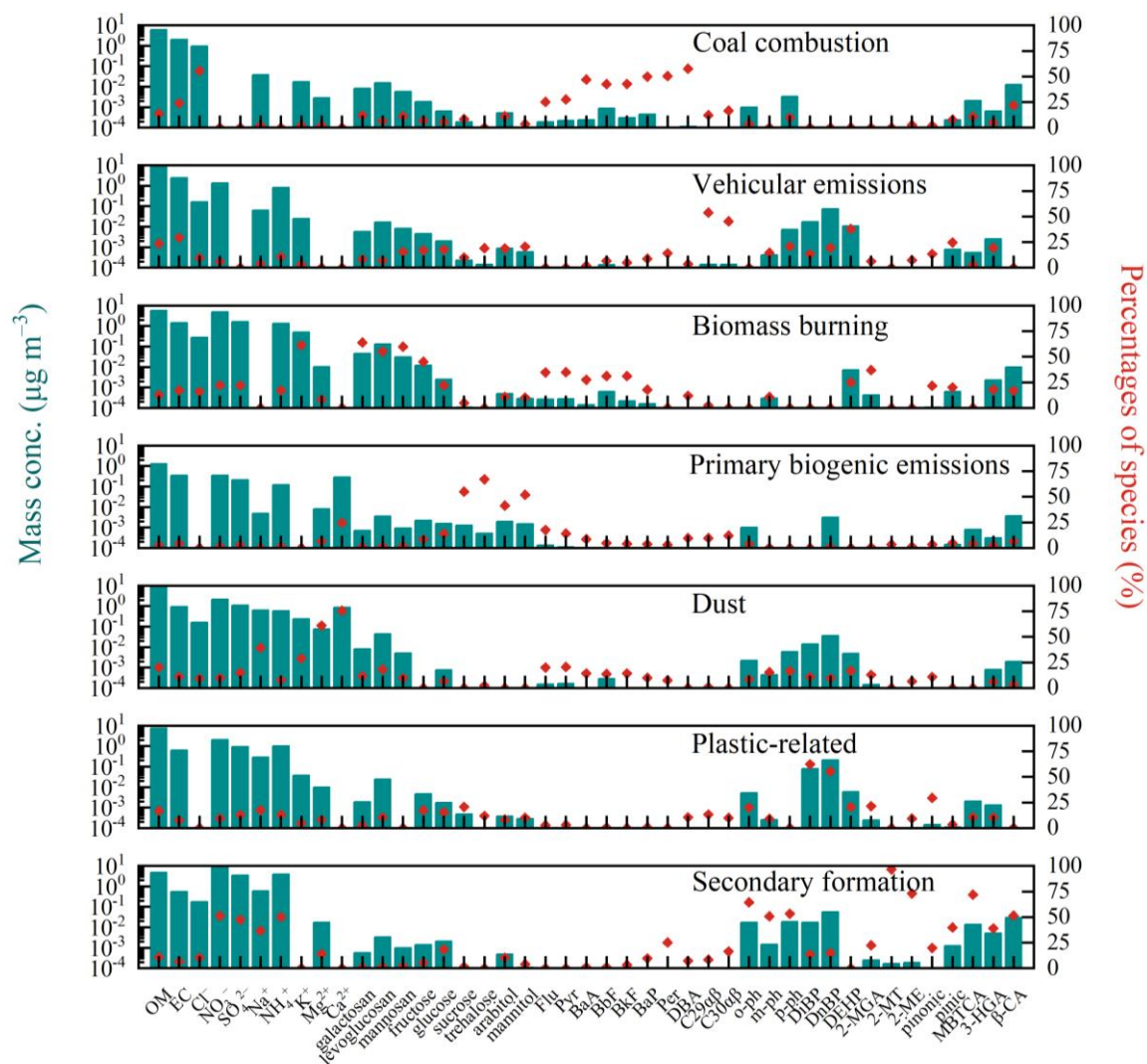


Figure S4: PMF source profiles for OC in terms of concentrations and percentages.

Table S1. Mass concentrations of the identified organic compounds in winter in Chengdu (ng m<sup>-3</sup>).

Compounds	Min	Max	Mean	SD	Daytime Mean	Nighttime Mean
<b>I. Aliphatic Lipids</b>						
<i>n</i> -Alkanes						
C <sub>18</sub>	0.06	2.48	0.86	0.46	0.82	0.91
C <sub>19</sub>	0.32	2.83	1.26	0.44	1.28	1.24
C <sub>20</sub>	1.13	4.74	2.72	0.81	2.70	2.74
C <sub>21</sub>	3.16	11.78	6.72	2.41	7.10	6.34
C <sub>22</sub>	3.21	15.79	7.13	2.61	7.25	7.02
C <sub>23</sub>	2.69	18.63	8.13	3.23	7.67	8.59
C <sub>24</sub>	1.99	22.97	9.76	4.67	9.39	10.12
C <sub>25</sub>	2.90	22.61	10.76	4.96	10.20	11.32
C <sub>26</sub>	1.62	19.04	9.06	4.54	8.54	9.58
C <sub>27</sub>	3.84	23.83	11.87	5.20	11.06	12.67
C <sub>28</sub>	1.49	15.50	7.35	3.61	6.96	7.74

C <sub>29</sub>	5.74	50.09	19.73	9.14	18.00	21.47
C <sub>30</sub>	0.91	14.11	5.76	3.38	5.24	6.29
C <sub>31</sub>	5.47	44.78	18.29	8.84	16.26	20.33
C <sub>32</sub>	0.46	11.09	4.44	2.64	3.95	4.94
C <sub>33</sub>	1.59	18.69	7.56	4.44	7.10	8.02
C <sub>34</sub>	0.04	7.04	3.13	1.86	2.96	3.30
C <sub>35</sub>	n.d.	8.81	4.10	2.24	3.66	4.56
C <sub>36</sub>	n.d.	4.67	1.48	1.21	1.36	1.62
<b>subtotal</b>	<b>49.0</b>	<b>286.8</b>	<b>139.9</b>	<b>60.0</b>	<b>131.3</b>	<b>148.4</b>
<b>Fatty Acids</b>						
C <sub>10:0</sub>	0.22	5.33	2.33	0.90	2.18	2.48
C <sub>11:0</sub>	0.06	3.83	0.70	0.69	0.60	0.79
C <sub>12:0</sub>	1.53	15.91	6.23	2.81	5.86	6.61
C <sub>13:0</sub>	0.35	5.40	2.21	1.01	2.20	2.23
C <sub>14:0</sub>	1.84	23.28	10.38	4.43	9.85	10.91
C <sub>15:0</sub>	0.49	22.19	3.83	2.75	3.25	4.41
C <sub>16:0</sub>	21.26	488.39	136.98	83.31	123.42	150.54
C <sub>17:0</sub>	0.80	9.24	3.54	1.87	3.13	3.95
C <sub>18:1</sub>	4.78	1155.48	143.08	274.56	34.30	251.86
C <sub>18:0</sub>	14.99	676.50	90.20	98.27	84.54	95.86
C <sub>19:0</sub>	0.52	6.66	2.24	1.28	1.95	2.53
C <sub>20:0</sub>	2.91	46.95	11.66	7.43	10.60	12.72
C <sub>21:0</sub>	0.95	15.75	5.21	2.77	4.83	5.59
C <sub>22:0</sub>	5.41	64.41	21.24	10.60	19.32	23.16
C <sub>23:0</sub>	2.79	27.27	11.58	5.30	10.86	12.29
C <sub>24:0</sub>	7.29	67.63	28.89	12.85	26.72	31.06
C <sub>25:0</sub>	0.83	14.80	6.08	3.02	5.81	6.36
C <sub>26:0</sub>	3.11	44.95	18.12	8.44	16.89	19.36
C <sub>27:0</sub>	0.29	9.79	3.74	1.93	3.66	3.82
C <sub>28:0</sub>	1.79	53.23	20.71	10.60	19.05	22.37
C <sub>29:0</sub>	0.26	15.03	5.55	3.21	5.09	6.01
C <sub>30:0</sub>	0.06	102.44	32.44	20.25	29.60	35.29
C <sub>31:0</sub>	n.d.	11.23	3.37	2.48	3.24	3.50
C <sub>32:0</sub>	n.d.	47.83	12.38	9.32	11.11	13.70
<b>subtotal</b>	<b>109.9</b>	<b>2099.5</b>	<b>582.0</b>	<b>458.4</b>	<b>437.6</b>	<b>726.3</b>
<b>Fatty Alcohols</b>						
C <sub>20</sub>	0.57	7.04	2.34	1.25	1.90	2.77
C <sub>22</sub>	1.67	11.41	5.38	2.31	4.72	6.04
C <sub>24</sub>	2.53	18.09	8.99	3.83	8.61	9.38
C <sub>26</sub>	3.22	25.29	11.25	4.84	10.03	12.46
C <sub>28</sub>	2.87	25.98	10.75	4.90	9.63	11.86
C <sub>30</sub>	1.33	24.39	9.42	5.27	8.34	10.50
C <sub>32</sub>	n.d.	20.85	6.29	4.44	5.12	7.49

<b>subtotal</b>	<b>15.8</b>	<b>127.0</b>	<b>54.1</b>	<b>25.2</b>	<b>48.2</b>	<b>60.0</b>
<b>II. Sugars</b>						
<b>Anhydrosugars</b>						
galactosan	3.01	178.60	70.00	36.18	59.94	80.06
mannosan	3.55	159.91	52.47	29.01	43.94	61.01
levoglucosan	37.78	452.77	239.81	100.14	220.72	258.90
<b>subtotal</b>	<b>44.3</b>	<b>791.3</b>	<b>362.3</b>	<b>162.1</b>	<b>324.6</b>	<b>400.0</b>
<b>Primary Saccharides</b>						
fructose	4.08	60.54	28.48	13.83	26.07	30.90
glucose	3.25	18.51	11.36	3.56	11.13	11.60
sucrose	0.75	6.51	2.41	1.02	2.65	2.17
trehalose	0.18	4.90	0.85	0.93	0.98	0.72
<b>subtotal</b>	<b>9.2</b>	<b>81.7</b>	<b>43.1</b>	<b>16.8</b>	<b>40.8</b>	<b>45.4</b>
<b>Sugar Alcohols</b>						
arabitol	1.16	16.40	5.33	2.89	4.98	5.68
mannitol	0.49	5.75	3.02	1.19	2.84	3.21
inositol	0.56	8.57	3.37	1.91	3.02	3.71
<b>subtotal</b>	<b>2.8</b>	<b>30.1</b>	<b>11.7</b>	<b>5.4</b>	<b>10.8</b>	<b>12.6</b>
<b>III. Hopanes</b>						
<i>C</i> <sub>27</sub> $\alpha$	0.01	0.25	0.09	0.06	0.09	0.09
<i>C</i> <sub>27</sub> $\beta$	0.00	0.41	0.08	0.06	0.07	0.09
<i>C</i> <sub>29</sub> $\alpha\beta$	0.05	0.84	0.28	0.18	0.29	0.27
<i>C</i> <sub>29</sub> $\beta\alpha$	0.01	0.41	0.10	0.07	0.09	0.11
<i>C</i> <sub>30</sub> $\alpha\beta$	0.10	1.05	0.33	0.19	0.29	0.36
<i>C</i> <sub>30</sub> $\beta\alpha$	0.01	0.24	0.06	0.04	0.05	0.06
<i>C</i> <sub>31</sub> $\alpha\beta$ S	0.01	0.39	0.11	0.08	0.10	0.12
<i>C</i> <sub>31</sub> $\alpha\beta$ R	0.01	0.23	0.08	0.05	0.08	0.08
<i>C</i> <sub>31</sub> $\beta\alpha$	0.00	0.25	0.06	0.05	0.05	0.08
<i>C</i> <sub>32</sub> $\alpha\beta$ S	n.d.	0.32	0.08	0.06	0.08	0.08
<i>C</i> <sub>32</sub> $\alpha\beta$ R	n.d.	0.13	0.05	0.03	0.04	0.06
<b>subtotal</b>	<b>0.3</b>	<b>3.7</b>	<b>1.3</b>	<b>0.7</b>	<b>1.2</b>	<b>1.4</b>
<b>IV. PAHs</b>						
Phenanthrene (Phe)	0.12	2.58	0.97	0.57	0.84	1.10
Anthracene (Ant)	n.d.	0.08	0.03	0.02	0.02	0.03
Fluoranthene (Flu)	0.28	1.83	0.81	0.39	0.71	0.91
Pyrene (Pyr)	0.31	1.97	0.83	0.38	0.73	0.94
Benz(a)anthracene (BaA)	0.10	2.74	0.56	0.44	0.40	0.72
Chrysene/triphenylene (CT)	0.27	4.66	1.17	0.76	0.89	1.45
Benzo(b)fluoranthene (BbF)	0.38	7.70	2.06	1.30	1.67	2.46
Benzo(k)fluoranthene (BkF)	0.11	2.80	0.72	0.46	0.57	0.87
Benzo(e)pyrene (BeP)	0.26	4.61	1.21	0.77	0.98	1.44
Benzo(a)pyrene (BaP)	0.16	5.38	0.95	0.84	0.64	1.26



Perylene (Per)	0.02	0.99	0.19	0.16	0.13	0.25
Indeno(1,2,3-cd)pyrene (IP)	0.16	5.93	1.53	1.07	1.25	1.80
Benzo(ghi)perylene (BghiP)	0.26	5.13	1.38	0.91	1.14	1.62
Dibenz(a,h)anthracene (DBA)	n.d.	0.81	0.23	0.16	0.18	0.27
Coronene (Cor)	0.08	2.57	0.66	0.55	0.58	0.75
<b>subtotal</b>	<b>2.8</b>	<b>48.9</b>	<b>13.3</b>	<b>8.2</b>	<b>10.7</b>	<b>15.8</b>
<b>V. Oxygenated PAHs (OPAHs)</b>						
1,4-Naphthoquinone	0.27	8.59	2.66	1.55	2.61	2.70
1-Naphthaldehyd	0.19	68.89	12.45	17.83	7.33	17.57
1-Ancenaphthenaquinone	0.03	0.57	0.19	0.10	0.20	0.18
9-Fluorenone	0.13	2.06	0.79	0.39	0.63	0.95
Ancenaphthenaquinone	0.55	8.89	2.21	1.53	2.16	2.26
Anthraquinone	1.03	12.11	4.30	2.48	3.82	4.79
Benzanthrone	0.60	15.50	3.79	2.77	2.85	4.74
Benzo(a)anthracene-7,12-dione	0.09	2.90	0.62	0.57	0.47	0.78
1,4-Chysenequione	n.d.	8.75	1.92	1.63	1.56	2.27
5,12-Naphthacenequione	n.d.	1.01	0.15	0.17	0.15	0.15
6H-Benzo(cd)pyrene-6-one	1.44	62.66	13.95	11.07	10.85	17.06
<b>subtotal</b>	<b>7.9</b>	<b>173.3</b>	<b>43.0</b>	<b>30.0</b>	<b>32.6</b>	<b>53.4</b>
<b>VI. Phthalic Acids</b>						
o-ph	3.40	67.39	27.73	12.54	26.40	29.07
m-ph	0.12	7.65	2.94	1.51	2.83	3.04
p-ph	1.95	99.92	38.19	22.95	33.91	42.47
<b>subtotal</b>	<b>5.5</b>	<b>164.5</b>	<b>68.9</b>	<b>34.2</b>	<b>63.1</b>	<b>74.6</b>
<b>VII. Phthalate Esters</b>						
Diisobutyl phthalates (DiBP)	32.43	329.23	139.49	68.41	157.35	121.64
Di- <i>n</i> -butyl phthalates (DnBP)	96.28	854.01	397.75	170.93	434.70	360.81
bis(2-ethylhexyl) phthalates (DEHP)	3.22	118.93	34.51	24.61	30.65	38.37
<b>subtotal</b>	<b>131.9</b>	<b>1205.8</b>	<b>571.8</b>	<b>246.7</b>	<b>622.7</b>	<b>520.8</b>
<b>VIII. Nitrophenols</b>						
4-nitrophenol (4NP)	0.35	7.31	2.05	1.41	1.25	2.84
3-methyl-4-nitrophenol (3M4NP)	0.03	1.16	0.23	0.19	0.13	0.34
4-nitroguaiacol (4NGA)	0.00	0.03	0.01	0.01	0.01	0.01
5-nitroguaiacol (5NGA)	0.00	0.03	0.01	0.01	0.01	0.01
4-nitrocatechol (4NC)	0.06	8.33	2.21	1.97	1.39	3.04
2,4-dinitrophenol (2,4-DNP)	0.00	0.20	0.06	0.04	0.05	0.07
4-methyl-5-nitrocatechol (4M5NC)	0.01	2.75	0.62	0.62	0.37	0.88
3-nitrosalicylic acid (3NSA)	0.00	0.02	0.01	0.00	0.01	0.01
3-nitrosalicylic acid (5NSA)	n.d.	0.03	0.01	0.00	0.01	0.01
<b>subtotal</b>	<b>0.5</b>	<b>17.7</b>	<b>5.2</b>	<b>3.8</b>	<b>3.2</b>	<b>7.2</b>

<b>IX. Biogenic SOA (BSOA) Tracers</b>						
<b>Isoprene SOA Tracers</b>						
2-methylglyceric acid (2-MGA)	0.07	2.84	1.27	0.69	1.22	1.32
2-methylthreitol (2MT)	0.01	0.87	0.18	0.15	0.15	0.22
2-methylerythritol (2ME)	0.02	0.77	0.27	0.16	0.24	0.30
cis-2-Methyl-1,3,4-trihydroxy-1-butene	0.07	2.63	1.18	0.59	1.19	1.16
3-Methyl-2,3,4-trihydroxy-1-butene	0.07	2.66	1.31	0.67	1.31	1.32
trans-2-Methyl-1,3,4-trihydroxy-1-butene	0.07	3.64	1.61	0.85	1.59	1.62
trans-3-Methyltetrahydrofuran-3,4-diol	n.d.	0.82	0.33	0.17	0.34	0.31
cis-3-Methyltetrahydrofuran-3,4-diol	n.d.	1.47	0.59	0.32	0.59	0.59
<b>subtotal</b>	<b>0.5</b>	<b>13.8</b>	<b>6.7</b>	<b>3.3</b>	<b>6.6</b>	<b>6.8</b>
<b>Monoterpene SOA Tracers</b>						
pinic acid (PA)	0.24	8.05	3.54	2.10	3.03	4.05
pinonic acid (PNA)	0.08	1.38	0.58	0.31	0.60	0.56
3-hydroxyglutaric acid (3-HGA)	0.85	30.78	13.77	7.34	13.15	14.39
MBTCA	n.d.	53.50	22.03	12.03	21.40	22.69
<b>subtotal</b>	<b>1.5</b>	<b>87.3</b>	<b>39.6</b>	<b>20.3</b>	<b>38.2</b>	<b>41.0</b>
<b>Sesquiterpene SOA Tracers</b>						
$\beta$ -Caryophyllinic acid	10.1	241.3	70.6	42.2	65.1	76.0

Note: In order to ensure accurate expression of the results for some low concentration OA species, all species concentration data were rounded to two decimal places, and the total concentration data for subtotal (including  $\beta$ -Caryophyllinic acid) were rounded to one decimal place.

**Table S2. Meteorological conditions and concentrations of gaseous pollutants during different pollution periods (C: clean, LP: lightly polluted, HP: heavily polluted).**

	C	LP	HP
T (°C)	7.3±3.3	6.9±3.4	7.7±2.6
RH (%)	72.4±15.2	74.7±15.8	85.8±9.3
CO (mg m <sup>-3</sup> )	0.6±0.2	0.8±0.3	1.1±0.1
SO <sub>2</sub> (μg m <sup>-3</sup> )	2.5±0.6	2.5±0.4	2.8±0.4
NO <sub>2</sub> (μg m <sup>-3</sup> )	24.3±5.9	39.2±11.6	49.5±10.5
O <sub>3</sub> (μg m <sup>-3</sup> )	34.9±12.0	28.4±15.8	25.3±16.7
PM <sub>2.5</sub> (μg m <sup>-3</sup> )	63.6±11.0	95.4±10.0	139.8±14.5

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