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Supplement of

In situ measurement of organic aerosol molecular markers in urban Hong Kong during a summer period: temporal variations and source apportionment

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Sect. S1. MDL calculation for AMS measurements

The MDLs of PM_1 components measured by AMS were determined. During the sampling period, we regularly installed an in-line HEPA filter at the inlet of the AMS to remove particulate matters. On the one hand, the concentrations of target species measured from the particle-free air represented the backgrounds, which were subtracted from all the measurement data. On the other hand, the background data was used to calculate the MDLs following the formula:

$$MDLs = t_{n-1,0.99} \times S$$

where n is the number of the background datasets; t is t-distribution (one-sided) with n-1 degrees of freedom and 99% confidence level; and S is the standard deviation of the background data. Generally, $t_{n-1,0.99}$ is approximately equal to 3.

Sect. S2. Normalization of diurnal profiles

The analysis of diurnal profiles focuses on the variations rather than magnitudes of the species. To accommodate the species with same patterns but different orders of magnitude in a same figure, we adopt a linear normalization approach to process the data, according to the formula:

$$Normalized\ value_t = \frac{x_t - min}{max - min}$$

where x_t is the mean (or median) value of the species in hour *t*; and min and max are the minimum and maximum of all the mean (or median) values throughout the day, respectively.

Supplemental Figures

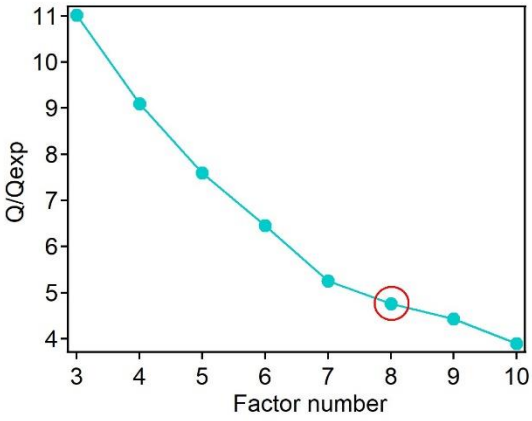

Figure S1. Change of Q/Q_{exp} ratio with the number of factors in PMF base runs. A solution with eight factors is adopted.

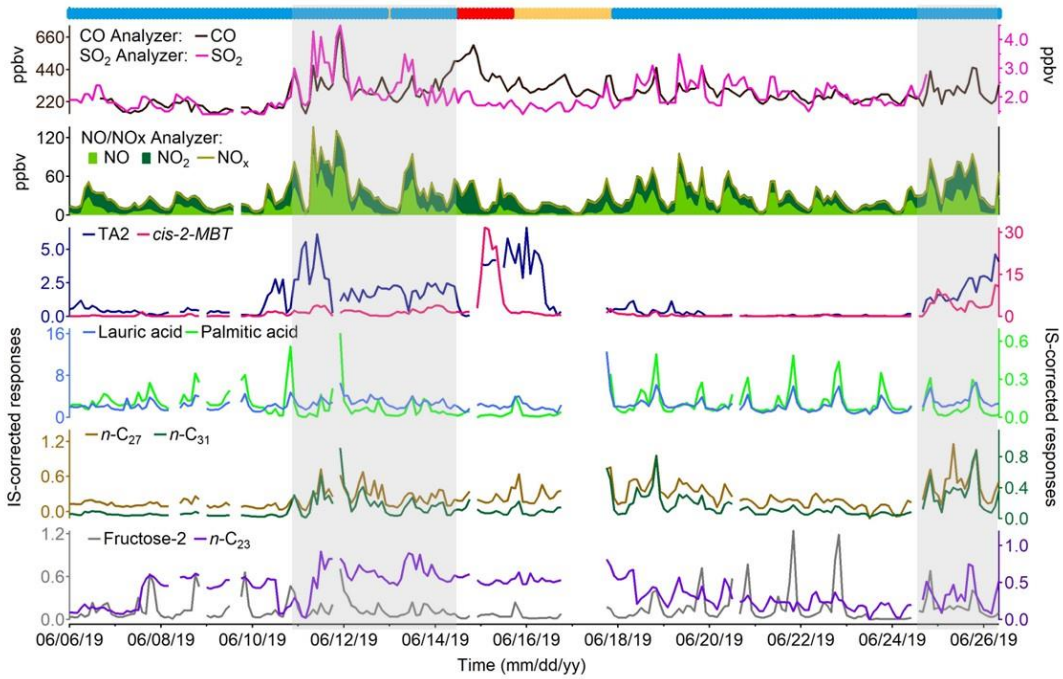

Figure S2. Time series of selected OA markers, CO, SO_2, and NO-NO_2-NO_x. Variations of OA markers are represented by IS-corrected response. Shaded areas represent the periods with troughs. Missing data are due to instrument maintenance.

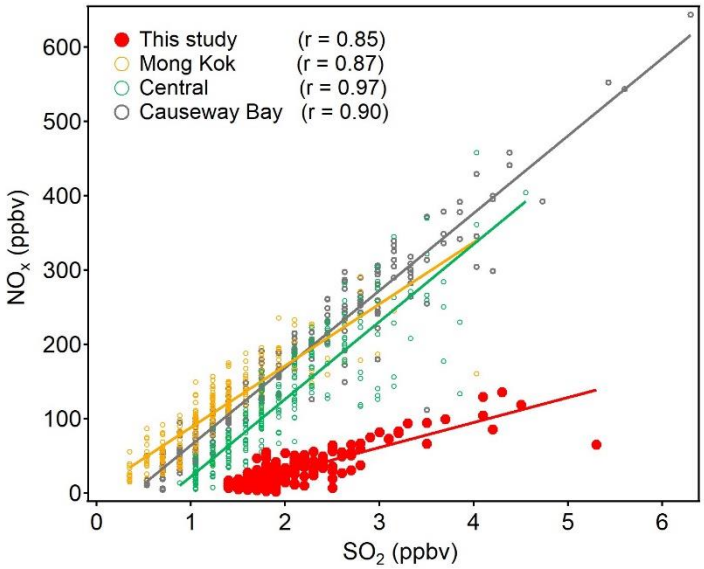

Figure S3. Correlations between NO_x and SO_2 at this site and three roadside sites in Hong Kong in the study period.

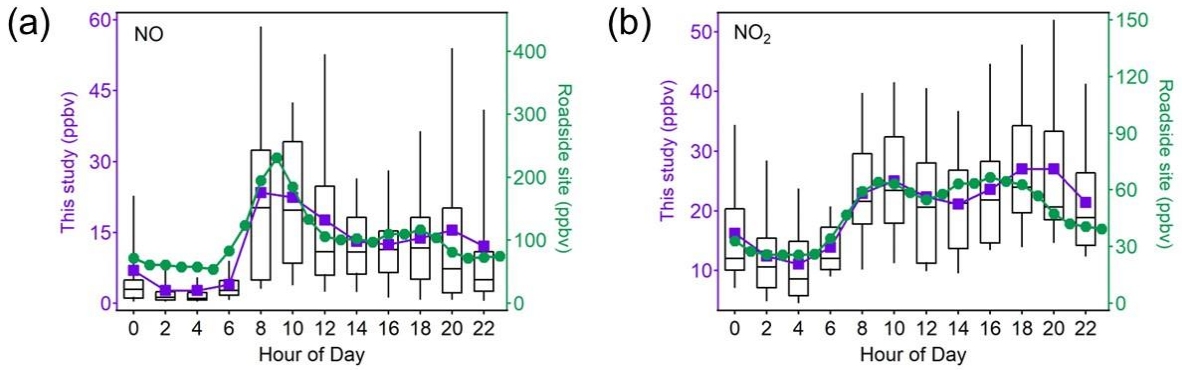

Figure S4. Diurnal patterns of NO and NO_2 at this site and a roadside site ~350 m away. Tip of the top (bottom) whisker is the 95th (5th) percentile. Top and bottom of the box denote the 75th and 25th percentiles, respectively. The mean value is indicated by purple square, and green circle represents the median value.

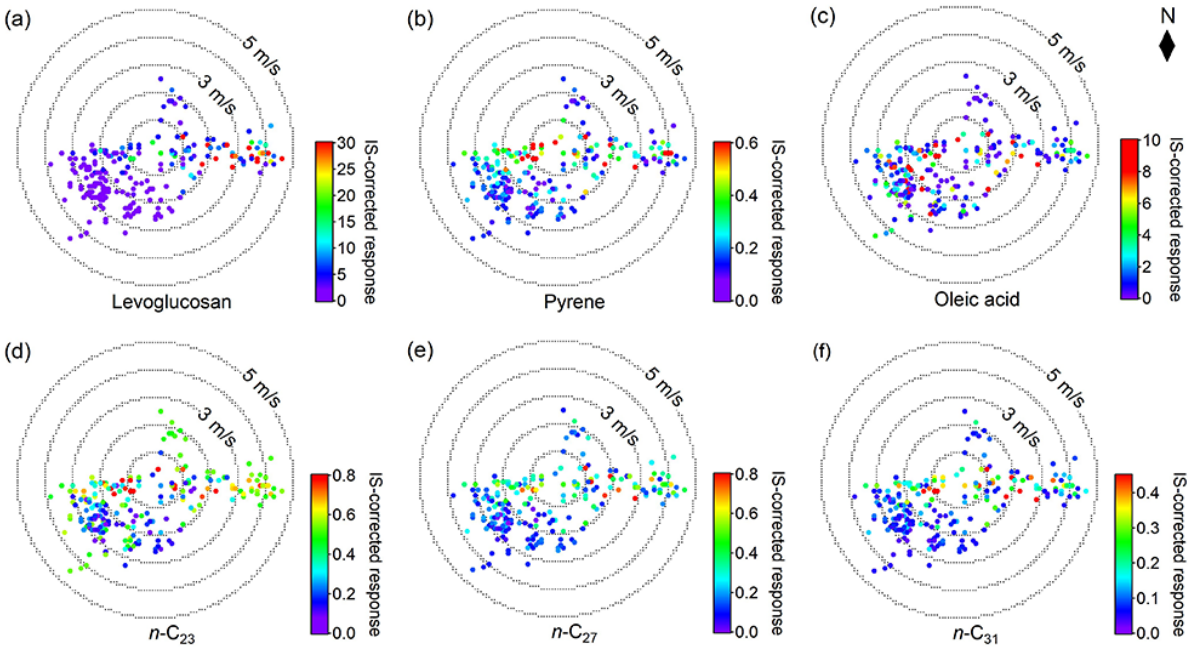

Figure S5. Wind roses color-coded by the IS-corrected response of levoglucosan (a), pyrene (b), oleic acid (c), *n*-C_{23} (d), *n*-C_{27} (e), and *n*-C_{31} (f).

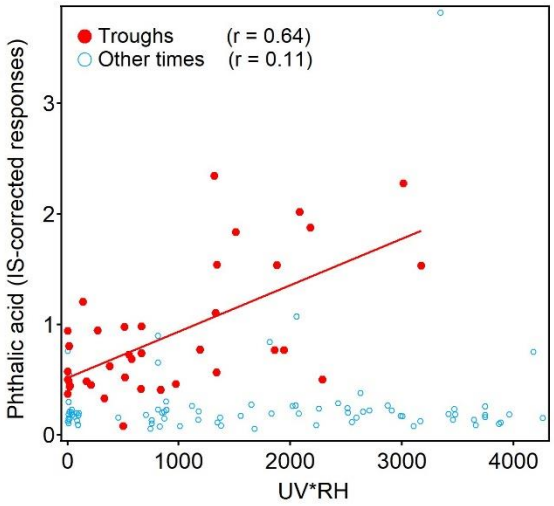

Figure S6. Correlations between phthalic acid and the product of UV and RH in presence of troughs and at other times with marine air.

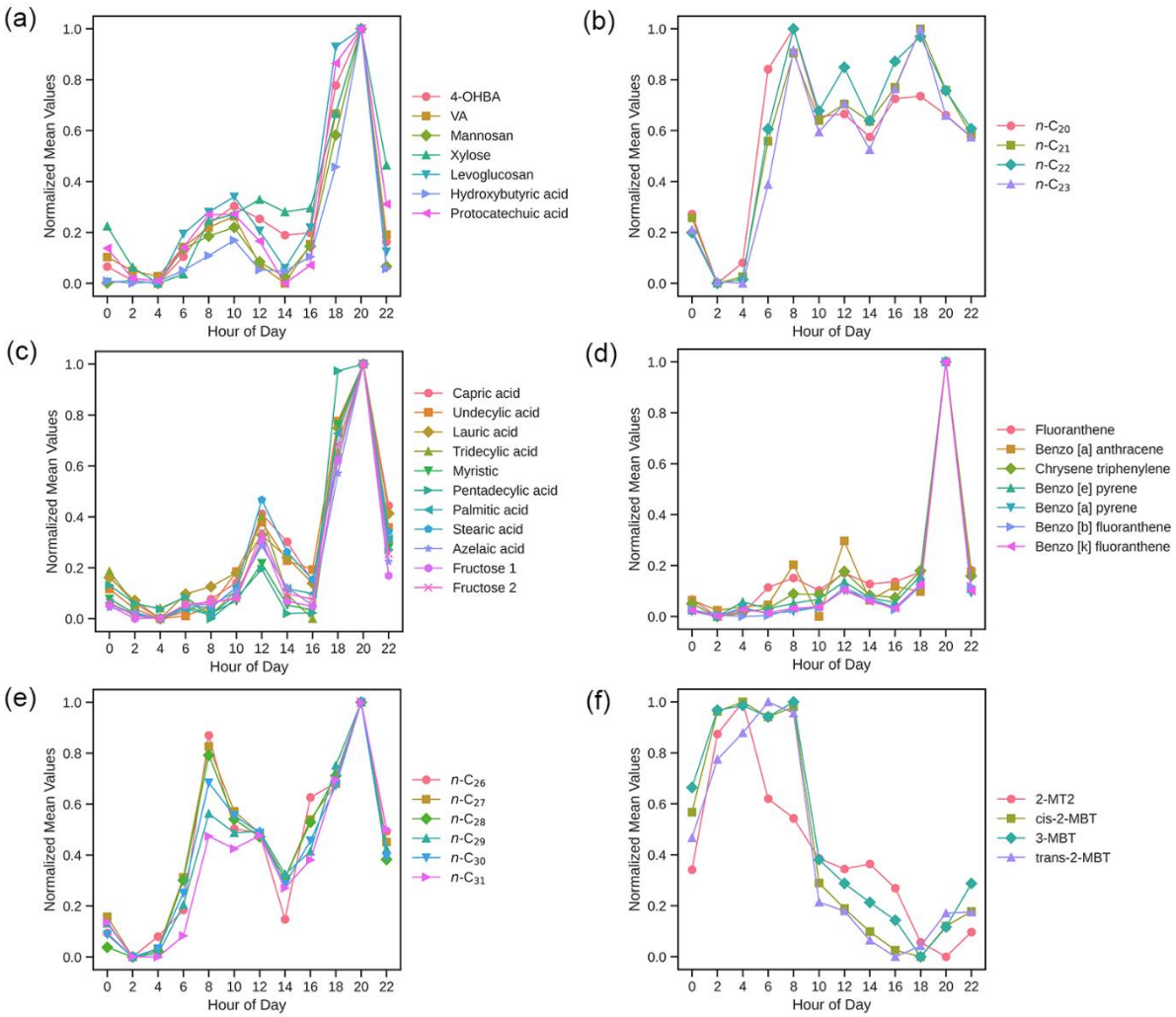

Figure S7. Diurnal patterns of selected OA markers represented by the normalized mean values of IS-corrected response (see Text S2 for normalization method). The species are grouped based on the similarity in patterns.

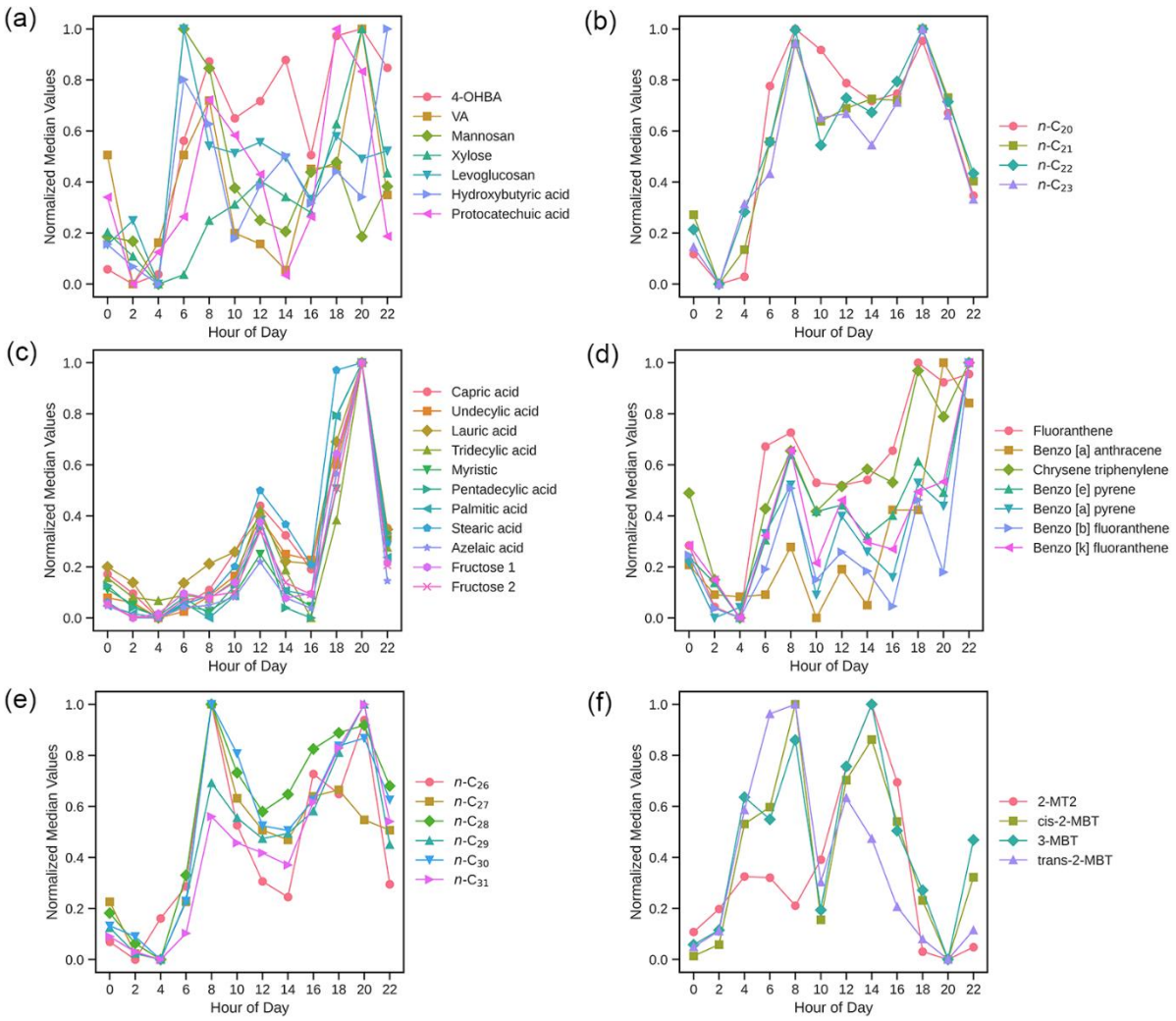

Figure S8. Same as Figure S7, but showing normalized median values (see Text S2 for normalization method).

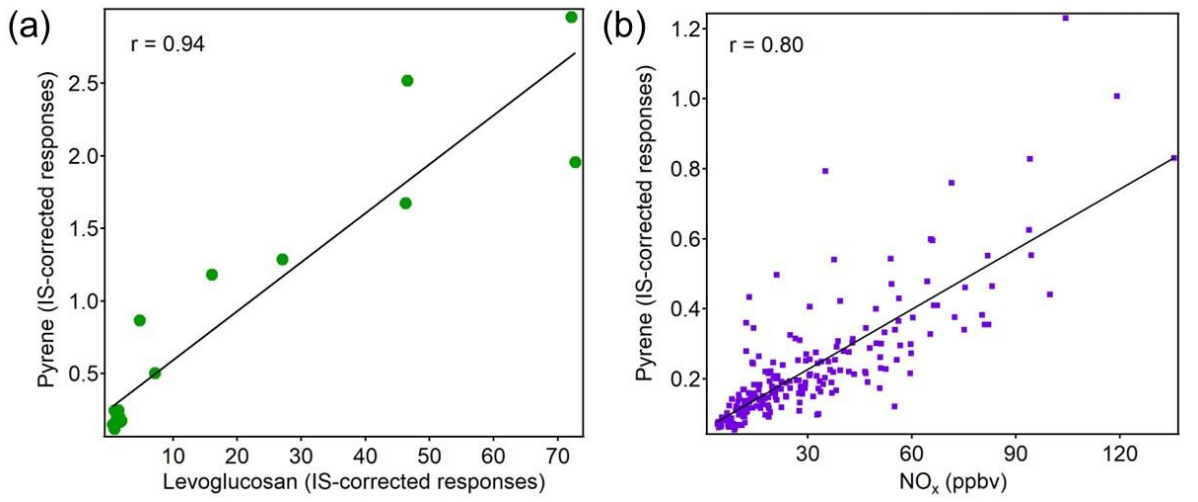

Figure S9. Correlations of pyrene (a representative of PAHs) *vs.* levoglucosan at 20:00 (a) and pyrene *vs.* NO_x at other times (b).

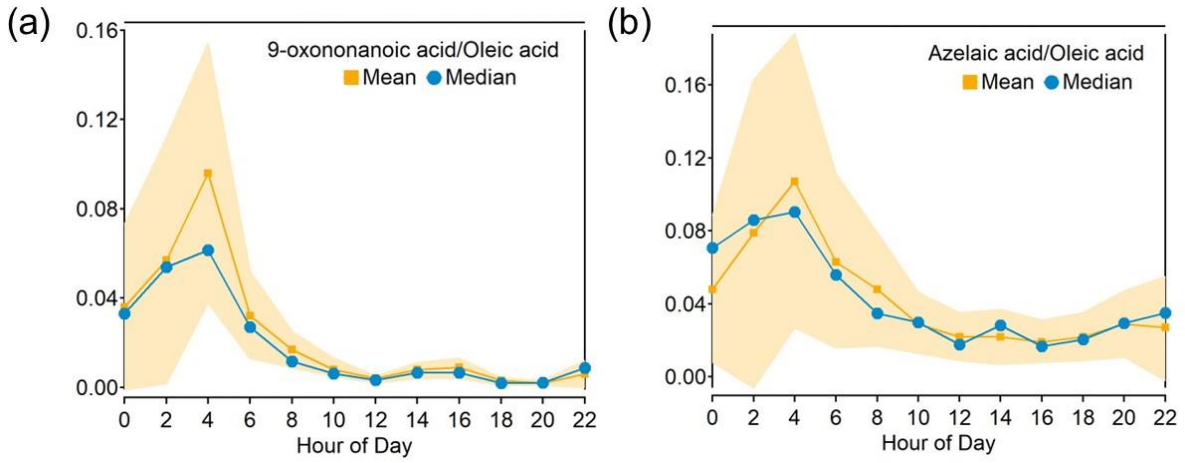

Figure S10. Diurnal variations in the ratio of 9-oxononanoic acid to oleic acid (a) and the ratio of azelaic acid to oleic acid (b). Shaded areas on both sides of the line with orange squares represent 95% confidence intervals.

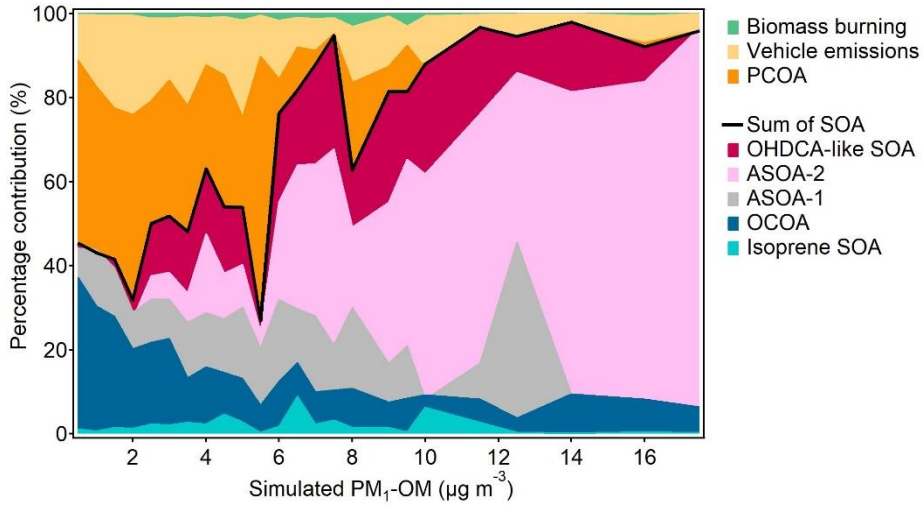

Figure S11. Changes of percentage contributions of individual OA sources to PM_1-OM with PM_1-OM concentration.

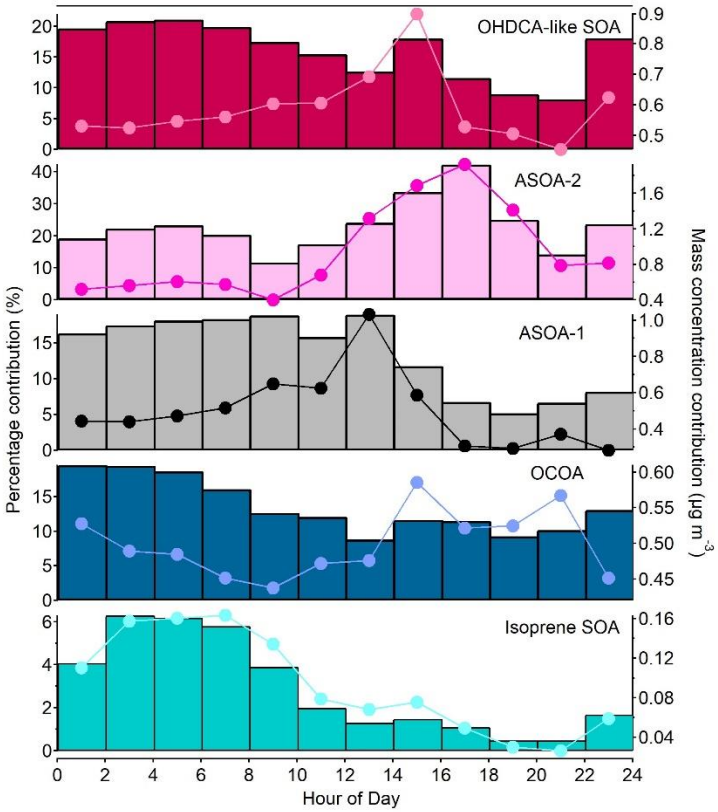

Figure S12. Average diurnal cycles of percentage contributions (columns) and mass concentration contributions (lines) to PM_1-OM of SOA factors.

Supplemental Tables

Table S1. Instruments and working principles for real-time measurement of trace gases.

Measurement species	Instrument	Model	Working principle
SO_2	Teledyne Advanced Pollution Instrumentation (API) SO_2 Analyzer	T100U	Ultraviolet fluorescence
CO	Teledyne Advanced Pollution Instrumentation (API) Gas Filter Correlation CO Analyzer	T300U	Infrared absorption
NO-NO_2-NO_x	Teledyne Advanced Pollution Instrumentation (API) NO/NO_x Analyzer	Model 200E	Chemiluminescence
O_3	Teledyne Advanced Pollution Instrumentation (API) O_3 Analyzer	T400	Ultraviolet absorption

Table S2. Statistics of trace gases, meteorological parameters and LWC throughout the study period.

Species / Parameters	Mean	Median	25th percentile	75th percentile	95% confidence interval
SO_2 (ppbv)	2.1	1.9	1.7	2.3	0.1
CO (ppbv)	282	271	226	317	12
O_3 (ppbv)	9.3	4.7	2.6	11.0	1.6
NO (ppbv)	10.7	4.6	0.6	15.0	1.9
NO_2 (ppbv)	20.2	18.3	11.6	26.3	1.4
Temp (°C)	28.6	28.7	27.3	29.7	0.2
RH (%)	82	83	78	88	1
UV (W m^{-2})	18.6	12.2	1.7	34.2	2.8
WS (m s^{-1})	2.4	2.4	1.8	3.0	0.1
LWC (μg m^{-3})	7.5	4.5	2.3	8.8	1.2

Table S3. Base ion, retention time, and internal standard for specific OA compounds. Bold are the representative species that we focus on in this study.

Sequence	Compound name	Base ion (m/z)	Retention time (s)	Internal standard
1	**2-methylglyceric acid (2-MGA)**	**219**	**426.1**	**PentaerythrItol-13C**
2	**2-methylerythritol (2-MT1)**	**219**	**495.9**	**Pentaerythritol-13C**
3	2-methylthreitol (2-MT2)	219	501.4	Pentaerythritol-13C
4	***cis*-2-methyl-1,3,4-trihydroxy-1-butene (*cis*-2-MBT)**	**231**	**442.5**	**Pentaerythritol-13C**
5	3-methyl-2,3,4-trihydroxy-1-butene (3-MBT)	231	450.3	Pentaerythritol-13C

6	*trans*-2-methyl-1,3,4-trihydroxy-1-butene (*trans*-2-MBT)	231	452.2	Pentaerythritol-13C
7	3-hydroxy-4,4-dimethylglutaric acid (HDMGA)	377	517.1	Pentaerythritol-13C
8	**2,3-dihydroxy-4-oxopentanoic acid (DHOPA)**	**321**	**490.5**	**Pentaerythritol-13C**
9	Tartaric acid isomer 1 (TA1)	292	510.0	Pentaerythritol-13C
10	**Tartaric acid isomer 2 (TA2)**	**292**	**523.5**	**Pentaerythritol-13C**
11	**Malic acid (MA)**	**233**	**481.1**	**Pentaerythritol-13C**
12	Citramalic acid (CMA)	247	477.4	Pentaerythritol-13C
13	2-hydroxyglutaric acid (2-HGA)	349	505.1	Pentaerythritol-13C
14	2-hydroxydicarboxylic acid	292	450.7	Pentaerythritol-13C
15	**Succinic acid**	**247**	**421.3**	**Pentaerythritol-13C**
16	Fumaric acid	245	433.1	Pentaerythritol-13C
17	Glutaric acid	261	453.1	D-adipic acid
18	Pimelic acid	289	511.2	D-adipic acid
19	Adipic acid	111	484.4	D-adipic acid
20	Azelaic acid	317	558.7	1-Pentadecan-d31-ol
21	Glyceric acid	292	430.0	Pentaerythritol-13C
22	Hydroxybutyric acid	233	490.7	Pentaerythritol-13C
23	Mannose	204	585.6	Pentaerythritol-13C
24	Glucose	204	603.1	Pentaerythritol-13C
25	Fructose isomer-1 (Fructose-1)	437	565.1	Pentaerythritol-13C
26	**Fructose isomer-2 (Fructose-2)**	**437**	**566.9**	**Pentaerythritol-13C**
27	Xylose	204	558.9	Pentaerythritol-13C
28	**Levoglucosan**	**204**	**541.5**	**Pentaerythritol-13C**
29	Mannosan	204	536.1	Pentaerythritol-13C
30	Erythritol	217	487.8	Pentaerythritol-13C
31	Arabinitol	319	544.8	Pentaerythritol-13C
32	Mannitol	319	595.1	Pentaerythritol-13C
33	Eicosane (*n*-C_{20})	57	603.0	Eicosane-d42
34	Heneicosane (*n*-C_{21})	57	624.4	Eicosane-d42
35	Docosane (*n*-C_{22})	57	645.4	Docosane-d46
36	**Tricosane (*n*-C_{23})**	**57**	**666.1**	**Docosane-d46**
37	Tetracosane (*n*-C_{24})	57	686.6	Tetracosane-d50
38	Pentacosane (*n*-C_{25})	57	707.2	Tetracosane-d50
39	Hexacosane (*n*-C_{26})	57	728.5	Hexacosane-d54
40	**Heptacosane (*n*-C_{27})**	**57**	**751.4**	**Hexacosane-d54**
41	Octacosane (*n*-C_{28})	57	776.2	Octacosane -d58
42	Nonacosane (*n*-C_{29})	57	803.5	Octacosane -d58
43	Triacontane (*n*-C_{30})	57	834.0	Triacontane-d62

44	**Hentriacontane (*n*-C_{31})**	**57**	**868.8**	**Triacontane-d62**
45	Dotriacontane (*n*-C_{32})	57	898.7	Dotriacontane-d66
46	Capric acid	229	469.0	D C10 acid
47	Undecylic acid	243	497.3	D C10 acid
48	**Lauric acid**	**257**	**523.1**	**1-Dodecan-d25-ol**
49	Tridecylic acid	271	547.0	1-Dodecan-d25-ol
50	Myristic acid	285	569.8	1-Pentadecan-d31-ol
51	Pentadecylic acid	299	591.8	1-Pentadecan-d31-ol
52	**Palmitic acid**	**313**	**613.21**	**1-Octadecad37-nol**
53	Stearic acid	341	654.72	Stearic-d35 acid
54	Underivatized palmitic acid	256	596.815	1-Octadecad37-nol
55	Underivatized stearic acid	284	639.315	Stearic-d35 acid
56	**9-oxononanoic acid**	**228**	**502.16**	**D-dodecanol**
57	**Oleic acid**	**339**	**650.12**	**Stearic-d35 acid**
58	Underivatized oleic acid	264	635.314	Stearic-d35 acid
59	Vanillic acid (VA)	297	553.2	1-Pentadecan-d31-ol
60	3-hydroxybenzoic acid (3-OHBA)	267	502.5	1-Dodecan-d25-ol
61	4-hydroxybenzoic acid (4-OHBA)	267	519.1	1-Dodecan-d25-ol
62	**Phthalic acid**	**295**	**537.612**	**D phthalic acid**
63	Isophthalic acid	295	551.2	D phthalic acid
64	Terephthalic acid	295	559.6	D phthalic acid
65	2,4-dyhydroxybenzoic acid	151	424.6	1-Dodecan-d25-ol
66	Protocatechuic acid	370	566.3	1-Pentadecan-d31-ol
67	Fluoranthene	202	631.6	D pyrene
68	**Pyrene**	**202**	**644.4**	**D pyrene**
69	Benzo [*a*] anthracene	228	716.8	D-chrysene
70	Chrysene triphenylene	228	719.3	D-chrysene
71	Benzo [*e*] pyrene	252	819.8	D-perylene
72	Benzo [*a*] pyrene	252	824.1	D-perylene
73	Benzo [*b*] fluoranthene	252	796.2	D-perylene
74	Benzo [*k*] fluoranthene	252	797.8	D-perylene

Table S4. Statistics of PM_1 compositions measured by AMS and selected OA markers measured by TAG throughout the study period.

Species / Parameters	Mean	Median	25th percentile	75th percentile	95% confidence interval	*p* value *
2-MGA (IS-corrected response, measured by TAG, same below)	0.059	0.032	0.010	0.077	0.011	0.000
2-MT1	1.20	0.48	0.19	1.32	0.27	0.000
cis-2-MBT	1.72	0.36	0.05	1.66	0.54	0.000
DHOPA	0.04	0.01	0.00	0.04	0.01	0.000
TA2	1.15	0.42	0.11	1.83	0.19	0.000
MA	4.50	1.79	0.86	7.56	0.61	0.000
Succinic acid	0.33	0.21	0.11	0.37	0.05	0.000
Fructose-2	0.033	0.021	0.012	0.040	0.005	0.000
Levoglucosan	6.42	1.76	0.70	5.60	1.69	0.000
n-C_{23}	0.39	0.42	0.20	0.55	0.03	0.000
n-C_{27}	0.24	0.19	0.12	0.32	0.02	0.000
n-C_{31}	0.15	0.09	0.05	0.18	0.02	0.000
Palmitic acid	2.48	1.71	1.01	3.13	0.33	0.000
Stearic acid	1.88	1.63	1.15	2.18	0.18	0.000
9-oxononanoic acid	0.019	0.013	0.010	0.018	0.003	0.000
Oleic acid	2.73	1.19	0.39	3.43	0.51	0.000
Phthalic acid	0.42	0.22	0.16	0.50	0.07	0.000
Pyrene	0.28	0.19	0.13	0.30	0.04	0.000
PM_1-OM ($\mu g\ m^{-3}$, measured by AMS, same below)	4.2	3.1	1.7	5.5	0.5	0.000
Nitrate	0.3	0.2	0.1	0.4	0.1	0.000
Sulfate	2.9	2.1	1.7	2.9	0.3	0.000
Ammonium	1.1	0.8	0.6	1.2	0.1	0.000
Chloride	0.04	0.02	0.02	0.04	0.01	0.000
SO_2 (ppbv)	2.1	1.9	1.7	2.3	0.1	0.000
CO (ppbv)	282	271	226	317	12	0.000
O_3 (ppbv)	9.3	4.7	2.6	11.0	1.6	0.000
NO (ppbv)	10.7	4.6	0.6	15.0	1.9	0.000
NO_2 (ppbv)	20.2	18.3	11.6	26.3	1.4	0.000
Temp (°C)	28.6	28.7	27.3	29.7	0.2	0.026
RH (%)	82	83	77	88	1	0.000
UV ($W\ m^{-2}$)	18.6	12.2	1.7	34.2	2.8	0.000
WS ($m\ s^{-1}$)	2.4	2.4	1.8	3.0	0.1	0.070
LWC ($\mu g\ m^{-3}$)	7.5	4.5	2.3	8.8	1.2	0.000

* *p* values derived from the Shapiro-Wilk tests (normal distribution: $p > 0.05$)

Table S5. Same as Table S4, but for the Case I periods.

Species / Parameters	Mean	Median	25th percentile	75th percentile	95% confidence interval	*p* value *
2-MGA (IS-corrected response, measured by TAG, same below)	0.252	0.198	0.138	0.288	0.093	0.000
2-MT1	5.56	3.04	1.23	8.88	2.81	0.011
cis-2-MBT	11.23	3.77	1.77	21.63	6.25	0.004
DHOPA	0.20	0.16	0.11	0.23	0.07	0.004
TA2	2.94	3.84	0.63	4.18	1.17	0.014
MA	12.51	12.09	11.29	13.33	0.89	0.020
Succinic acid	1.05	0.92	0.50	1.47	0.38	0.026
Fructose-2	0.023	0.022	0.017	0.024	0.006	0.001
Levoglucosan	5.67	3.03	1.97	4.26	4.48	0.000
n-C_{23}	0.53	0.53	0.49	0.56	0.02	0.370
n-C_{27}	0.23	0.19	0.18	0.26	0.04	0.008
n-C_{31}	0.10	0.09	0.07	0.12	0.03	0.013
Palmitic acid	0.55	0.44	0.33	0.63	0.17	0.109
Stearic acid	1.78	1.36	1.22	2.33	0.53	0.040
9-oxononanoic acid	0.022	0.019	0.014	0.026	0.005	0.071
Oleic acid	0.78	0.44	0.21	0.95	0.42	0.002
Phthalic acid	1.02	0.65	0.55	1.07	0.71	0.000
Pyrene	0.15	0.12	0.10	0.19	0.03	0.014
PM_1-OM (μg m^{-3}, measured by AMS, same below)	11.1	8.3	7.0	15.1	2.9	0.031
Nitrate	1.2	0.6	0.5	1.6	0.6	0.001
Sulfate	4.7	4.6	3.8	5.5	0.6	0.897
Ammonium	1.9	2.0	1.8	2.2	0.2	0.949
Chloride	0.04	0.02	0.03	0.05	0.01	0.015
SO_2 (ppbv)	1.8	1.8	1.7	1.9	0.1	0.026
CO (ppbv)	436	413	367	524	49	0.399
O_3 (ppbv)	30.94	25.21	21.32	36.25	7.30	0.010
NO (ppbv)	4.7	4.3	1.4	6.5	2.9	0.003
NO_2 (ppbv)	28.6	28.3	17.4	39.4	7.3	0.590
Temp (°C)	29.0	29.4	27.8	30.2	0.7	0.345
RH (%)	67	67	62	71	3	0.756
UV (W m^{-2})	29.3	36.4	12.3	47.4	13.0	0.180
WS (m s^{-1})	2.6	2.3	1.8	3.5	0.5	0.062
LWC (μg m^{-3})	2.6	1.0	0.8	2.2	2.4	0.000

* *p* values derived from the Shapiro-Wilk tests (normal distribution: $p > 0.05$)

Table S6. Same as Table S4, but for the Case II periods.

Species / Parameters	Mean	Median	25th percentile	75th percentile	95% confidence interval	*p* value *
2-MGA (IS-corrected response, measured by TAG, same below)	0.125	0.128	0.100	0.150	0.023	0.993
2-MT1	0.79	0.71	0.48	1.17	0.19	0.099
cis-2-MBT	1.04	1.09	0.48	1.39	0.31	0.134
DHOPA	0.11	0.12	0.09	0.14	0.02	0.194
TA2	2.56	2.44	0.60	4.13	1.05	0.089
MA	11.37	12.42	11.29	14.33	2.13	0.004
Succinic acid	0.88	0.87	0.69	1.15	0.16	0.271
Fructose-2	0.021	0.012	0.011	0.024	0.009	0.000
Levoglucosan	21.40	8.46	5.58	25.12	12.14	0.000
n-C_{23}	0.56	0.52	0.51	0.58	0.05	0.002
n-C_{27}	0.34	0.28	0.17	0.41	0.10	0.040
n-C_{31}	0.16	0.09	0.06	0.15	0.09	0.000
Palmitic acid	1.30	0.37	0.27	0.81	1.11	0.000
Stearic acid	2.34	2.05	1.38	2.60	0.94	0.000
9-oxononanoic acid	0.033	0.014	0.017	0.045	0.015	0.000
Oleic acid	2.54	0.89	0.36	3.83	1.72	0.000
Phthalic acid	0.53	0.51	0.23	0.76	0.18	0.263
Pyrene	0.50	0.17	0.11	0.30	0.43	0.000
PM_1-OM (μg m^{-3}, measured by AMS, same below)	7.0	6.3	4.4	9.4	1.3	0.096
Nitrate	0.6	0.6	0.4	0.7	0.1	0.051
Sulfate	6.6	6.7	4.8	8.9	1.1	0.112
Ammonium	2.5	2.5	1.8	3.3	0.4	0.318
Chloride	0.07	0.04	0.06	0.08	0.02	0.001
SO_2 (ppbv)	1.7	1.7	1.6	1.8	0.1	0.003
CO (ppbv)	318	308	283	344	18	0.065
O_3 (ppbv)	26.19	27.71	19.62	34.90	4.17	0.188
NO (ppbv)	3.4	1.8	0.8	2.9	2.9	0.000
NO_2 (ppbv)	15.5	14.4	10.3	18.5	3.1	0.335
Temp (°C)	27.3	27.1	26.8	27.5	0.3	0.022
RH (%)	83	83	80	85	2	0.262
UV (W m^{-2})	15.2	10.1	1.3	23.3	7.8	0.015
WS (m s^{-1})	3.6	3.8	3.4	4.2	0.3	0.017
LWC (μg m^{-3})	14.0	14.0	8.4	16.6	3.7	0.001

* *p* values derived from the Shapiro-Wilk tests (normal distribution: $p > 0.05$)

Table S7. Same as Table S4, but for the periods with marine air.

	Marine air						Marine air without troughs						Marine air with troughs					
Species	Mean	Median	Q1#	Q3†	95% CI^	*p* value *	Mean	Median	Q1	Q3	95% CI	*p* value	Mean	Median	Q1	Q3	95% CI	*p* value
2-MGA (IS-corrected response, measured by TAG, same below)	0.040	0.020	0.009	0.061	0.006	0.000	0.017	0.012	0.007	0.021	0.003	0.000	0.087	0.074	0.058	0.098	0.010	0.000
2-MT1	0.92	0.41	0.17	1.26	0.18	0.000	0.42	0.22	0.14	0.46	0.08	0.000	1.97	1.56	0.98	2.45	0.43	0.000
cis-2-MBT	1.10	0.19	0.04	1.44	0.26	0.000	0.27	0.08	0.03	0.26	0.07	0.000	2.84	2.07	1.38	3.56	0.60	0.000
DHOPA	0.02	0.00	0.00	0.02	0.00	0.000	0.00	0.00	0.00	0.00	0.00	0.000	0.04	0.03	0.02	0.05	0.01	0.000
TA2	0.93	0.38	0.09	1.58	0.16	0.000	0.32	0.17	0.05	0.41	0.08	0.000	2.22	2.07	1.52	2.70	0.29	0.000
MA	3.26	1.38	0.78	5.83	0.48	0.000	1.33	1.00	0.60	1.48	0.23	0.000	7.36	7.25	5.48	8.91	0.69	0.557
Succinic acid	0.24	0.17	0.10	0.28	0.03	0.000	0.16	0.12	0.08	0.19	0.02	0.000	0.42	0.30	0.22	0.53	0.07	0.000
Fructose-2	0.035	0.021	0.012	0.042	0.005	0.000	0.033	0.018	0.010	0.037	0.007	0.000	0.038	0.032	0.019	0.045	0.007	0.000
Levoglucosan	5.24	1.37	0.63	5.03	1.54	0.000	2.69	0.78	0.46	1.54	1.17	0.000	10.67	5.48	3.54	9.13	3.80	0.000
n-C_{23}	0.37	0.33	0.19	0.54	0.03	0.000	0.30	0.25	0.16	0.44	0.03	0.000	0.50	0.53	0.32	0.67	0.06	0.112
n-C_{27}	0.24	0.18	0.11	0.31	0.03	0.000	0.19	0.15	0.10	0.22	0.03	0.000	0.34	0.29	0.17	0.48	0.06	0.000
n-C_{31}	0.15	0.09	0.05	0.19	0.02	0.000	0.10	0.07	0.05	0.12	0.02	0.000	0.24	0.19	0.11	0.33	0.05	0.000
Palmitic acid	2.72	1.99	1.26	3.18	0.35	0.000	3.10	2.29	1.58	3.53	0.41	0.000	1.90	1.14	0.51	1.98	0.62	0.000
Stearic acid	1.85	1.62	1.13	2.16	0.18	0.000	1.72	1.55	1.13	1.94	0.19	0.000	2.12	1.79	1.19	2.56	0.41	0.000
9-oxononanoic acid	0.018	0.012	0.010	0.017	0.003	0.000	0.014	0.011	0.009	0.014	0.002	0.000	0.015	0.014	0.012	0.017	0.002	0.000
Oleic acid	2.89	1.33	0.39	3.73	0.57	0.000	2.83	1.25	0.39	3.72	0.69	0.000	3.02	1.65	0.46	3.71	1.01	0.000
Phthalic acid	0.38	0.21	0.15	0.46	0.06	0.000	0.17	0.17	0.11	0.21	0.01	0.059	0.77	0.54	0.45	0.93	0.13	0.000
Pyrene	0.27	0.19	0.14	0.30	0.04	0.000	0.20	0.17	0.12	0.22	0.03	0.000	0.42	0.33	0.23	0.47	0.08	0.000
PM_1-OM (μg m^{-3}, measured by AMS, same below)	3.2	2.5	1.6	4.3	0.3	0.000	2.2	1.9	1.4	2.8	0.2	0.000	5.6	5.1	4.0	7.2	0.6	0.002
Nitrate	0.2	0.1	0.1	0.2	0.0	0.000	0.1	0.1	0.1	0.1	0.0	0.000	0.5	0.3	0.2	0.6	0.1	0.000

Sulfate	2.2	1.9	1.6	2.5	0.2	0.000	2.0	1.9	1.7	2.4	0.1	0.000	2.5	2.1	1.3	2.9	0.5	0.000
Ammonium	0.8	0.7	0.6	1.0	0.1	0.000	0.8	0.7	0.6	1.0	0.1	0.000	0.9	0.8	0.5	1.1	0.2	0.000
Chloride	0.03	0.01	0.02	0.03	0.01	0.000	0.02	0.01	0.02	0.02	0.00	0.000	0.07	0.02	0.04	0.08	0.02	0.000
SO_2 (ppbv)	2.1	1.9	1.7	2.3	0.1	0.000	2.0	1.9	1.7	2.1	0.1	0.000	2.6	2.3	2.0	3.0	0.2	0.000
CO (ppbv)	264	249	217	301	12	0.000	238	237	203	271	10	0.000	318	299	260	346	24	0.000
O_3 (ppbv)	4.37	3.69	2.24	5.62	0.51	0.000	4.08	3.83	2.64	5.55	0.43	0.062	4.79	2.79	2.11	6.50	1.07	0.00
NO (ppbv)	12.7	6.0	1.6	17.8	2.2	0.000	9.1	5.0	1.3	13.0	1.9	0.000	20.2	14.5	2.7	31.4	5.3	0.000
NO_2 (ppbv)	20.2	18.6	11.6	26.1	1.5	0.000	16.0	15.0	10.6	20.1	1.2	0.000	29.1	28.3	21.1	37.4	2.8	0.672
Temp (°C)	28.8	28.9	27.7	29.8	0.2	0.060	29.5	29.4	28.5	30.6	0.2	0.018	27.2	27.0	26.3	28.0	0.3	0.056
RH (%)	83	83	79	89	1	0.003	81	81	77	85	1	0.070	89	91	86	93	2	0.000
UV (W m^{-2})	18.1	11.2	1.5	32.7	3.0	0.000	21.8	17.9	2.4	37.2	3.9	0.000	10.1	6.0	1.0	16.0	3.5	0.000
WS (m s^{-1})	2.2	2.3	1.6	2.8	0.1	0.058	2.4	2.4	1.9	2.8	0.1	0.078	1.9	1.8	1.0	2.5	0.2	0.010
LWC (μg m^{-3})	6.9	4.4	2.5	7.0	1.3	0.000	3.9	3.9	1.4	5.3	0.5	0.000	13.3	8.4	4.5	17.4	3.4	0.000

Q1: 25th percentile; † Q3:75th percentile; ^ 95% CI: 95% confidence interval; * *p* values derived from the Shapiro-Wilk tests (normal distribution: $p > 0.05$)

Table S8. Values of r, slope, and intercept for the linear regressions between the modelling and observations.

Species	Intercept	Slope	Standard error	r
PM_1-OM	0.54	0.82	0.92	0.95
MA	0.21	0.93	1.60	0.94
2-HGA	0.06	0.89	0.17	0.99
2-MT1	-0.04	1.00	0.69	0.95
cis-2-MBT	0.21	0.72	0.47	0.99
Levoglucosan	-0.02	1.00	0.72	1.00
Fructose-2	8.34	0.65	10.25	0.96
Palmitic acid	-0.19	1.06	0.71	0.96
Oleic acid	0.66	0.66	0.93	0.93
DHOPA	4.06	0.97	90.71	0.99
Phthalic acid	0.01	0.98	0.03	0.99
2-MGA	0.02	0.61	0.03	0.84
9-oxononanoic acid	0.00	0.87	0.00	0.99
NO_x	0.69	0.97	4.01	0.98
HDMGA	0.00	0.70	0.01	0.88