Supplement to the manuscript

An overview of organic aerosols at an urban site in Hong Kong: insights from in-situ measurement of molecular markers

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Supplemental Figures

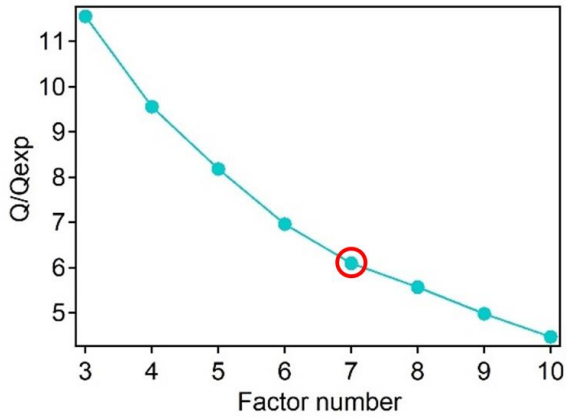

Figure S1. Change of Q/Q_{exp} ratio with the number of factors in PMF base runs. A seven-factor solution is adopted, as highlighted in red circle.

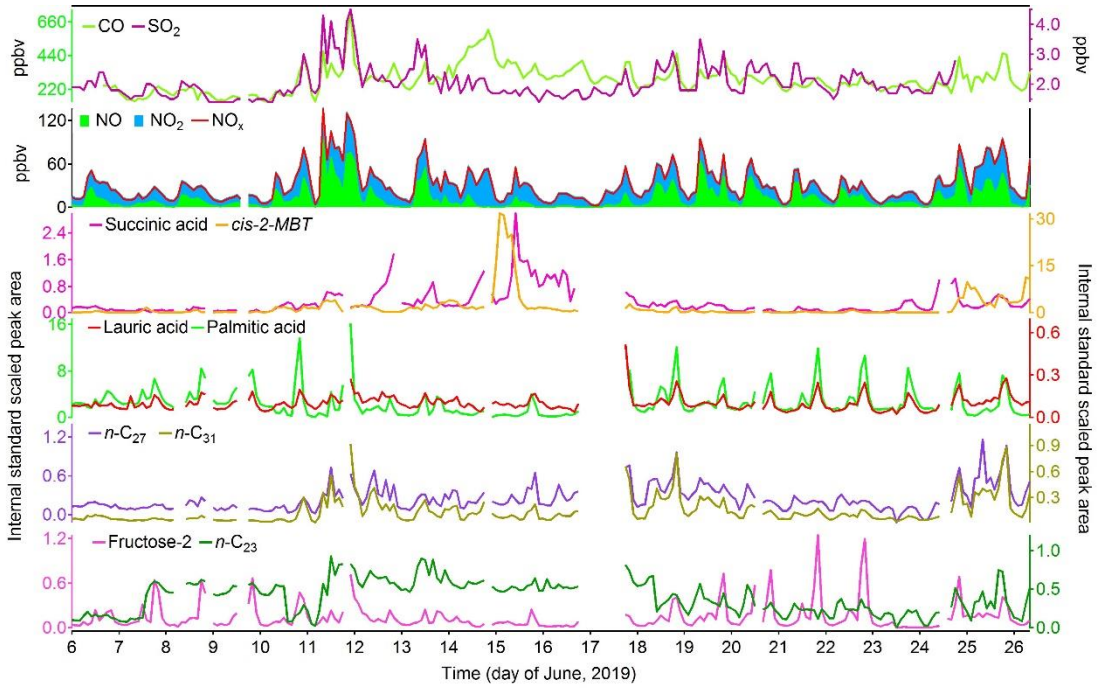

Figure S2. Time series of selected OA markers, CO, SO_2, and NO-NO_2-NO_x. Variations of OA markers are represented by internal standard scaled peak areas. Missing data are due to instrument maintenance.

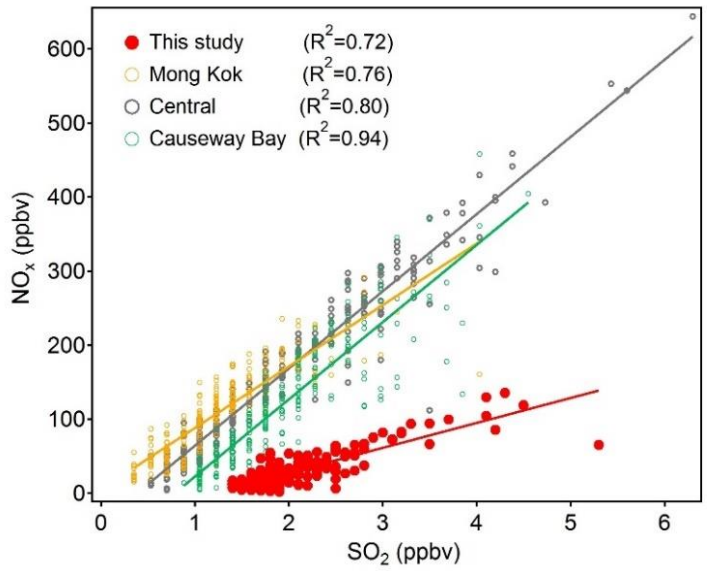

Figure S3. Correlations between NO_x and SO_2 at this site and three roadside sites in Hong Kong in the study period.

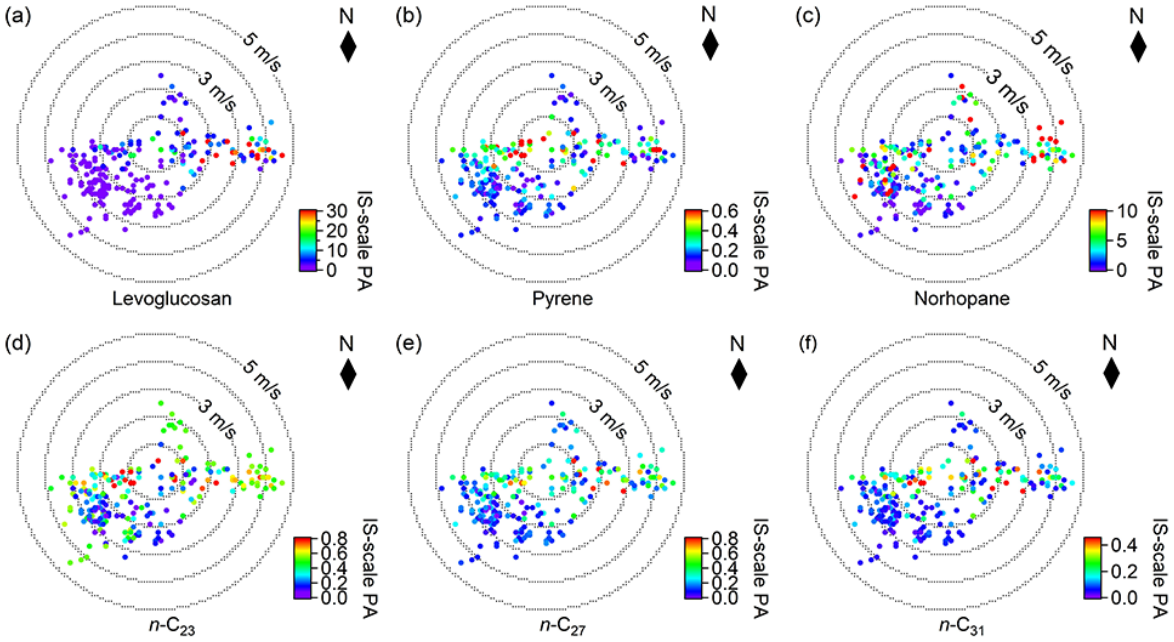

Figure S4. Wind roses colored by the IS-scaled PA of levoglucosan (a), pyrene (b), norhopane (c), *n*-C_{23} (d), *n*-C_{27} (e), and *n*-C_{31} (f).

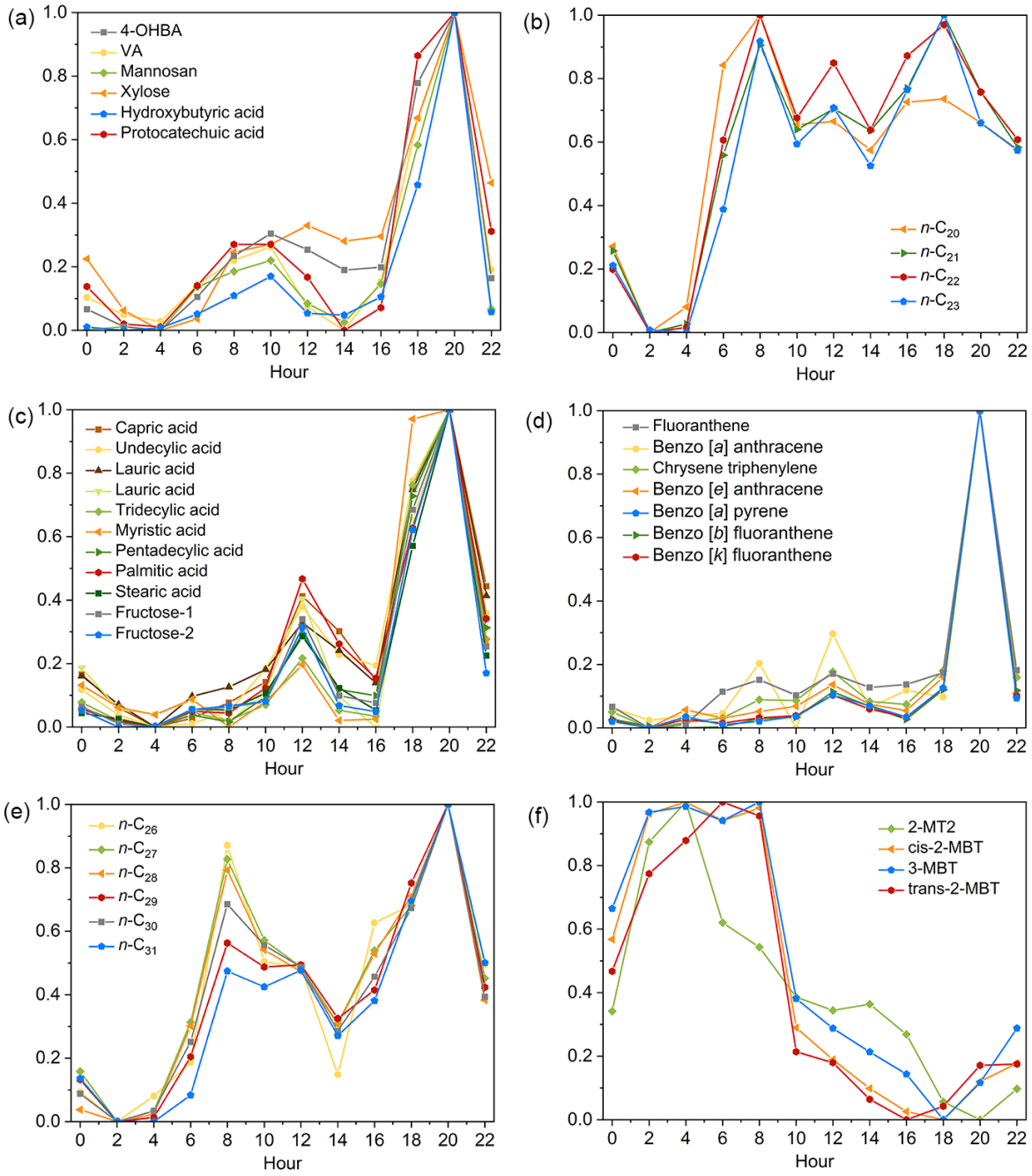

Figure S5. Diurnal patterns of selected OA markers represented by the normalized IS-scaled PA. The species are grouped based on the similarity in patterns.

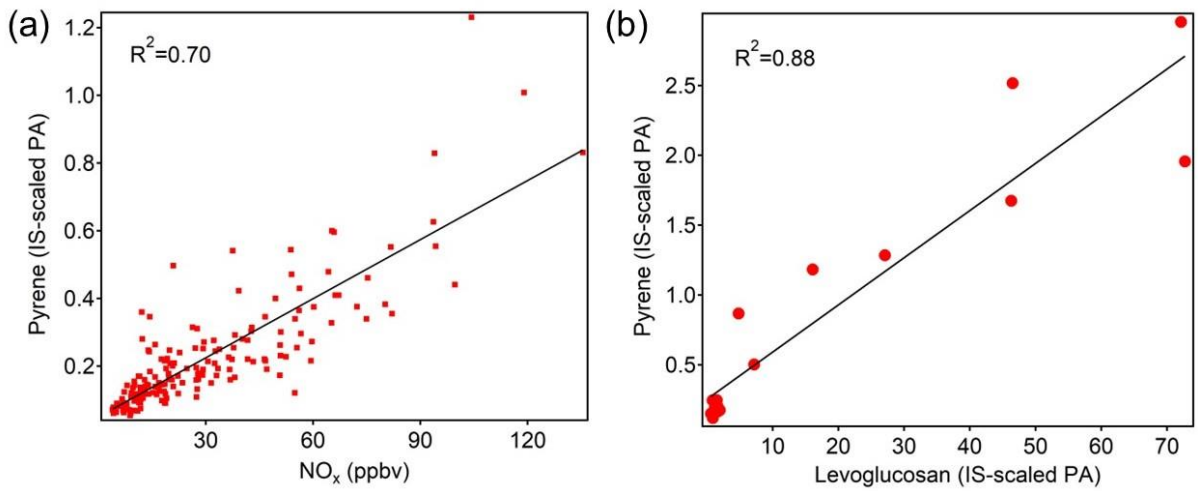

Figure S6. Correlations of pyrene (a representative of PAHs) *vs.* levoglucosan at 20:00 (a) and pyrene *vs.* NO_x at other times excluding 14:00 – 16:00 (b).

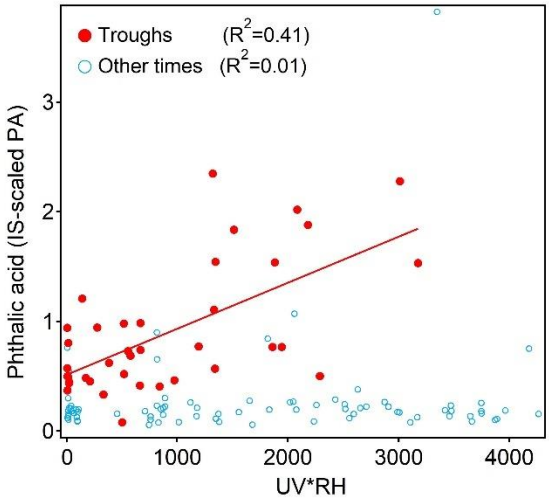

Figure S7. Correlations between phthalic acid and the product of UV and RH in presence of troughs and at other times with marine air.

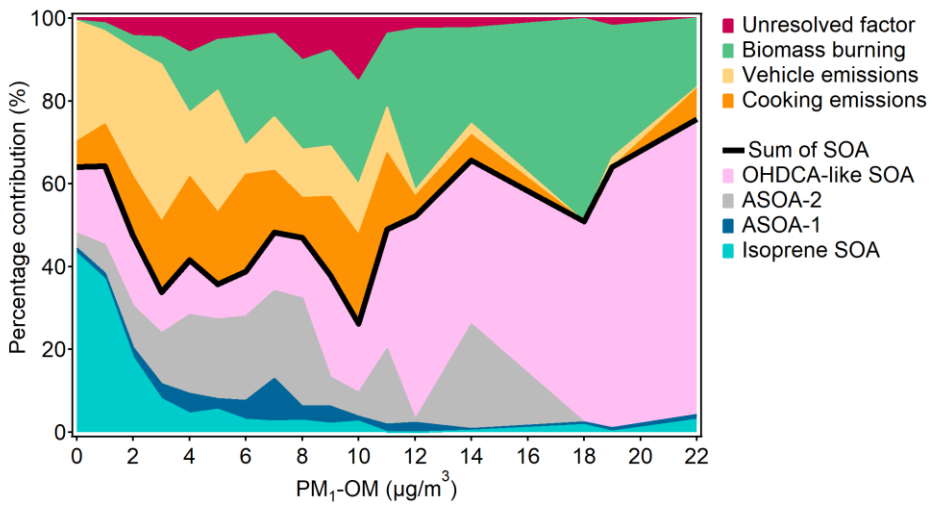

Figure S8. Changes of percentage contributions of individual OA sources to PM_1-OM with PM_1-OM concentration.

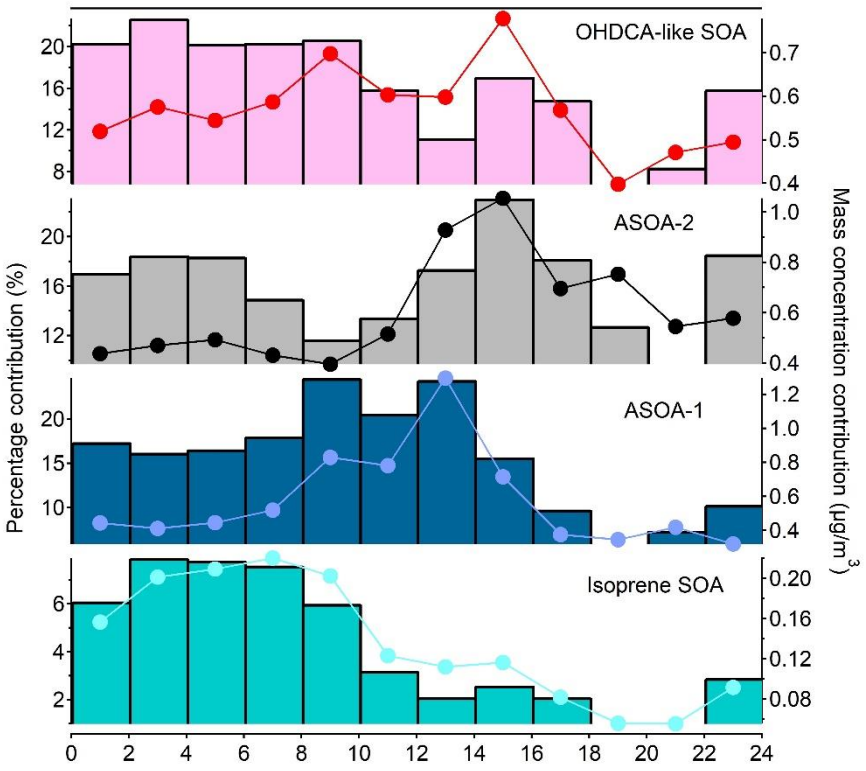

Figure S9. Average diurnal cycles of percentage contributions (columns) and mass concentration contributions (lines) to PM_1-OM of SOA factors.

Supplemental Tables

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

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

Table S2. 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	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	**17 alpha (H),28-norhopane (Norhopane)**	**191**	**917.9**	**D-cholesterol**
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	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 S3. Mean levels of PM_1 compositions and trace gases by air mass origins.

Species	Marine air without troughs	Marine air with troughs	Continental air	Coastal air
CO (ppb)	264±12	290±24	436±49	318±18
O_3 (ppb)	4.4±0.5	4.6±1.0	30.9±7.3	26.2±4.2
SO_2 (ppb)	2.1±0.1	2.5±0.2	1.8±0.1	1.7±0.1
NO (ppb)	12.7±2.2	19.2±5.0	2.2±2.1	1.0±1.5
NO_2 (ppb)	20.2±1.5	27.3±2.9	28.6±7.3	15.5±3.1
NO_x (ppb)	32.9±3.5	46.5±7.5	30.8±8.1	16.5±4.4
O_x (ppb)	26.4±1.6	33.6±2.3	59.6±12.3	41.7±3.1
PM_1-OM (μg/m^3)	3.2±0.3	5.0±0.6	11.1±2.9	7.0±1.3
NO_3^- (μg/m^3)	0.2±0.0	0.4±0.1	1.2±0.6	0.6±0.1
SO_4^{2-} (μg/m^3)	2.2±0.2	2.3±0.5	4.7±0.6	6.6±1.1
NH_4^+ (μg/m^3)	0.8±0.1	0.9±0.2	1.9±0.2	2.5±0.4

Table S4. Values of R^2, slope, and intercept for the linear regressions between the simulations and observations.

Species	Intercept	Slope	Standard error	R^2	*p* value
PM_1-OM	0.68	0.76	1.08	0.86	0.106
MA	0.23	0.92	1.12	0.94	0.007

CMA	0.04	0.86	0.07	0.93	0.040
2-HGA	0.04	0.92	0.27	0.94	0.000
2-MT1	0.01	0.93	0.69	0.89	0.000
cis-2-MBT	0.23	0.75	0.43	0.98	0.002
Levoglucosan	-0.12	1.02	0.70	1.00	0.000
Fructose-2	0.04	0.65	0.05	0.84	0.021
Palmitic acid	0.11	0.92	0.65	0.92	0.107
Norhopane	0.74	0.75	4.13	0.76	0.000
Oleic acid	0.42	0.77	1.15	0.86	0.078
DHOPA	0.01	0.74	0.03	0.79	0.000
Phthalic acid	0.00	1.00	0.02	1.00	0.649
2-MGA	0.02	0.57	0.03	0.66	0.000