

Supporting information

**Molecular characteristics and diurnal variations of organic aerosols
at a rural site in the North China Plain with implications for the
influence of regional biomass burning**

Jianjun Li^{1,4}, Gehui Wang^{2,3*}, Qi Zhang^{4*}, Jin Li¹, Can Wu², Wenqing Jiang⁴, Tong
Zhu⁵, and Limin Zeng⁵

¹Key Lab of Aerosol Chemistry & Physics, SKLLQG, Institute of Earth Environment,
Chinese Academy of Sciences, Xi'an, 710061, China

²Key Laboratory of Geographic Information Science of the Ministry of Education,
School of Geographic Sciences, East China Normal University, Shanghai 200241,
China

³Institute of Eco-Chongming, 3663 N. Zhongshan Rd., Shanghai 200062, China

⁴Department of Environmental Toxicology, University of California, Davis, CA
95616, USA

⁵BIC-ESAT and SKL-ESPC, College of Environmental Sciences and Engineering,
Peking University, Beijing, China

*Corresponding authors:

Prof. Gehui Wang, E-mail: ghwang@geo.ecnu.edu.cn;

Prof. Qi Zhang, E-mail: dkwzhang@ucdavis.edu

Table S1 Concentrations of total measured organic compounds (ng m⁻³) in the time-resolved (3-h) PM_{2.5} samples in the rural site of NCP during the whole sampling period, Period 1 (P1) and Period 2 (P2).

Compounds	Whole period (N=117)				Period 1 (N=28)				Period 2 (N=13)			
	min	max	Mean	SD	min	max	Mean	SD	min	max	Mean	SD
I. n-alkanes												
C ₁₈	0.76	7.82	3.05	1.35	1.70	6.42	3.55	1.22	1.16	4.58	2.26	0.96
C ₁₉	0.73	6.83	2.66	1.28	0.81	5.83	3.03	1.19	1.02	3.72	2.04	0.86
C ₂₀	0.69	5.44	2.08	0.96	0.80	5.44	2.69	1.02	0.69	2.69	1.46	0.57
C ₂₁	1.12	9.47	4.35	1.93	2.50	9.47	5.93	1.83	1.46	4.06	2.49	0.75
C ₂₂	0.72	8.85	3.25	1.68	1.53	8.85	4.62	1.89	0.75	2.72	1.58	0.55
C ₂₃	0.78	18.9	6.56	3.74	3.37	18.93	9.77	3.95	1.31	4.58	2.80	1.10
C ₂₄	0.62	17.1	4.75	3.07	2.46	12.6	6.47	2.31	1.03	2.60	1.87	0.54
C ₂₅	0.77	25.2	8.10	5.41	3.62	20.4	12.0	4.27	1.48	3.84	2.50	0.80
C ₂₆	0.84	22.4	6.35	4.63	3.21	15.7	9.11	3.66	1.21	3.52	2.17	0.82
C ₂₇	0.92	52.2	16.2	11.7	7.79	44.7	28.3	9.70	1.65	6.03	3.50	1.27
C ₂₈	0.55	26.9	7.85	5.55	3.88	18.8	11.9	4.13	0.55	5.25	2.35	1.25
C ₂₉	0.76	249.3	44.6	39.3	16.9	135.1	80.2	31.5	2.66	25.9	7.39	5.94
C ₃₀	0.24	49.1	8.67	6.91	4.95	26.1	13.6	4.70	0.57	6.16	2.61	1.34
C ₃₁	0.18	317.5	42.7	46.7	11.8	317.5	79.1	61.3	2.47	27.7	8.11	7.20
C ₃₂	0.40	61.5	9.65	8.07	6.12	31.3	14.9	5.08	0.40	6.69	2.65	1.72
C ₃₃	0.95	63.4	15.4	11.6	7.32	42.5	24.5	8.54	0.95	7.30	3.53	2.08
C ₃₄	0.28	51.1	7.77	6.70	5.53	24.4	12.2	4.36	0.28	4.62	1.93	1.20
C ₃₅	0.24	44.5	7.19	6.09	5.04	23.1	11.9	4.38	0.24	3.60	1.53	1.05
C ₃₆	0.49	37.9	6.4	5.19	3.92	18.3	9.94	3.80	0.49	2.65	1.49	0.77
subtotal	9.97	722.2	206.9	149.3	94.7	722.3	343.7	134.1	25.1	103.2	54.3	22.4
II. Fatty acids												
C _{12:0}	1.67	35.7	10.6	5.69	5.75	25.7	13.8	4.53	3.40	11.57	6.43	2.23
C _{13:0}	0.84	18.8	6.52	3.64	3.23	16.2	9.16	3.75	1.66	5.42	3.19	1.02
C _{14:0}	3.13	153.9	35.9	22.2	17.2	85.3	51.2	18.0	6.92	37.3	14.3	8.33
C _{15:0}	1.30	22.8	9.12	4.6	5.82	22.8	13.3	4.30	2.12	7.70	4.60	1.62
C _{16:0}	11.9	286.0	76.4	48.5	38.0	286.0	111.8	47.7	11.9	56.8	28.6	10.3
C _{17:0}	0.96	18.6	5.38	3.52	2.14	18.6	8.19	3.79	1.08	9.81	2.87	2.15
C _{18:0}	7.20	136.2	34.2	23.7	24.0	136.2	53.3	23.2	7.20	24.4	12.6	4.75
C _{19:0}	0.51	9.65	3.01	2.14	1.20	9.65	5.02	2.39	0.54	2.01	1.10	0.35
C _{20:0}	1.31	27.3	8.61	6.20	3.90	27.3	14.2	6.48	1.31	4.81	2.71	0.91
C _{21:0}	0.77	21.9	5.20	4.51	1.79	21.9	9.55	5.45	0.77	3.09	1.49	0.57
C _{22:0}	2.76	103.4	25.7	21.6	6.78	93.3	43.2	23.6	3.32	42.2	9.72	10.2
C _{23:0}	1.36	74.2	16.5	15.7	6.55	74.2	32.0	19.3	1.44	9.71	3.91	2.08
C _{24:0}	2.78	122.0	29.4	25.9	9.80	122.0	55.6	31.6	3.22	14.2	7.21	2.81
C _{25:0}	0.96	42.6	10.6	9.72	3.45	42.6	21.9	11.3	1.33	4.35	2.87	0.93
C _{26:0}	2.22	118.2	30.4	27.5	10.3	118.2	60.2	30.6	2.70	11.0	5.82	1.98
C _{27:0}	0.71	52.3	12.1	12.4	3.39	52.3	27.2	14.8	1.07	3.24	1.95	0.64
C _{28:0}	2.49	319.7	77.9	79.0	15.5	319.7	162.3	84.3	5.00	28.7	10.6	6.71
C _{29:0}	1.19	46.7	13.8	12.2	3.57	46.7	26.9	12.7	1.44	5.73	3.20	1.12
C _{30:0}	1.84	523.4	87.8	88.1	22.5	291.9	159.1	69.9	5.44	48.1	13.9	11.9
C _{16:1}	0.83	13.1	4.13	2.52	2.41	11.0	6.05	1.93	0.83	11.6	2.52	2.70
C _{18:1}	0.63	25.0	4.69	3.81	2.94	14.9	6.74	2.72	0.95	7.28	2.30	1.66

C _{18:2}	1.37	30.1	6.65	5.10	5.29	20.4	9.73	3.83	1.37	14.50	3.50	3.28
subtotal	64.6	1777	514.4	384.3	206.7	1528	900.3	358.3	81.4	234.4	145.3	47.7
III. Fatty alcohols												
C ₂₂	0.36	18.9	4.55	3.53	2.33	14.0	6.74	3.32	0.36	3.01	1.38	0.63
C ₂₃	0.15	11.2	2.70	2.29	1.15	8.53	4.12	2.06	0.37	1.44	0.87	0.32
C ₂₄	0.33	45.2	7.33	7.18	1.76	41.3	12.5	7.00	0.86	4.27	1.60	0.93
C ₂₅	0.13	12.6	2.99	2.73	0.88	11.90	4.85	2.30	0.24	1.70	0.77	0.34
C ₂₆	0.34	73.1	17.4	15.3	6.35	63.2	29.4	15.0	1.82	9.60	3.73	1.99
C ₂₇	0.25	17.00	4.71	3.96	1.52	17.00	8.84	3.96	0.62	1.72	1.06	0.31
C ₂₈	0.78	667.7	110.5	122.0	23.0	421.0	178.9	98.7	8.30	66.4	17.8	15.9
C ₂₉	0.19	26.2	5.45	5.15	1.70	21.3	9.85	5.12	0.49	2.44	1.10	0.48
C ₃₀	0.63	139.4	36.9	33.3	20.0	135.4	66.8	30.4	2.45	12.0	5.55	3.23
subtotal	3.18	975.9	192.6	187.4	62.4	638.2	322.0	150.7	16.6	100.2	33.9	22.6
IV. Sugar compounds												
<i>Anhydrosugars</i>												
galactosan	1.03	97.78	18.5	20.6	2.16	97.8	29.5	27.9	1.45	13.3	4.61	3.13
mannosan	0.69	54.82	9.78	10.4	1.61	54.8	15.0	13.3	0.96	6.63	2.83	1.43
levoglucosan	5.56	1447	240.1	287.8	29.3	1428	404.0	344.0	11.2	123.0	47.8	26.2
<i>Sugars</i>												
fructose	0.48	98.6	8.96	10.4	4.15	23.6	13.9	5.12	0.90	4.28	1.90	0.94
glucose	1.29	315.9	48.9	50.2	17.4	245.9	90.7	49.0	3.49	37.4	11.0	9.51
sucrose	0.13	20.3	3.57	3.33	1.53	9.38	4.99	1.96	0.20	1.57	0.70	0.36
trehalose	0.06	25.3	4.23	4.91	1.59	25.3	9.46	5.91	0.18	3.75	0.88	0.98
<i>Sugar alcohols</i>												
arabitol	0.72	852.2	40.6	83.8	6.67	115.0	55.4	29.2	1.34	26.3	6.65	6.68
mannitol	0.43	669.6	56.6	81.6	12.9	211.9	92.7	53.4	1.09	107.3	16.4	29.1
inositol	0.08	7.08	1.67	1.40	0.74	5.93	2.94	1.48	0.19	1.24	0.48	0.25
subtotal	15.9	2228	432.8	428.9	151.9	1727	718.0	403.1	39.7	241.3	93.2	52.9
V. PAHs												
phenanthrene	0.21	6.21	1.62	1.36	0.78	6.21	2.69	1.58	0.22	0.73	0.41	0.16
anthracene	0.04	0.38	0.14	0.08	0.09	0.36	0.20	0.07	0.05	0.09	0.07	0.01
fluoranthene	0.07	4.80	0.92	0.83	0.42	2.68	1.50	0.71	0.07	0.28	0.15	0.05
pyrene	0.09	3.87	0.90	0.79	0.43	2.89	1.52	0.80	0.09	0.36	0.18	0.06
benz(a)anthracene	0.03	2.30	0.49	0.48	0.15	1.80	0.82	0.54	0.05	0.21	0.09	0.04
chrysene / triphenylene	0.09	5.92	1.16	1.15	0.40	4.02	1.83	1.08	0.09	0.35	0.18	0.08
benzo(b)fluoranthene	0.07	9.14	1.82	1.91	0.45	6.23	2.75	1.81	0.13	0.77	0.31	0.19
benzo(k)fluoranthene	0.03	2.58	0.56	0.55	0.15	1.97	0.84	0.56	0.04	0.26	0.10	0.06
benzo(e)pyrene	0.07	6.26	1.23	1.28	0.36	4.28	1.82	1.15	0.09	0.51	0.22	0.12
benzo(a)pyrene	0.02	3.66	0.69	0.70	0.16	2.43	1.08	0.77	0.05	0.23	0.10	0.05
perylene	0.00	0.89	0.18	0.18	0.06	0.63	0.29	0.19	0.02	0.07	0.03	0.01
indeno[123-cd]pyrene	0.03	5.60	1.04	1.17	0.15	3.57	1.46	1.10	0.05	0.59	0.21	0.15
dibenz(a,h)anthracene	0.01	1.22	0.20	0.20	0.07	0.55	0.28	0.16	0.02	0.16	0.05	0.04
benzo(ghi)perylene	0.03	4.89	1.01	1.05	0.25	4.01	1.50	1.10	0.07	0.64	0.22	0.17
subtotal	1.11	48.5	12.0	11.0	4.21	37.7	18.6	11.0	1.25	5.01	2.33	0.98
VI. Hopanes												
C ₂₉ αβ	0.30	2.77	1.05	0.61	0.42	2.77	1.47	0.59	0.30	0.68	0.52	0.10
C ₂₉ βα	ND ^a	1.20	0.37	0.26	ND	1.20	0.68	0.20	ND	0.23	0.15	0.04
C ₃₀ αβ	0.29	3.15	1.17	0.64	0.44	2.54	1.55	0.57	0.41	0.79	0.63	0.12
C ₃₀ βα	ND	1.91	0.46	0.33	ND	1.91	0.82	0.37	ND	0.22	0.17	0.04

C ₃₁ αβS	ND	2.14	0.59	0.49	ND	2.14	0.91	0.58	ND	0.28	0.19	0.05
C ₃₁ αβR	ND	0.90	0.40	0.24	ND	0.84	0.56	0.15	ND	0.26	0.17	0.05
subtotal	0.66	10.81	3.46	2.38	0.86	9.97	4.40	2.48	1.14	2.28	1.81	0.31
VII. Phthalate esters												
dimethyl	0.10	14.6	4.17	2.82	1.38	14.6	5.34	3.31	0.20	4.74	2.46	1.36
diethyl	0.36	9.72	3.03	1.94	1.19	9.72	3.89	2.38	0.80	2.40	1.42	0.44
diisobutyl	4.86	49.3	22.7	9.45	17.3	45.7	27.3	6.42	9.40	20.3	14.6	3.67
isobutylbutyl	0.32	3.97	1.71	0.79	0.85	3.71	2.03	0.64	0.74	2.06	1.15	0.38
dibutyl	4.02	46.0	18.4	8.78	10.8	37.9	21.3	6.19	6.92	18.9	11.2	3.51
bis (2-ethylhexyl)	6.46	137.4	34.9	24.7	26.5	137.4	51.7	25.8	6.46	74.8	20.3	18.2
Subtotal	17.7	219.9	84.9	41.3	68.8	183.1	111.5	32.7	31.5	100.8	51.1	18.1
VIII. Phthalic acids												
<i>o</i> -ph	12.3	400.2	100.6	56.8	52.5	208.6	115.6	40.9	12.6	71.1	35.8	15.7
<i>m</i> -ph	0.60	19.6	3.77	3.74	1.27	19.02	5.75	4.32	0.60	8.97	1.77	2.12
<i>p</i> -ph	2.77	248.00	50.1	52.0	16.7	248.0	89.6	67.5	2.77	23.6	8.73	5.50
Subtotal	17.1	487.2	154.5	93.9	91.3	388.6	211.0	87.1	17.1	81.0	46.3	17.1
IX. Biogenic SOA tracers												
<i>Isoprene SOA tracers</i>												
MeTHFdiols	0.73	31.8	7.04	5.93	2.61	31.8	12.6	8.38	2.26	5.54	3.64	1.04
C5-triols	4.29	218.8	40.7	41.3	16.7	218.8	85.4	58.4	9.39	25.5	15.7	4.42
MTs	3.98	134.7	45.0	32.7	17.9	134.7	74.6	35.4	12.5	74.5	28.7	19.3
2-MGA	2.00	60.0	19.2	13.4	9.89	60.0	35.9	13.2	4.08	24.2	8.93	5.51
Σisoprene SOA tracers	11.1	404.1	111.9	85.8	48.3	404.1	208.5	104.9	34.8	127.5	57.0	29.4
<i>α-/β-Pinene SOA tracers</i>												
<i>cis</i> -pinonic acid	1.13	29.9	10.6	6.6	4.06	29.9	14.4	6.25	2.34	10.8	4.86	2.36
pinic acid	1.94	37.4	10.5	6.74	4.92	35.8	15.3	8.07	2.61	37.4	7.09	8.83
3-hydroxyglutaric acid	1.21	51.1	14.0	11.4	8.6	51.1	26.4	13.4	1.51	6.87	3.20	1.41
MBTCA	6.86	81.1	31.3	13.8	15.7	50.1	29.3	9.58	18.4	49.8	29.8	9.28
Σmonoterpene SOA tracers	11.1	166.2	66.1	31.2	37.3	166.2	85.3	34.9	26.7	64.5	44.6	12.6
<i>β-Caryophyllene SOA tracers</i>												
<i>β</i> -caryophyllinic acid	0.49	77.7	17.4	17.1	4.60	77.8	34.7	20.8	2.44	6.28	4.08	1.21
subtotal	22.7	618.1	195.2	125.9	107.6	618.1	328.4	152.0	65.6	193.4	105.6	38.3
IX. Toluene SOA tracers												
DHOPA	1.59	35.3	9.36	7.15	4.06	35.3	15.6	9.80	2.70	6.99	4.16	1.42

^a ND: not detected.

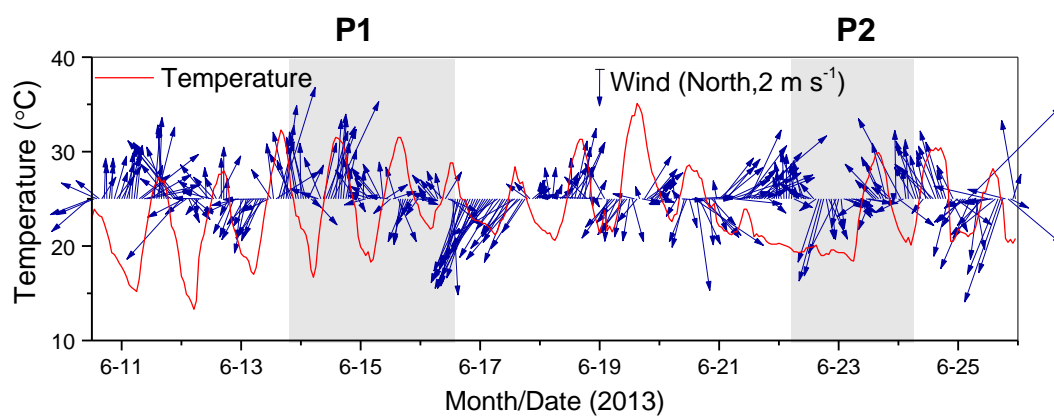


Figure S1 Temporal variations of temperature, wind speed, and wind direction at Gucheng during the study period.

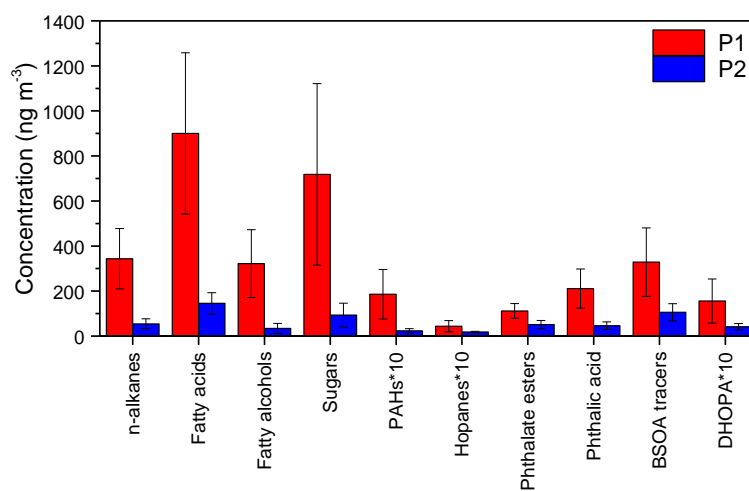


Figure S2. A comparison of the average concentrations of different organic compound classes in PM_{2.5} during P1 and P2.

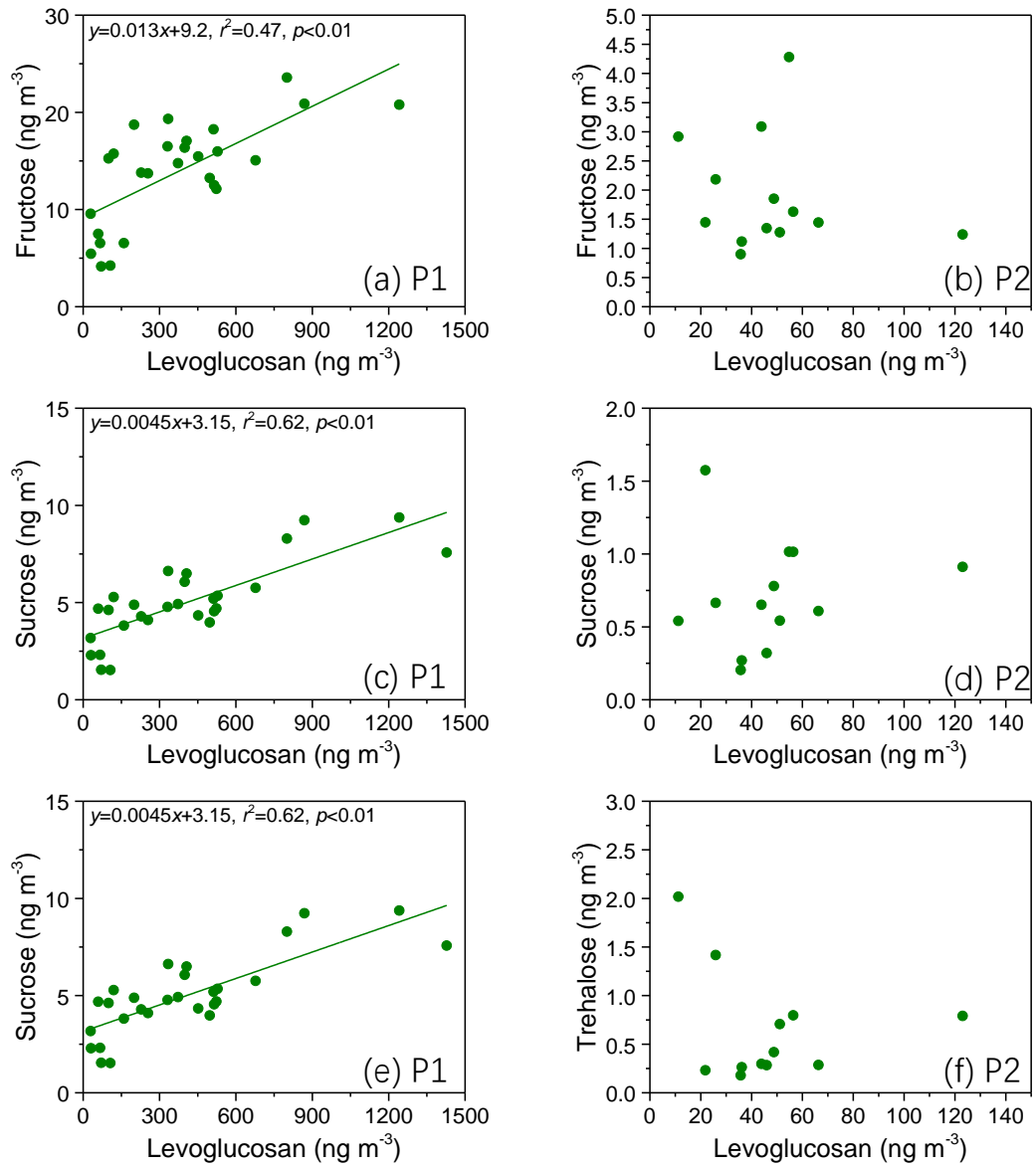


Figure S3 Relationships of fructose, sucrose, and trehalose with levoglucosan during P1 and P2.

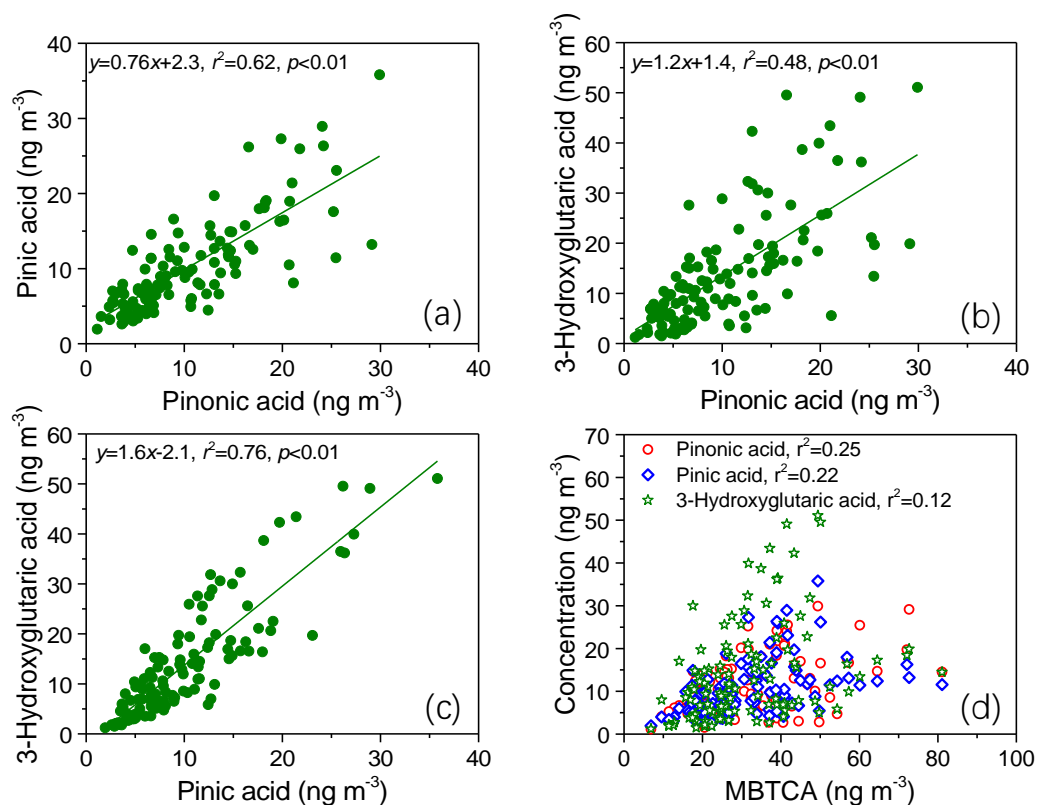


Figure S4 Relationships of the four α -/ β -pinene-derived products, i.e., pinonic acid, pinic acid, 3-hydroxyglutaric acid, and MBTCA, during the study period.

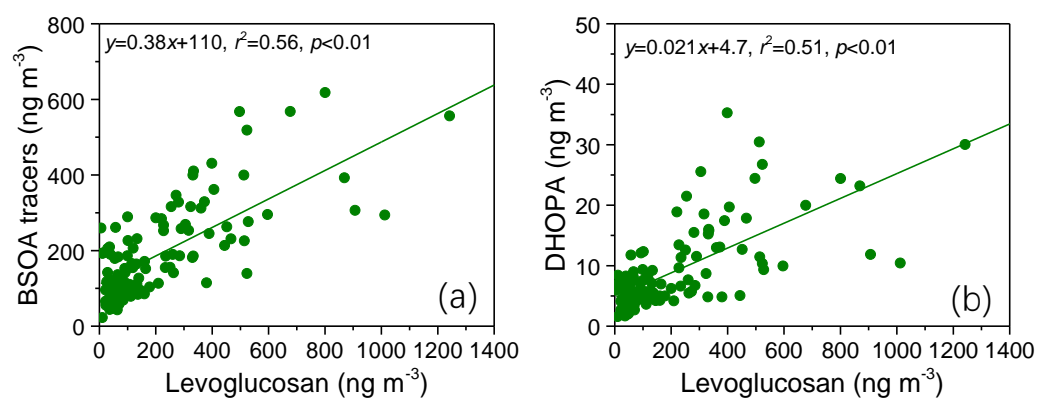


Figure S5 Relationships of the sum of BSOA tracers, and toluene-derived DHOPA with levoglucosan during the study period.