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Supplement of

Volatility parameterization of ambient organic aerosols at a rural site of the North China Plain

Siman Ren et al.

Correspondence to: Lin Wang (lin_wang@fudan.edu.cn)

Table S1. T_{max} and C^* of 91 CHO compounds.

Molecular formula	Molecular weight (Da)	T_{max} (°C)	log(C*)
$C_2H_2O_4$	89.9953	85.19	-2.53
$C_3H_6O_3$	90.0317	76.86	-1.74
$C_4H_6O_3$	102.0317	53.02	0.55
$C_3H_4O_4$	104.0110	62.59	-0.34
$C_3H_6O_4$	106.0266	58.74	0.03
$C_6H_6O_2$	110.0368	60.83	-0.15
$C_5H_8O_3$	116.0473	57.01	0.23
$C_4H_6O_4$	118.0266	69.60	-0.94
$C_4H_8O_4$	120.0423	60.13	-0.05
$C_7H_8O_2$	124.0524	62.92	-0.30
$C_6H_8O_3$	128.0473	68.29	-0.79
$C_5H_6O_4$	130.0266	69.65	-0.91
$C_5H_8O_4$	132.0423	59.19	0.08
$C_4H_6O_5$	134.0215	85.22	-2.36
$C_5H_{10}O_4$	134.0579	64.84	-0.44
$C_8H_8O_2$	136.0524	54.83	0.50
$C_8H_{10}O_2$	138.0681	63.02	-0.26
$C_6H_8O_4$	144.0423	70.29	-0.92
$C_6H_{10}O_4$	146.0579	71.49	-1.03
$C_8H_8O_3$	152.0473	57.96	0.26
$C_6H_8O_5$	160.0372	59.97	0.09
$C_7H_{12}O_4$	160.0736	74.83	-1.30
$C_6H_{10}O_5$	162.0528	70.76	-0.92
$C_7H_{14}O_4$	162.0892	77.78	-1.57
$C_6H_{12}O_5$	164.0685	71.40	-0.97
$C_7H_8O_5$	172.0372	87.61	-2.47
$C_8H_{12}O_4$	172.0736	67.08	-0.54
$C_{11}H_{12}O_2$	176.0837	71.73	-0.97
$C_{10}H_{10}O_3$	178.0630	76.28	-1.39
$C_{10}H_{14}O_3$	182.0943	63.91	-0.22
$C_8H_8O_5$	184.0372	62.42	-0.08
$C_5H_{12}O_7$	184.0583	62.65	-0.10
$C_{10}H_{16}O_3$	184.1099	66.60	-0.47
$C_6H_{12}O_7$	196.0583	90.54	-2.69
$C_7H_{16}O_6$	196.0947	75.50	-1.28
$C_6H_{14}O_7$	198.0740	80.87	-1.78
$C_{13}H_{12}O_2$	200.0837	82.75	-1.95
$C_{11}H_{20}O_3$	200.1412	74.11	-1.14
$C_9H_{14}O_5$	202.0841	90.32	-2.66
$C_{10}H_{18}O_4$	202.1205	87.91	-2.43
$C_8H_{12}O_6$	204.0634	80.57	-1.74
$C_8H_{14}O_6$	206.0790	90.41	-2.66
$C_7H_{14}O_7$	210.0740	94.76	-3.06
$C_8H_{18}O_6$	210.1103	73.29	-1.04

$C_7H_{16}O_7$	212.0896	89.09	-2.52
$C_9H_{10}O_6$	214.0477	98.16	-3.37
$C_{14}H_{14}O_2$	214.0994	82.22	-1.87
$C_{13}H_{16}O_3$	220.1099	84.65	-2.09
$C_8H_{14}O_7$	222.0740	94.55	-3.01
$C_9H_{18}O_6$	222.1103	83.27	-1.95
$C_{10}H_{10}O_6$	226.0477	98.84	-3.41
$C_7H_{14}O_8$	226.0689	100.28	-3.54
$C_{15}H_{14}O_2$	226.0994	92.14	-2.78
$C_{11}H_{16}O_5$	228.0998	92.71	-2.83
$C_{12}H_{20}O_4$	228.1362	87.15	-2.31
$C_{10}H_{14}O_6$	230.0790	94.56	-3.00
$C_{10}H_{16}O_6$	232.0947	94.37	-2.98
$C_9H_{18}O_7$	238.1053	95.59	-3.08
$C_{13}H_{20}O_4$	240.1362	93.67	-2.90
$C_{15}H_{28}O_2$	240.2089	64.65	-0.17
$C_{14}H_{26}O_3$	242.1882	69.47	-0.62
$C_{15}H_{30}O_2$	242.2246	69.97	-0.67
$C_{11}H_{16}O_6$	244.0947	102.22	-3.69
$C_{12}H_{20}O_5$	244.1311	91.12	-2.65
$C_{11}H_{20}O_6$	248.1260	89.62	-2.50
$C_{15}H_{24}O_3$	252.1725	87.32	-2.28
$C_{16}H_{28}O_2$	252.2089	72.46	-0.88
$C_9H_{18}O_8$	254.1002	100.63	-3.53
$C_{16}H_{30}O_2$	254.2246	66.04	-0.28
$C_{14}H_{24}O_4$	256.1675	87.53	-2.29
$C_{16}H_{32}O_2$	256.2402	60.40	0.26
$C_{17}H_{32}O_2$	268.2402	69.64	-0.59
$C_{17}H_{34}O_2$	270.2559	73.91	-0.99
$C_{18}H_{30}O_2$	278.2246	64.42	-0.09
$C_{18}H_{32}O_2$	280.2402	69.07	-0.52
$C_{18}H_{34}O_2$	282.2559	76.70	-1.23
$C_{18}H_{36}O_2$	284.2715	60.75	0.27
$C_{18}H_{34}O_3$	298.2508	82.58	-1.76
$C_{19}H_{38}O_2$	298.2872	79.85	-1.50
$C_{17}H_{34}O_4$	302.2457	87.55	-2.22
$C_{20}H_{36}O_2$	308.2715	84.89	-1.96
$C_{20}H_{38}O_2$	310.2872	88.15	-2.27
$C_{20}H_{40}O_2$	312.3028	77.77	-1.29
$C_{18}H_{36}O_4$	316.2614	91.83	-2.60
$C_{20}H_{32}O_3$	320.2351	94.83	-2.88
$C_{19}H_{36}O_4$	328.2614	93.15	-2.71
$C_{20}H_{26}O_4$	330.1831	96.12	-2.99
$C_{19}H_{38}O_4$	330.2770	95.76	-2.96
$C_{20}H_{38}O_4$	342.2770	95.04	-2.87
$C_{20}H_{40}O_4$	344.2927	92.03	-2.59
$C_{21}H_{40}O_4$	356.2927	97.53	-3.09

Table S2. T_{max} and C^* of 90 CHON compounds.

Molecular formula	Molecular weight (Da)	T_{max} (°C)	log(C*)
$C_3H_5NO_3$	103.0269	65.53	-0.62
$C_3H_7NO_3$	105.0426	45.23	1.29
$C_4H_7NO_3$	117.0426	73.60	-1.32
C_7H_5NO	119.0371	54.30	0.50
$C_2H_6N_2O_4$	122.0328	50.48	0.87
$C_6H_5NO_2$	123.0320	69.98	-0.96
$C_5H_8N_2O_2$	128.0586	96.77	-3.46
$C_6H_5NO_3$	139.0269	57.86	0.23
$C_4H_8N_2O_4$	148.0484	68.01	-0.70
$C_7H_7NO_3$	153.0426	57.95	0.26
$C_6H_5NO_4$	155.0219	75.37	-1.37
$C_8H_7NO_3$	165.0426	79.33	-1.71
$C_8H_9NO_3$	167.0582	54.22	0.65
$C_7H_7NO_4$	169.0375	76.44	-1.43
$C_9H_{17}NO_2$	171.1259	99.47	-3.59
$C_6H_{13}NO_5$	179.0794	85.70	-2.28
$C_9H_{12}N_2O_2$	180.0899	56.23	0.49
$C_9H_{11}NO_3$	181.0739	56.98	0.43
$C_8H_9NO_4$	183.0532	76.10	-1.36
$C_7H_{10}N_2O_4$	186.0641	80.82	-1.80
$C_9H_{17}NO_3$	187.1208	95.93	-3.22
$C_7H_{14}N_2O_4$	190.0954	76.72	-1.41
$C_6H_{12}N_2O_5$	192.0746	89.21	-2.58
$C_8H_6N_2O_4$	194.0328	95.75	-3.19
$C_9H_{10}N_2O_3$	194.0691	87.07	-2.37
$C_6H_{13}NO_6$	195.0743	78.17	-1.53
$C_9H_{13}N_3O_2$	195.1008	60.31	0.15
$C_8H_{10}N_2O_4$	198.0641	72.67	-1.01
$C_{11}H_{21}NO_2$	199.1572	97.99	-3.38
$C_{11}H_{12}N_2O_2$	204.0899	87.26	-2.37
$C_{12}H_{16}N_2O$	204.1263	80.85	-1.76
$C_{11}H_{14}N_2O_2$	206.1055	86.08	-2.25
$C_7H_{13}NO_6$	207.0743	87.30	-2.36
$C_{10}H_{12}N_2O_3$	208.0848	83.09	-1.97
$C_{14}H_{11}NO$	209.0841	86.51	-2.28
$C_9H_9NO_5$	211.0481	85.78	-2.21
$C_{10}H_{13}NO_4$	211.0845	92.91	-2.88
$C_{12}H_{21}NO_2$	211.1572	94.73	-3.05
$C_{12}H_8N_2O_2$	212.0586	96.28	-3.20
$C_{12}H_{10}N_2O_2$	214.0742	94.01	-2.98
$C_{12}H_{12}N_2O_2$	216.0899	91.65	-2.75
$C_{13}H_{16}N_2O$	216.1263	89.29	-2.53
$C_{11}H_{10}N_2O_3$	218.0691	93.80	-2.95
$C_8H_{14}N_2O_5$	218.0903	88.40	-2.44

$C_{10}H_{13}NO_5$	227.0794	96.68	-3.20
$C_{13}H_{25}NO_2$	227.1885	101.28	-3.64
$C_9H_{12}N_2O_5$	228.0746	98.58	-3.38
$C_{13}H_{14}N_2O_2$	230.1055	92.88	-2.84
$C_{10}H_{17}NO_5$	231.1107	87.69	-2.35
$C_8H_{12}N_2O_6$	232.0695	98.86	-3.40
$C_9H_{15}NO_6$	233.0899	89.60	-2.53
$C_{14}H_{19}NO_2$	233.1416	79.43	-1.57
$C_{11}H_{23}NO_4$	233.1627	57.12	0.52
$C_8H_{14}N_2O_6$	234.0852	95.71	-3.10
$C_{14}H_{21}NO_2$	235.1572	81.80	-1.79
$C_8H_{16}N_2O_6$	236.1008	94.68	-3.00
$C_{15}H_{18}N_2O$	242.1419	85.89	-2.16
$C_{13}H_{25}NO_3$	243.1834	97.12	-3.22
$C_{10}H_{15}NO_6$	245.0899	93.55	-2.88
$C_9H_{14}N_2O_6$	246.0852	100.38	-3.52
$C_{10}H_{18}N_2O_5$	246.1216	94.64	-2.98
$C_{10}H_{17}NO_6$	247.1056	88.84	-2.43
$C_{12}H_{25}NO_4$	247.1784	47.48	1.45
$C_{14}H_{25}NO_3$	255.1834	90.15	-2.54
$C_{15}H_{16}N_2O_2$	256.1212	97.68	-3.25
$C_{10}H_{14}N_2O_6$	258.0852	108.82	-4.29
$C_{11}H_{18}N_2O_5$	258.1216	100.38	-3.50
$C_{12}H_{21}NO_5$	259.1420	82.79	-1.84
$C_{13}H_{27}NO_4$	261.1940	48.73	1.36
$C_{10}H_{20}N_2O_6$	264.1321	91.45	-2.65
$C_{14}H_{29}NO_4$	275.1944	50.46	1.22
$C_{11}H_{20}N_2O_6$	276.1321	98.48	-3.29
$C_{15}H_{31}NO_4$	289.2253	53.08	1.00
$C_{17}H_{32}N_2O_2$	296.2464	74.90	-1.04
$C_{18}H_{26}N_2O_2$	302.1994	83.15	-1.81
$C_{16}H_{33}NO_4$	303.2415	77.67	-1.29
$C_{17}H_{32}N_2O_3$	312.2413	91.24	-2.55
$C_{20}H_{30}N_2O$	314.2358	93.39	-2.75
$C_{17}H_{35}NO_4$	317.2566	59.75	0.41
$C_{21}H_{22}N_2O$	318.1732	94.57	-2.86
$C_{18}H_{33}NO_4$	327.2410	86.00	-2.04
$C_{19}H_{37}NO_3$	327.2773	92.77	-2.68
$C_{18}H_{20}N_2O_4$	328.1423	109.88	-4.28
$C_{16}H_{28}N_2O_5$	328.1998	93.91	-2.78
$C_{18}H_{35}NO_4$	329.2566	88.85	-2.31
$C_{19}H_{37}NO_4$	343.2723	69.94	-0.51
$C_{19}H_{39}NO_4$	345.2879	64.44	0.01
$C_{20}H_{38}N_2O_3$	354.2882	97.76	-3.11
$C_{20}H_{39}NO_4$	357.2879	90.47	-2.42
$C_{23}H_{40}N_2O$	360.3141	90.37	-2.41

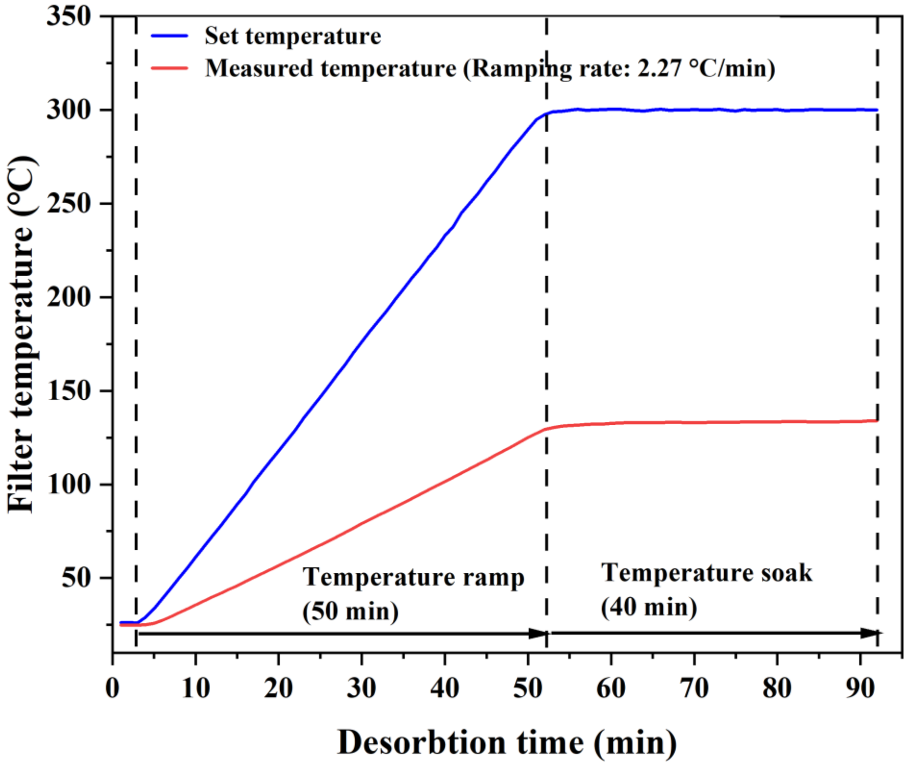


Figure S1. The desorption procedure for the calibration experiments and the field filter measurements.

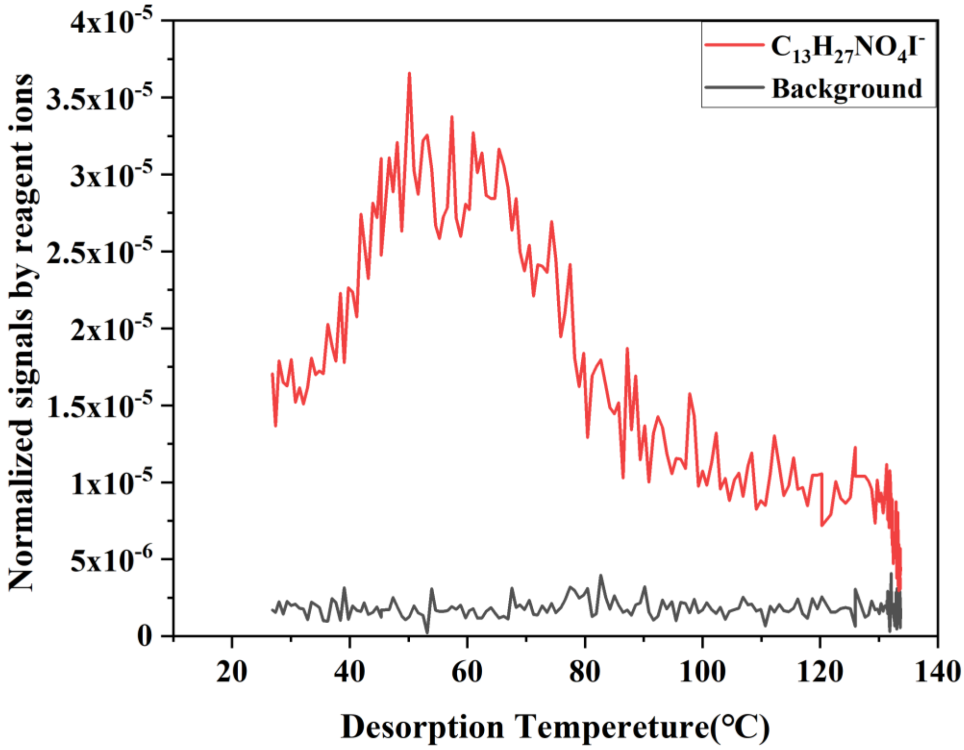


Figure S2. An example of the background and desorption signals of an identified compound, $C_{13}H_{27}NO_4I^-$.

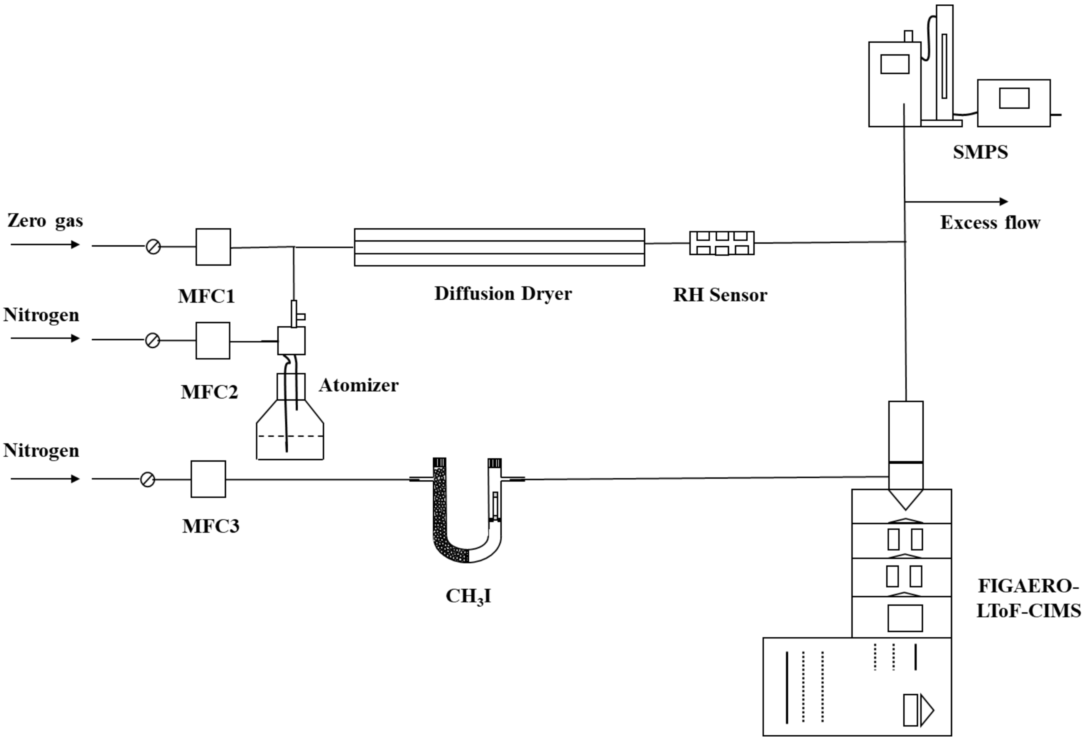


Figure S3. Schematics of the atomization method setup.

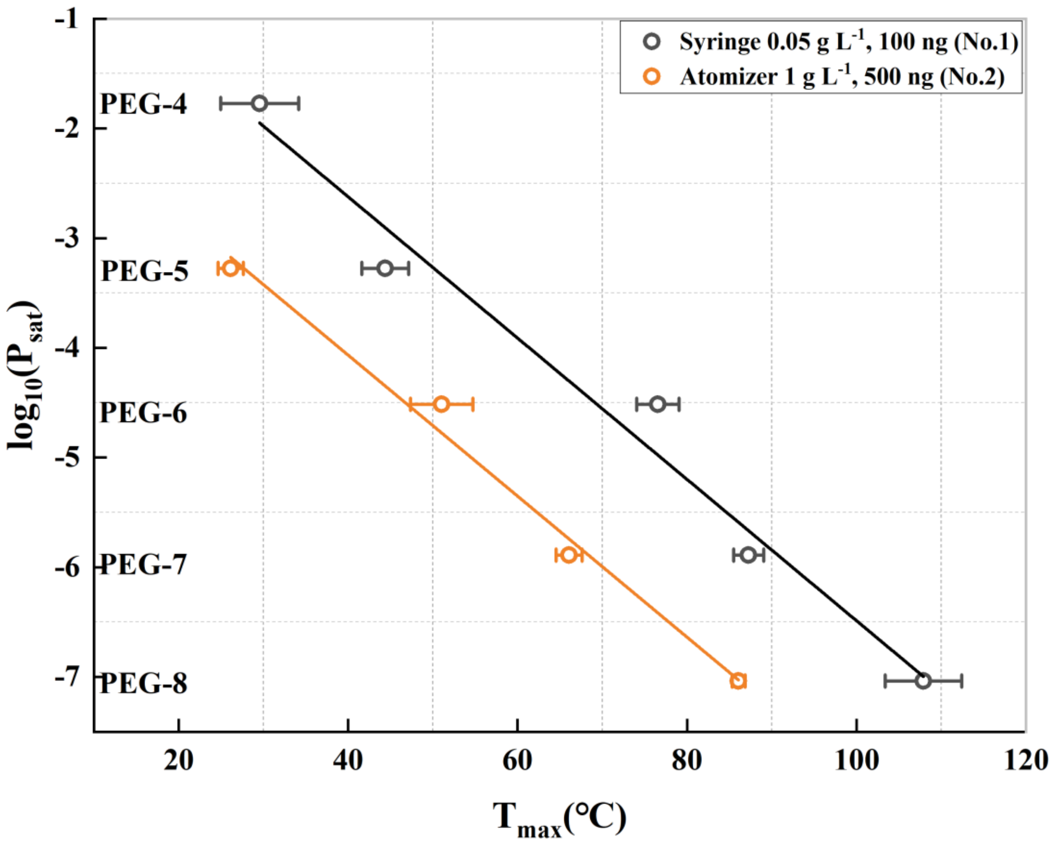


Figure S4. Comparison of T_{max} of different authentic organic standards between the syringe deposition method and the atomization method. Logarithm of literature-based P_{sat} are plotted against measured T_{max} for PEG compounds. Error bars represent ± 1 standard deviation of T_{max} from four replicate experiments.

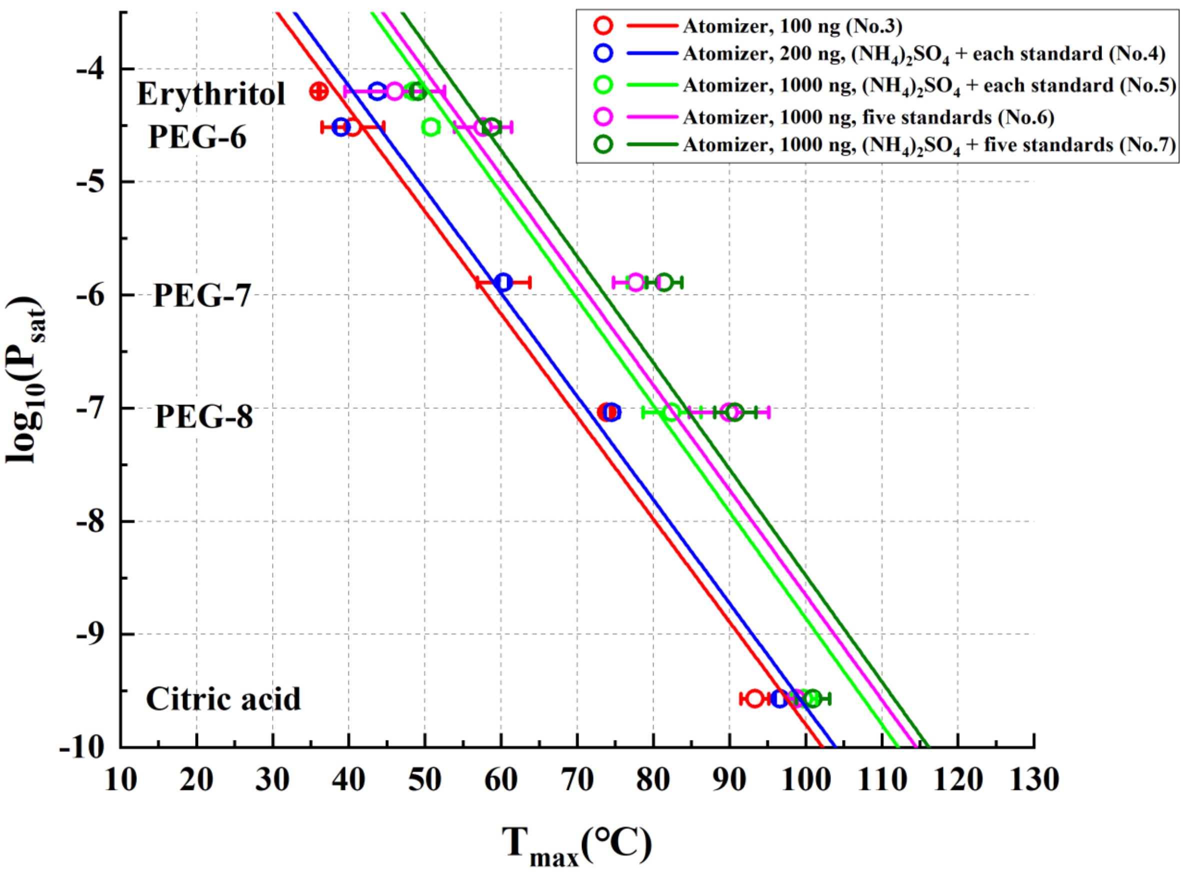


Figure S5. Influence of addition of ammonium sulfate and mixing of organic compounds on T_{max} of organic standards. The red, blue, light green, magenta, and dark green lines denote calibration results of no.3-7 sets of experiments, respectively. Error bars represent ± 1 standard deviation of T_{max} from four replicate experiments.

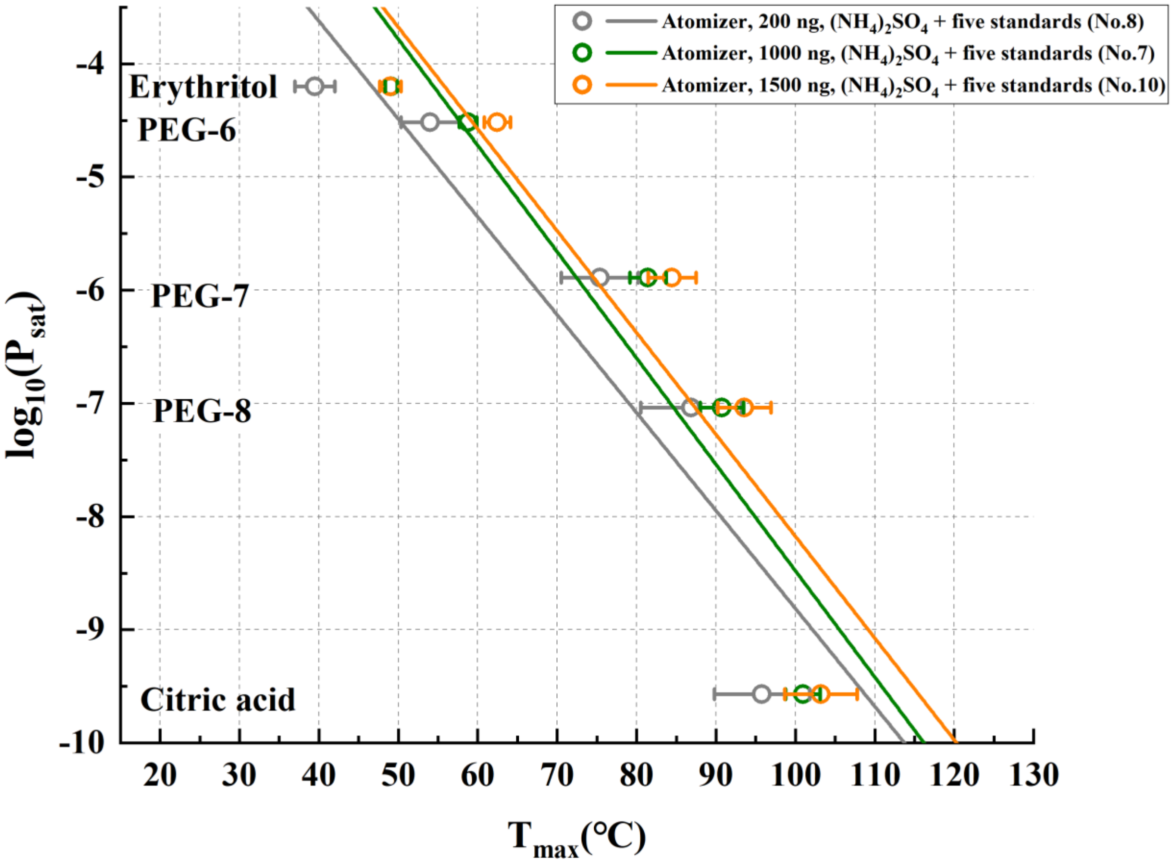


Figure S6. Influence of mass loading on filters on the T_{max} of organic standards. The grey, dark green, and orange lines denote calibration results of no.8, no.7, and no.10 sets of experiments, respectively. Error bars represent ± 1 standard deviation of T_{max} from four replicate experiments.

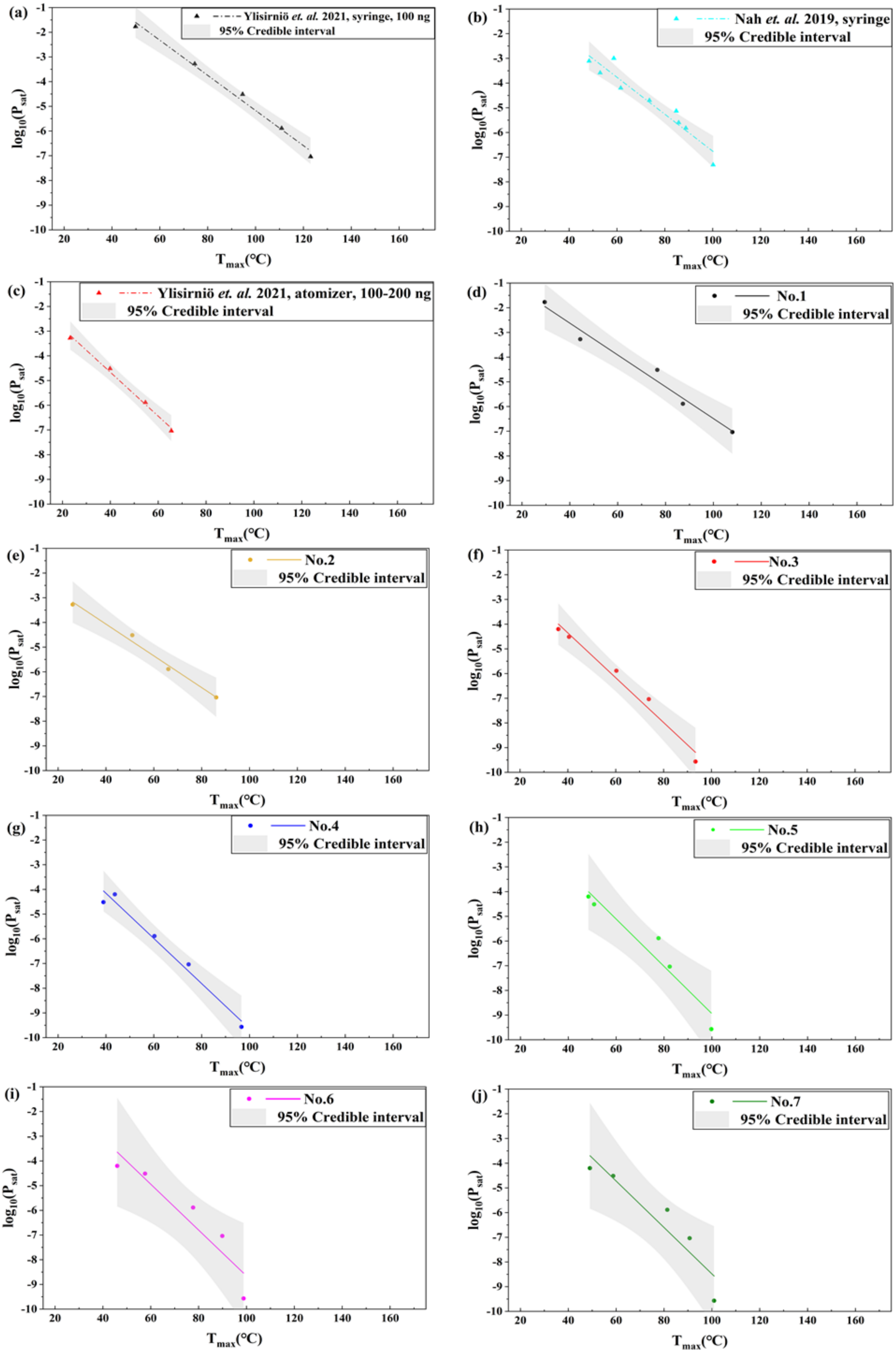


Figure S7. The 95% credible intervals of the fitted lines obtained in this study and previous studies.

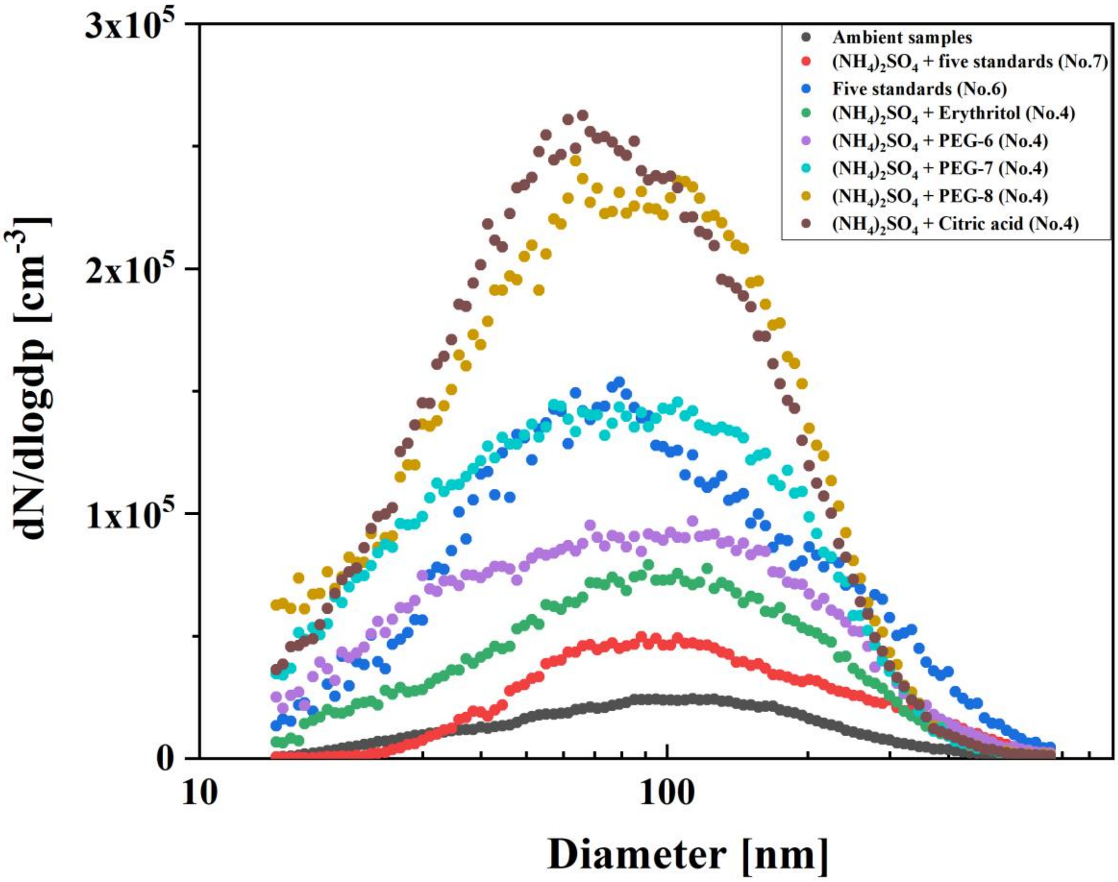


Figure S8. The particle size distributions of calibration experiments (no.4, no.6, and no.7 sets of experiments) and ambient samples.

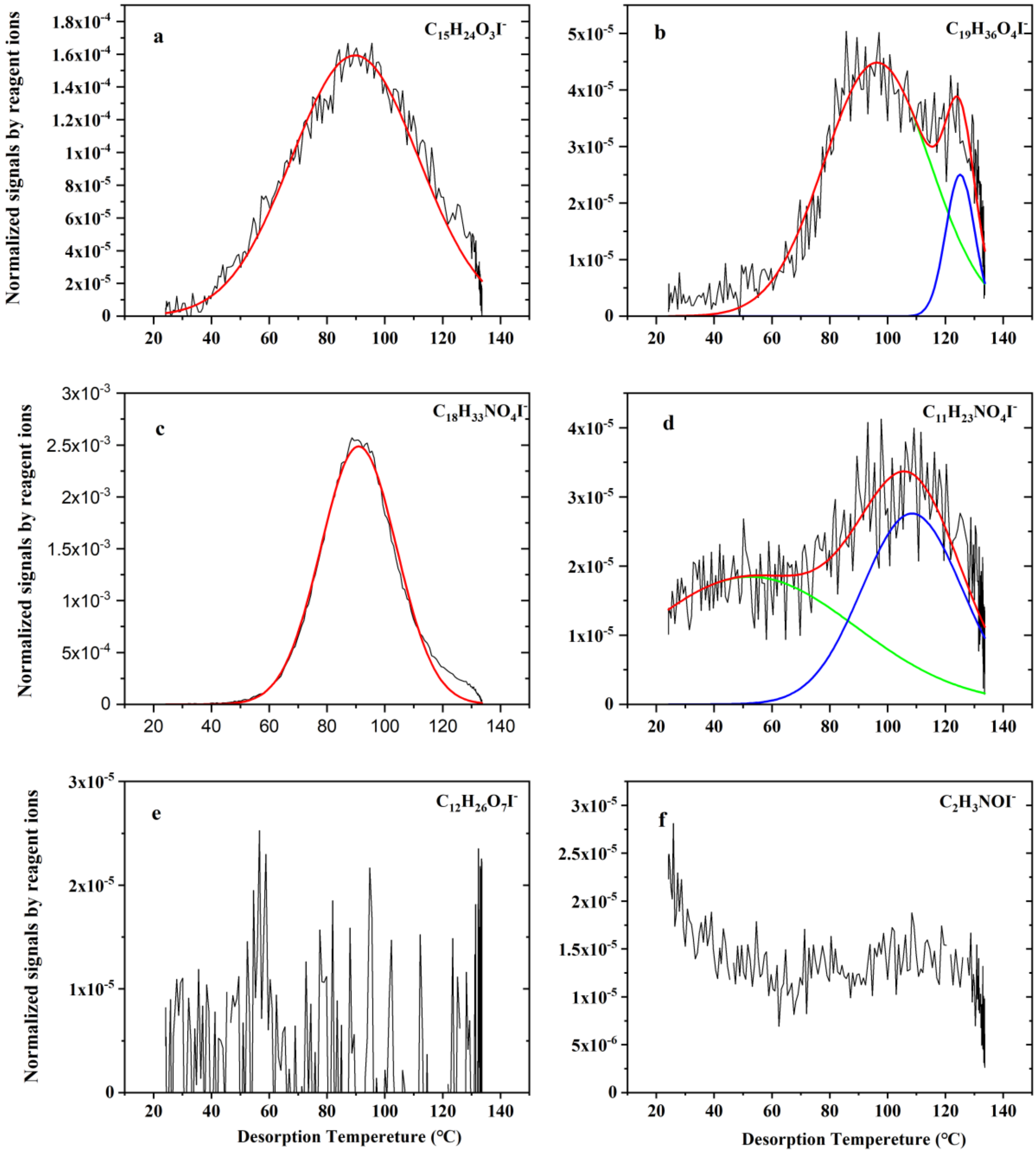
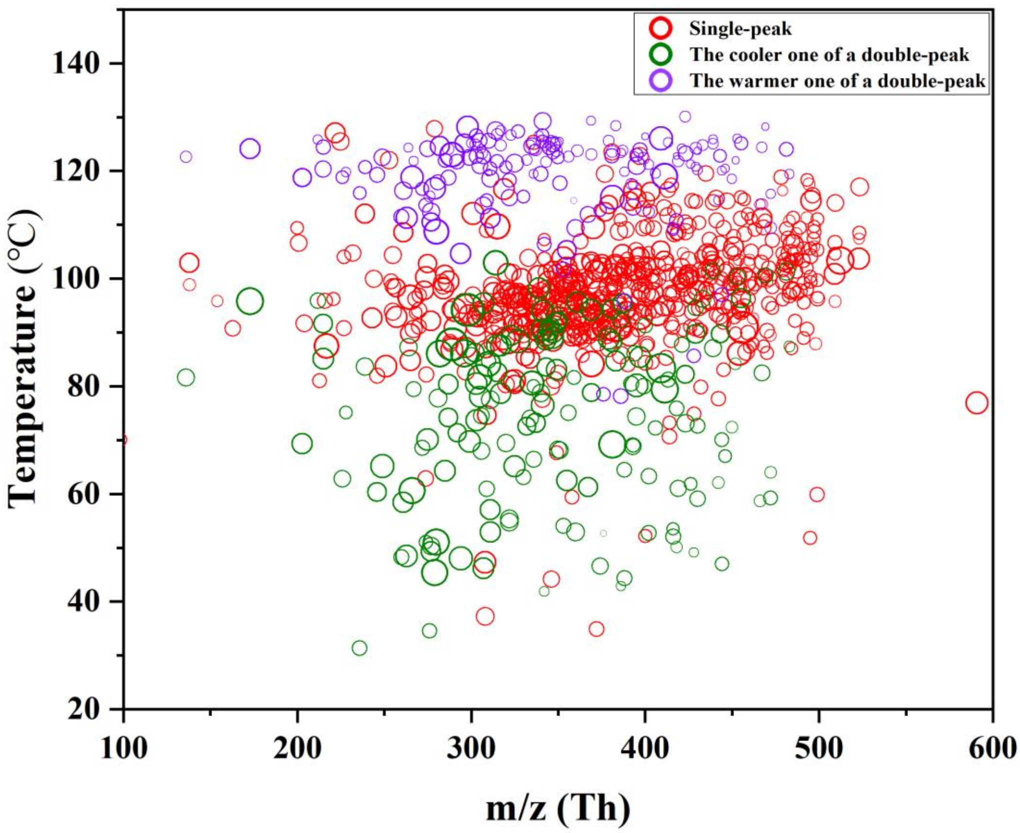


Figure S9. Four representative types of thermograms. Red, green, and blue lines represent fitting curves for the overall thermogram, the first desorption peak, and the second desorption peak, respectively.



35 **Figure S10.** The peak temperatures of thermograms of 765 organic compounds. The mass of reagent ion I^- was not removed from the m/z shown in the plot. The single peaks, the cooler peaks, and the warmer peaks of double peaks are denoted by red, green, and purple circles, respectively. The symbol size is proportional to the logarithm of the total signal.

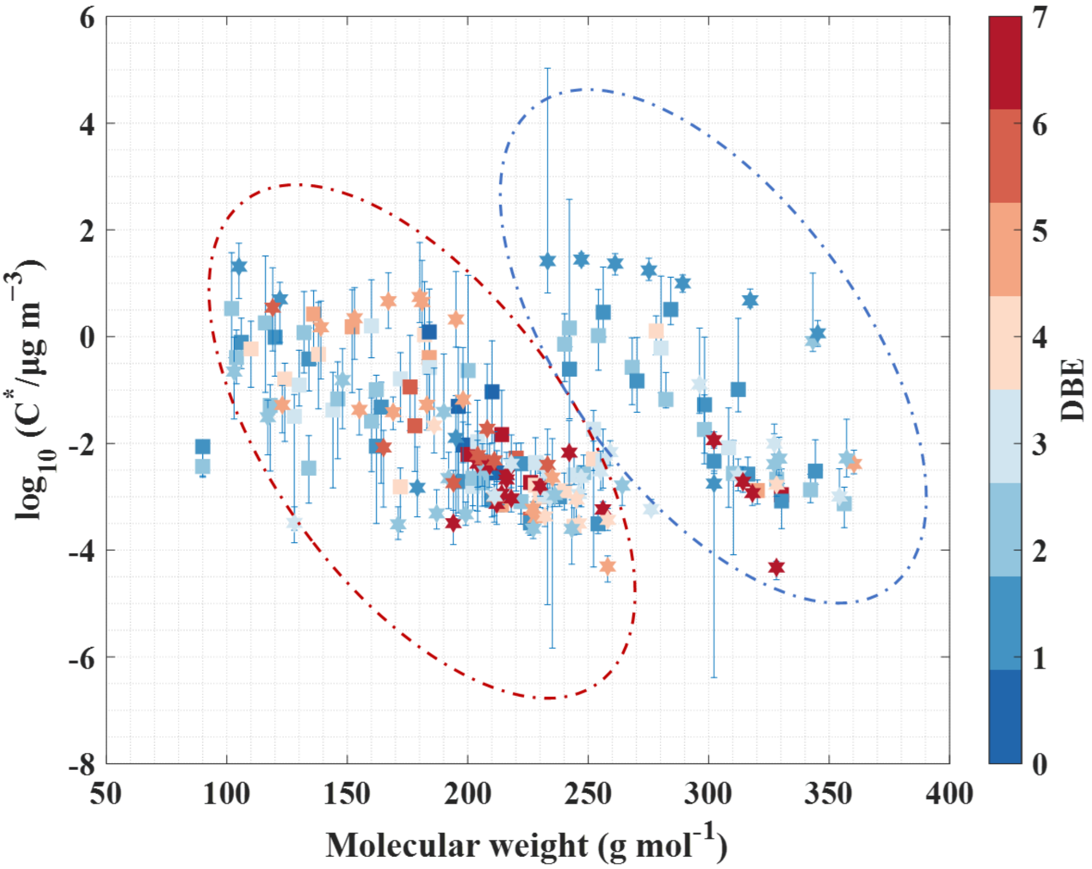


Figure S11. Saturation mass concentration of CHO and CHON compounds against their molecular weights, as color-coded by DBE. Note that compounds with DBE equal to or greater than 7 are marked with the same color. The CHO and CHON compounds are denoted by squares and hexagrams, respectively. Whiskers denote 25th and 75th percentile values of measured saturation mass concentration from 30 ambient samples and whiskers are ultimately due to variability in the measured T_{max} of CHO and CHON compounds.

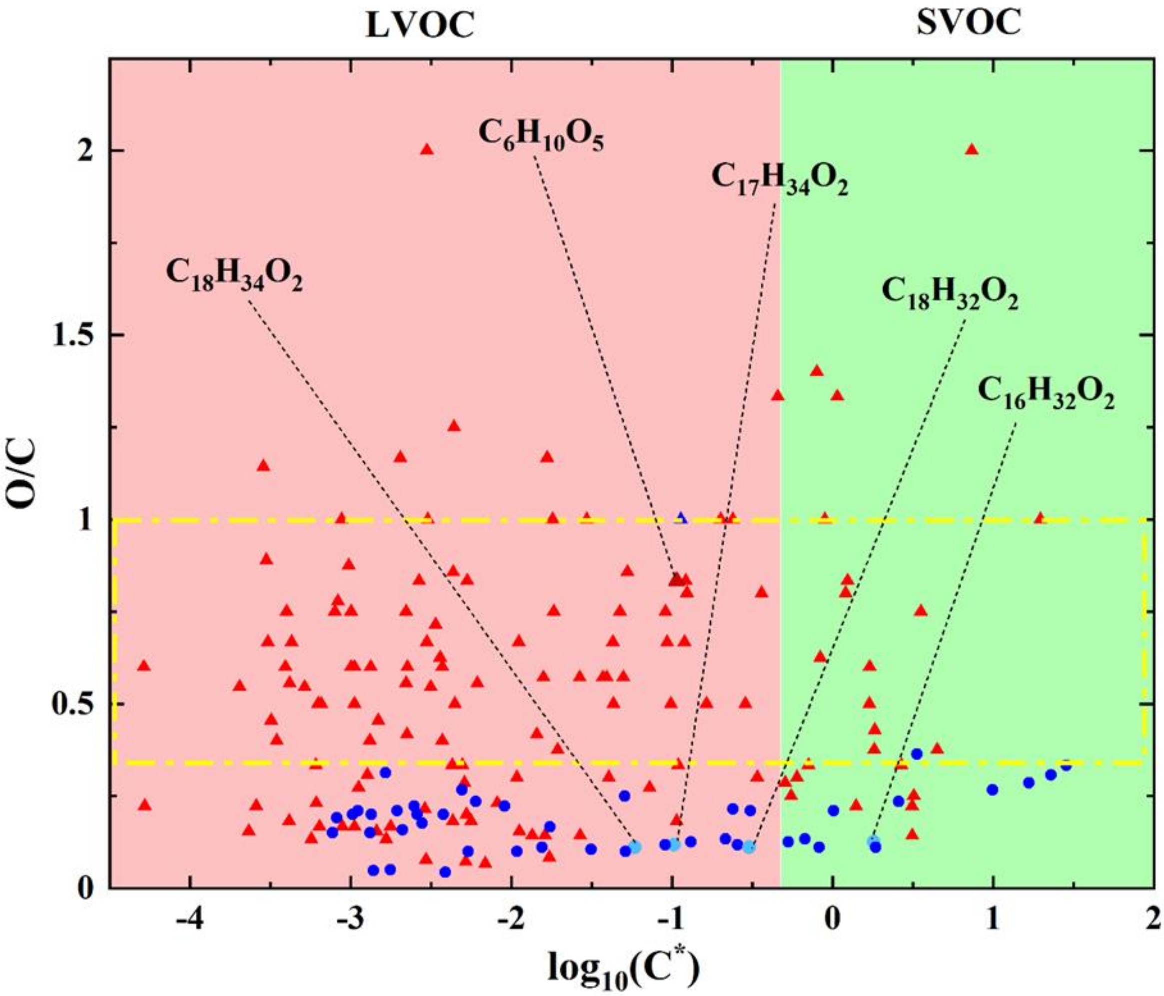


Figure S12. The volatility ($\log_{10}(C^{*})$) for 90 CHO and 91 CHNO species versus O/C ratios. Red triangles and blue circles denote the compounds in the dashed red and blue ellipses in Figure 4, respectively. Marked compounds are oleic acid ($C_{18}H_{34}O_2$), levoglucosan or related isomers ($C_6H_{10}O_5$), margaric acid ($C_{17}H_{34}O_2$), linoleic acid ($C_{18}H_{32}O_2$), and palmitic acid ($C_{16}H_{32}O_2$), respectively.

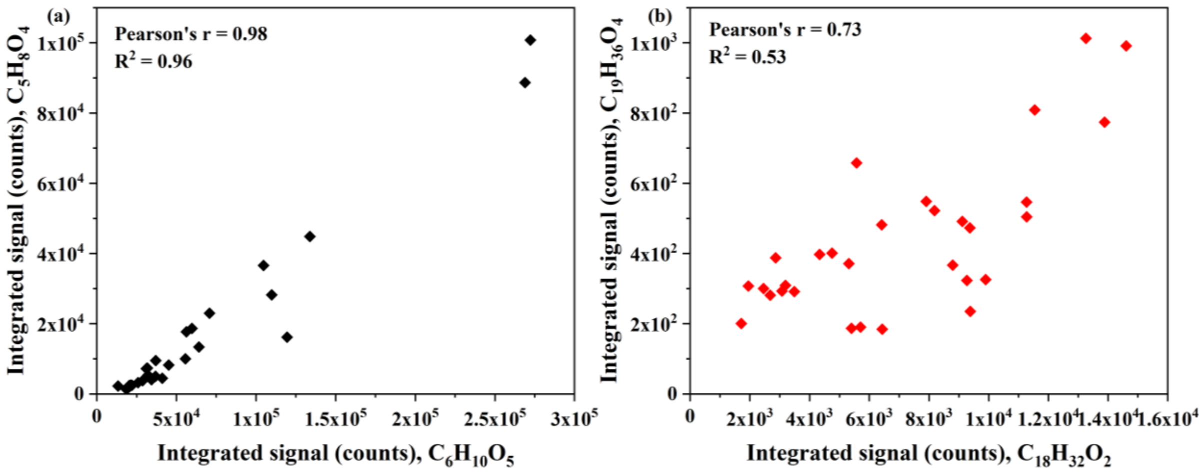


Figure S13. (a) An example of the correlation of $C_6H_{10}O_5$ and $C_5H_8O_4$ in the dashed red ellipse of Figure 4 in main text, **(b)** An example of the correlation of $C_{18}H_{32}O_2$ and $C_{19}H_{36}O_4$ in the dashed blue ellipse of Figure 4 in main text.

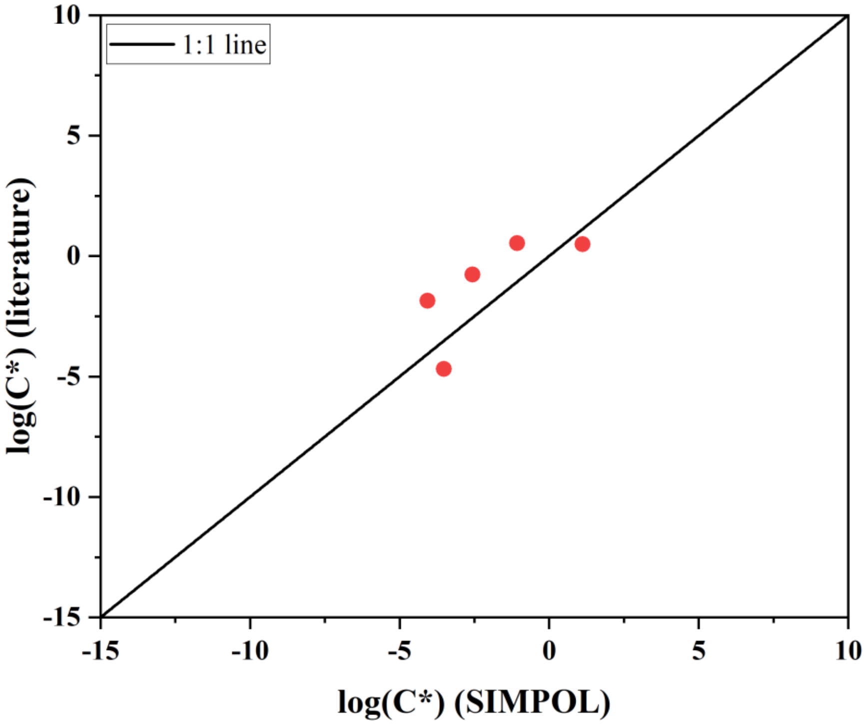


Figure S14. Saturation mass concentration (C^*) of five organic compounds (i.e., erythritol, PEG-6, PEG-7, PEG-8, and citric acid) from Krieger et al. (2018), Emanuelsson et al. (2016), and Ye et al. (2019) against those calculated by SIMPOL.

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