



Supplement of

Measurement report: Collocated speciation and potential mechanisms of gaseous adsorption for integrated filter-based sampling and analysis of water-soluble organic molecular markers in the atmosphere

Wei Feng et al.

Correspondence to: Mingjie Xie (mingjie.xie@nuist.edu.cn, mingjie.xie@colorado.edu)

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Table S1. Summaries of sampling date, meteorological conditions, and treatment types of Q_{bb} in Sampler I and II.

Date	Temperature (°C) ^a	Relative humidity (%) ^b	Sampler I	Sampler II
2021/8/4 N ^c	28.0	81	KOH	No treatment
2021/8/5 D ^d	31.5	67	KOH	No treatment
2021/8/5 N	28.4	80	(NH ₄) ₂ SO ₄	No treatment
2021/8/6 D	32.0	63	(NH ₄) ₂ SO ₄	No treatment
2021/8/6 N	28.0	88	KOH	No treatment
2021/8/7 D	31.4	61	KOH	No treatment
2021/8/8 N	25.8	89	(NH ₄) ₂ SO ₄	No treatment
2021/8/9 D	29.5	74	(NH ₄) ₂ SO ₄	No treatment
2021/8/17 N	24.2	98	KOH	No treatment
2021/8/18 D	29.5	71	KOH	No treatment
2021/9/5 N	23.5	89	(NH ₄) ₂ SO ₄	No treatment
2021/9/6 D	25.6	79	(NH ₄) ₂ SO ₄	No treatment
2021/9/6 N	23.4	88	KOH	No treatment
2021/9/7 D	25.1	78	KOH	No treatment
2021/9/7 N	22.2	93	(NH ₄) ₂ SO ₄	No treatment
2021/9/8 D	27.8	67	(NH ₄) ₂ SO ₄	No treatment
2021/9/9 N	24.9	94	KOH	No treatment
2021/9/10 D	31.9	52	KOH	No treatment
2021/9/10 N	24.8	94	(NH ₄) ₂ SO ₄	No treatment
2021/9/11 D	30.9	64	(NH ₄) ₂ SO ₄	No treatment
2021/9/21 N	22.7	89	KOH	No treatment
2021/9/22 D	30.5	56	KOH	No treatment
2021/9/22 N	21.8	91	(NH ₄) ₂ SO ₄	No treatment
2021/9/23 D	32.1	37	(NH ₄) ₂ SO ₄	No treatment

^a Mean temperature during each sampling interval; ^b mean relative humidity (RH, %) during each sampling interval; ^c night; ^d day.

Table S2. Mean concentration of bulk components in collocated Q_f , Q_b and Q_{bb} samples ($\mu\text{g m}^{-3}$).

Species	Q_f		Q_b		Q_{bb}^a
	Sampler I	Sampler II	Sampler I	Sampler II	Sampler II
Total sample ($N=24$)					
NH_4^+	1.74 ± 1.25^b	1.93 ± 1.46	0.030 ± 0.027	0.022 ± 0.021	0.019 ± 0.013
NO_3^-	3.12 ± 2.78	3.32 ± 3.04	0.67 ± 0.70	0.51 ± 0.60	0.30 ± 0.37
SO_4^{2-}	5.73 ± 1.91	5.90 ± 2.12	0.17 ± 0.18	0.099 ± 0.049	0.11 ± 0.065
Ca^{2+}	1.36 ± 0.84	1.55 ± 0.98	0.13 ± 0.12	0.095 ± 0.13	0.11 ± 0.14
Mg^{2+}	0.082 ± 0.046	0.094 ± 0.045	0.018 ± 0.012	0.016 ± 0.010	0.017 ± 0.019
K^+	0.28 ± 0.10	0.27 ± 0.11	/	/	/
OC	6.01 ± 2.22	6.49 ± 2.67	2.54 ± 6.40	0.35 ± 0.20	0.16 ± 0.13
EC	1.63 ± 0.59	1.78 ± 0.69	/	/	/
WSOC	3.39 ± 1.45	3.55 ± 1.46	1.63 ± 1.94	0.82 ± 0.70	0.32 ± 0.33
(NH_4)$_2\text{SO}_4$ treatment periods ($N=12$)					
NH_4^+	1.91 ± 1.09	2.02 ± 1.18	0.033 ± 0.026	0.024 ± 0.022	0.018 ± 0.012
NO_3^-	3.24 ± 1.85	3.41 ± 1.98	0.48 ± 0.65	0.51 ± 0.76	0.31 ± 0.42
SO_4^{2-}	6.05 ± 2.08	6.31 ± 2.24	0.13 ± 0.056	0.10 ± 0.040	0.098 ± 0.054
Ca^{2+}	1.50 ± 0.91	1.72 ± 1.02	0.16 ± 0.15	0.12 ± 0.20	0.20 ± 0.31
Mg^{2+}	0.10 ± 0.050	0.11 ± 0.050	0.022 ± 0.012	0.022 ± 0.0074	0.019 ± 0.022
OC	6.32 ± 2.16	6.79 ± 2.50	0.28 ± 0.14	0.34 ± 0.20	0.15 ± 0.12
EC	1.74 ± 0.55	1.89 ± 0.69	/	/	/
WSOC	3.17 ± 1.39	3.53 ± 1.51	1.02 ± 1.07	0.93 ± 0.88	0.43 ± 0.40
KOH treatment periods ($N=12$)					
NH_4^+	1.57 ± 1.43	1.84 ± 1.76	0.027 ± 0.029	0.019 ± 0.020	0.021 ± 0.012
NO_3^-	2.99 ± 3.57	3.23 ± 3.92	0.92 ± 0.73	0.52 ± 0.40	0.27 ± 0.25
SO_4^{2-}	5.42 ± 1.77	5.45 ± 2.00	0.34 ± 0.39	0.095 ± 0.058	0.11 ± 0.074
Ca^{2+}	1.18 ± 0.77	1.39 ± 0.95	0.11 ± 0.099	0.074 ± 0.058	0.17 ± 0.20
Mg^{2+}	0.063 ± 0.032	0.078 ± 0.035	0.010 ± 0.0085	0.013 ± 0.010	0.021 ± 0.022
OC	5.71 ± 2.32	6.18 ± 2.90	5.24 ± 8.99	0.35 ± 0.21	0.17 ± 0.14
EC	1.51 ± 0.63	1.66 ± 0.69	/	/	/
WSOC	3.62 ± 1.53	3.57 ± 1.48	2.19 ± 2.41	0.71 ± 0.48	0.23 ± 0.26

^a Q_{bb} samples in Sampler I were not analyzed, as the filters were treated with (NH_4) $_2\text{SO}_4$ or KOH; ^b mean $\pm$ standard deviation.

Figure S1

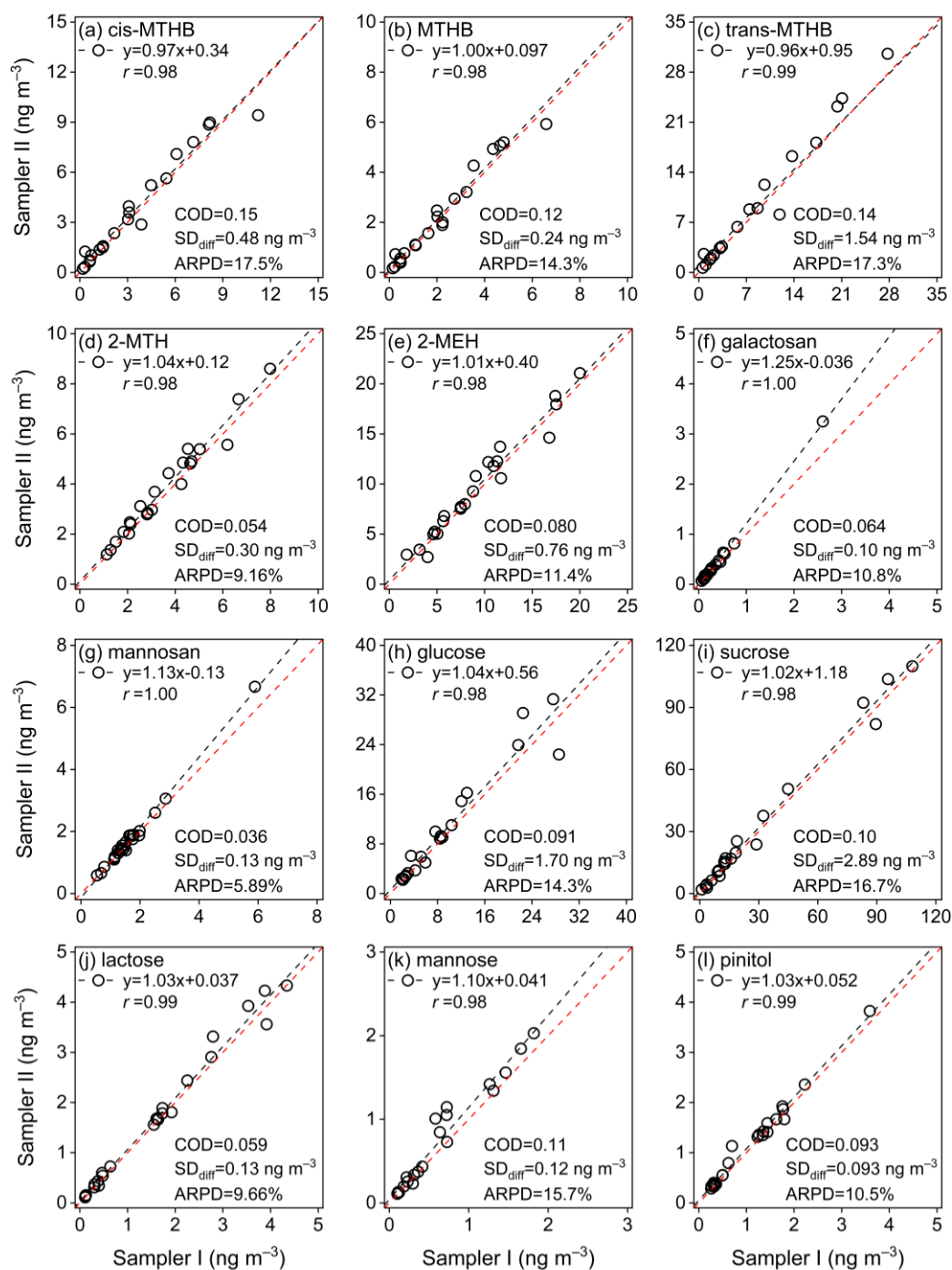


Figure S1. Comparisons between collocated Q_f samples for concentrations of individual WSOMMs (the red dashed line represents $y=x$).

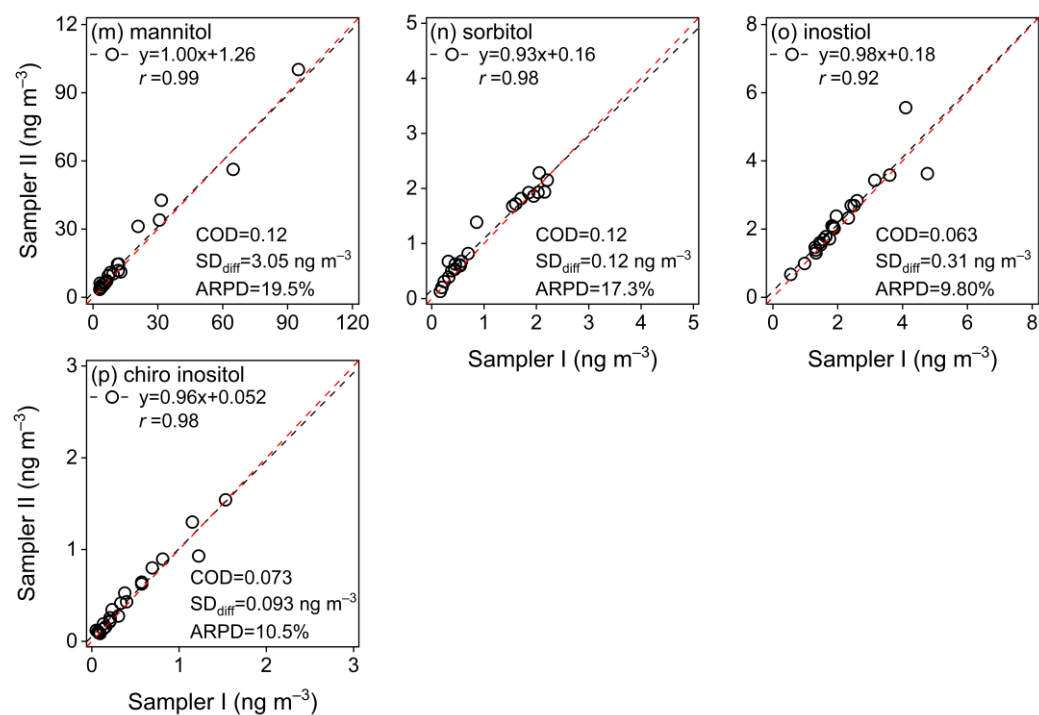


Figure S1. Continue.

Figure S2

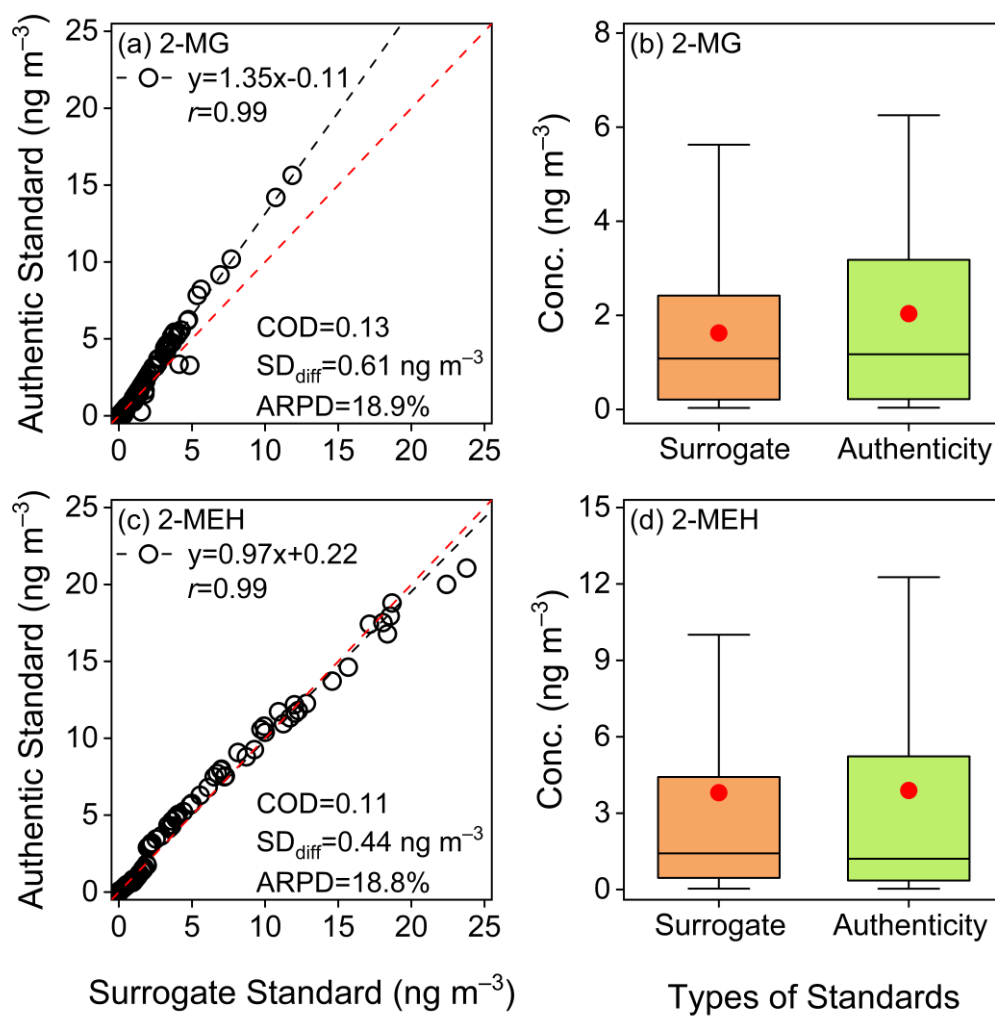


Figure S2. Comparisons of the concentrations of 2-MG and 2-MEH between quantification results using authentic standards and meso-erythritol (surrogate).

Figure S3

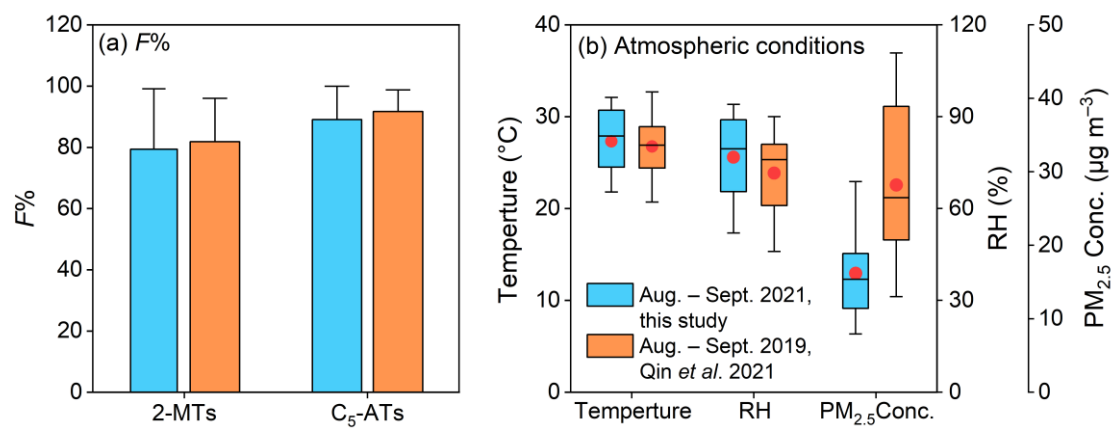


Figure S3. Comparisons of $F\%$ of 2-MTs and C₅-ATs and atmospheric conditions between this study and Qin et al. (2021).

Figure S4

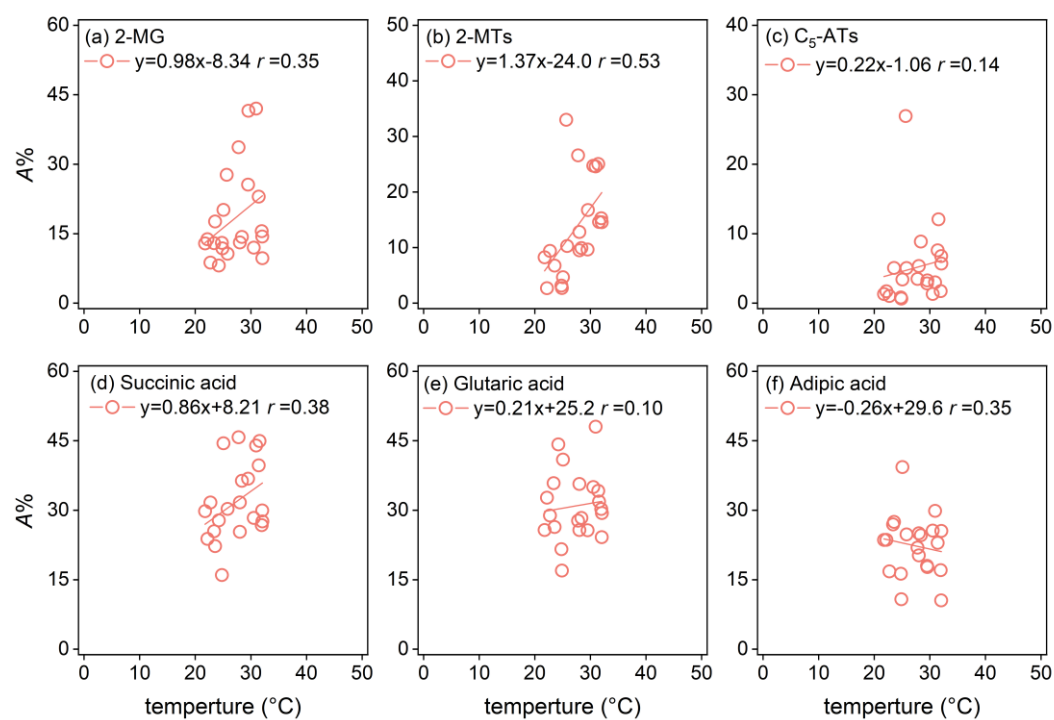


Figure S4. Linear regressions between A% of individual WSOMMs and temperature.

Figure S5

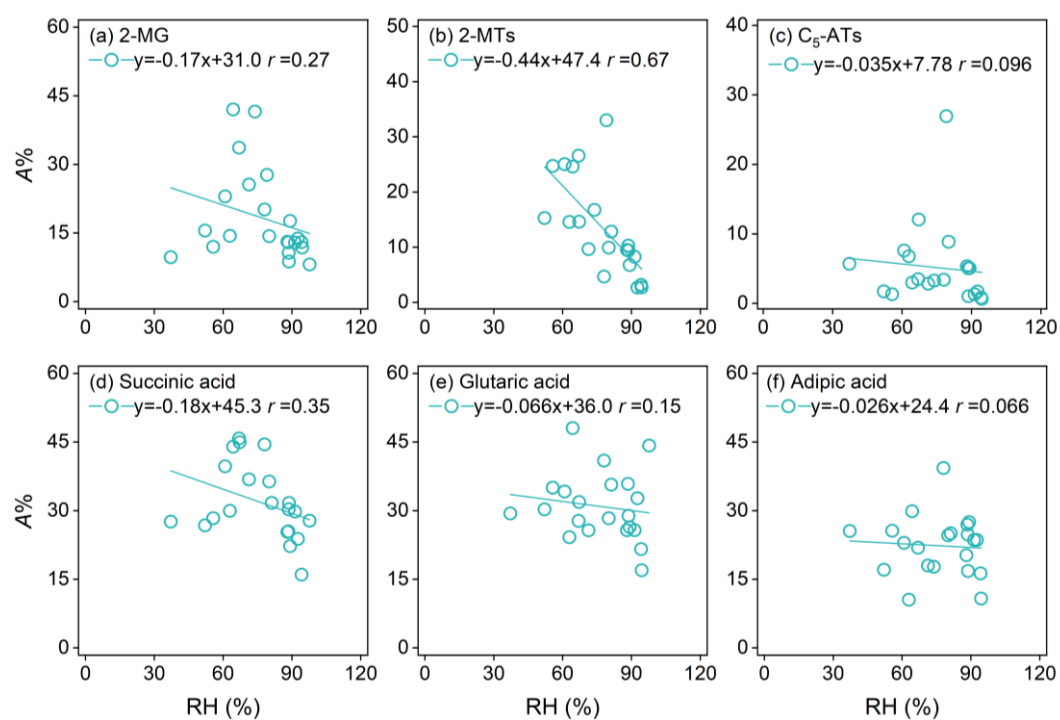


Figure S5. Linear regressions between A% of individual WSOMMs and relative humidity (RH, %).

Figure S6

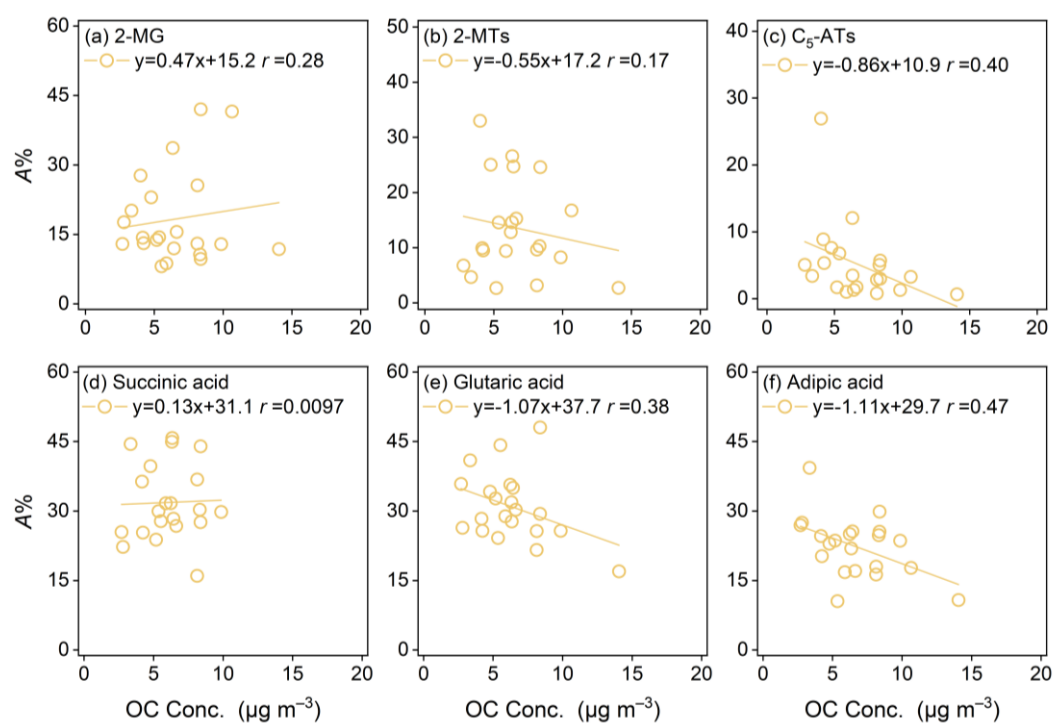


Figure S6. Linear regressions between A% of individual WSOMMs and OC concentrations.

Figure S7

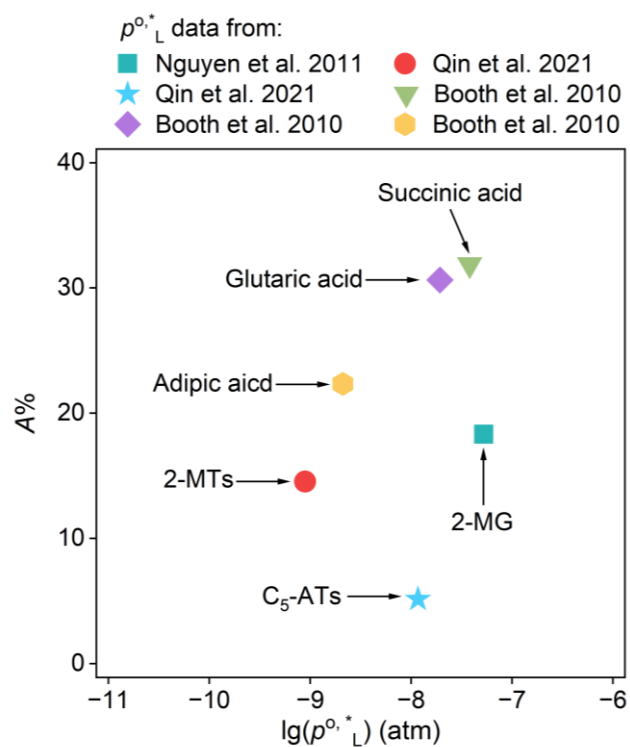


Figure S7. Changes in mean $A\%$ with the vapor pressure of individual WSOMMs. The $p^{0,*}_L$ data are obtained from Booth et al. (2010), Nguyen et al. (2011), and Qin et al. (2021).

Reference

- Booth, A., Barley, M., Topping, D., McFiggans, G., Garforth, A., and Percival, C.: Solid state and sub-cooled liquid vapour pressures of substituted dicarboxylic acids using Knudsen Effusion Mass Spectrometry (KEMS) and Differential Scanning Calorimetry, *Atmos. Chem. Phys.*, 10(10), 4879-4892, <https://doi.org/10.5194/acp-10-4879-2010>, 2010.
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- Qin, C., Gou, Y., Wang, Y., Mao, Y., Liao, H., Wang, Q. g., and Xie, M.: Gas–particle partitioning of polyol tracers at a suburban site in Nanjing, east China: increased partitioning to the particle phase, *Atmos. Chem. Phys.*, 21(15), 12141-12153, <https://doi.org/10.5194/acp-21-12141-2021>, 2021.