

## Supplement Information

# Advances in characterization of black carbon particles and their associated coatings using the soot particle aerosol mass spectrometer in Singapore, a complex city environment

Mutian Ma<sup>1\*</sup>, Laura-Hélène Rivellini<sup>2</sup>, Yichen Zong<sup>3,4</sup>, Markus Kraft<sup>4,5</sup>, Liya E. Yu<sup>1,2</sup>, Alex King Yin Lee<sup>6</sup>

<sup>1</sup>Department of Civil and Environmental Engineering, National University of Singapore, Singapore

<sup>2</sup>NUS Environmental Research Institute, National University of Singapore, Singapore

<sup>3</sup>Department of Mechanical Engineering, National University of Singapore, Singapore

<sup>4</sup>Cambridge Centre of Advance Research and Education in Singapore, Singapore

<sup>5</sup>Department of Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom'

<sup>6</sup>Air Quality Processes Research Section, Environment and Climate Change Canada, ON, Toronto, Canada

*\* now at Cambridge Centre of Advance Research and Education in Singapore, Singapore*

*Correspondence to: Alex King Yin, Lee (alex.lee@ec.gc.ca)*

Table S1. Detection limit for metal and metal ions.

<b>Metal/metal salt</b>	<b>Na<sup>+</sup></b>	<b>K<sup>+</sup></b>	<b>Rb<sup>+</sup></b>	<b>V<sup>+</sup></b>	<b>Ni<sup>+</sup></b>	<b>K<sub>3</sub>SO<sub>4</sub><sup>+</sup></b>
<b>Detection limit (Hz)</b>	7.33	40.36	0.52	0.50	0.35	0.23
<b>Campaign average (Hz)</b>	26.70	500.20	1.85	1.74	0.64	5.16

Table S2. The Org/rBC ratios for factors identified by PMF<sub>base-4</sub>, PMF<sub>metal-7</sub> and PMF<sub>all-8</sub>

	<b>PMF<sub>base-4</sub></b>	<b>PMF<sub>metal-7</sub></b>	<b>PMF<sub>all-8</sub></b>
<b>HOA</b>	6.6	11.3	13.9
<b>rBC-rich*</b>	0.1	0.1	0.1
<b>LO-OOA</b>	61.0	17.8	18.3
<b>MO-OOA</b>	6.8	9.4	7.4
<b>IOA*</b>	NA	0.2	0.2
<b>BBOA</b>	NA	2.8	3.7
<b>A-BBOA</b>	NA	2.8	6.9
<b>Night-IA- BBOA</b>	NA	NA	2.3

\*All CO<sup>+</sup>, CO<sub>2</sub><sup>+</sup> and C<sub>3</sub>O<sub>2</sub><sup>+</sup> signals are considered as rBC mass as rBC-rich and IOA are largely dominated by rBC mass.

Table S3. Mass spectra and time series correlations of PMF<sub>base-4</sub> factors against to those from PMF<sub>metal-4</sub> and PMF<sub>all-4</sub>.

PMF factors	Mass spectra correlations with PMF <sub>base-4</sub> ( $R_{m/z}$ )				Time series correlations ( $R_{ts}$ ) with PMF <sub>base-4</sub>			
	HOA	rBC-rich	LO-OOA	MO-OOA	HOA	rBC-rich	LO-OOA	MO-OOA
<b>HOA</b> <sub>metal-4</sub>	<b>1.00</b>	0.38	0.40	0.24	<b>0.96</b>	0.78	0.52	0.07
<b>rBC-rich</b> <sub>metal-4</sub>	0.41	<b>1.00</b>	0.44	0.77	0.78	<b>0.94</b>	0.45	0.04
<b>LO-OOA</b> <sub>metal-4</sub>	0.34	0.54	<b>0.98</b>	0.89	0.42	0.38	<b>0.97</b>	0.70
<b>MO-OOA</b> <sub>metal-4</sub>	0.25	0.80	0.75	<b>1.00</b>	0.03	0.00	0.47	<b>0.97</b>
<b>HOA</b> <sub>all-4</sub>	<b>1.00</b>	0.44	0.41	0.28	<b>1.00</b>	0.79	0.52	0.07
<b>rBC-rich</b> <sub>all-4</sub>	0.43	<b>1.00</b>	0.46	0.78	0.71	<b>0.98</b>	0.37	0.01
<b>LO-OOA</b> <sub>all-4</sub>	0.35	0.56	<b>0.98</b>	0.89	0.45	0.41	<b>0.99</b>	0.66
<b>MO-OOA</b> <sub>all-4</sub>	0.25	0.79	0.77	<b>1.00</b>	0.03	-0.01	0.48	<b>0.98</b>

Table S4. Mass spectra and time series correlations of PMF<sub>metal-7</sub> factors against to those from PMF<sub>metal-4</sub>.

Mass spectra correlations ( $R_{m/z}$ )								
PMF solution		HOA	rBC-rich	LO-OOA	MO-OOA	IOA	A-BBOA	BBOA
HOA	Slope	1.06	0.84	0.48	0.31	0.79	0.47	0.54
	R	<b>0.99</b>	0.35	0.50	0.24	0.48	0.28	0.50
rBC-rich	Slope	0.14	1.05	0.09	0.17	0.71	0.30	0.37
	R	0.24	<b>1.00</b>	0.17	0.34	0.98	0.42	0.80
LO-OOA	Slope	0.50	0.80	0.93	1.08	0.68	0.69	0.67
	R	0.34	0.29	<b>0.94</b>	0.94	0.35	0.37	0.55
MO-OOA	Slope	0.35	1.23	0.56	0.86	0.91	1.24	0.88
	R	0.25	0.54	0.60	<b>0.84</b>	0.57	0.83	0.88
Time series correlations ( $R_{ts}$ )								
PMF solution		HOA	rBC-rich	LO-OOA	MO-OOA	IOA	A-BBOA	BBOA
HOA	Slope	0.46	0.63	0.23	0.21	0.22	0.07	0.14
	R	<b>0.99</b>	0.71	0.58	0.10	0.68	0.05	0.27
rBC-rich	Slope	0.27	0.50	0.15	0.15	0.13	0.05	0.10
	R	0.77	<b>0.97</b>	0.49	0.07	0.61	0.03	0.23
LO-OOA	Slope	0.31	0.48	0.32	0.51	0.16	0.12	0.22
	R	0.40	0.32	<b>0.92</b>	0.78	0.36	0.48	0.61
MO-OOA	Slope	0.14	0.25	0.14	0.49	0.07	0.14	0.21
	R	0.01	-0.03	0.30	<b>0.94</b>	0.06	0.92	0.80

Table S5. Mass spectra and time series correlations of PMF<sub>all-8</sub> factors against to those from PMF<sub>all-4</sub>.

Mass spectra correlations ( $R_{m/z}$ )									
PMF solution		HOA	rBC-rich	LO-OOA	MO-OOA	IOA	A-BBOA	BBOA	Night-IA-BBOA
HOA	Slope	1.04	0.43	0.40	0.29	0.47	0.29	0.43	0.35
	R	<b>0.97</b>	0.16	0.42	0.24	0.26	0.13	0.38	0.24
rBC-rich	Slope	0.36	1.45	0.34	0.52	1.08	0.68	0.72	0.61
	R	0.35	<b>0.75</b>	0.43	0.62	0.79	0.48	0.85	0.60
LO-OOA	Slope	0.49	0.44	0.93	0.98	0.43	0.49	0.56	0.58
	R	0.33	0.13	<b>0.96</b>	0.88	0.18	0.22	0.43	0.38
MO-OOA	Slope	0.31	0.44	0.65	0.91	0.42	1.08	0.70	0.61
	R	0.19	0.15	0.69	<b>0.88</b>	0.20	0.61	0.62	0.44
Time series correlations ( $R_{ts}$ )									
PMF solution		HOA	rBC-rich	LO-OOA	MO-OOA	IOA	A-BBOA	BBOA	Night-IA-BBOA
HOA	Slope	0.41	0.50	0.22	0.17	0.21	0.03	0.11	0.10
	R	<b>0.99</b>	0.69	0.58	0.06	0.68	0.06	0.28	0.09
rBC-rich	Slope	0.29	0.50	0.17	0.15	0.15	0.04	0.10	0.10
	R	0.70	<b>0.96</b>	0.43	0.01	0.53	0.06	0.23	0.10
LO-OOA	Slope	0.29	0.40	0.33	0.44	0.16	0.06	0.19	0.11
	R	0.43	0.32	<b>0.94</b>	0.68	0.36	0.44	0.67	0.21
MO-OOA	Slope	0.12	0.20	0.14	0.49	0.07	0.08	0.19	0.10
	R	-0.01	-0.04	0.28	<b>0.96</b>	0.07	0.88	0.86	0.26

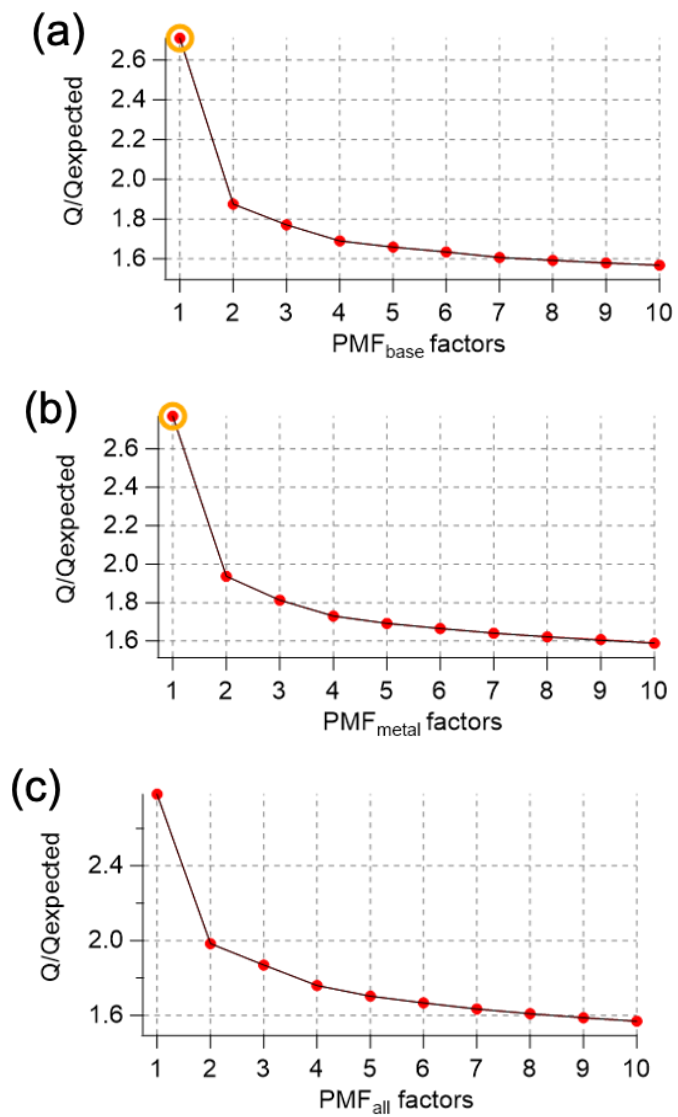


Figure S1.  $Q/Q_{\text{expected}}$  plots for different PMF scenarios up to 10-factor solution.

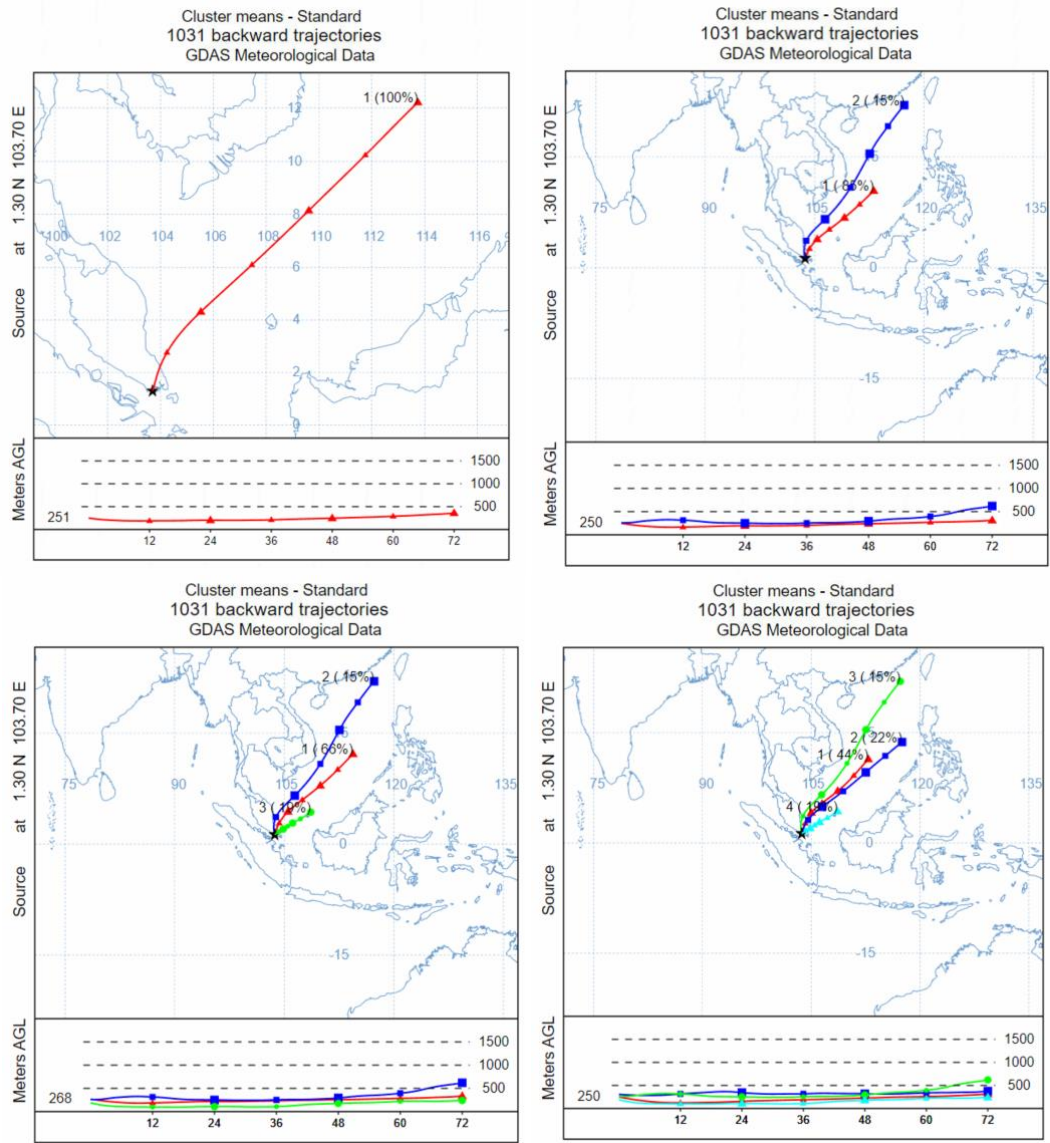


Figure S2. Results of cluster analysis (from 1 to 4 clusters) of 72-hours air mass back trajectory.

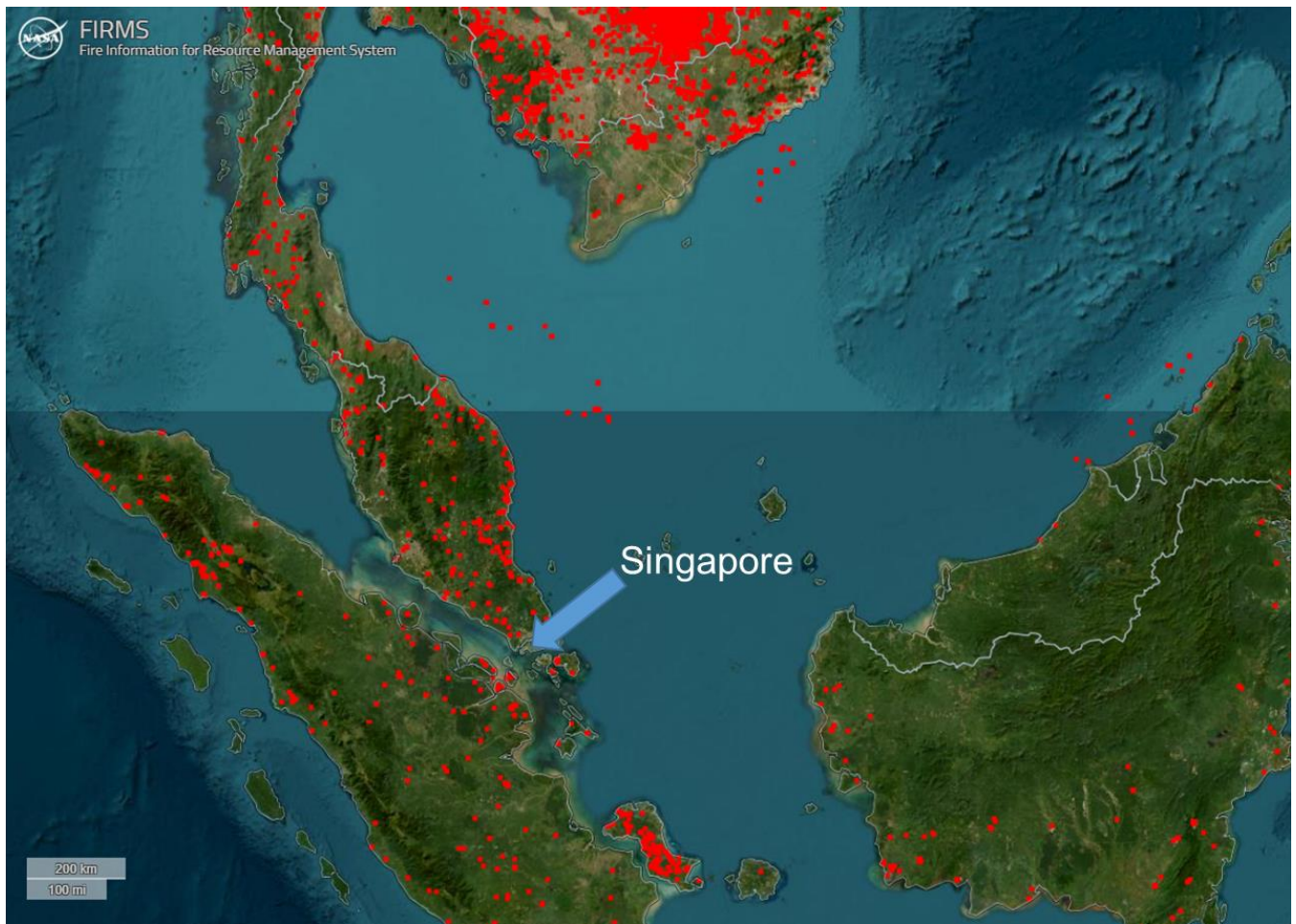


Figure S3. Regional fire counts from 2022/01/22-2022/01/29 (red dots in the map, <https://firms.modaps.eosdis.nasa.gov/map/>).



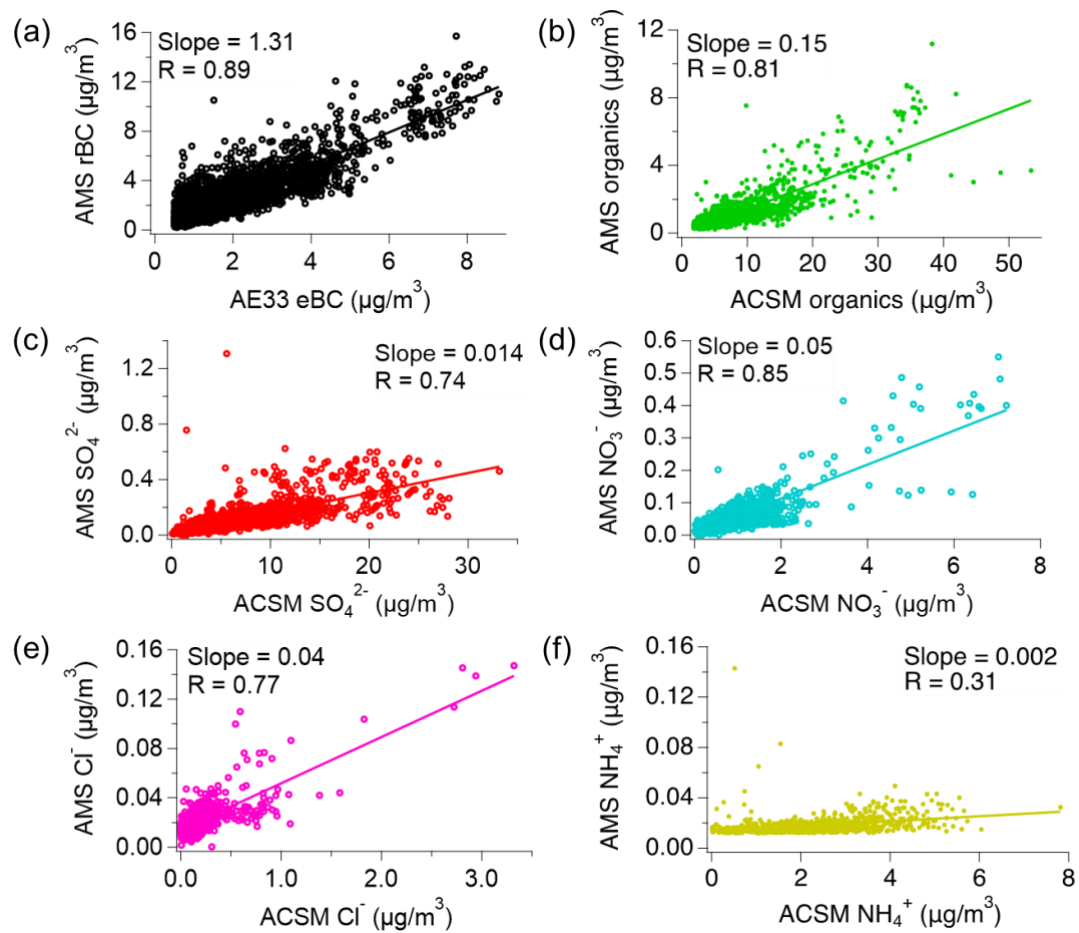


Figure S4. Time series correlation between bulk SP-AMS measurements against aethalometer (a) and ToF-ACSM (b-f) measurements.

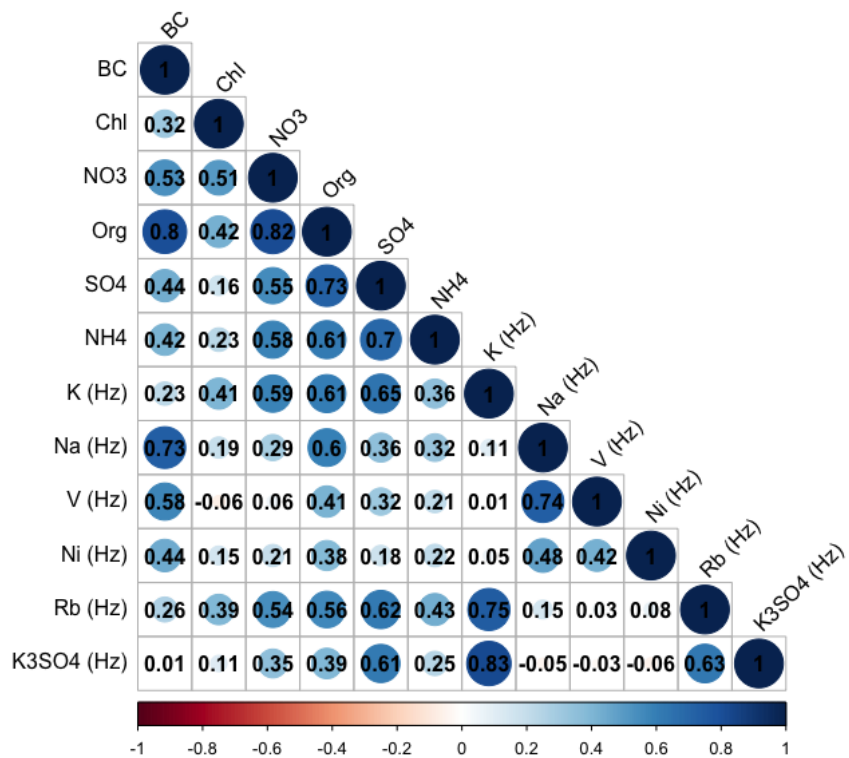


Figure S5. Time series correlation coefficients between major species measured by SP-AMS. Pearson correlation (R) values are shown in corresponding cells. The R values are also shown by the size and color of the circle in the cells.

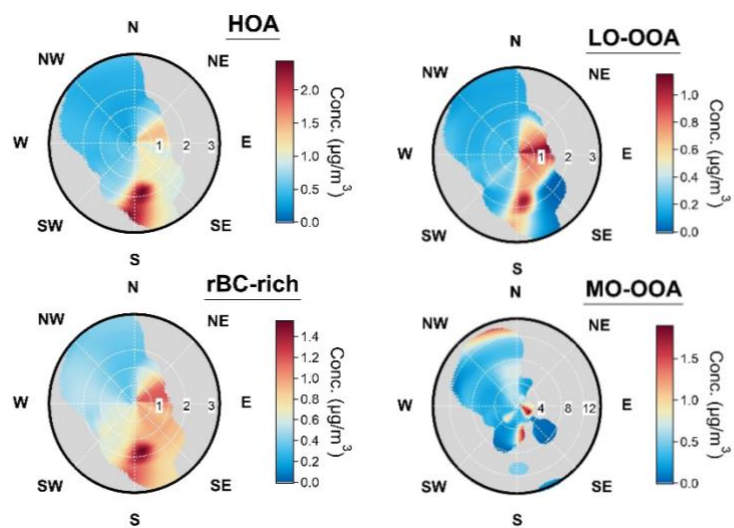


Figure S6. The NWR plots of factors identified by PMF<sub>base-4</sub>.

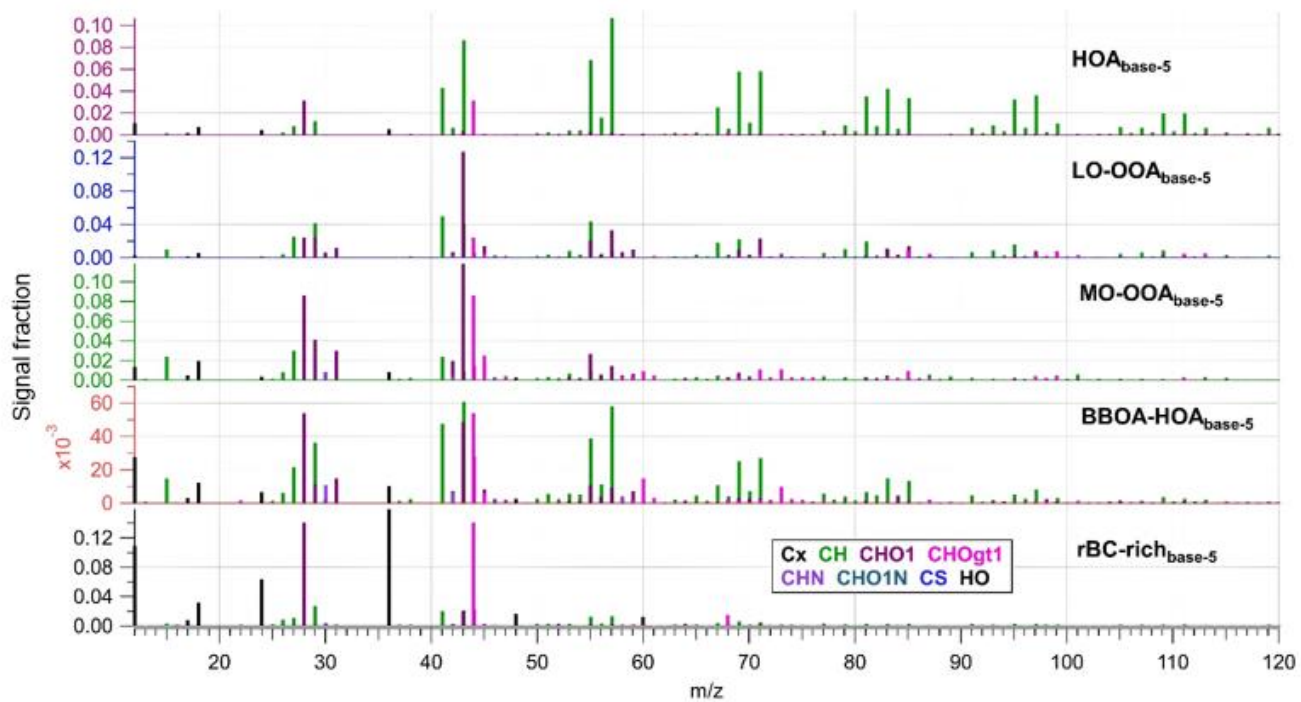


Figure S7. Summary of the 5-factor solutions of PMF<sub>base-5</sub>.

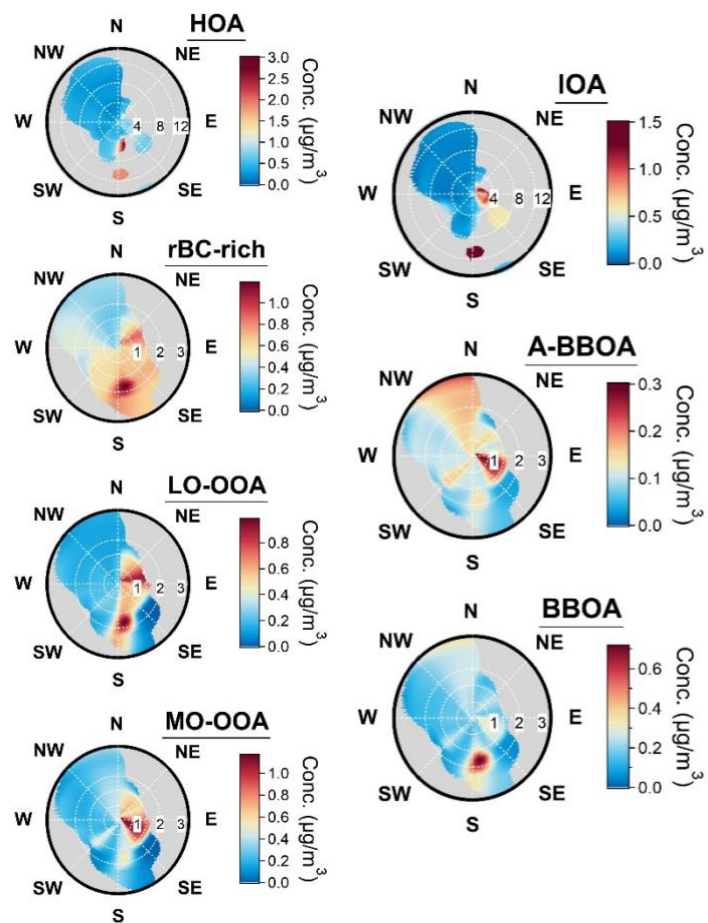


Figure S8. The NWR plots of factors identified by PMF<sub>metal-7</sub>.

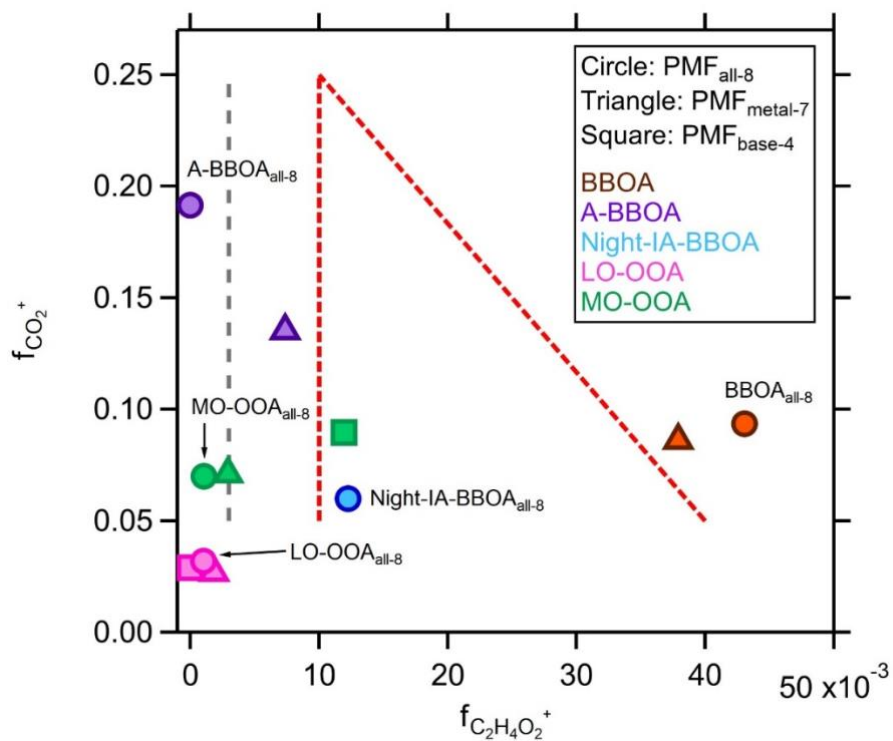


Figure S9. The  $f_{CO_2^+}$  vs.  $f_{C_2H_4O_2^+}$  plot for evaluating OOA and biomass burning-related OA factors derived from different PMF scenarios. Correction factor was not applied for  $f_{C_2H_4O_2^+}$  in this plot. Grey dashed line represents background level (0.3%) of  $f_{C_2H_4O_2^+}$  for OA without significant biomass burning signature reported by Cubison et al. (2011). Red dashed lines represent the boundaries of triangular region that cover BBOA observed by Cubison et al. (2011).

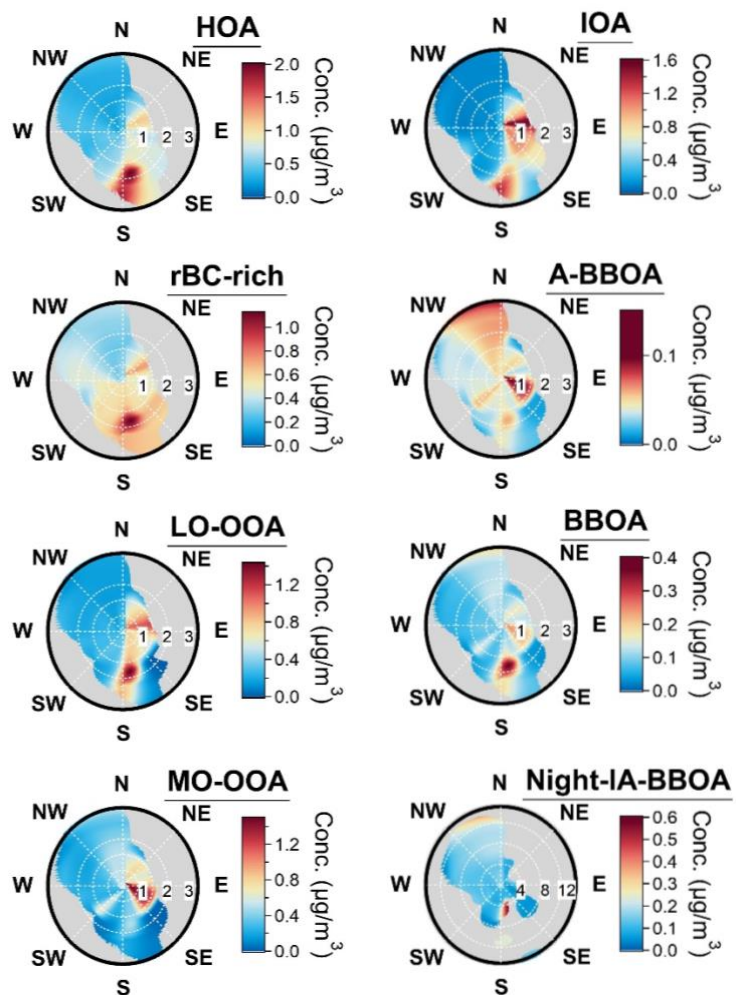


Figure S10. The NWR plots of factors identified by PMF<sub>all-8</sub>.