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Chemical composition, sources, and processes of urban aerosols during summertime in northwest China: insights from high-resolution aerosol mass spectrometry

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1 Table S1. Overview of the studies using Aerodyne AMS in China. The list is based on the sampling date.

Sampling Site	Location	Sampling period	Instrument	Mass Loading (μg m^{-3})	PM_1 Composition	Organic Components	Elemental Ratio	References
Lanzhou (Urban site)	36.1N, 103.9E	Jul. 12–Aug. 7, 2012	HR-ToF-AMS	24.5	Organics (47%), Sulfate (16%), Nitrate (10%), Ammonium (11%), Chloride (4%), BC (12%)	HOA (16%), COA (24%), SV-OOA (27%), LV-OOA (32%)	HOA (O/C: 0.10, H/C: 1.84, N/C: 0.015, OM/OC: 1.31) COA (O/C: 0.10, H/C: 1.69, N/C: 0.001, OM/OC: 1.28) SV-OOA (O/C: 0.28, H/C: 1.34, N/C: 0.015, OM/OC: 1.78) LV-OOA (O/C: 0.68, H/C: 1.30, N/C: 0.016, OM/OC: 2.03)	This study
Beijing (Urban site)		Jul. 9–21, 2006	Q-AMS	80±40.6	Organics (35%), Sulfate (25%), Nitrate (22%), Ammonium (16%), Chloride (1.4%)	HOA (40%), SV-OOA (20%), LV-OOA (40%)		(Sun et al., 2010)
Back-Garden (Urban downwind site)	113.03E, 23.49N	Jul. 12–30, 2006	Q-AMS	30.0	Organics (44%), Sulfate (38%), Nitrate (5%), Ammonium (12%), Chloride	HOA (34%), SV-OOA (28%), LV-OOA (38%)		(Xiao et al., 2011)

					(1%)			
Beijing (Urban downwind site)	39.5N, 116.3E	Aug. 15–Sep. 10, 2006	Q-AMS	~2–100				(Takegawa et al., 2009)
Beijing (Urban site)	116.33E, 39.99N	Jun. 5–Sep. 22, 2008	Q-AMS					(Zhang et al., 2011)
Beijing (Urban site)		Jul. 24–Sept. 20, 2008	HR-ToF-AMS	63.1 (2.47–356)	Organics (37.9%), Sulfate (26.7%), Ammonium (15.9%), Nitrate (15.8%), BC (3.1%), Chloride (0.87%).	HOA (18.1%), COA (24.4%), SV-OOA (23.7%), LV-OOA (33.7%)	HOA (O/C: 0.17, H/C: 1.58, N/C: 0.02, OM/OC: 1.38) COA (O/C: 0.11, H/C: 1.73, N/C: 0.012, OM/OC: 1.30) SV_OOA (O/C: 0.47, H/C: 1.33, N/C: 0.033, OM/OC: 1.78) LV_OOA (O/C: 0.48, H/C: 1.38, N/C: 0.011, OM/OC: 1.78)	(Huang et al., 2010)
Kaiping (Urban downwind site)	113.9E, 22.6N	Oct. 12–Nov. 18, 2008	HR-ToF-AMS	33.1 (2.4–150)	Organics (34%), Sulfate (34%), Ammonium (14%), Nitrate (10.7%), Chloride (1.1%), BC (6.7).	BBOA (24.5%), SV-OOA (35.8%), LV-OOA (39.6%)	BBOA (O/C: 0.26, H/C: 1.62, N/C: 0.06, OM/OC: 1.55) SV-OOA (O/C: 0.39, H/C: 1.48, N/C: 0.01, OM/OC: 1.65) LV-OOA (O/C: 0.64, H/C: 1.30, N/C: 0.02, OM/OC: 1.99)	(Huang et al., 2011)
Shenzhen (Urban site)		Oct. 25–Dec. 2, 2009	HR-ToF-AMS	44.5 ±34.0 (3.0–219)	Organics (39.7%), Sulfate	HOA (29.5%) BBOA	HOA (O/C: 0.11, H/C: 1.70, N/C: 0.01, OM/OC: 1.3) BBOA (O/C: 0.32, H/C:	(He et al., 2011)

					(24.5%), Ammonium (10.2%), Nitrate (10.0%), Chloride (1.6%), BC (14%).	(24.1%) SV-OOA (27.6%) LV-OOA (18.8%)	1.47, N/C: 0.06, OM/OC: 1.62) SV-OOA (O/C: 0.45, H/C: 1.45, N/C: 0.02, OM/OC: 1.75) LV-OOA (O/C: 0.59, H/C: 1.26, N/C: 0.03, OM/OC: 1.92)	
Shanghai (Urban site)	121.90E, 31.38N	May 15–Jun. 10, 2010	HR-ToF-AMS	29.2 (5.5–155)	Organics (28.7%), Sulfate (33.3%), Nitrate (16.3%), Ammonium (13.4%), Chloride (1.6%), BC (6.7%)	HOA (24%), SV-OOA (46.8%), LV-OOA (29.2%).	HOA (O/C: 0.16, H/C: 1.77, N/C: 0.01, OM/OC: 1.38) SV-OOA (O/C: 0.35, H/C:1.48, N/C: 0.02, OM/OC: 1.61) LV-OOA (O/C: 0.65, H/C: 1.49, N/C: 0.02, OM/OC: 2.02)	(Huang et al., 2012)
Jiaxing (Urban downwind site)	120.8E, 30.8N	Jun. 29–Jul. 15, 2010	HR-ToF-AMS	32.9 (4.6–104)	Organics (32.1%), Sulfate (25.2%), Nitrate (18.0%), Ammonium (12.6%), Chloride (3%), BC (9.1%)	HOA (31.7%) OOA (68.3%)	HOA (O/C: 0.13, H/C: 1.77, N/C: 0.01, OM/OC: 1.38) OOA (O/C: 0.41, H/C: 1.47, N/C: 0.02, OM/OC: 1.70)	(Huang et al., 2013)
Jiaxing (Urban downwind site)	120.8E, 30.8N	Dec. 11–23, 2010	HR-ToF-AMS	41.9 (5.8–160)	Organics (30.3%), Sulfate (17.0%),	HOA (39.7%), BBOA (30.1%),	HOA (O/C: 0.11, H/C: 1.85, N/C: 0.02, OM/OC: 1.32) BBOA (O/C: 0.27, H/C: 1.51, N/C: 0.03, OM/OC:	(Huang et al., 2013)

					Nitrate (17.8%), Ammonium (11.6%), Chloride (6.5%), BC (16.9%)	OOA (30.2%),	1.93) OOA (O/C: 0.59, H/C: 1.29, N/C: 0.03, OM/OC: 1.93)	
Changdao (Urban downwind site)	37.99N, 120.70E	Mar. 21–Apr. 24, 2011	HR-ToF-AMS	47±36	Organics (30%), Sulfate (19%), Nitrate (28%), Ammonium (14.7%), Chloride (3.0%), BC (5.6%)	HOA (23%), SV-OOA (24%), LV-OOA (44%), CCOA (9%)	HOA (O/C: 0.34, H/C: 1.52, , N/C: 0.01, OM/OC: 1.56) CCOA (O/C: 0.17 H/C: 1.40, , N/C: 0.016, OM/OC: 1.37) SV-OOA (O/C: 0.62, H/C: 1.33, N/C: 0.041, OM/OC: 1.99) LV-OOA (O/C: 0.78, H/C: 1.27, N/C: 0.016, OM/OC: 2.17)	(Hu et al., 2013)
Hongkong (Urban downwind site)	22.3N, 114.3E	Apr. 26–Jun. 1, 2011	HR-ToF-AMS	14.5±9.7	Organics (28.2%), Sulfate (51.0%), Nitrate (4.1%), Ammonium (16.4%), Chloride (0.3%)	HOA (23.2), SV-OOA (22.6%), LV-OOA (54.2%)	HOA (O/C: 0.15, H/C: 1.71, N/C: 0.006, OM/OC: 1.36) SV-OOA (O/C: 0.16, H/C: 1.59, N/C: 0.009, OM/OC: 1.36 LV-OOA (O/C: 0.80, H/C: 1.21, N/C: 0.018, OM/OC: 2.20)	(Lee et al., 2013)
Beijing (Urban site)	39.98N, 116.37E	Jun. 26–Aug. 28, 2011	ACSM	50 (±30)	Organics (40%), Sulfate (18%), Nitrate	HOA (36%) OOA (64%)		(Sun et al., 2012)

					(25%), Ammonium (16%), Chloride (1%)			
Beijing (Urban site)	39.98N, 116.37E	Nov. 21– Jan. 20, 2011/2012	ACSM	66.8 ±55	Organics (52%), Sulfate (14%), Nitrate (16%), Ammonium (13%), Chloride (5%)	HOA (17%) COA (19%) CCOA (33%) OOA (31%)		(Sun et al., 2013)

Table S2 Comparison between the detection limits (DLs) of HR-ToF-AMS measurements in different studies

Avg. time	**Organics**	**Sulfate**	**Nitrate**	**Ammonium**	**Chloride**	**References**
min	**(μg m^{-3})**					
2.5	0.066	0.008	0.0054	0.008	0.013	This study
1	0.022	0.0052	0.0029	0.038	0.012	(DeCarlo et al., 2006)
5	0.057	0.005	0.004	0.023	0.005	(Sun et al., 2011)
2.5	0.075	0.011	0.018	0.01	0.017	(Setyan et al., 2012)
5	0.06	0.011	0.008	0.03	0.012	(Ge et al., 2012)

Figures

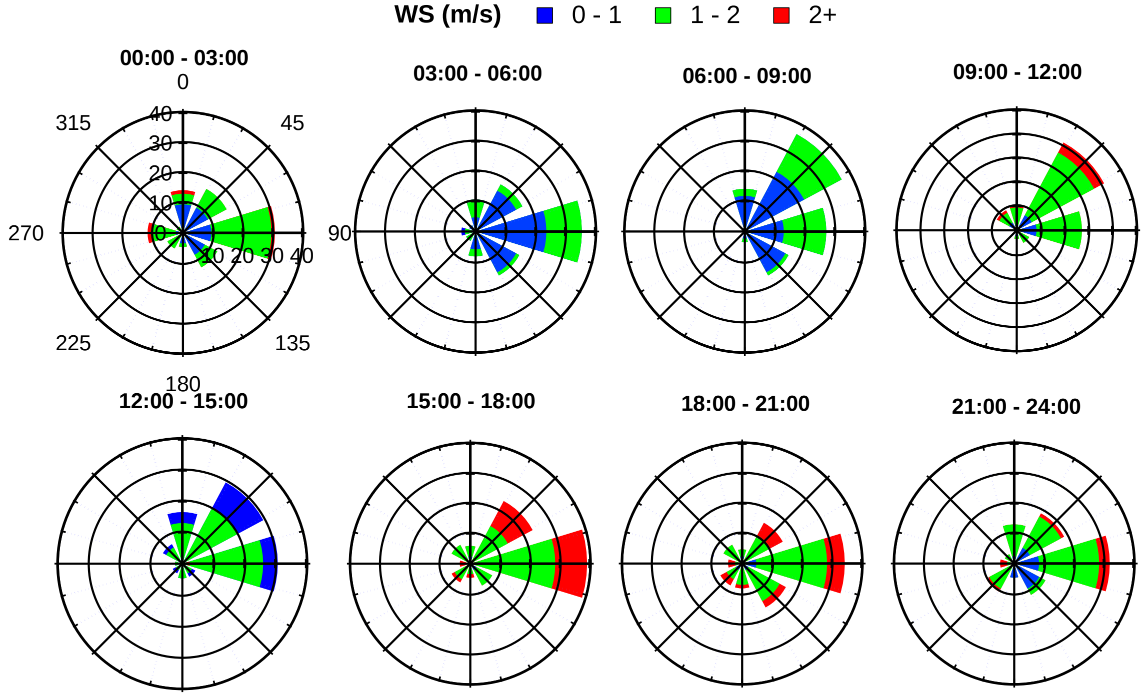


Fig. S1. 3-hour internal wind rose plot in Lanzhou during summer 2012.

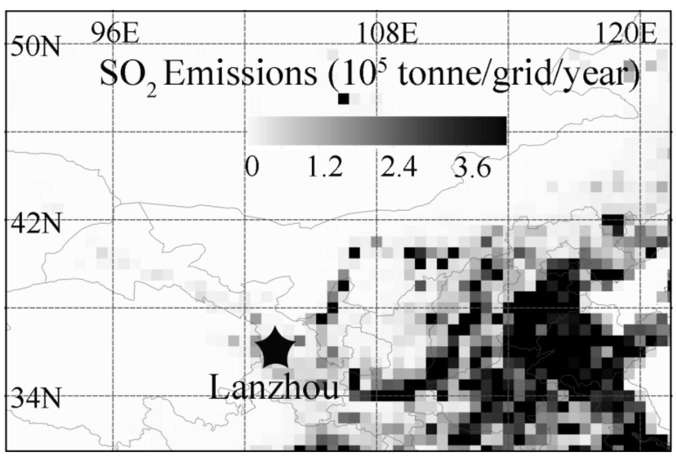


Fig. S2. The estimated anthropogenic SO2 emissions in 2006 for part of China (Zhang et al., 2009)

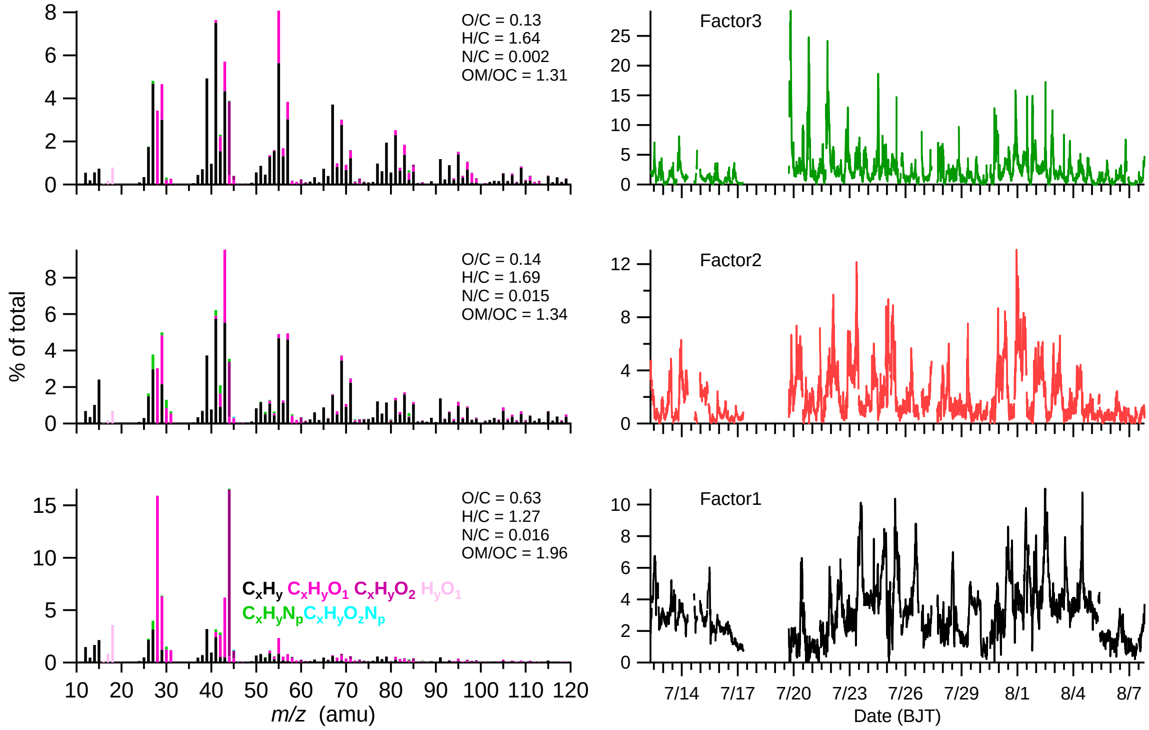


Fig. S3. 3-factor solution performed by PMF on organic high resolution mass spectra.

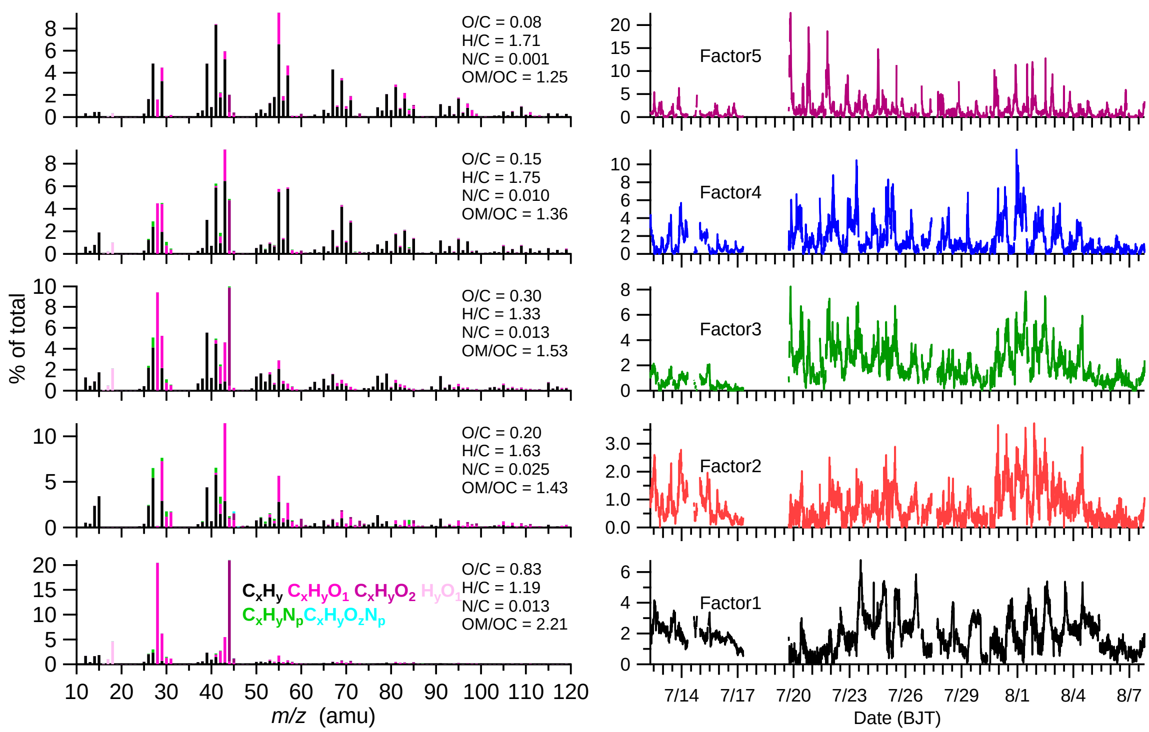


Fig. S4. 5-factor solution performed by PMF on organic high resolution mass spectra.

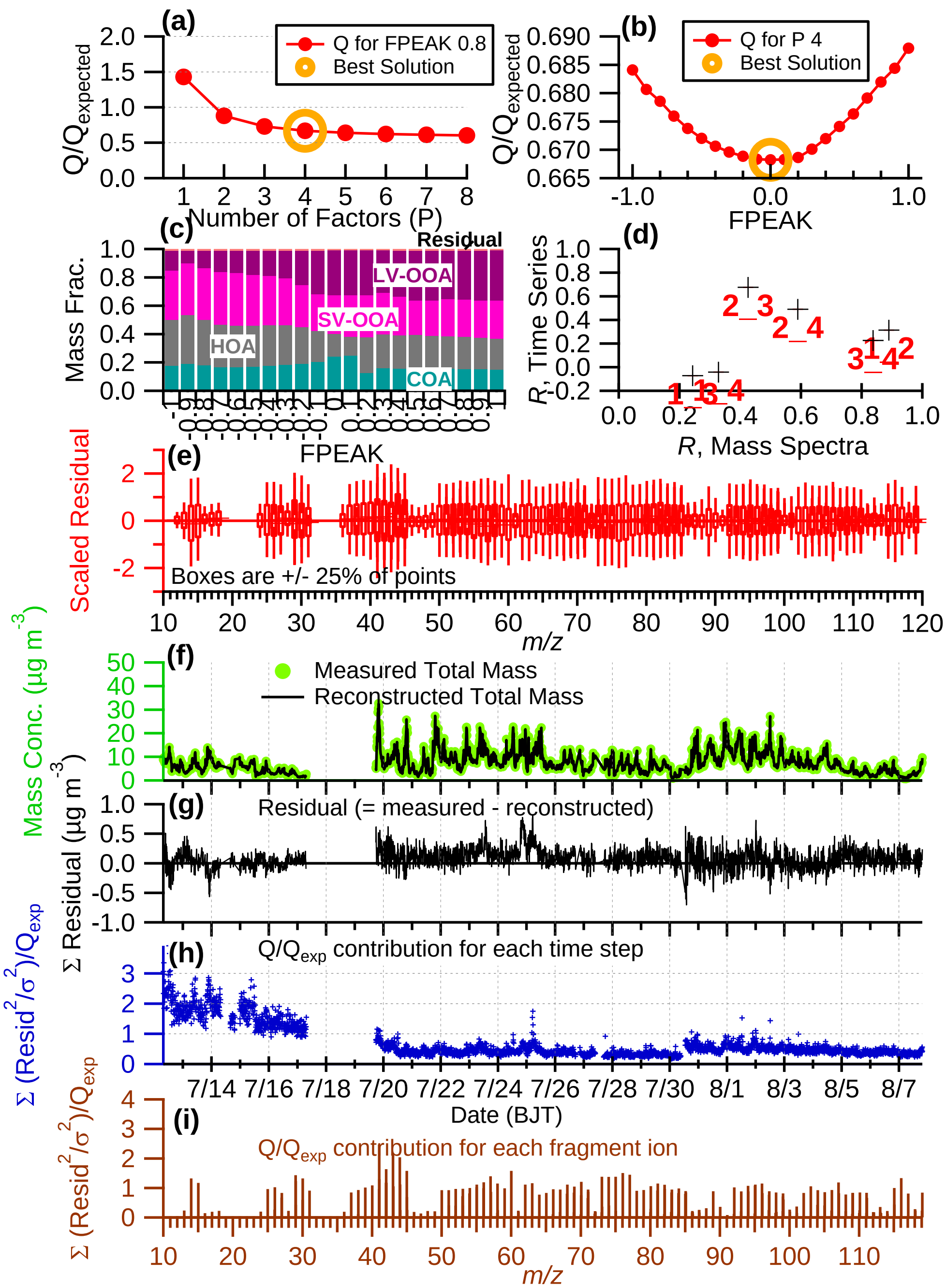


Fig. S5. Summary of key diagnostic plots of the PMF results: (a) Q/Q_{exp} as a function of number of factors (p) selected for PMF analysis. For the best solution (4-factor solution): (b) Q/Q_{exp} as a function of FPEAK, (c) fractions of OA factors vs. FPEAK, (d) correlations among PMF factors, (e) the box and whiskers plot showing the distributions of scaled residuals for each m/z, (f) time series of the measured organic mass and the reconstructed organic mass (COA + HOA + SV-OOA + LV-OOA), (g) variations of the residual (=measured − reconstructed) of the fit, (h) the Q/Q_{exp} for each point in time, and (i) the Q/Q_{exp} values for each ion.

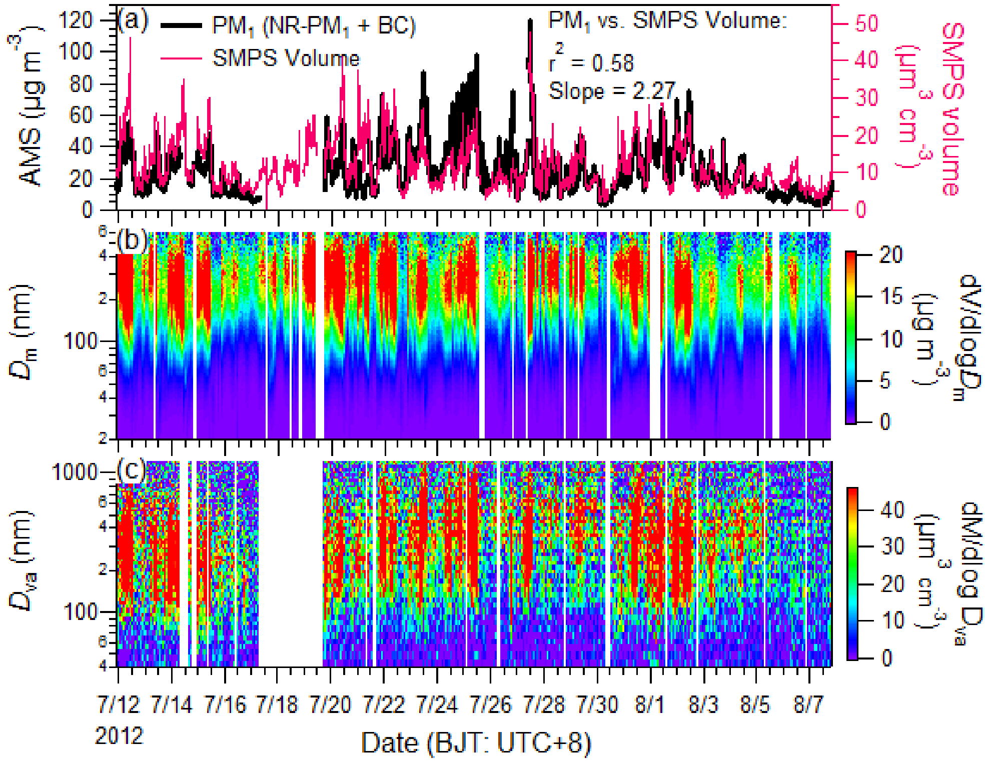


Fig. S6. Comparisons between (a) PM_1 mass concentrations ($NR\text{-}PM_1$ + BC) and particle volumes from the SMPS by assuming spherical particles, (b) particle volume distributions by the SMPS and (c) mass-based sized distributions by the AMS.

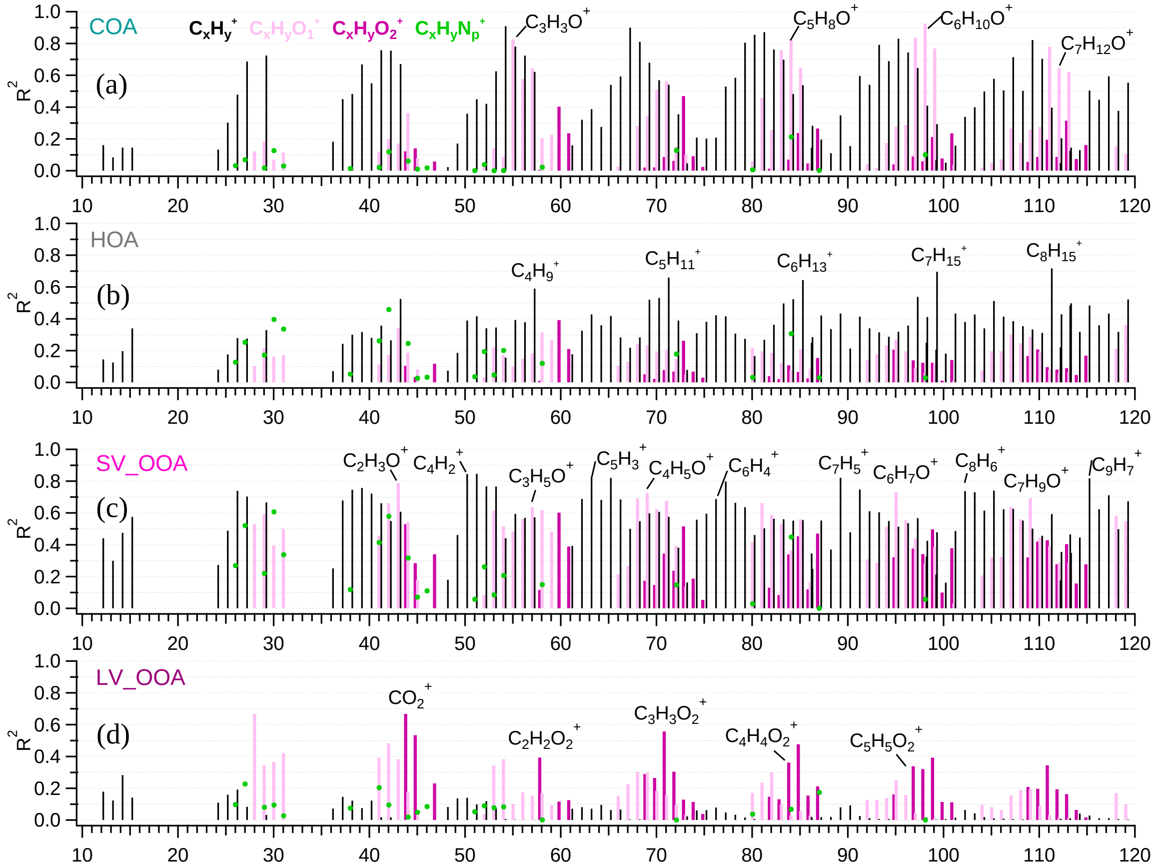
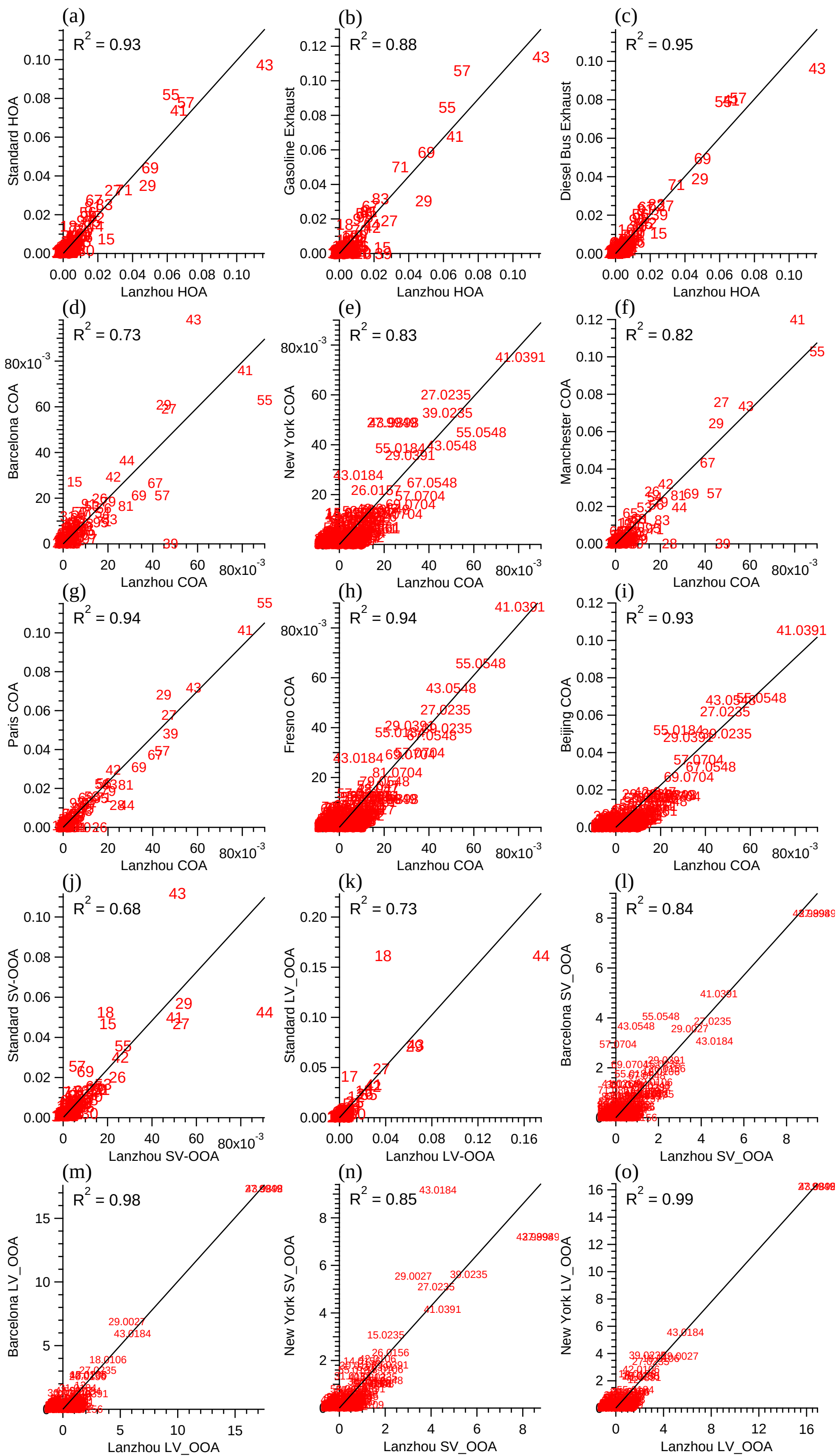


Fig. S7. Correlations of each OA component with ions colored by four ion categories. The ions that show strong correlations with individual OA components are marked by their formulas.



(a)
R^2 = 0.93
Standard HOA
Lanzhou HOA
(b)
R^2 = 0.88
Gasoline Exhaust
Lanzhou HOA
(c)
R^2 = 0.95
Diesel Bus Exhaust
Lanzhou HOA
(d)
R^2 = 0.73
Barcelona COA
Lanzhou COA
(e)
R^2 = 0.83
New York COA
Lanzhou COA
(f)
R^2 = 0.82
Manchester COA
Lanzhou COA
(g)
R^2 = 0.94
Paris COA
Lanzhou COA
(h)
R^2 = 0.94
Fresno COA
Lanzhou COA
(i)
R^2 = 0.93
Beijing COA
Lanzhou COA
(j)
R^2 = 0.68
Standard SV-OOA
Lanzhou SV-OOA
(k)
R^2 = 0.73
Standard LV_OOA
Lanzhou LV-OOA
(l)
R^2 = 0.84
Barcelona SV_OOA
Lanzhou SV_OOA
(m)
R^2 = 0.98
Barcelona LV_OOA
Lanzhou LV_OOA
(n)
R^2 = 0.85
New York SV_OOA
Lanzhou SV_OOA
(o)
R^2 = 0.99
New York LV_OOA
Lanzhou LV_OOA

Fig. S8. Scatter plots of mass spectra of OA components in Lanzhou study with referenced spectra determined from other studies (details in the main text).

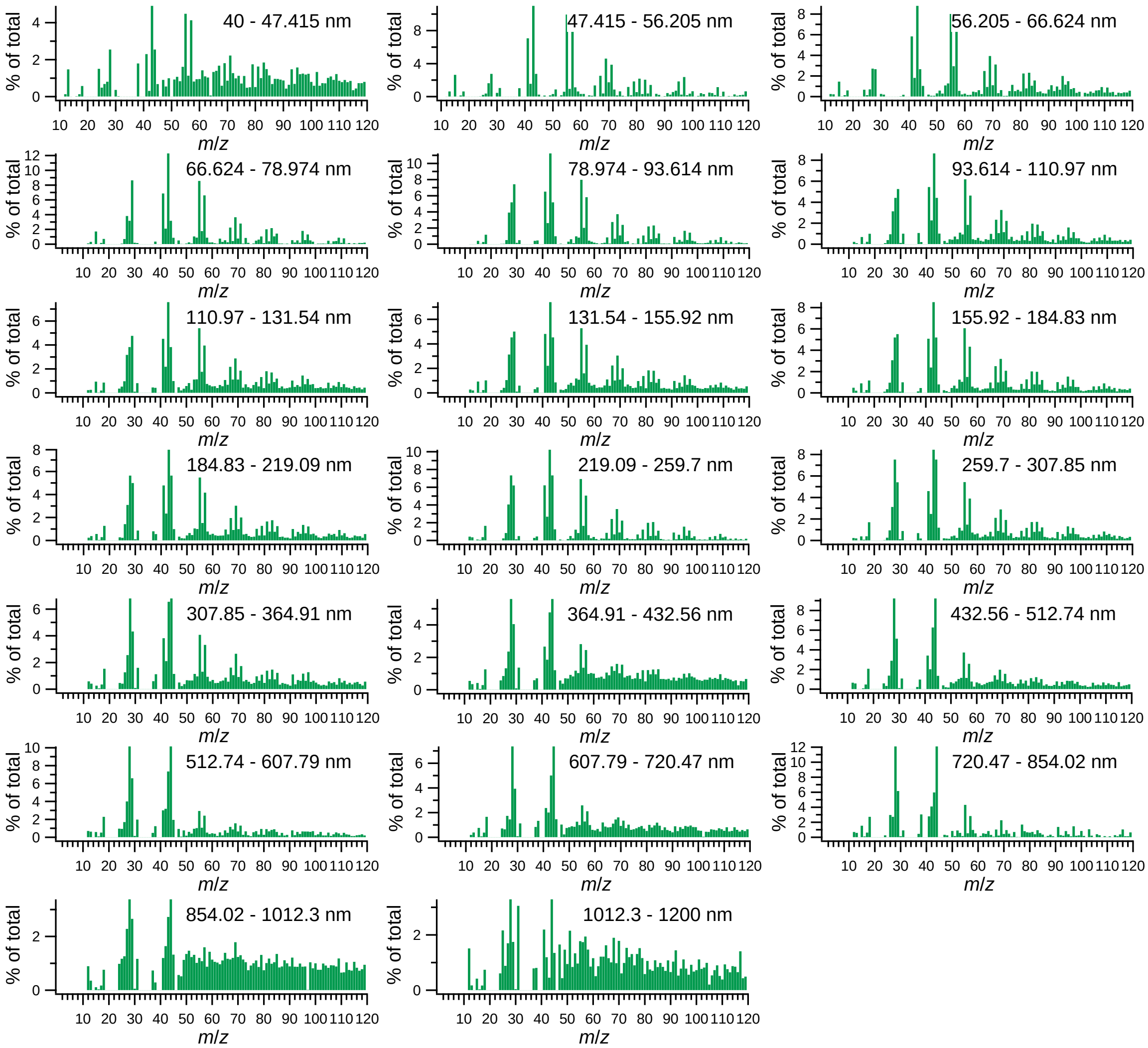


Fig. S9. Average mass spectrum of the total OA at each size bin used for the multilinear fitting for the size distributions of individual OA component.

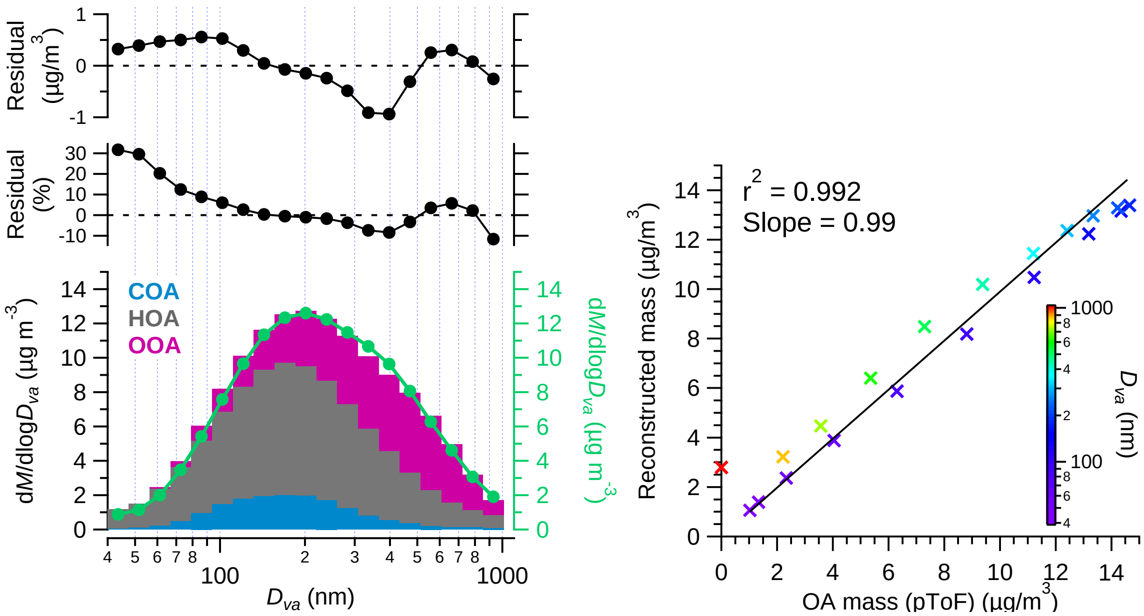


Fig. S10. Diagnostics plots for the multilinear fitting for the size distributions of individual OA component.

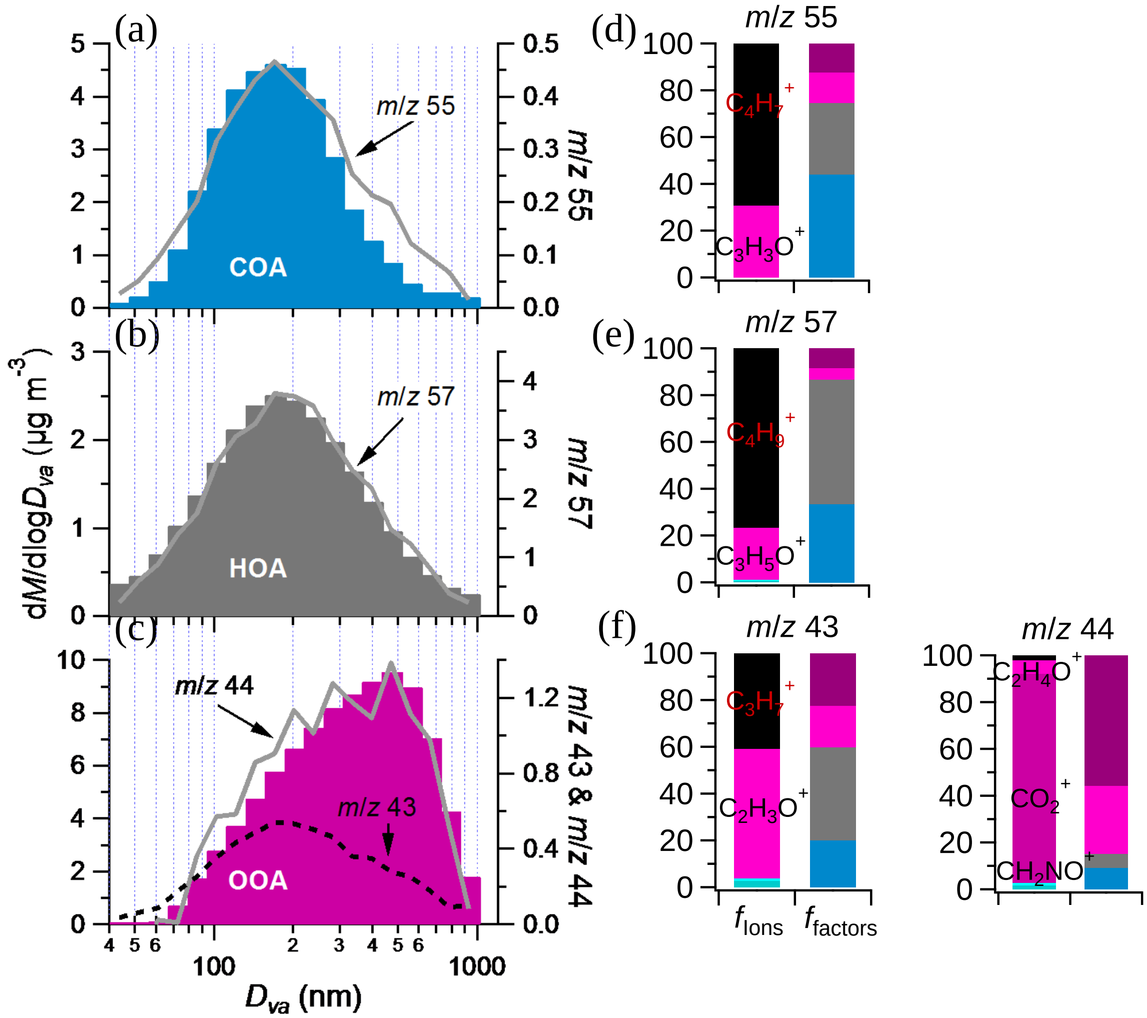


Fig. S11. Average size distributions of individual OA factors and relevant tracer *m/z*'s: (a) COA and *m/z* 57, (b) HOA and *m/z* 55, and (c) OOA and *m/z* 44 and 43. Fractional contributions of different ions (f_{ion}) and the four OA factors (f_{factors}) to the average mass of (d) *m/z* 55, (e) *m/z* 57, and (f) *m/z* 44 and 43. The size distributions of SV-OOA and LV-OOA are merged into one factor (OOA).

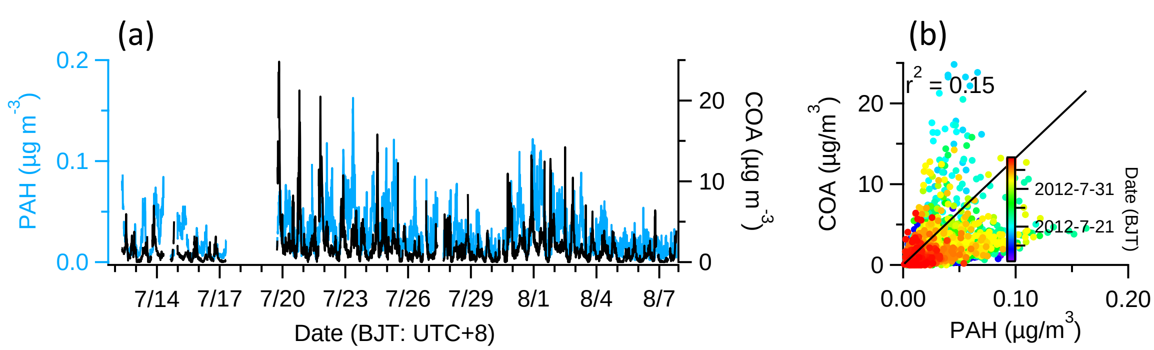


Fig. S12. (a) Time series of PAHs and COA, and (b) scatter plots of PAHs with COA. The data points are colored by measurement time.

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