Simultaneous factor analysis of organic particle and gas mass spectra: AMS and PTR-MS measurements at an urban site

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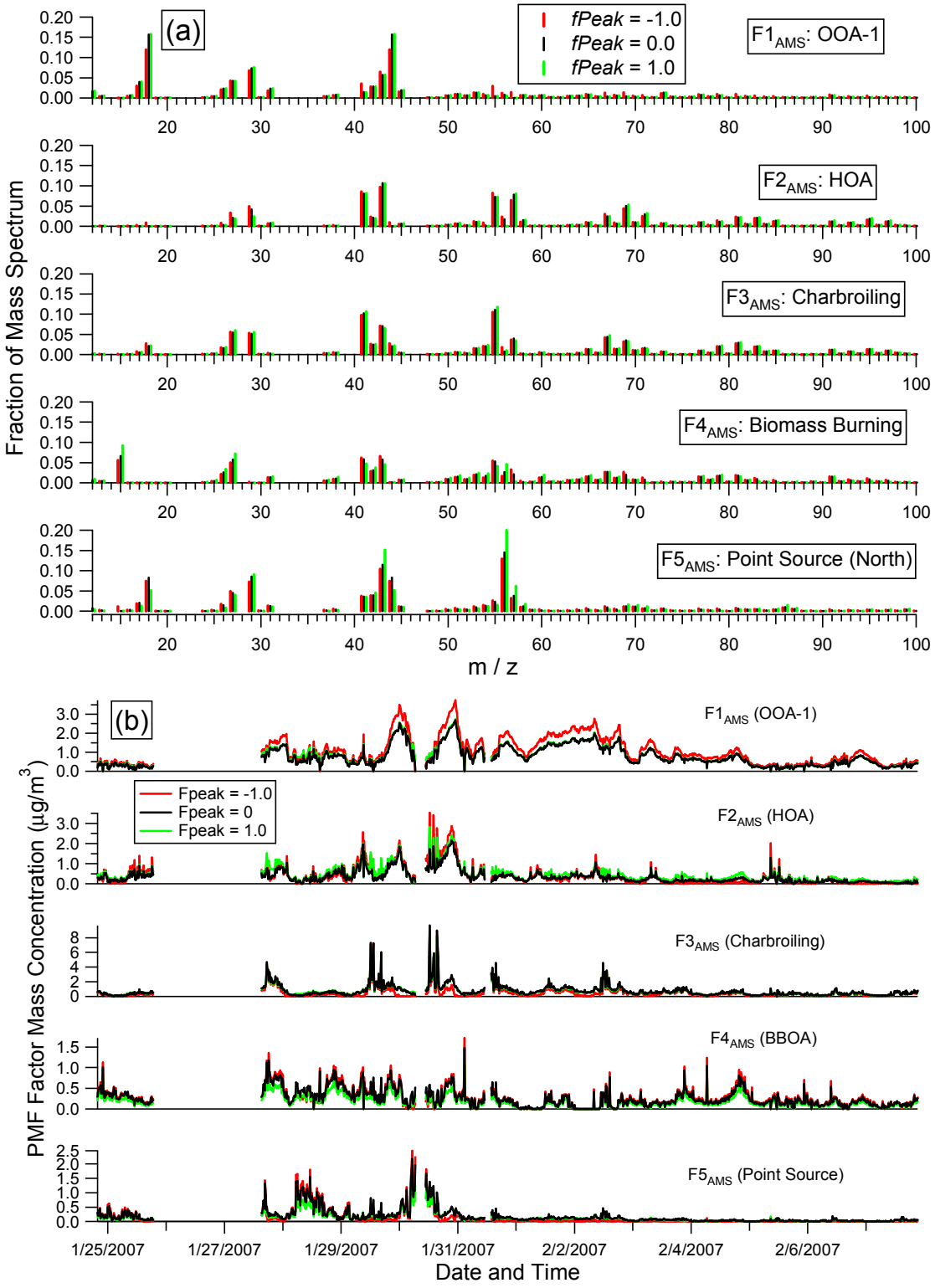
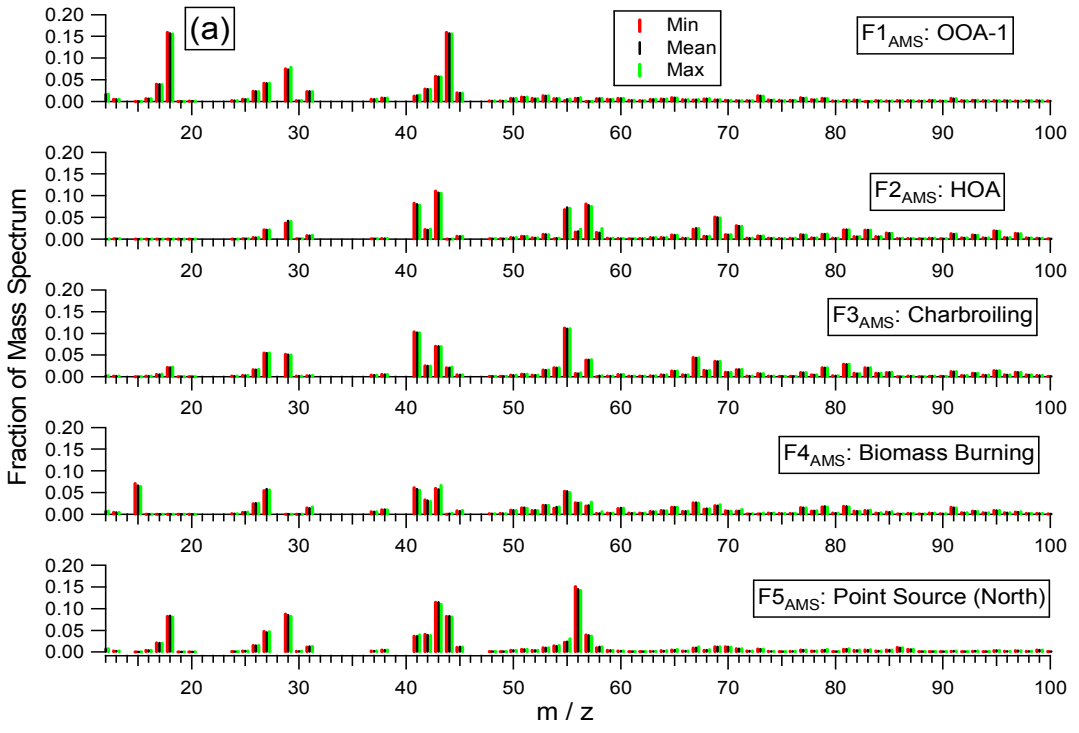


Figure S1. Factor mass spectra (a) and time series (b) for the solutions to the AMS dataset at *fPeak* = -1.0 (red), 0 (black), and 1.0 (green).



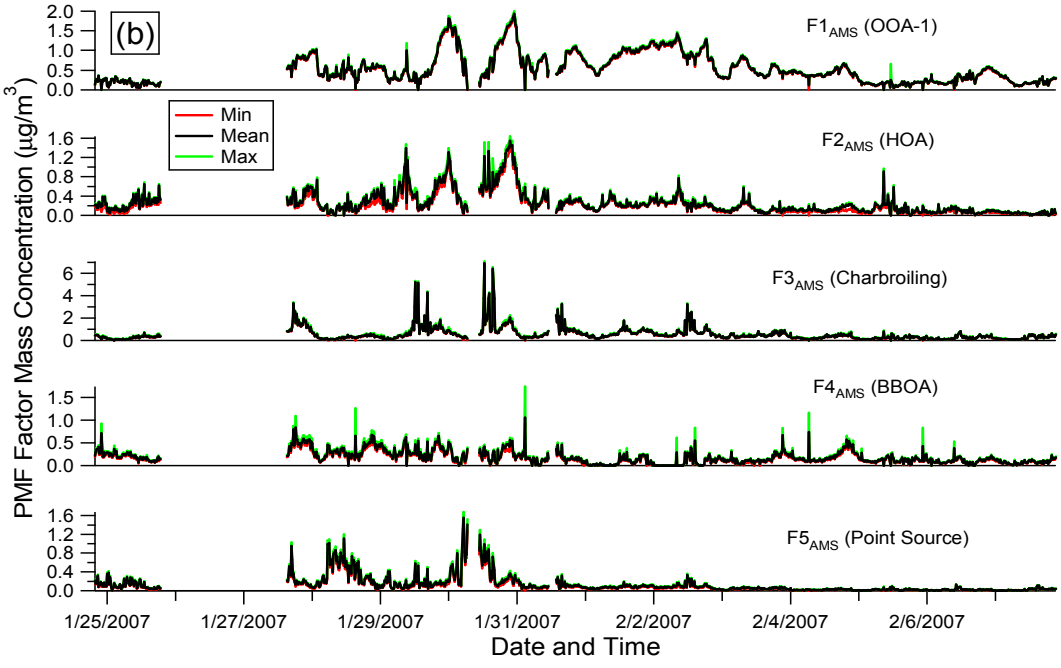


Figure S2. Factor mass spectra (a) and time series (b) for the 5-factor solution to the AMS dataset for 98 convergent runs generated from 100 random starting points. The mean, maximum, and minimum values for each *m/z* and time point are shown.

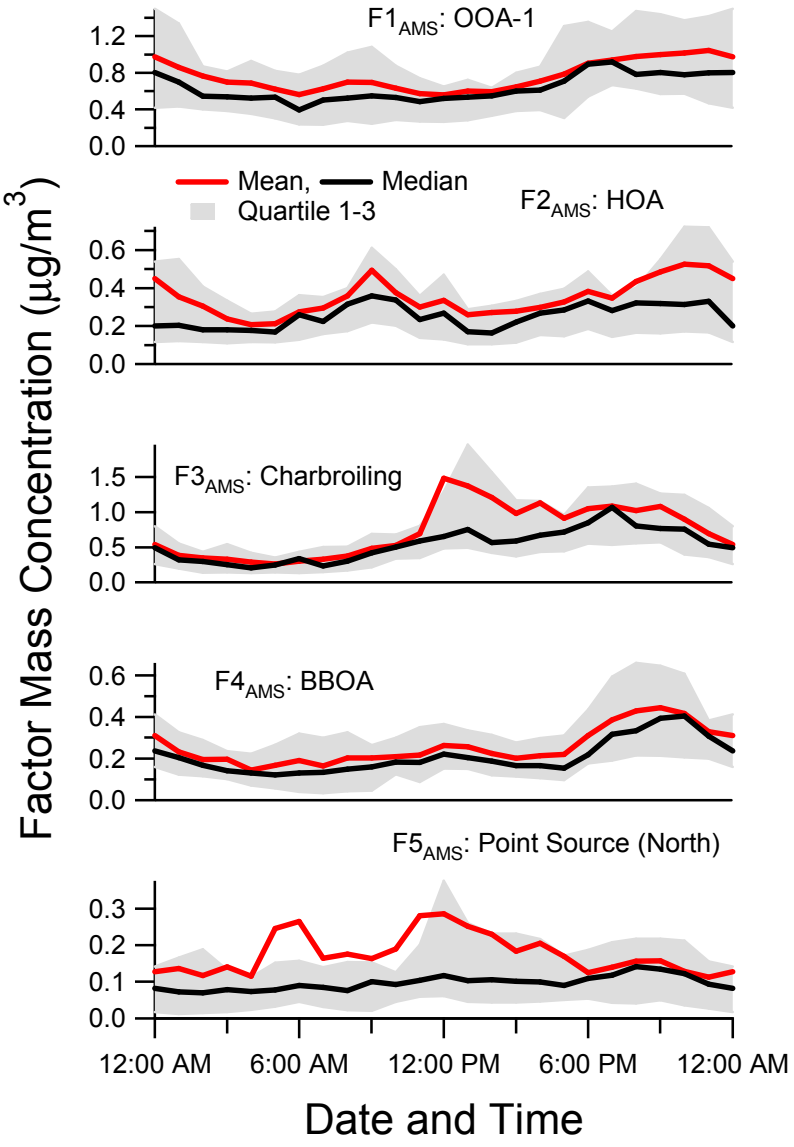
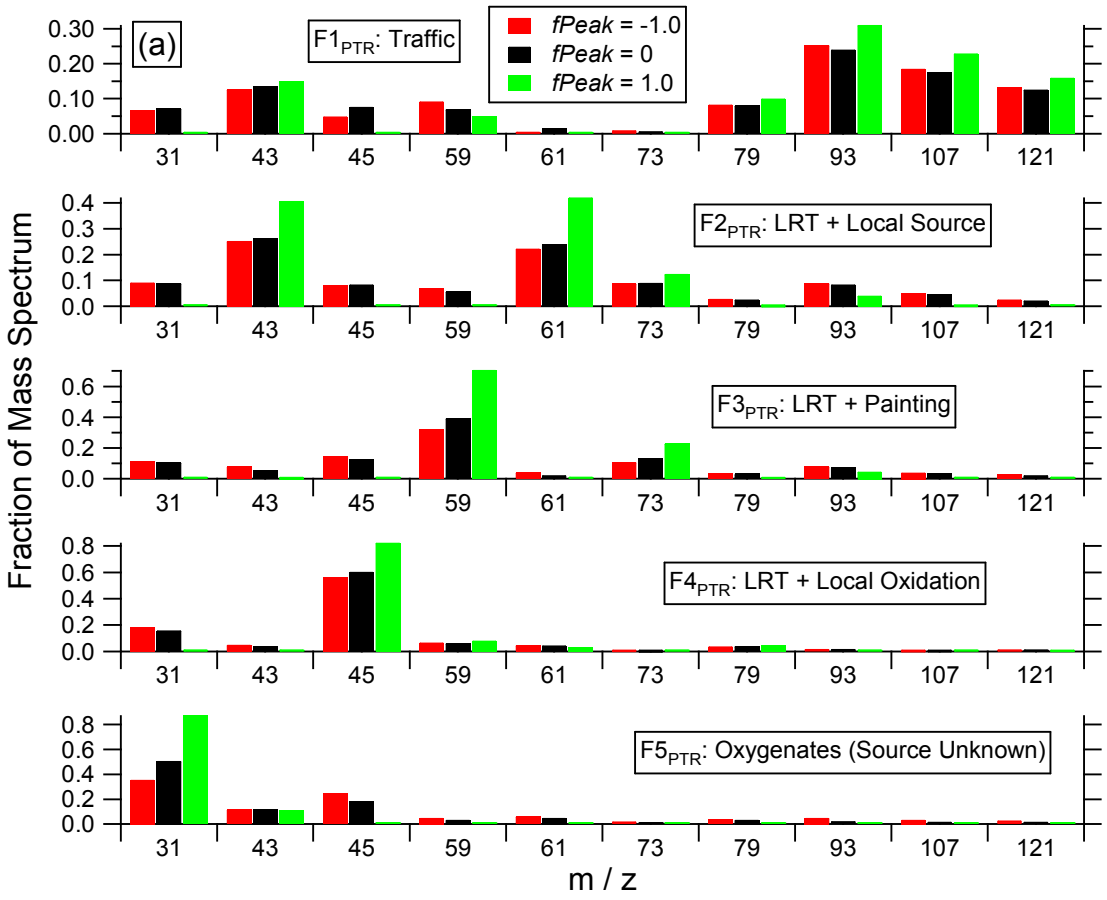


Figure S3. Hourly mean (red) and median (black) factor concentrations for the AMS dataset. Gray shading indicates the region bounded by the 1st and 3rd quartiles.


(a)
F1PTR: Traffic
fPeak = -1.0
fPeak = 0
fPeak = 1.0
F2PTR: LRT + Local Source
F3PTR: LRT + Painting
F4PTR: LRT + Local Oxidation
F5PTR: Oxygenates (Source Unknown)
Fraction of Mass Spectrum
m / z
31
43
45
59
61
73
79
93
107
121

1

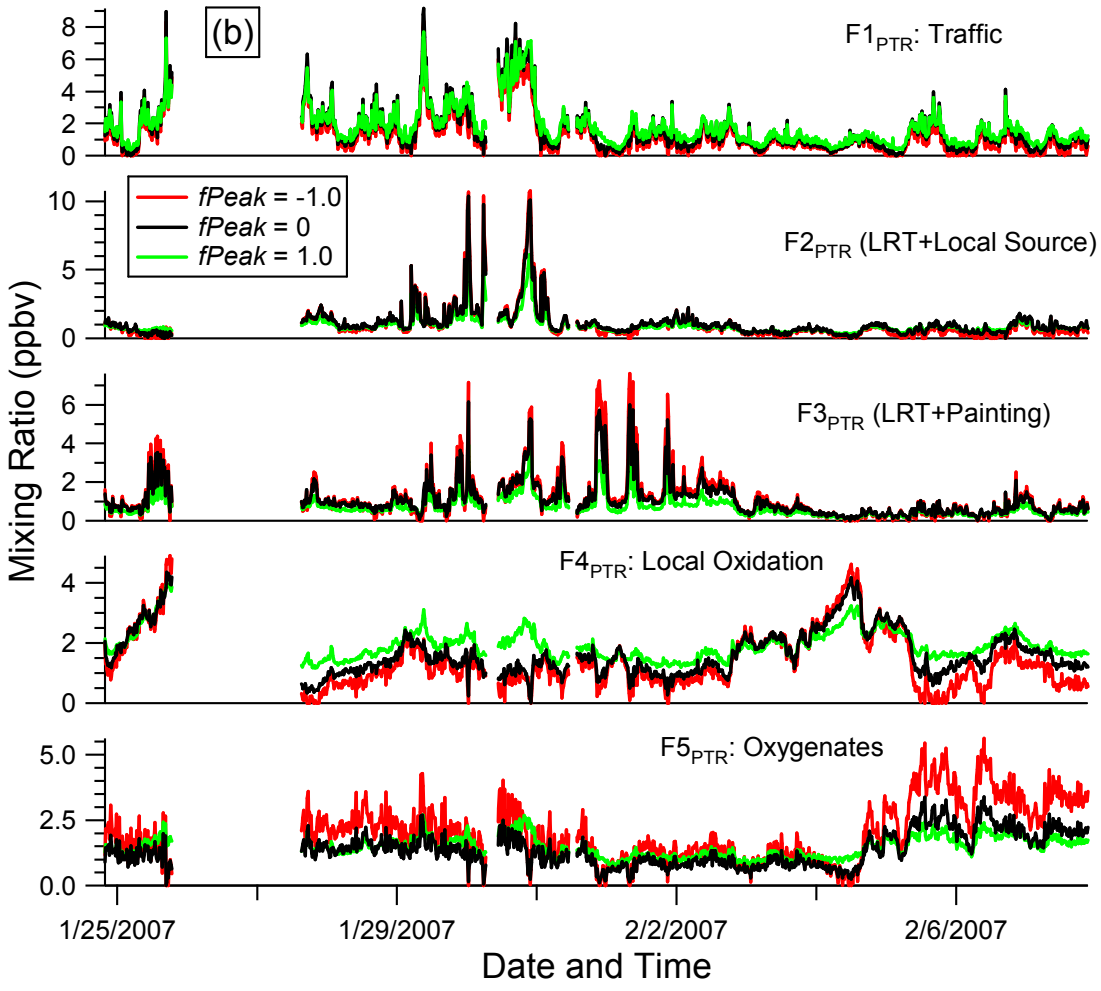
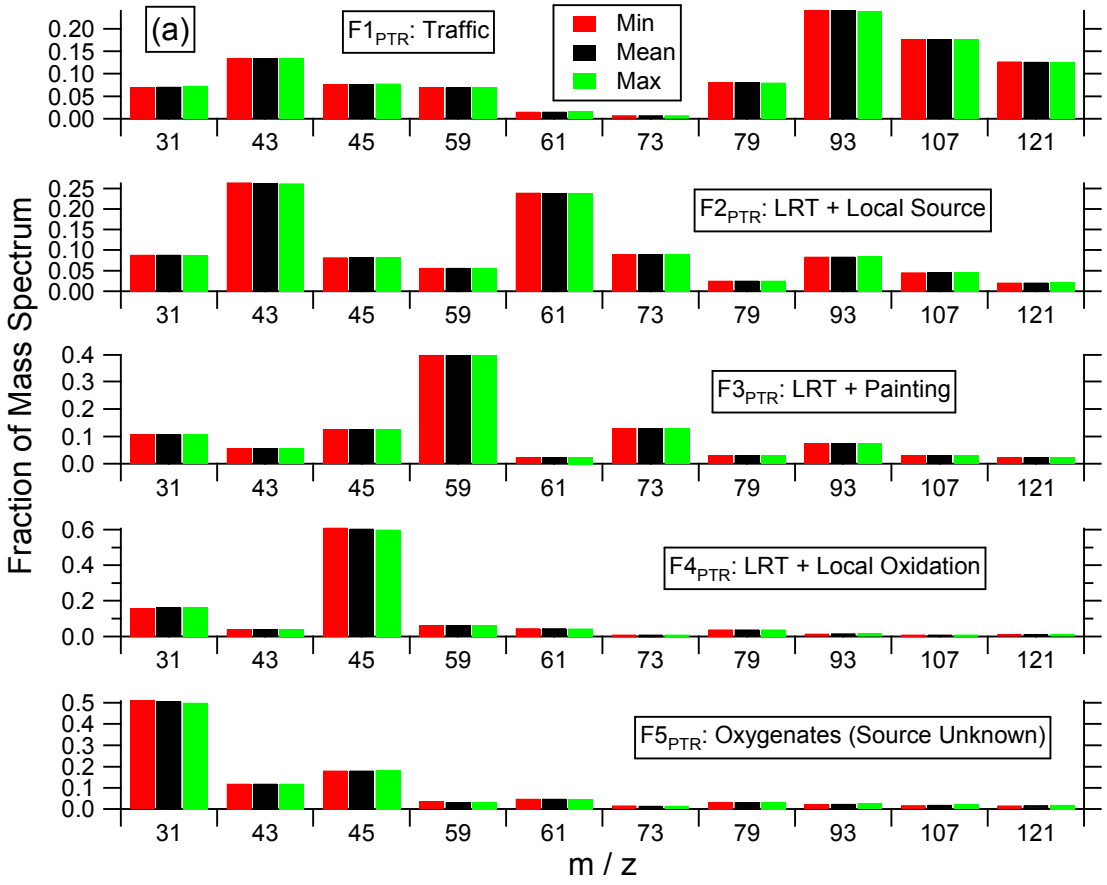


Figure S4. Factor mass spectra (a) and time series (b) for the solutions to the PTR-MS dataset at *fPeak* = -1.0 (red), 0 (black), and 1.0 (green). Differences between the solutions occur primarily in the apportionment of acetaldehyde (*m/z* 45), which in the *fPeak* = 1.0 solution is attributed more strongly to the local oxidation factor.


(a)
F1PTR: Traffic
Min
Mean
Max
F2PTR: LRT + Local Source
F3PTR: LRT + Painting
F4PTR: LRT + Local Oxidation
F5PTR: Oxygenates (Source Unknown)
Fraction of Mass Spectrum
m / z
31
43
45
59
61
73
79
93
107
121

1

2

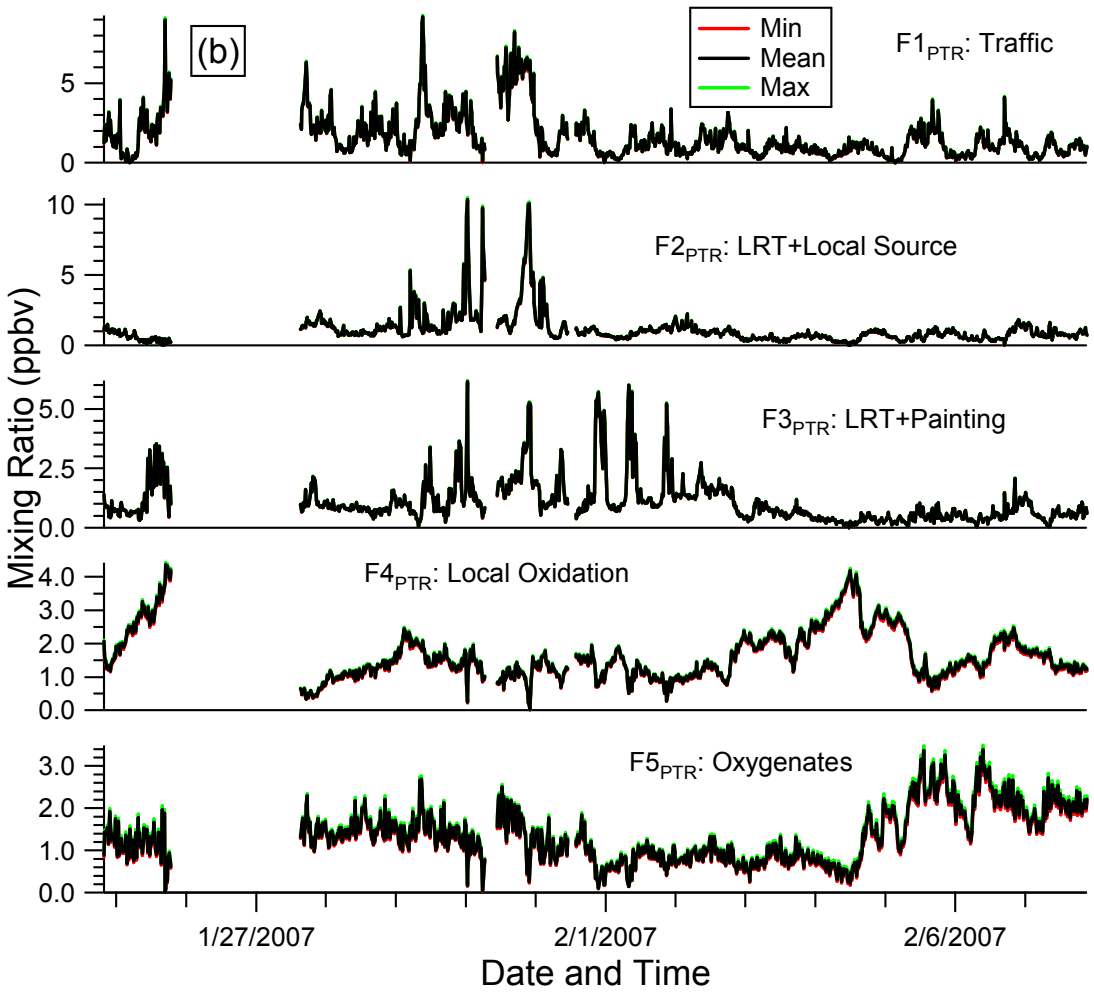


Figure S5. Factor mass spectra (a) and time series (b) for the 5-factor solution to the PTR-MS dataset generated from 100 random starting points. The mean, maximum, and minimum values for each *m/z* and time point are shown.

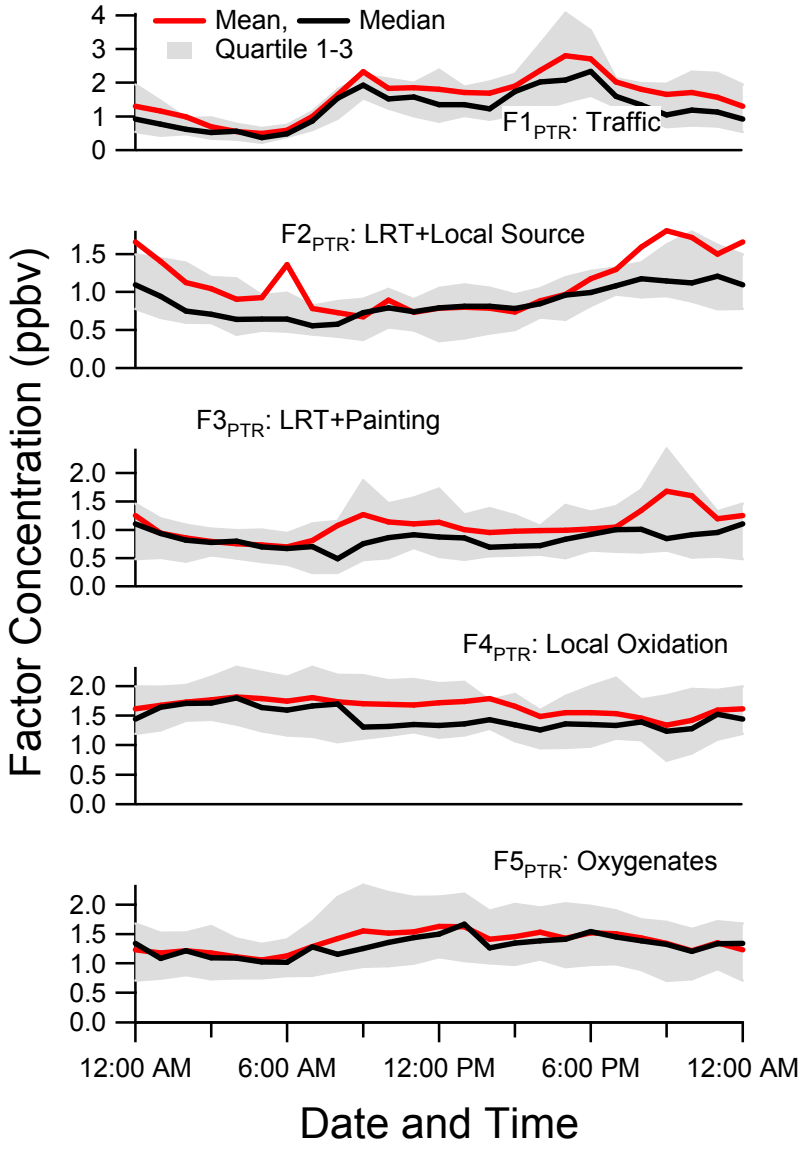
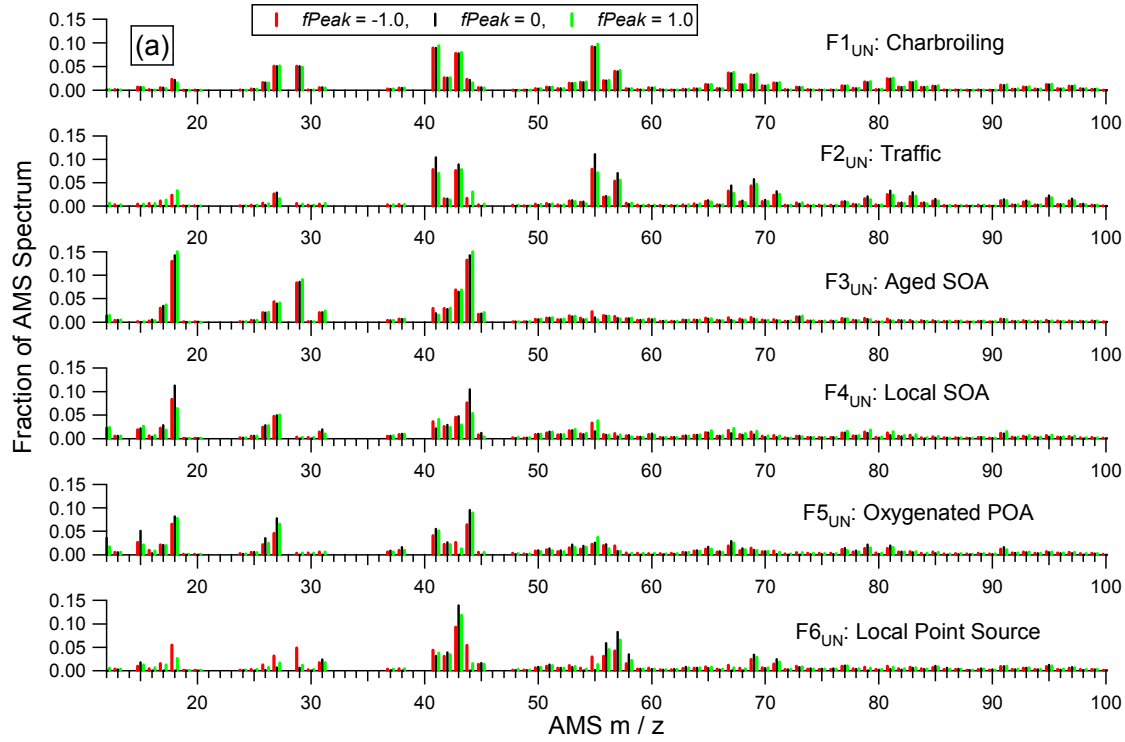
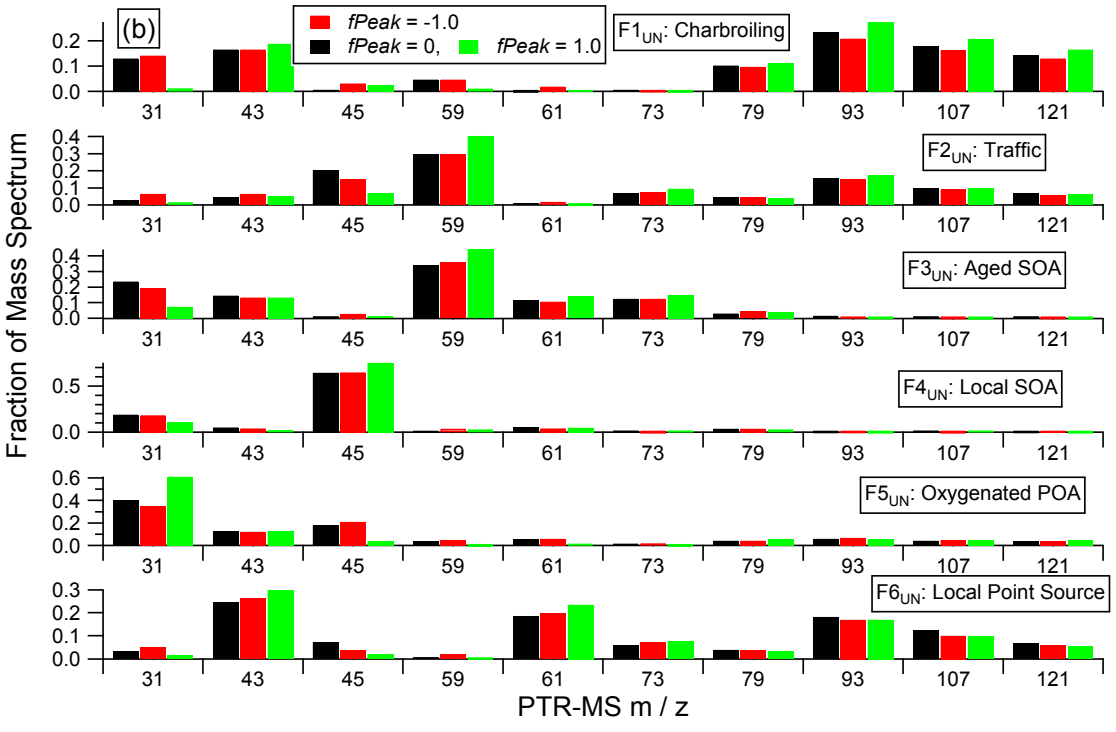


Figure S6. Hourly mean (red) and median (black) factor concentrations for the PTR-MS dataset. Gray shading indicates the region bounded by the 1st and 3rd quartiles.


(a)
fPeak = -1.0, fPeak = 0, fPeak = 1.0
F1UN: Charbroiling
F2UN: Traffic
F3UN: Aged SOA
F4UN: Local SOA
F5UN: Oxygenated POA
F6UN: Local Point Source
Fraction of AMS Spectrum
AMS m / z

1


(b)
fPeak = -1.0
fPeak = 0, fPeak = 1.0
F1UN: Charbroiling
F2UN: Traffic
F3UN: Aged SOA
F4UN: Local SOA
F5UN: Oxygenated POA
F6UN: Local Point Source
Fraction of Mass Spectrum
PTR-MS m / z

2

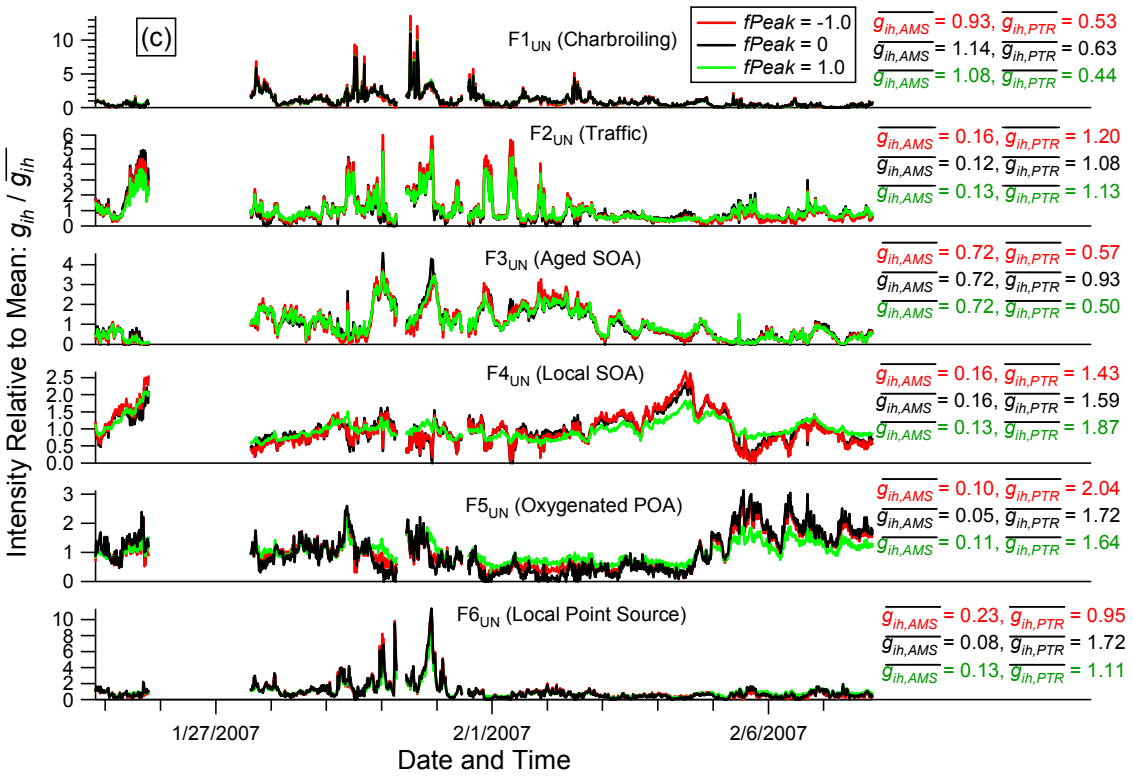
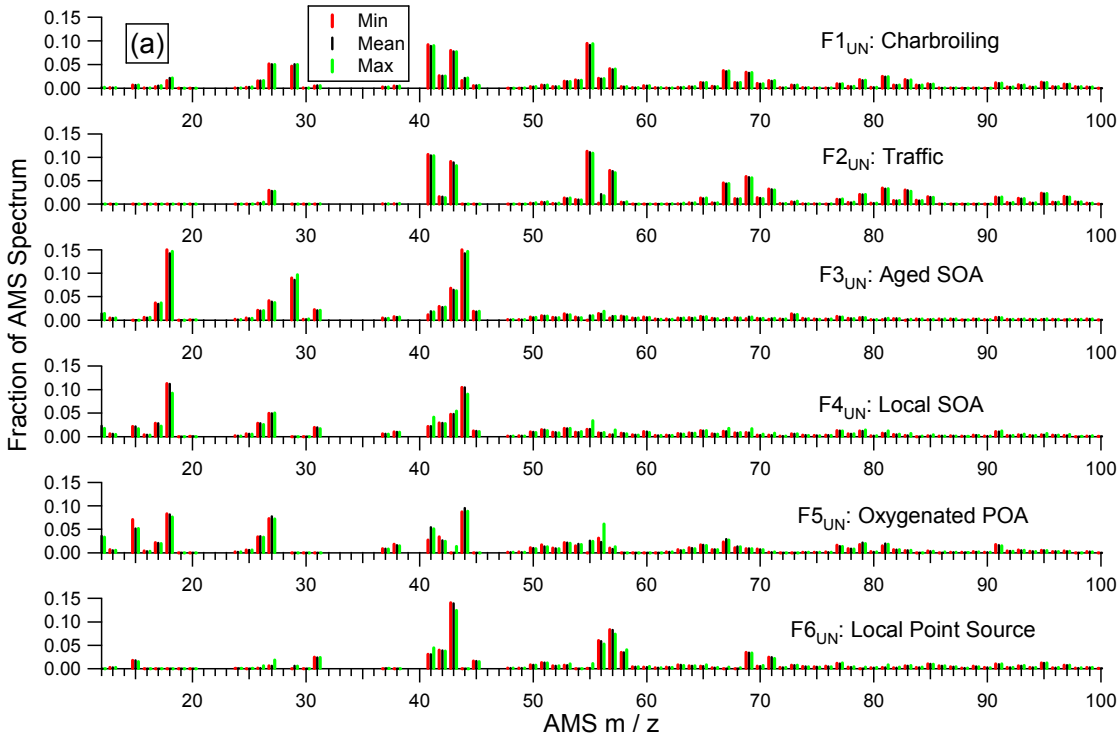
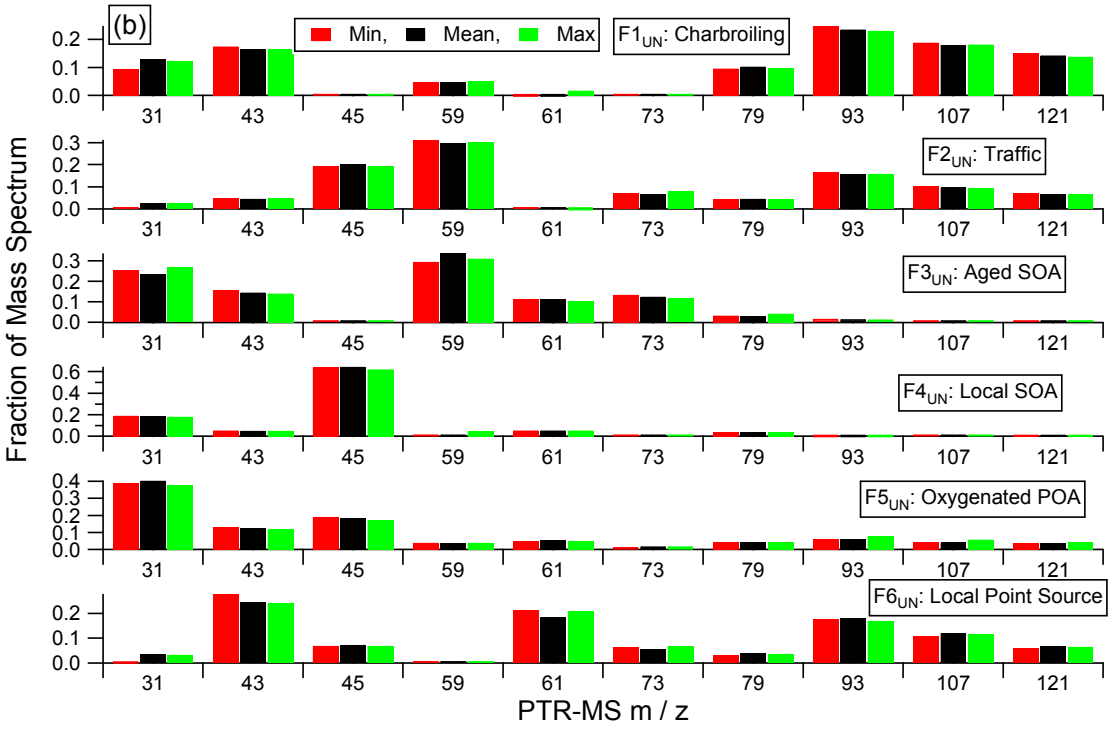


Figure S7. Factor mass spectra (a,b) and time series (c) as a function of *fPeak* for the 6-factor solution to the unified dataset. Units for $\overline{g_{ih,AMS}}$ and $\overline{g_{ih,PTR}}$ are μg/m^3 and ppbv, respectively. Solutions are similar, independent of *fPeak*.


(a)
Min
Mean
Max
F1UN: Charbroiling
F2UN: Traffic
F3UN: Aged SOA
F4UN: Local SOA
F5UN: Oxygenated POA
F6UN: Local Point Source
Fraction of AMS Spectrum
AMS m / z

1


(b)
Min, Mean, Max
F1UN: Charbroiling
F2UN: Traffic
F3UN: Aged SOA
F4UN: Local SOA
F5UN: Oxygenated POA
F6UN: Local Point Source
Fraction of Mass Spectrum
PTR-MS m / z

2

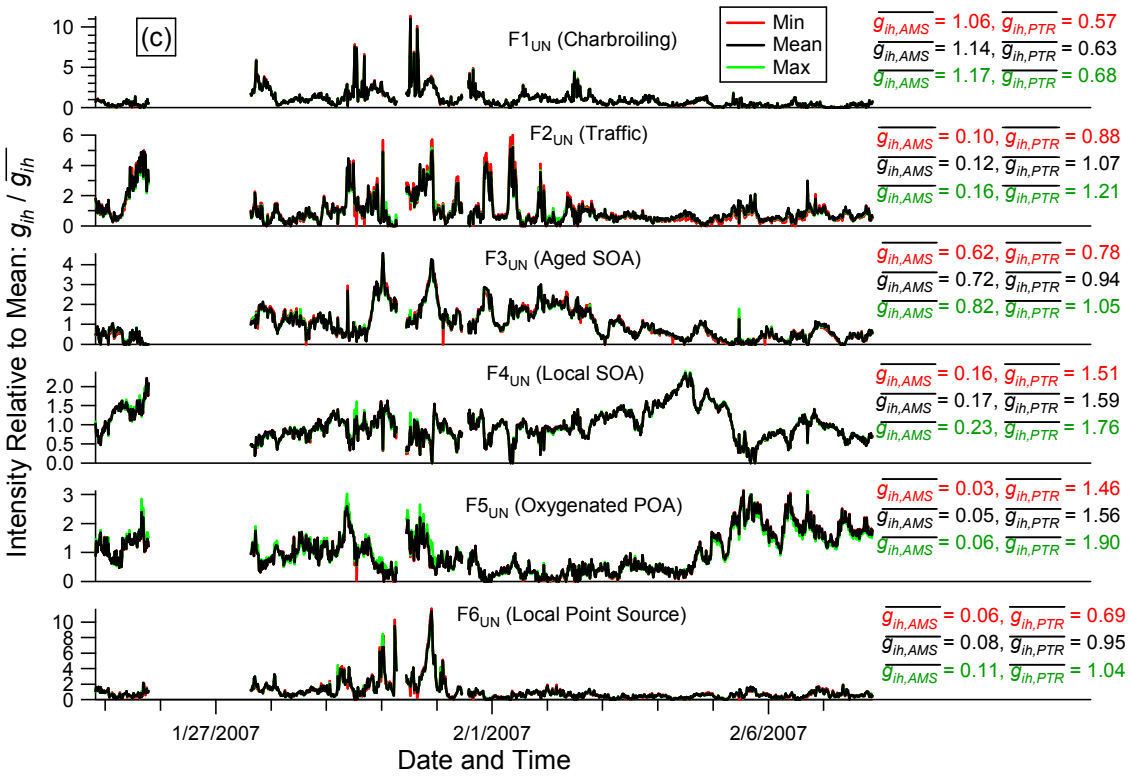


Figure S8. Factor mass spectra (a,b) and time series (c) for the 6-factor solution to the unified dataset for 98 convergent runs generated from 100 random starting points. The mean, maximum, and minimum values for each *m/z* and time point are shown. Units for $\overline{g_{ih,AMS}}$ and $\overline{g_{ih,PTR}}$ are μg/m^3 and ppbv, respectively.

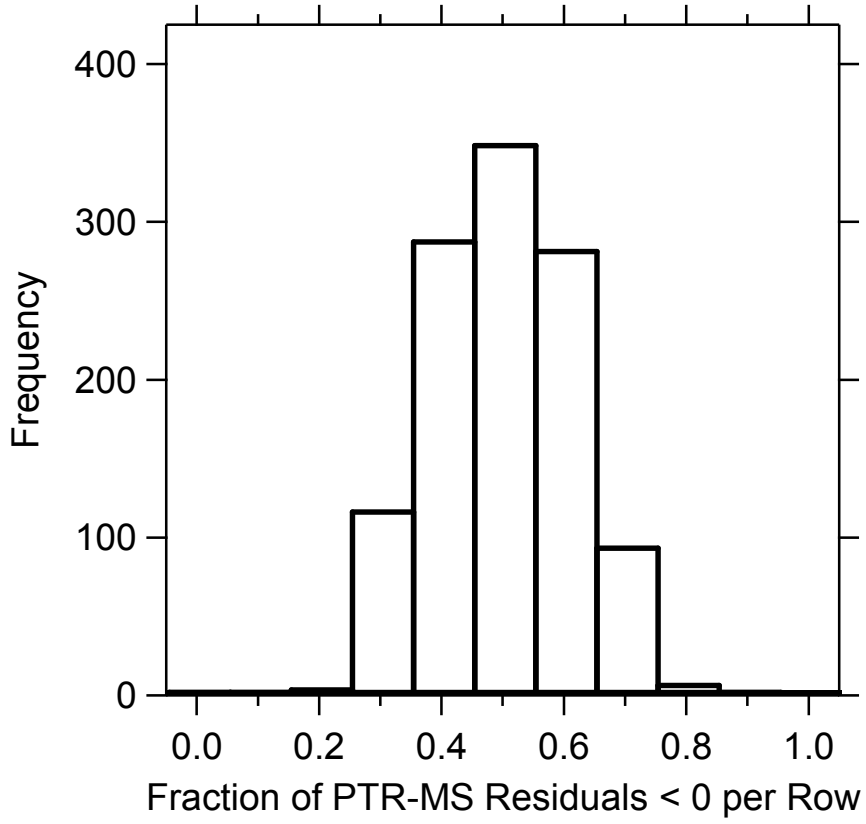


Figure S9. Frequency of negative PTR-MS residuals per row (i.e. time point) of residual matrix **E**, for the solution at $p = 6$, $C_{PTR} = 10$ in the unified dataset.

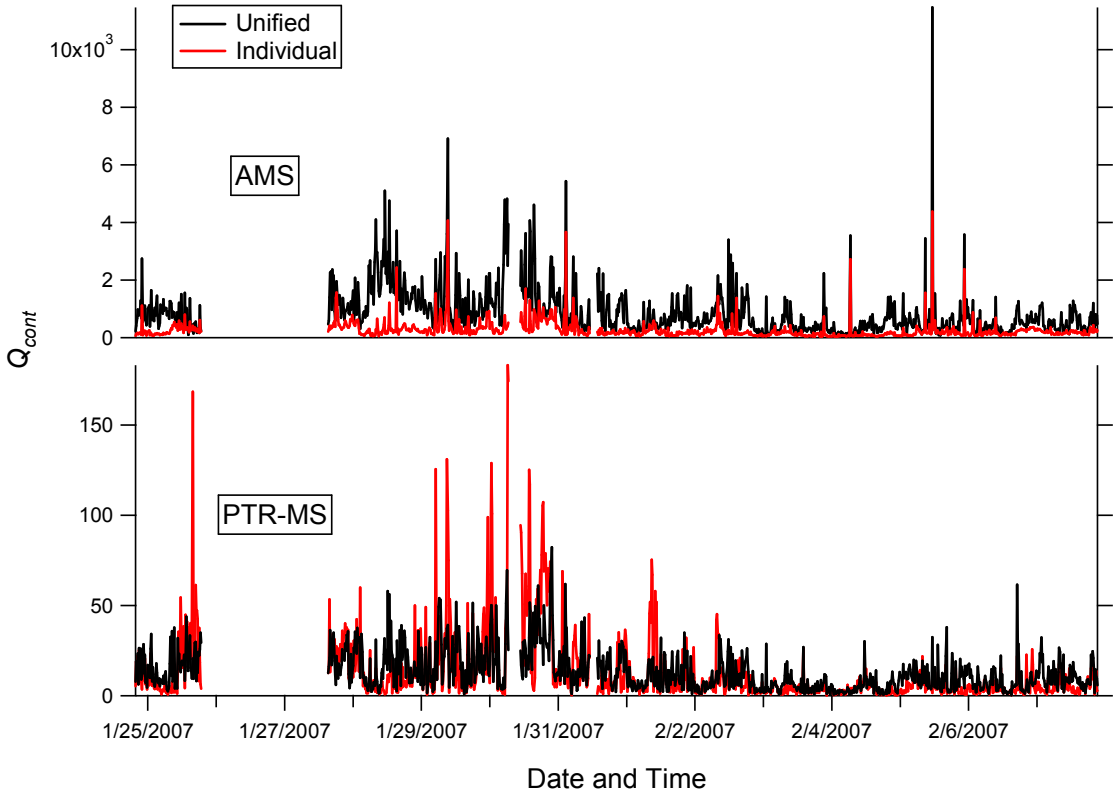
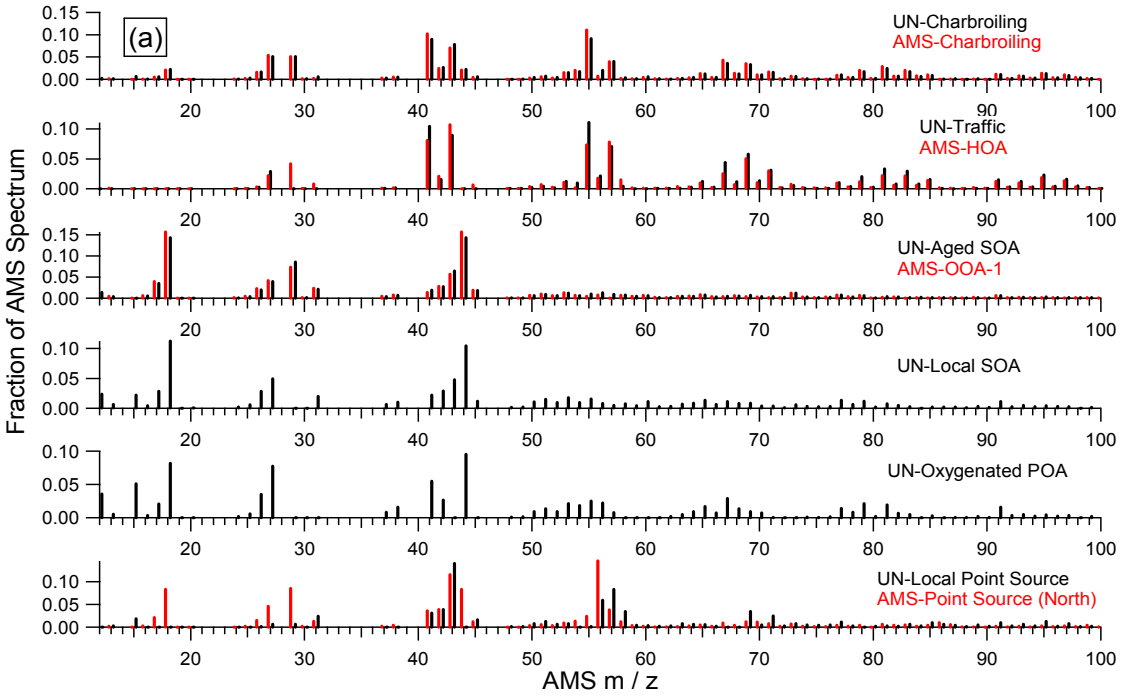
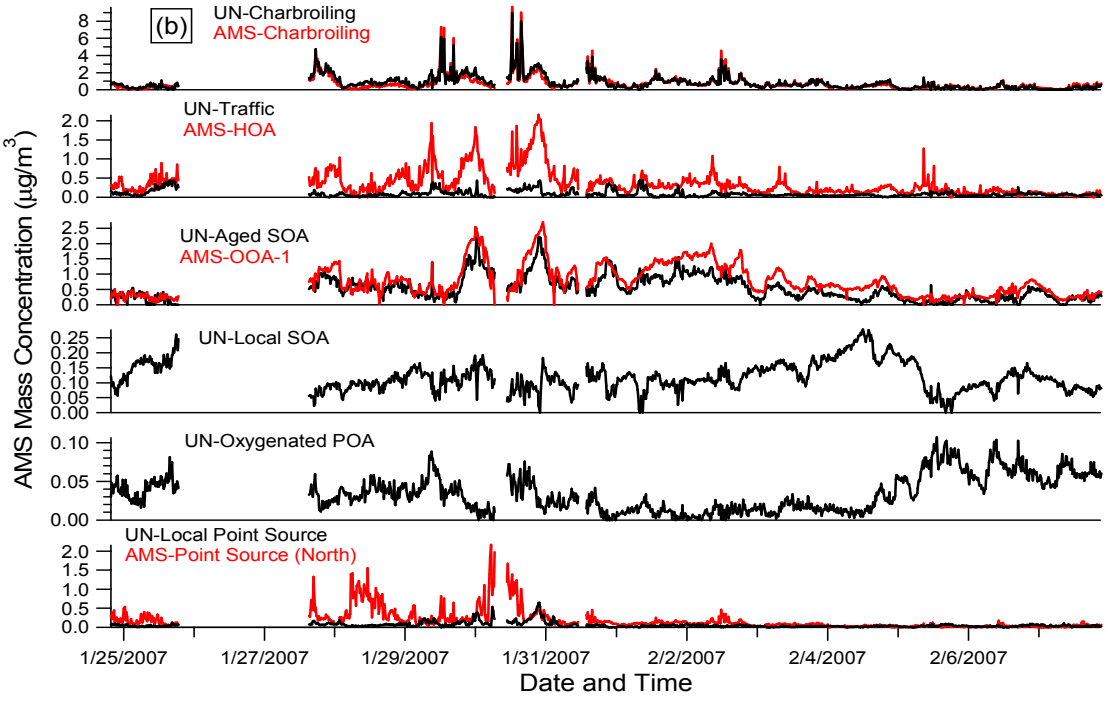


Figure S10. Comparison of Q_{cont} time series between the unified and individual datasets. For comparison purposes, C_{PTR} has been removed from the unified dataset uncertainties in the calculation of Q_{cont}.



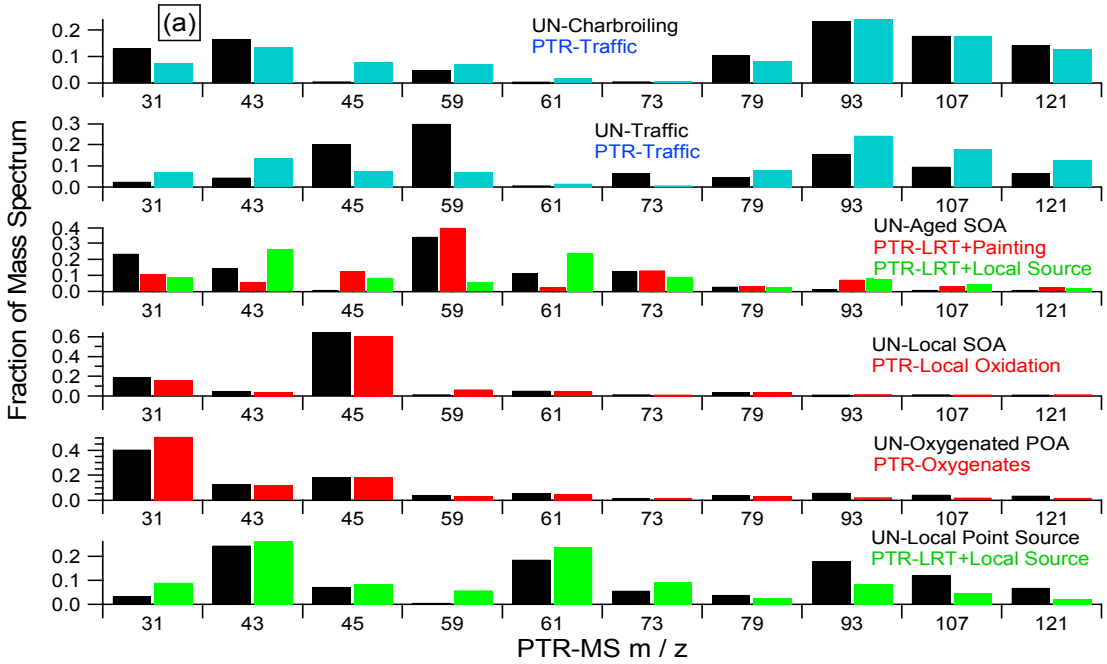
1



2

3 Figure S11. Comparison of solutions to the AMS (p = 5) and unified (p = 6) dataset
4 solutions. Note that the unified dataset traces shown here are in µg m^{-3} and are calculated
5 as the product of the normalized intensity and the AMS normalization factor reported in

Fig. 11. The AMS-biomass burning factor is not related to any factor in the unified dataset and is therefore excluded from this comparison.



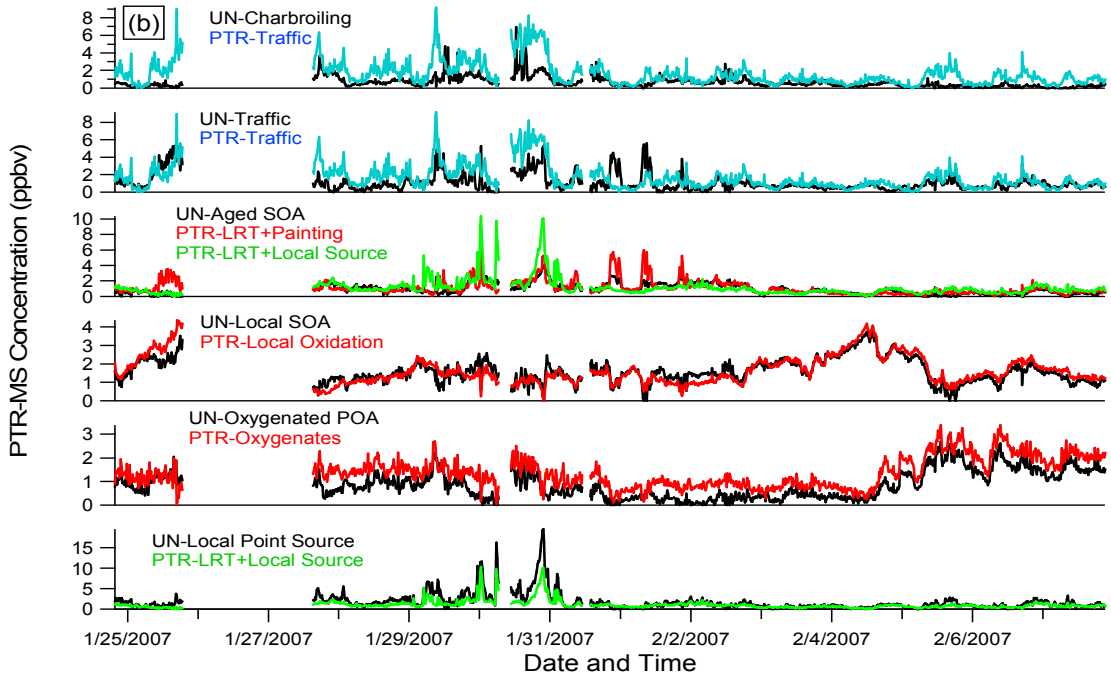


Figure S12. Comparison of solutions to the PTR-MS (p = 5) and unified (p = 6) dataset solutions. Note that the PTR-Traffic (blue) and PTR-LRT+Local Source factors are compared to multiple UN factors. The unified dataset time series shown here are reported in ppbv and are calculated as the product of the normalized intensity and the PTR-MS normalization factor reported in Fig. 11.

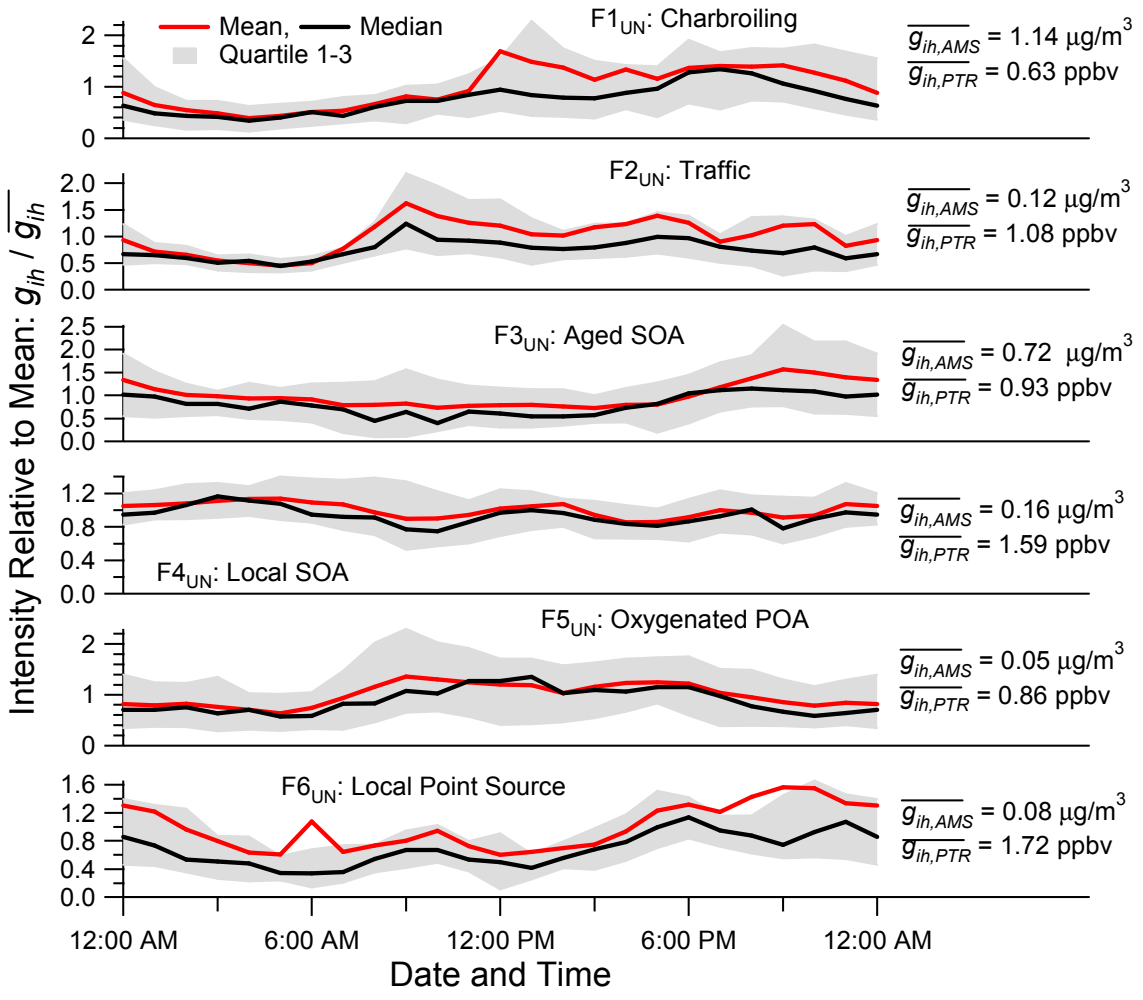
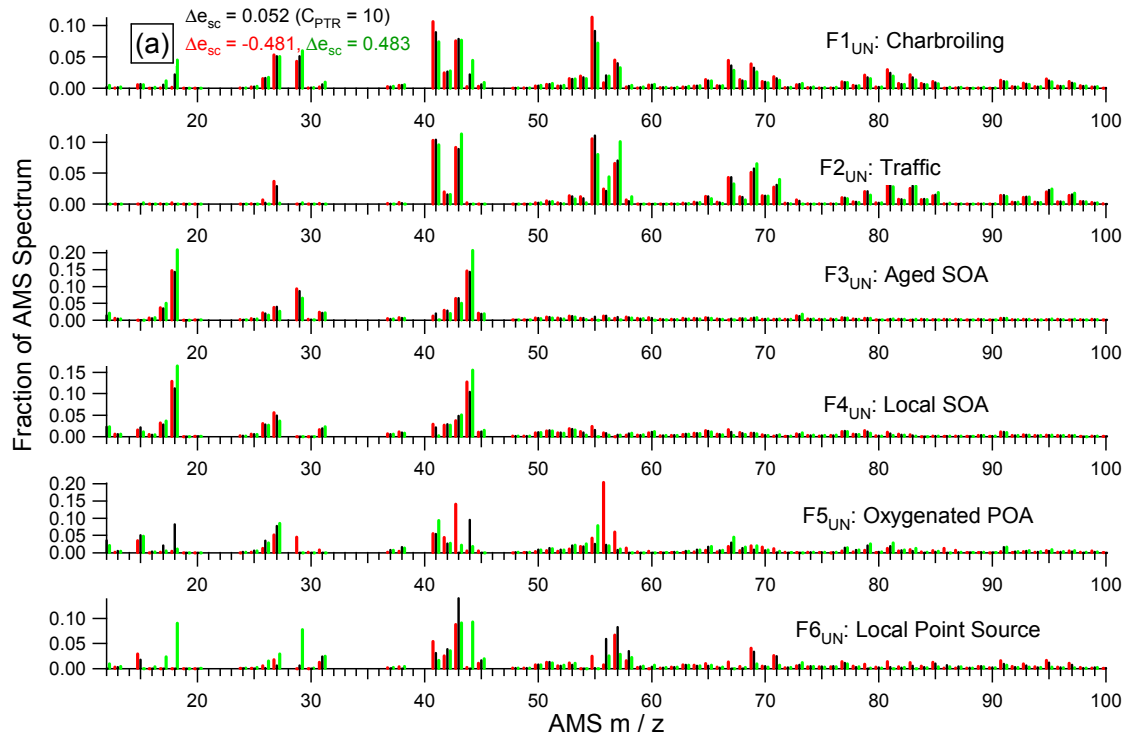
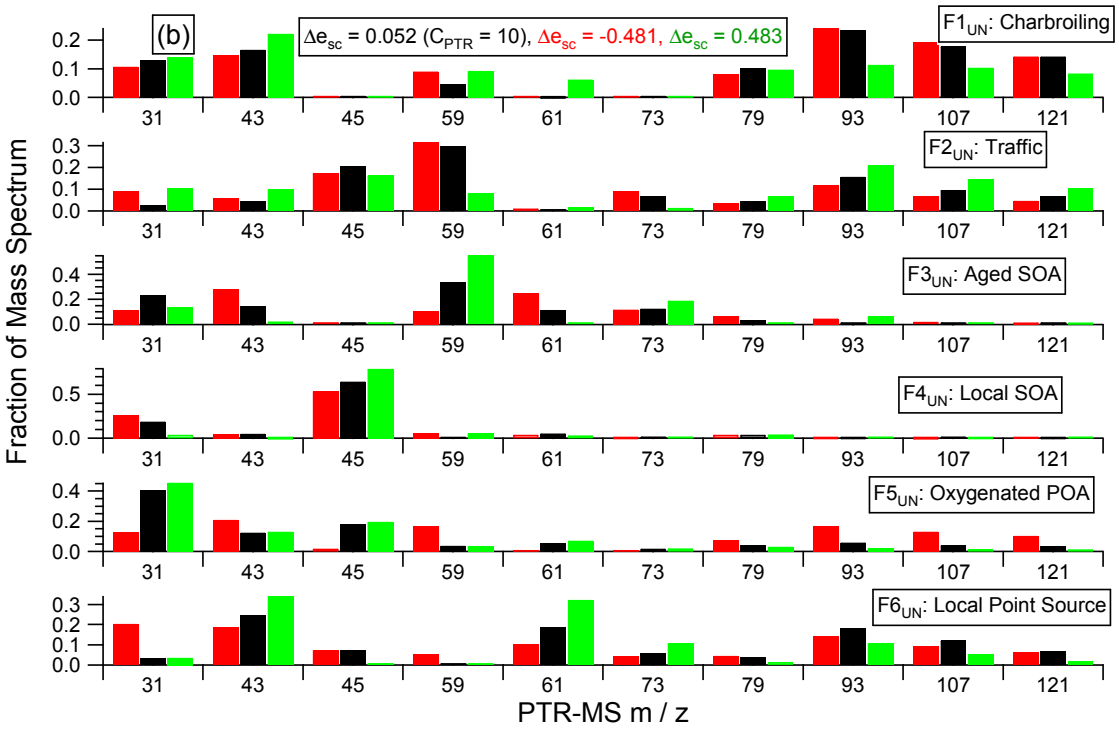


Figure S13. Hourly mean (red) and median (black) factor concentrations for the unified dataset. Gray shading indicates the region bounded by the 1st and 3rd quartiles.


(a)
Δe_sc = 0.052 (C_PTR = 10)
Δe_sc = -0.481, Δe_sc = 0.483
F1_UN: Charbroiling
F2_UN: Traffic
F3_UN: Aged SOA
F4_UN: Local SOA
F5_UN: Oxygenated POA
F6_UN: Local Point Source
Fraction of AMS Spectrum
AMS m / z

1


(b)
Δe_sc = 0.052 (C_PTR = 10), Δe_sc = -0.481, Δe_sc = 0.483
F1_UN: Charbroiling
F2_UN: Traffic
F3_UN: Aged SOA
F4_UN: Local SOA
F5_UN: Oxygenated POA
F6_UN: Local Point Source
Fraction of Mass Spectrum
PTR-MS m / z

2

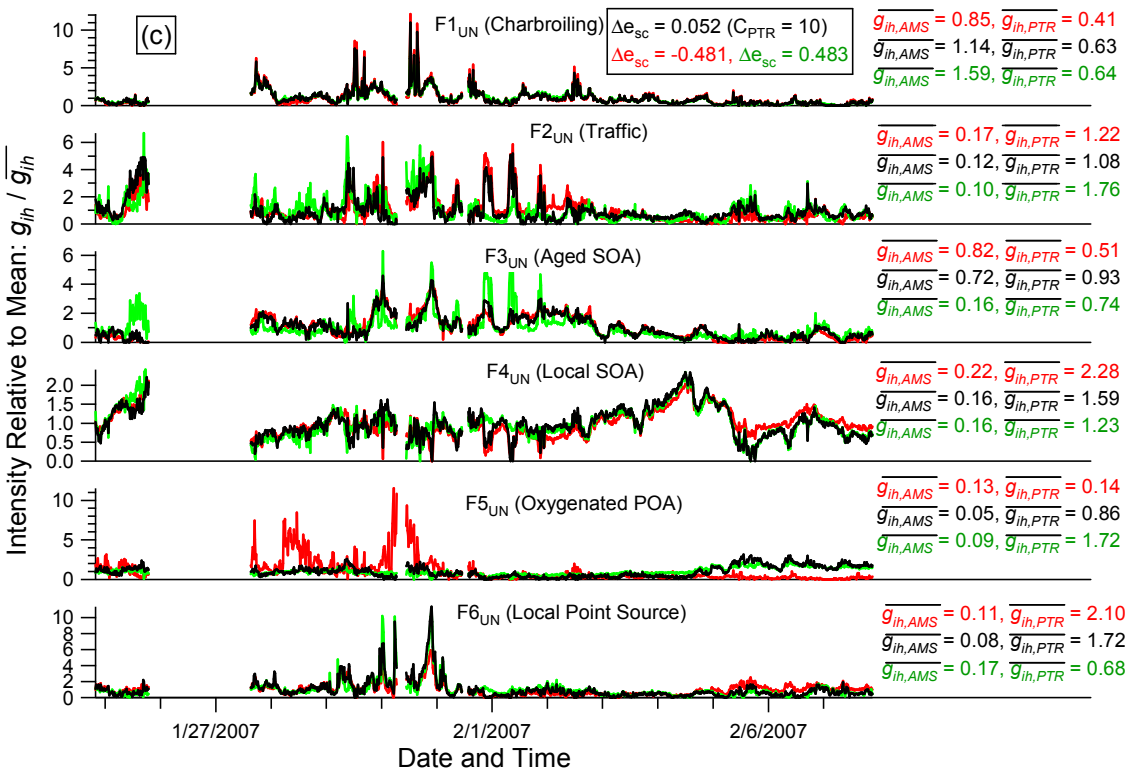
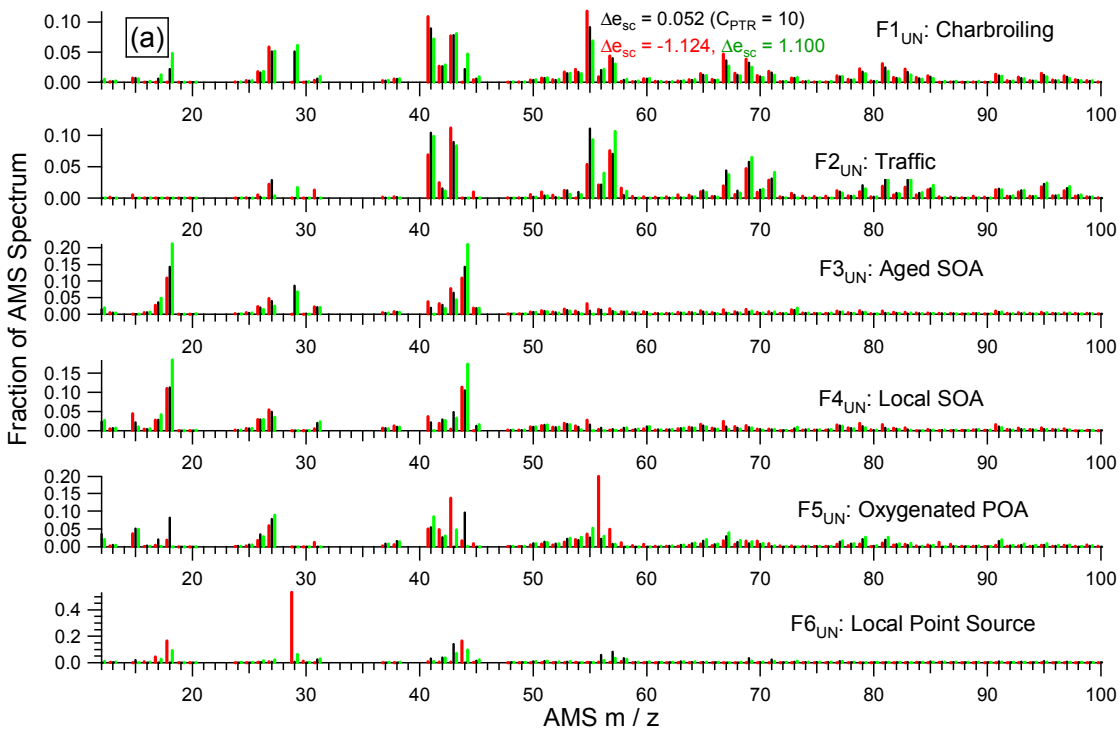
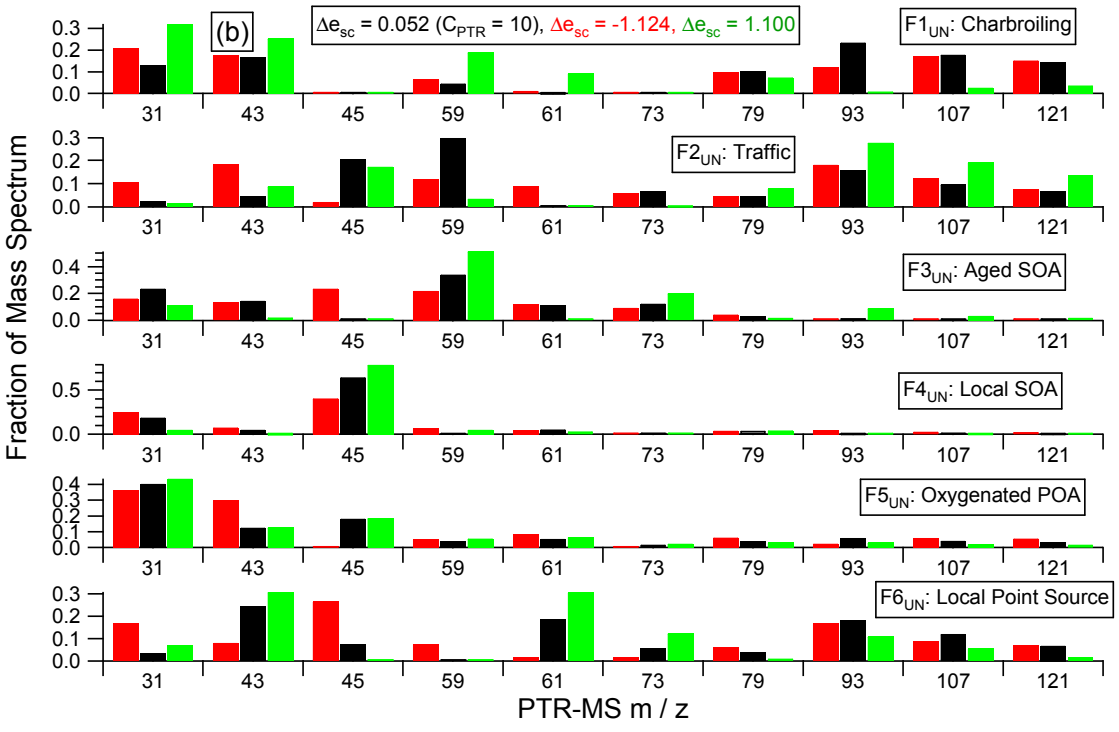


Figure S14. Factor mass spectra (a,b) and time series (c) for the 6-factor solution to the unified dataset at $\overline{\Delta e_{sc}}$ = -0.481 (C_{PTR} = 4, red), $\overline{\Delta e_{sc}}$ = 0.052 (C_{PTR} = 10, black), and $\overline{\Delta e_{sc}}$ = 0.483 (C_{PTR} = 30, green). Units for $\overline{g_{ih,AMS}}$ and $\overline{g_{ih,PTR}}$ are μg/m^3 and ppbv, respectively.


(a)
Δe_sc = 0.052 (C_PTR = 10)
Δe_sc = -1.124, Δe_sc = 1.100
F1_UN: Charbroiling
F2_UN: Traffic
F3_UN: Aged SOA
F4_UN: Local SOA
F5_UN: Oxygenated POA
F6_UN: Local Point Source
Fraction of AMS Spectrum
AMS m / z

1


(b)
Δe_sc = 0.052 (C_PTR = 10), Δe_sc = -1.124, Δe_sc = 1.100
F1_UN: Charbroiling
F2_UN: Traffic
F3_UN: Aged SOA
F4_UN: Local SOA
F5_UN: Oxygenated POA
F6_UN: Local Point Source
Fraction of Mass Spectrum
PTR-MS m / z

2

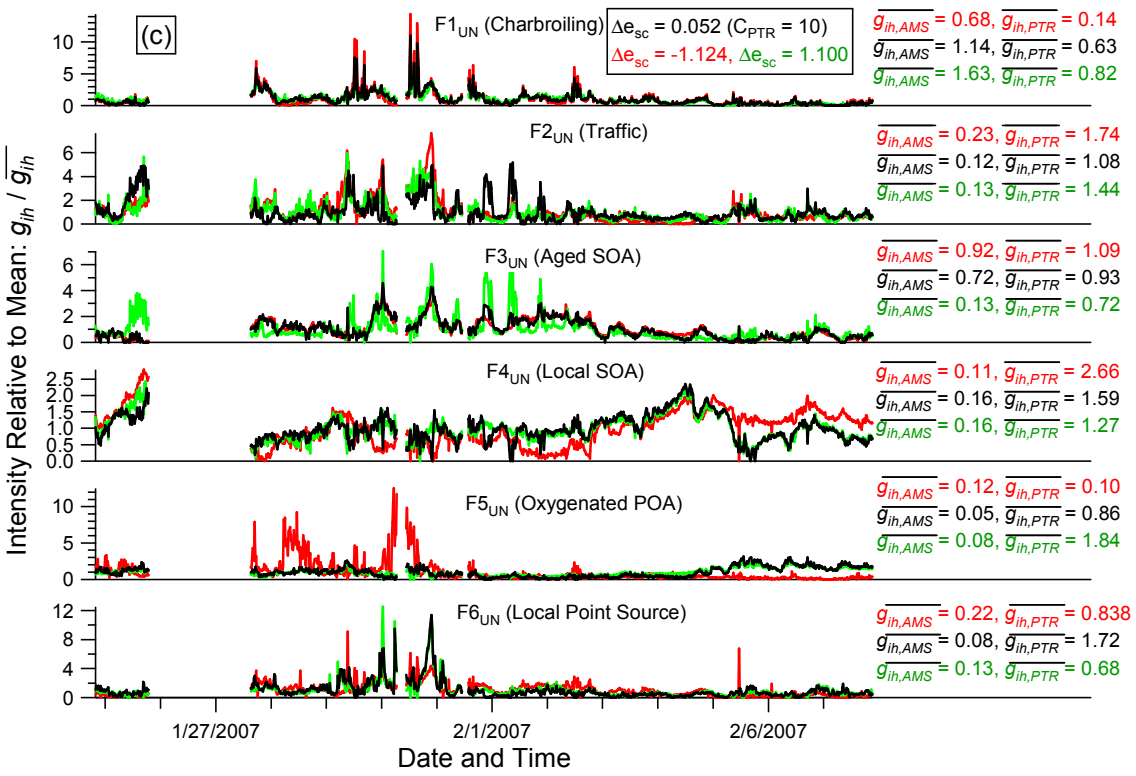


Figure S15. Factor mass spectra (a,b) and time series (c) for the 6-factor solution to the unified dataset at $\Delta\overline{e_{sc}}$ = -1.124 (C_{PTR} = 2, red), $\Delta\overline{e_{sc}}$ = 0.052 (C_{PTR} = 10, black), and $\Delta\overline{e_{sc}}$ = 1.100 (C_{PTR} = 52, green). Units for $\overline{g_{ih,AMS}}$ and $\overline{g_{ih,PTR}}$ are μg/m^3 and ppbv, respectively.

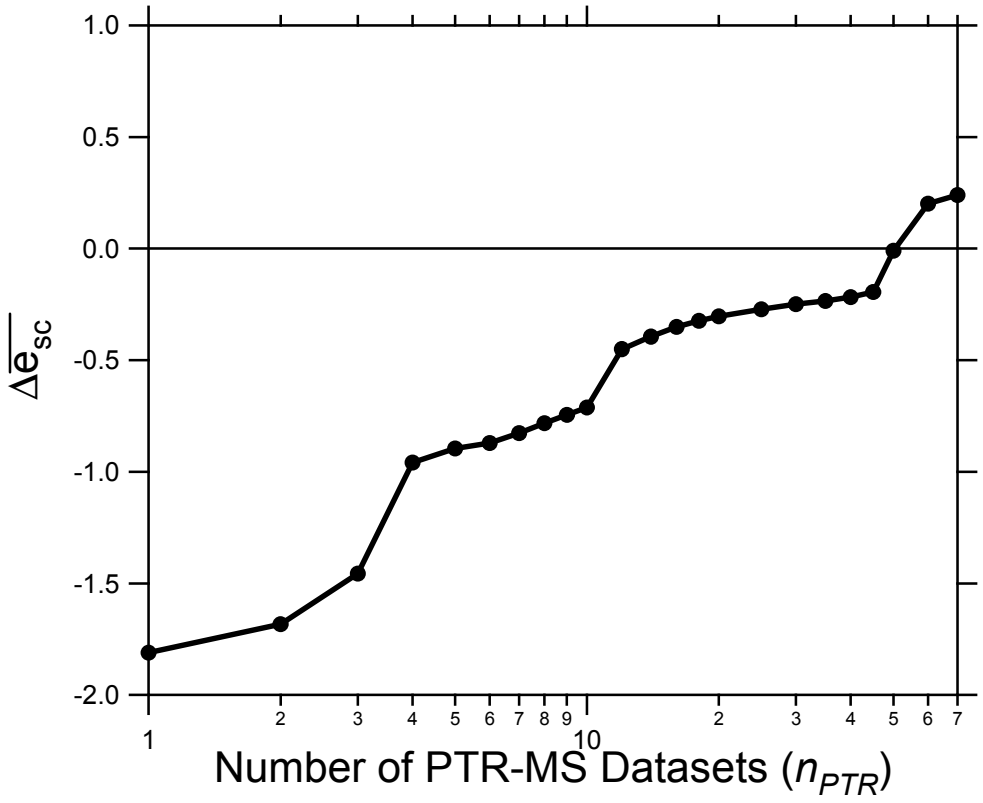


Figure S16. $\Delta\overline{e_{sc}}$ as a function of the number of included PTR-MS datasets (n_{PTR}) for the PTR-redundancy method.

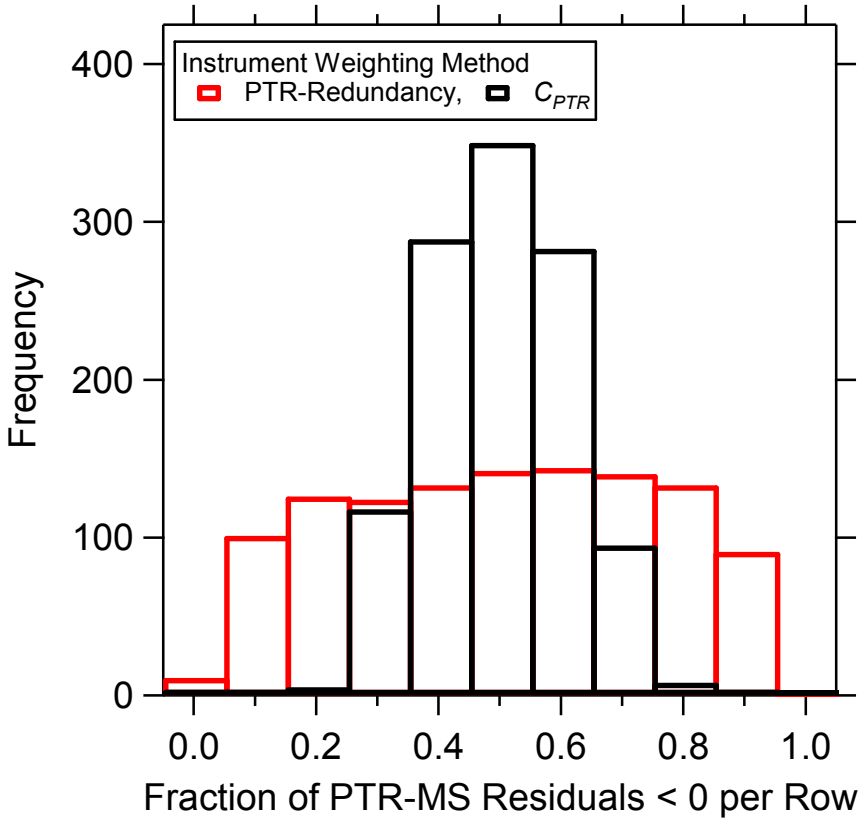
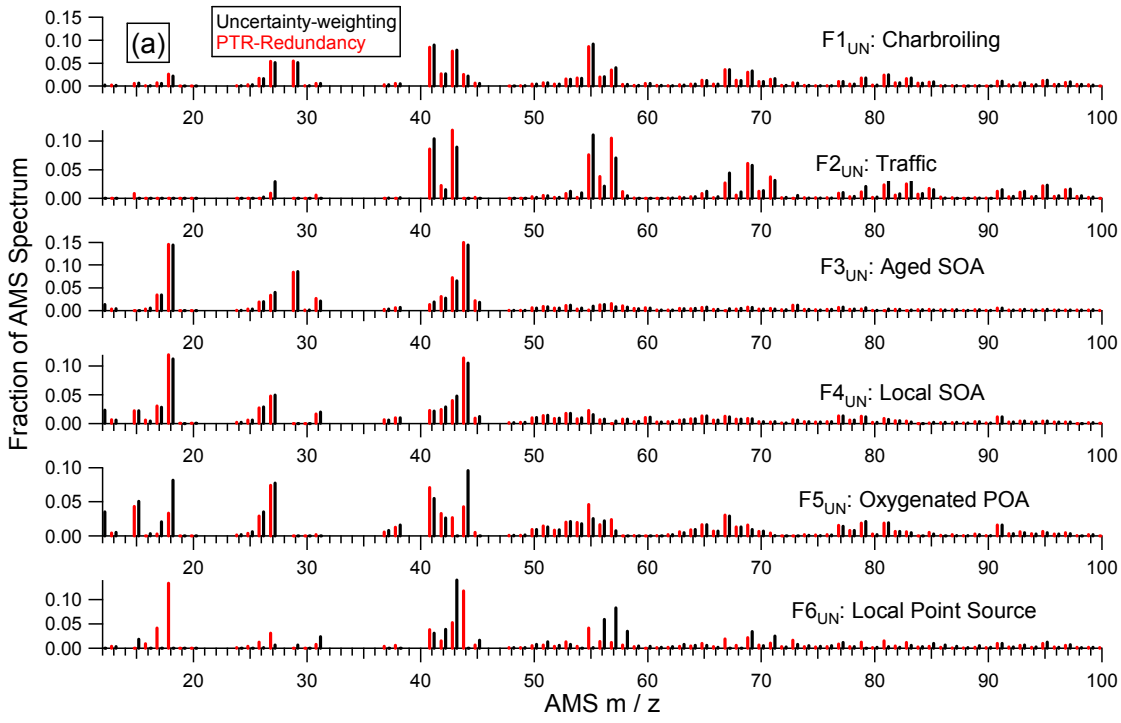
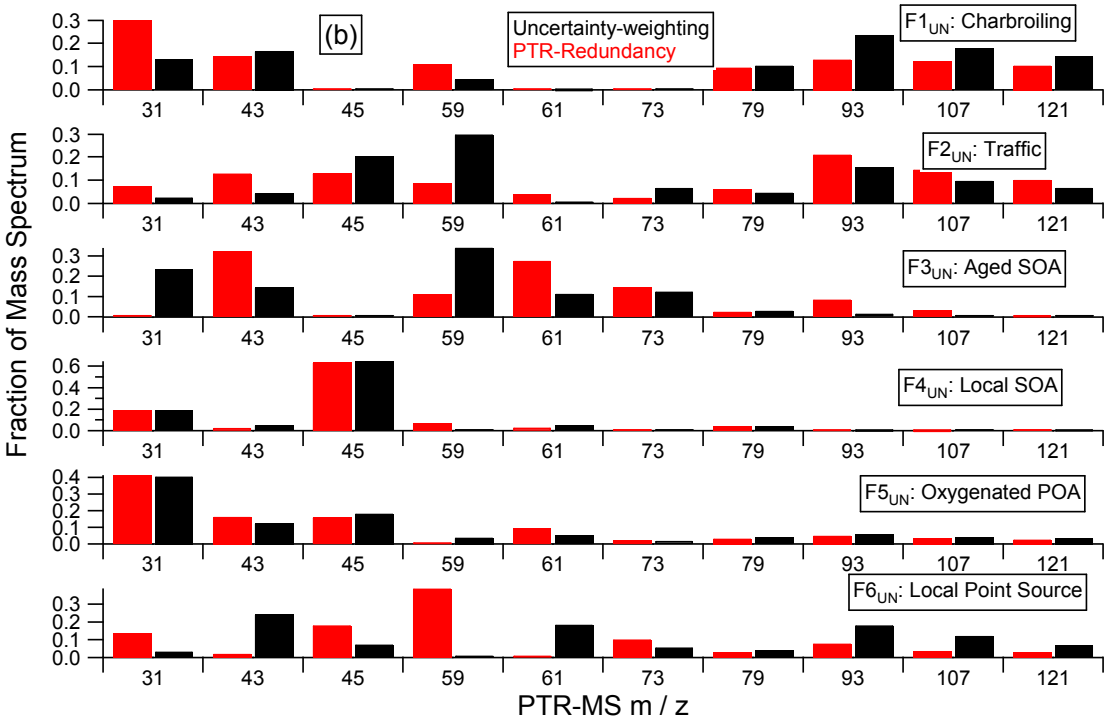


Figure S17. Frequency of negative PTR-MS residuals per row (i.e. time point) of residual matrix **E**. Shown are 6-factor solutions for n_{PTR} = 50 (PTR-redundancy method) and C_{PTR} = 10 (uncertainty-weighting method) for the unified dataset.


(a)
Uncertainty-weighting
PTR-Redundancy
F1UN: Charbroiling
F2UN: Traffic
F3UN: Aged SOA
F4UN: Local SOA
F5UN: Oxygenated POA
F6UN: Local Point Source
Fraction of AMS Spectrum
AMS m / z

1


(b)
Uncertainty-weighting
PTR-Redundancy
F1UN: Charbroiling
F2UN: Traffic
F3UN: Aged SOA
F4UN: Local SOA
F5UN: Oxygenated POA
F6UN: Local Point Source
Fraction of Mass Spectrum
PTR-MS m / z

2

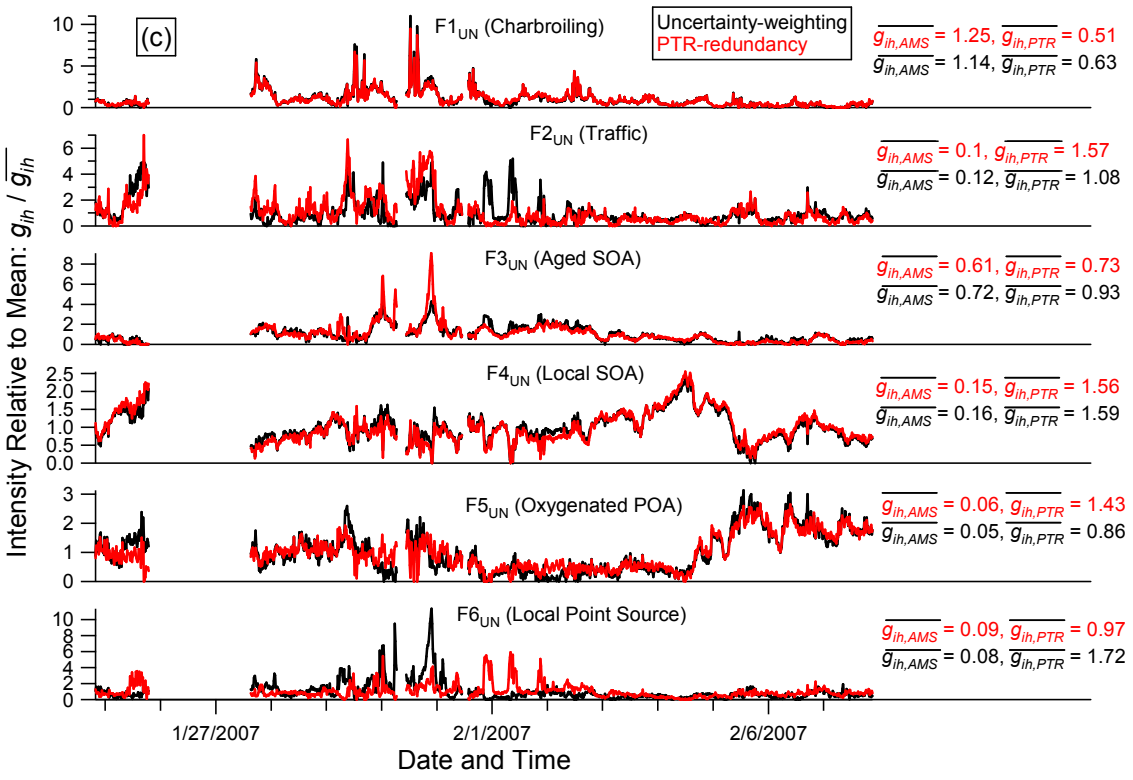


Figure S18. Comparison of factor mass spectra (a,b) and time series (c) for the 6-factor solution to the unified dataset obtained from the uncertainty-weighting method at $\overline{\Delta e_{sc}}$ = 0.052 (C_{PTR} = 10) and the PTR-redundancy method at $\overline{\Delta e_{sc}}$ = -0.0098 (n_{PTR} = 50).

1

m/z	AMS-OOA-1	AMS-HOA	AMS-Charbroiling	AMS-BBOA	AMS-Point Source (North)
12	1.69E-02	2.10E-08	6.86E-03	1.88E-03	7.58E-03
13	5.01E-03	8.66E-04	4.28E-03	1.19E-03	2.22E-03
15	2.53E-10	9.39E-10	6.60E-02	6.46E-10	4.66E-09
16	6.29E-03	8.40E-07	2.03E-07	8.33E-04	3.33E-03
17	3.93E-02	3.38E-07	6.05E-08	5.22E-03	2.08E-02
18	1.57E-01	8.01E-08	1.03E-07	2.09E-02	8.32E-02
19	1.87E-04	9.84E-07	6.99E-07	2.46E-05	9.87E-05
20	3.14E-04	6.89E-07	4.20E-07	4.15E-05	1.66E-04
24	1.68E-03	5.92E-06	1.33E-03	6.58E-04	5.35E-04
25	4.85E-03	2.99E-04	4.80E-03	2.62E-03	2.03E-03
26	2.31E-02	3.29E-03	2.59E-02	1.59E-02	1.44E-02
27	4.20E-02	2.16E-02	5.81E-02	5.40E-02	4.52E-02
29	7.35E-02	4.21E-02	3.65E-08	5.07E-02	8.52E-02
30	1.74E-03	5.18E-04	9.76E-09	1.09E-03	1.86E-03
31	2.32E-02	7.91E-03	1.36E-02	2.43E-03	1.28E-02
37	4.63E-03	8.05E-04	5.83E-03	2.86E-03	2.17E-03
38	7.66E-03	1.85E-03	1.08E-02	4.78E-03	4.08E-03
41	1.40E-02	8.09E-02	5.85E-02	1.02E-01	3.62E-02
42	2.84E-02	2.10E-02	3.13E-02	2.43E-02	3.90E-02
43	5.71E-02	1.07E-01	5.74E-02	7.02E-02	1.15E-01
44	1.57E-01	1.76E-07	1.42E-03	2.08E-02	8.28E-02
45	1.93E-02	6.31E-03	7.39E-03	4.22E-03	1.16E-02
48	1.16E-03	6.86E-04	1.36E-03	3.69E-04	4.19E-04
49	1.38E-03	5.24E-04	1.56E-03	4.95E-04	5.83E-04
50	6.91E-03	3.79E-03	9.63E-03	3.24E-03	3.55E-03
51	1.00E-02	6.81E-03	1.50E-02	5.69E-03	5.53E-03
52	6.57E-03	2.82E-03	9.41E-03	3.46E-03	3.80E-03
53	1.34E-02	1.06E-02	2.10E-02	1.50E-02	9.40E-03
54	6.98E-03	1.95E-03	1.72E-02	2.01E-02	1.34E-02
55	4.89E-03	7.30E-02	5.28E-02	1.10E-01	2.37E-02
56	8.22E-03	1.77E-02	2.61E-02	7.39E-03	1.45E-01
57	1.30E-08	7.81E-02	2.08E-02	3.94E-02	3.82E-02
58	7.20E-03	1.51E-02	2.07E-03	2.09E-03	1.22E-02
59	4.67E-03	1.92E-03	2.51E-03	1.07E-03	3.52E-03
60	7.10E-03	1.24E-03	1.46E-02	4.67E-03	2.09E-03
61	2.43E-03	8.81E-04	3.05E-03	1.29E-03	8.17E-04
62	2.32E-03	1.36E-03	2.74E-03	7.33E-04	8.34E-04
63	5.02E-03	3.57E-03	6.44E-03	1.89E-03	1.50E-03
64	5.47E-03	3.40E-03	8.71E-03	3.80E-03	2.78E-03
65	8.45E-03	9.40E-03	1.66E-02	1.30E-02	4.90E-03
66	3.79E-03	2.28E-03	7.15E-03	4.25E-03	1.93E-03
67	3.90E-03	2.50E-02	2.76E-02	4.36E-02	9.36E-03
68	5.85E-03	6.73E-03	1.29E-02	1.39E-02	4.10E-03
69	3.75E-03	5.01E-02	2.00E-02	3.53E-02	1.21E-02
70	3.13E-03	1.01E-02	7.54E-03	1.03E-02	1.14E-02
71	1.58E-03	3.00E-02	8.01E-03	1.66E-02	7.50E-03

72	2.33E-03	2.16E-03	7.48E-04	1.32E-03	2.25E-03
73	1.27E-02	7.36E-03	1.27E-03	7.05E-03	6.89E-03
74	3.44E-03	2.14E-03	2.43E-03	1.20E-03	1.82E-03
75	2.35E-03	1.87E-03	1.73E-03	6.02E-04	1.03E-03
76	2.98E-03	1.89E-03	2.17E-03	5.17E-04	1.20E-03
77	8.36E-03	9.80E-03	1.54E-02	9.46E-03	4.35E-03
78	3.95E-03	2.93E-03	7.89E-03	4.45E-03	1.98E-03
79	6.83E-03	1.18E-02	1.81E-02	2.06E-02	4.25E-03
80	1.35E-03	2.15E-03	2.82E-03	2.12E-03	4.84E-04
81	2.78E-03	2.20E-02	1.81E-02	2.86E-02	6.36E-03
82	3.44E-03	5.67E-03	6.90E-03	7.52E-03	3.92E-03
83	3.33E-08	2.13E-02	8.82E-03	2.05E-02	4.76E-03
84	2.34E-03	5.76E-03	3.04E-03	7.64E-03	2.29E-03
85	1.13E-03	1.40E-02	4.81E-03	9.79E-03	4.21E-03
86	1.99E-03	1.76E-03	9.73E-04	6.68E-09	9.84E-03
87	2.19E-03	1.22E-03	1.78E-03	7.69E-04	5.59E-03
88	8.94E-04	5.89E-04	8.10E-04	1.45E-04	7.86E-04
89	2.45E-03	2.03E-03	3.03E-03	6.65E-04	7.58E-04
90	1.31E-03	9.12E-04	1.13E-03	2.43E-04	5.28E-04
91	6.56E-03	1.22E-02	1.55E-02	1.17E-02	2.07E-03
92	2.01E-03	2.84E-03	3.80E-03	2.65E-03	6.71E-04
93	2.46E-03	9.40E-03	6.89E-03	7.80E-03	2.00E-03
94	1.79E-03	2.84E-03	3.75E-03	2.84E-03	6.47E-04
95	1.70E-03	1.88E-02	8.56E-03	1.38E-02	3.35E-03
96	2.18E-03	3.41E-03	3.78E-03	3.83E-03	1.35E-03
97	1.08E-03	1.30E-02	4.95E-03	9.83E-03	3.12E-03
98	1.65E-03	3.21E-03	2.01E-03	4.39E-03	1.34E-03
99	2.16E-03	2.09E-03	1.92E-03	2.54E-03	4.39E-03
100	8.99E-04	5.36E-04	6.42E-04	4.40E-04	8.62E-04

1 Table S1. Factor profiles for the 5-factor solution to the AMS dataset, $m/z \leq 100$.

1

m/z	PTR-Traffic	PTR-LRT + Local Source	PTR-LRT + Painting	PTR-LRT + Local Oxidation	PTR-Oxygenates
31	7.23E-02	8.90E-02	1.07E-01	1.60E-01	5.07E-01
43	1.35E-01	2.63E-01	5.79E-02	4.12E-02	1.18E-01
45	7.60E-02	8.33E-02	1.26E-01	6.06E-01	1.83E-01
59	6.99E-02	5.69E-02	3.94E-01	6.40E-02	3.38E-02
61	1.57E-02	2.39E-01	2.43E-02	4.48E-02	4.79E-02
73	7.33E-03	9.06E-02	1.30E-01	4.10E-03	1.61E-02
79	8.04E-02	2.61E-02	3.22E-02	3.93E-02	3.26E-02
93	2.41E-01	8.40E-02	7.29E-02	1.84E-02	2.38E-02
107	1.76E-01	4.62E-02	3.18E-02	7.73E-03	1.95E-02
121	1.26E-01	2.17E-02	2.42E-02	1.49E-02	1.79E-02

2 Table S2. Factor profiles for the 5-factor solution to the PTR-MS dataset.

1

PTR-MS m/z	UN-Charbroiling	UN-Traffic	UN-Aged SOA	UN-Local SOA	UN-Oxygenated POA	UN-Local Point Source
31	1.30E-01	2.51E-02	2.34E-01	1.88E-01	4.04E-01	3.38E-02
43	1.66E-01	4.52E-02	1.44E-01	5.06E-02	1.25E-01	2.44E-01
45	2.72E-04	2.02E-01	8.60E-09	6.45E-01	1.82E-01	7.27E-02
59	4.59E-02	2.97E-01	3.39E-01	1.37E-02	3.80E-02	3.26E-10
61	1.08E-03	1.50E-10	1.13E-01	5.25E-02	5.46E-02	1.85E-01
73	1.56E-10	6.60E-02	1.25E-01	1.28E-10	1.87E-02	5.65E-02
79	1.03E-01	4.57E-02	2.92E-02	3.74E-02	4.09E-02	3.90E-02
93	2.34E-01	1.56E-01	1.55E-02	5.87E-03	5.96E-02	1.81E-01
107	1.78E-01	9.64E-02	4.51E-10	3.61E-10	4.17E-02	1.21E-01
121	1.42E-01	6.64E-02	1.04E-10	6.73E-03	3.57E-02	6.79E-02

AMS m/z	UN-Charbroiling	UN-Traffic	UN-Aged SOA	UN-Local SOA	UN-Oxygenated POA	UN-Local Point Source
12	2.24E-03	5.50E-09	1.39E-02	2.31E-02	3.55E-02	8.16E-09
13	1.60E-03	1.54E-09	4.38E-03	6.21E-03	5.32E-03	2.92E-03
15	6.71E-03	4.23E-10	7.08E-11	2.20E-02	5.07E-02	1.80E-02
16	9.37E-04	1.34E-08	5.58E-03	4.43E-03	3.39E-03	2.29E-05
17	5.82E-03	2.74E-09	3.50E-02	2.82E-02	2.08E-02	2.06E-07
18	2.22E-02	3.20E-09	1.43E-01	1.12E-01	8.18E-02	9.63E-09
19	2.78E-05	4.93E-08	1.66E-04	1.38E-04	9.36E-05	2.55E-07
20	4.65E-05	2.19E-08	2.80E-04	2.32E-04	1.58E-04	1.49E-07
24	6.72E-04	2.71E-09	1.36E-03	2.10E-03	2.00E-03	2.42E-04
25	2.70E-03	1.41E-04	4.12E-03	5.98E-03	6.06E-03	2.30E-05
26	1.63E-02	2.38E-03	2.01E-02	2.86E-02	3.51E-02	1.42E-03
27	5.12E-02	2.87E-02	3.96E-02	4.94E-02	7.75E-02	6.65E-03
29	5.12E-02	2.34E-10	8.57E-02	1.92E-10	3.29E-10	6.60E-03
30	1.12E-03	3.94E-09	1.82E-03	1.87E-09	3.05E-09	1.63E-07
31	6.18E-03	6.62E-10	2.12E-02	1.98E-02	1.20E-09	2.41E-02
37	2.98E-03	6.19E-04	4.08E-03	6.16E-03	8.36E-03	2.08E-04
38	5.25E-03	1.38E-03	6.88E-03	1.02E-02	1.59E-02	9.60E-09
41	8.92E-02	1.04E-01	1.93E-02	2.18E-02	5.48E-02	3.13E-02
42	2.66E-02	1.55E-02	2.78E-02	2.90E-02	2.63E-02	3.90E-02
43	7.83E-02	8.92E-02	6.49E-02	4.79E-02	1.83E-08	1.39E-01
44	2.23E-02	1.39E-09	1.43E-01	1.04E-01	9.55E-02	1.60E-09
45	6.25E-03	3.30E-10	1.83E-02	1.21E-02	2.27E-09	1.62E-02
48	4.99E-04	2.83E-04	1.05E-03	1.65E-03	1.00E-03	1.63E-03
49	6.19E-04	3.08E-04	1.22E-03	1.91E-03	1.28E-03	1.26E-03
50	4.04E-03	2.00E-03	6.17E-03	1.05E-02	9.41E-03	8.12E-03
51	6.95E-03	4.24E-03	9.06E-03	1.47E-02	1.35E-02	1.29E-02
52	4.20E-03	1.51E-03	5.84E-03	9.52E-03	9.03E-03	5.89E-03
53	1.50E-02	1.25E-02	1.24E-02	1.78E-02	2.14E-02	7.61E-03
54	1.72E-02	9.50E-03	6.20E-03	9.71E-03	1.83E-02	2.67E-10
55	9.14E-02	1.11E-01	1.02E-02	1.59E-02	2.56E-02	1.52E-03
56	2.05E-02	2.14E-02	1.34E-02	7.82E-03	2.22E-02	5.89E-02
57	4.00E-02	7.03E-02	8.86E-03	4.61E-03	7.81E-03	8.25E-02

58	3.79E-03	4.42E-03	8.15E-03	7.45E-03	4.62E-10	3.45E-02
59	1.61E-03	9.21E-10	4.57E-03	4.06E-03	9.17E-05	4.55E-03
60	5.77E-03	4.13E-10	6.02E-03	1.11E-02	5.02E-10	3.77E-03
61	1.50E-03	2.12E-04	2.22E-03	2.87E-03	2.05E-04	1.81E-03
62	1.02E-03	5.33E-04	2.11E-03	3.29E-03	2.00E-03	3.10E-03
63	2.54E-03	1.14E-03	4.68E-03	6.62E-03	5.02E-03	7.83E-03
64	4.15E-03	2.72E-03	4.95E-03	8.38E-03	9.42E-03	6.01E-03
65	1.24E-02	1.26E-02	7.76E-03	1.33E-02	1.69E-02	5.76E-03
66	4.18E-03	2.87E-03	3.41E-03	6.00E-03	7.03E-03	1.83E-03
67	3.61E-02	4.38E-02	4.54E-03	1.14E-02	2.94E-02	8.78E-10
68	1.23E-02	1.16E-02	5.42E-03	7.88E-03	1.35E-02	1.29E-09
69	3.27E-02	5.76E-02	7.43E-03	8.68E-03	9.54E-03	3.41E-02
70	1.00E-02	1.34E-02	4.16E-03	3.68E-03	7.17E-03	5.27E-03
71	1.59E-02	3.13E-02	3.97E-03	3.57E-03	8.77E-04	2.46E-02
72	1.47E-03	1.56E-03	2.45E-03	1.19E-03	5.35E-09	2.73E-03
73	6.75E-03	5.09E-03	1.24E-02	5.96E-03	4.65E-09	7.76E-03
74	1.50E-03	8.18E-04	3.29E-03	3.24E-03	9.99E-04	4.90E-03
75	8.60E-04	6.87E-04	2.25E-03	2.57E-03	9.52E-04	4.34E-03
76	8.62E-04	5.90E-04	2.80E-03	3.26E-03	1.28E-03	4.96E-03
77	9.74E-03	1.02E-02	7.73E-03	1.32E-02	1.41E-02	1.14E-02
78	4.47E-03	3.63E-03	3.52E-03	6.22E-03	8.30E-03	3.30E-03
79	1.76E-02	2.06E-02	6.39E-03	1.18E-02	2.12E-02	4.65E-05
80	2.04E-03	2.32E-03	1.30E-03	2.15E-03	2.18E-03	2.09E-03
81	2.45E-02	3.34E-02	3.88E-03	7.25E-03	1.93E-02	3.02E-03
82	6.95E-03	8.01E-03	3.48E-03	4.94E-03	6.94E-03	2.02E-03
83	1.74E-02	2.94E-02	1.94E-03	2.76E-03	5.02E-03	6.17E-03
84	6.66E-03	8.10E-03	2.56E-03	4.85E-10	3.19E-09	3.03E-03
85	9.18E-03	1.52E-02	2.13E-03	1.94E-03	3.01E-03	1.00E-02
86	1.02E-03	7.07E-04	2.17E-03	1.94E-03	4.49E-09	6.52E-03
87	1.35E-03	1.26E-09	2.33E-03	1.87E-03	9.56E-04	4.36E-03
88	3.14E-04	3.14E-09	8.78E-04	1.05E-03	4.74E-04	1.72E-03
89	1.04E-03	5.26E-04	2.31E-03	3.39E-03	1.88E-03	4.98E-03
90	4.30E-04	2.46E-04	1.22E-03	1.45E-03	6.74E-04	2.33E-03
91	1.12E-02	1.50E-02	6.29E-03	1.13E-02	1.61E-02	9.78E-03
92	2.62E-03	3.40E-03	1.89E-03	2.74E-03	3.43E-03	2.85E-03
93	7.25E-03	1.21E-02	2.74E-03	4.53E-03	5.00E-03	6.46E-03
94	2.75E-03	3.18E-03	1.71E-03	2.82E-03	2.79E-03	2.65E-03
95	1.25E-02	2.28E-02	2.94E-03	4.15E-03	4.76E-03	1.24E-02
96	3.58E-03	4.32E-03	2.11E-03	3.04E-03	2.68E-03	2.20E-03
97	8.90E-03	1.59E-02	1.90E-03	2.66E-03	3.28E-03	7.51E-03
98	3.86E-03	4.68E-03	1.70E-03	5.33E-09	5.03E-05	1.59E-03
99	2.62E-03	2.18E-03	2.31E-03	1.65E-03	2.29E-03	2.30E-03
100	5.29E-04	3.94E-04	8.91E-04	6.86E-04	1.76E-04	9.92E-04

Table S1. Factor profiles for the 6-factor solution to the UN dataset. AMS $m/z \leq 100$ are shown.