SUPPLEMENTAL INFORMATION

For the paper

Interpretation and Sensitivity Analysis of Organic Components Extracted by Positive Matrix Factorization of Aerosol Mass Spectrometric Data

I. M. Ulbrich,[1,2] M. Canagaratna,[3] Q. Zhang,[4] D. Worsnop,[3] and J. L. Jimenez[1,2,*]

[1]Cooperative Institute for Research in the Environmental Sciences (CIRES), and [2]Department of Chemistry and Biochemistry, University of Colorado, Boulder, CO, 80309

[3]Aerodyne Research, Inc., Billerica, MA, 01821-3976

[4]Atmospheric Sciences Research Center, University at Albany, State University of New York, Albany, NY 12203

[*]Corresponding author: email jose.jimenez@colorado.edu

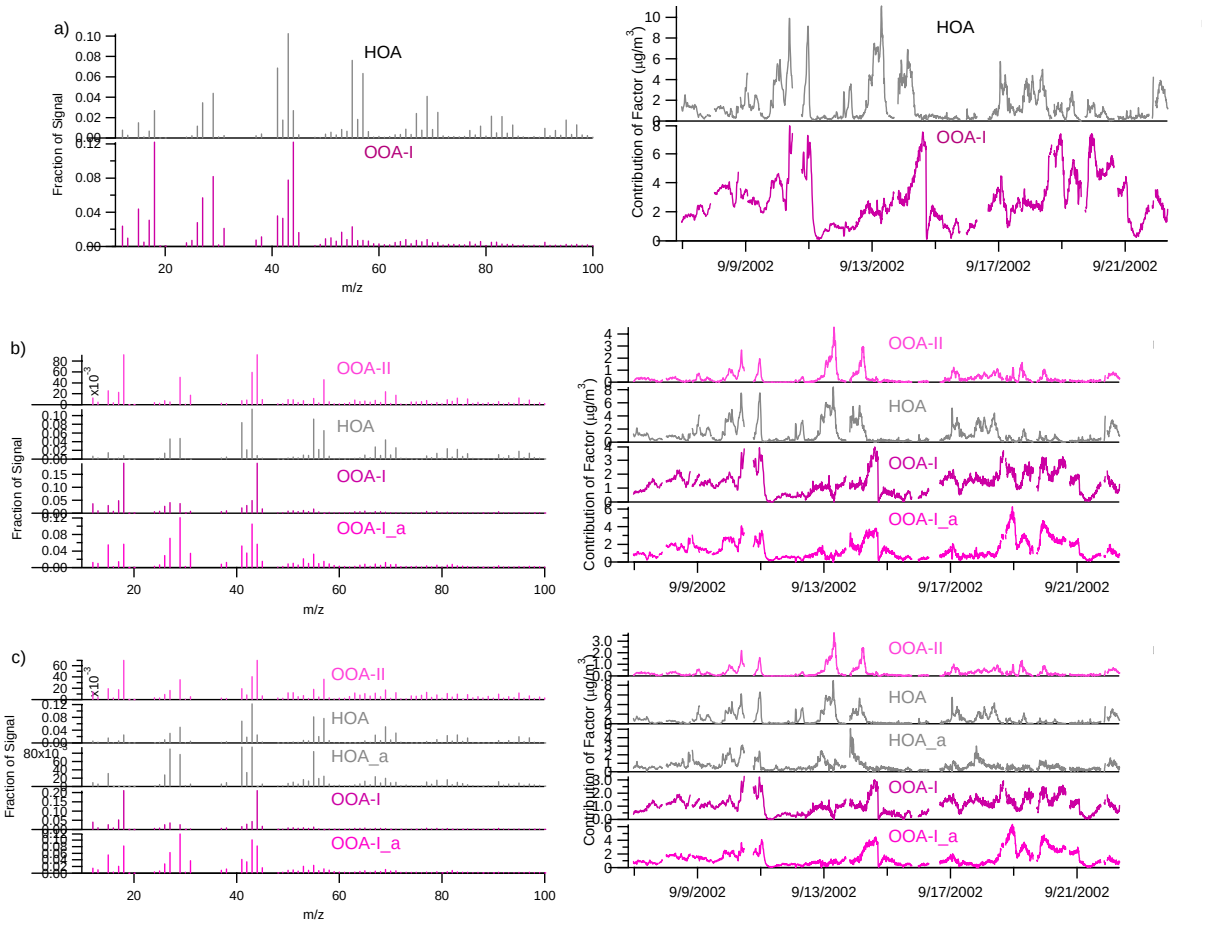

Figure S1. PMF solutions of the real Pittsburgh case with a) 2 factors, b) 4 factors, and c) 5 factors.

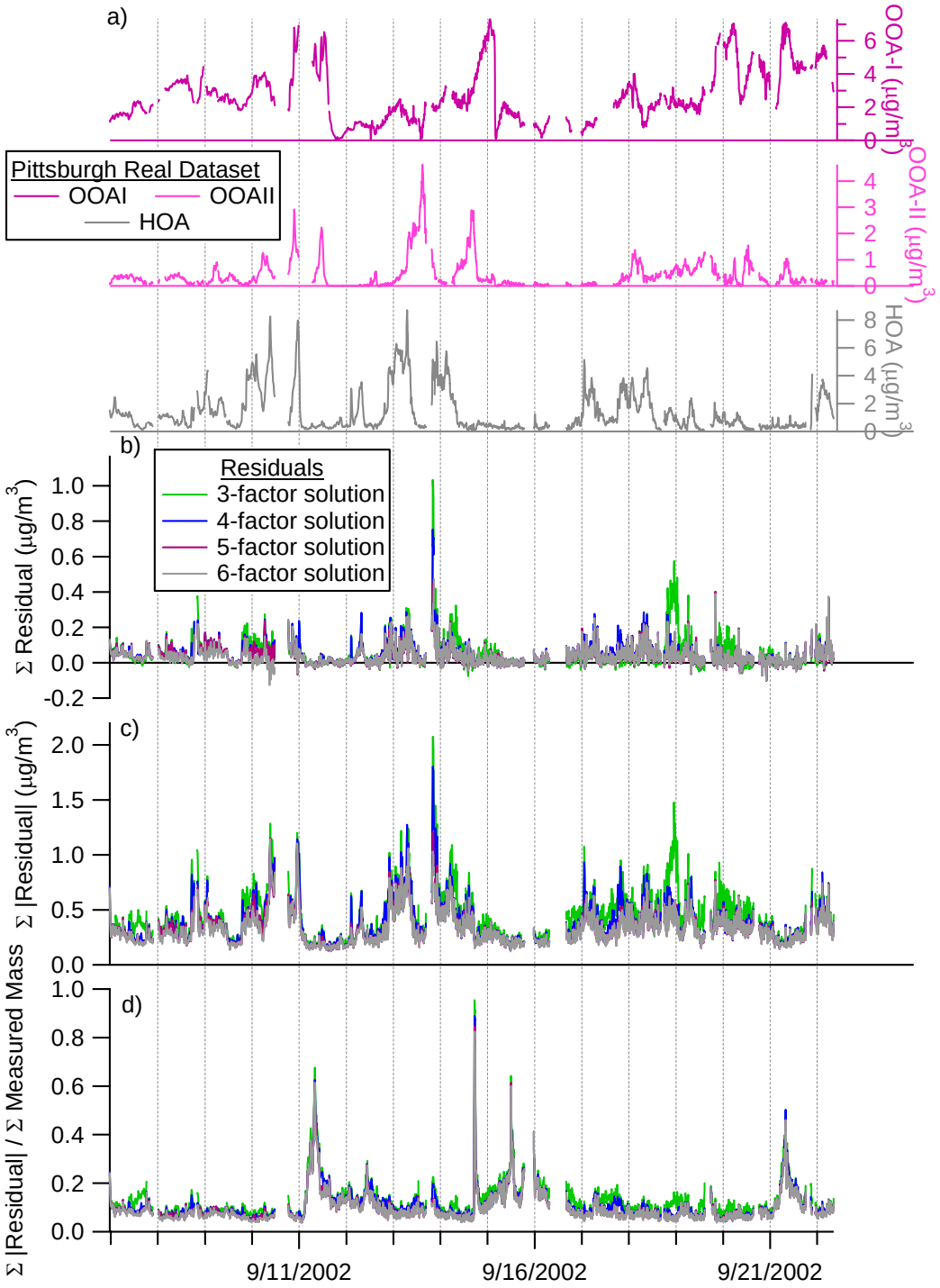

Figure S2. a) OOA-I, OOA-II, and HOA time series from the 3-factor solution of the real Pittsburgh dataset. b) Total Residual, c) Total absolute residual, and d) absolute residual normalized by total signal for the 3- to 6-factor solutions of the real Pittsburgh case.

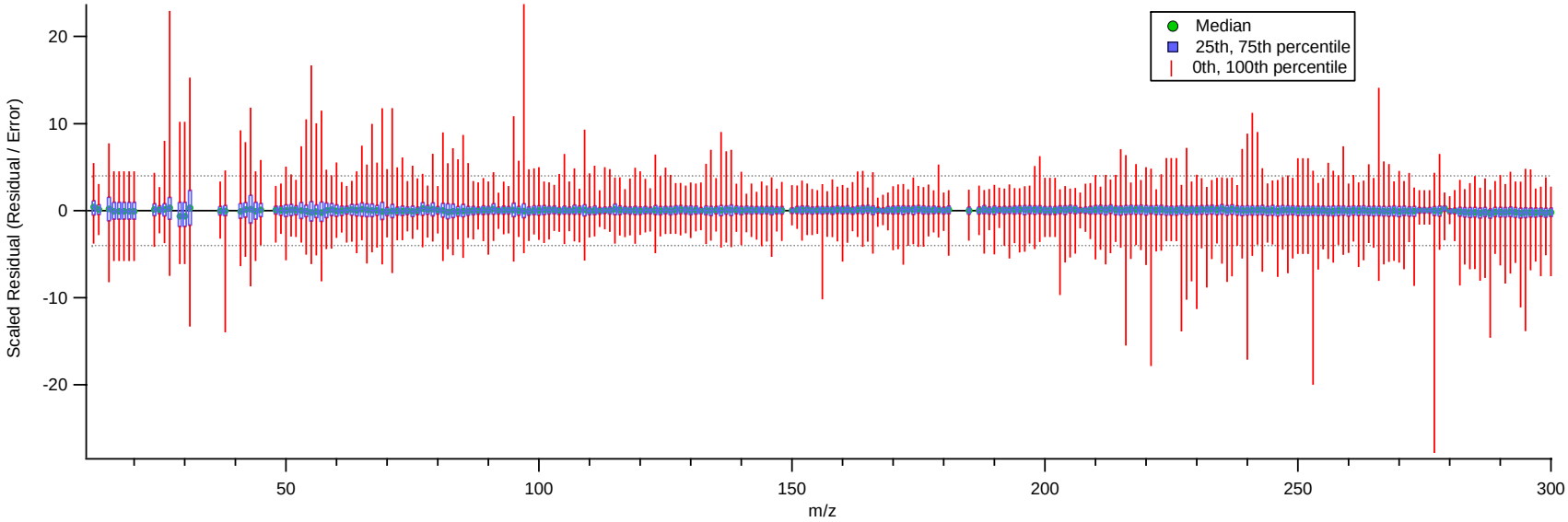

Figure S3. Distributions of residuals for each *m/z* for the 3-factor solution of the real Pittsbugh case.

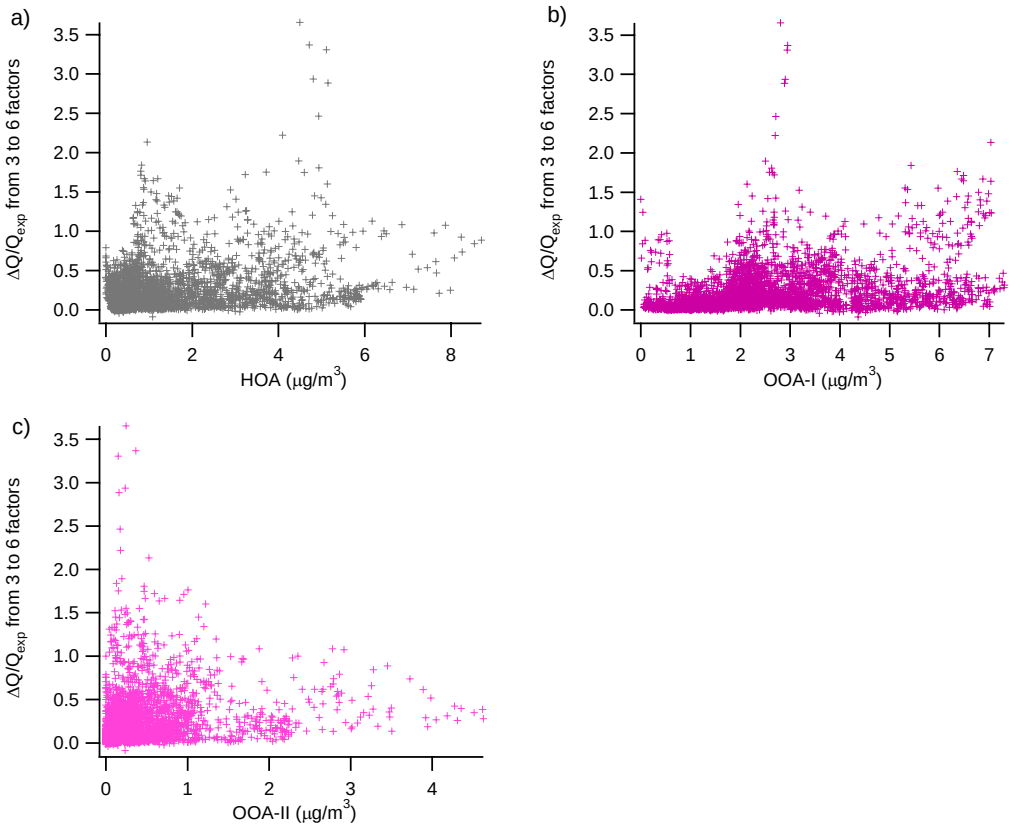

Figure S4. Change in Q/Q_{exp} in the real Pittsburgh dataset from 3 to 6 factors vs. a) HOA contribution, b) OOA-I contribution, and c) OOA-II contribution from the 3-factor solution.

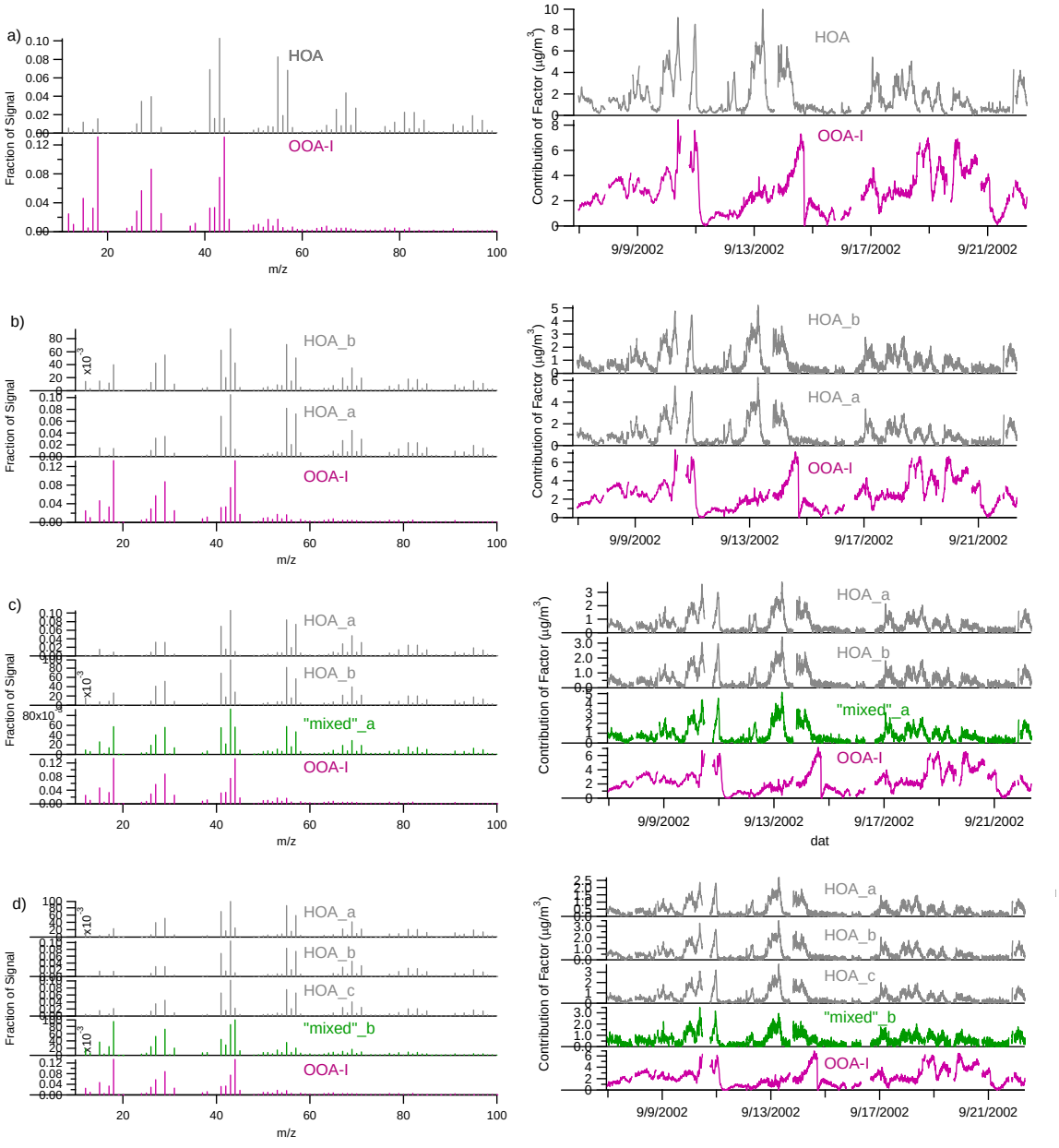

Figure S5. PMF solutions of the 2-factor synthetic base case with a) 2 factors, b) 3 factors, c) 4 factors, and d) 5 factors.

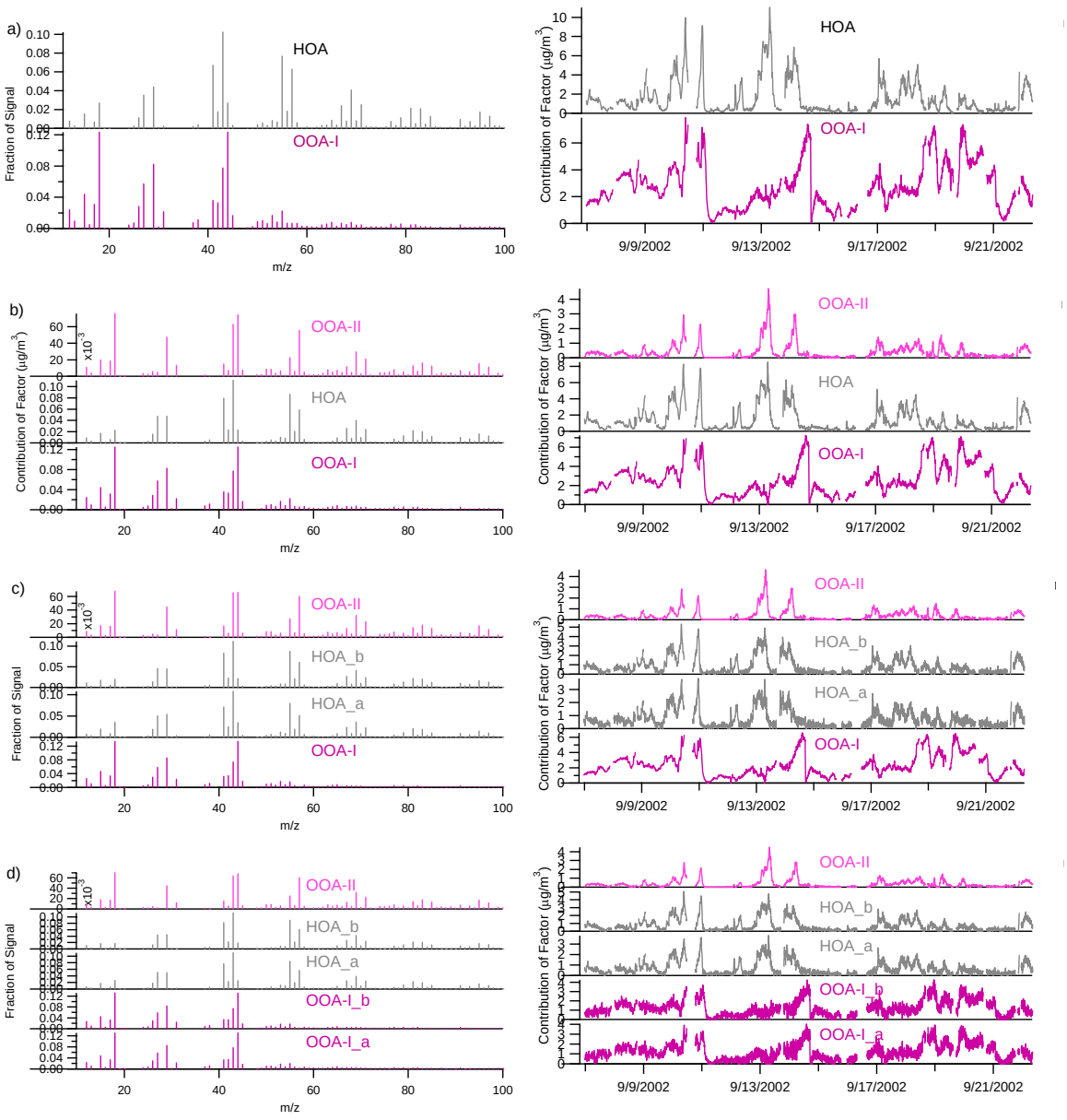

Figure S6. PMF solutions of the 3-factor synthetic base case with a) 2 factors, b) 3 factors, c) 4 factors, and d) 5 factors.

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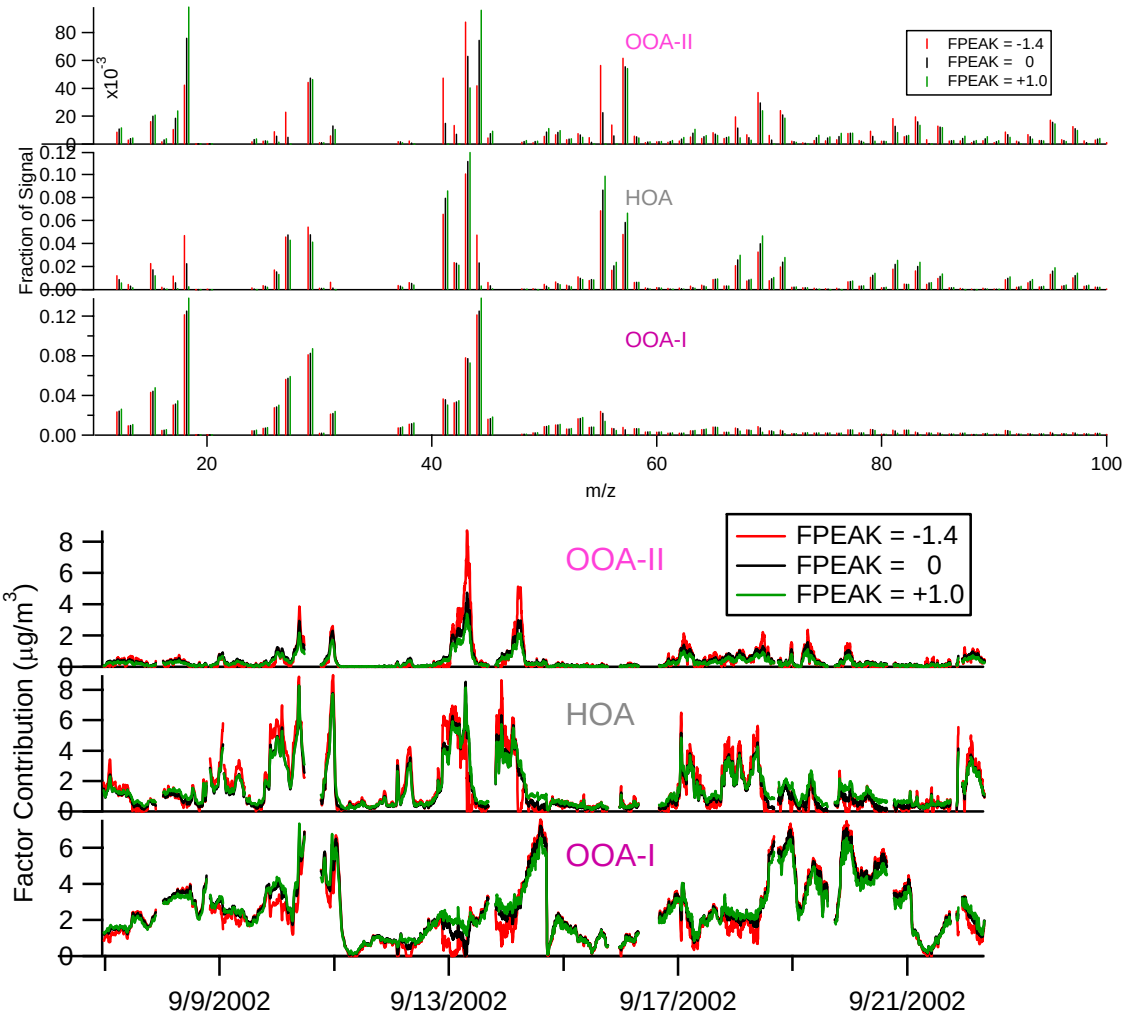

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1320 Figure S7. 3-factor solutions of the 3-factor synthetic base case for selected "good" FPEAK

1321 values.

Table S1. Scaling vectors and equations used to create 2-factor synthetic input cases with selected correlation.

	R_{MS} = 0.02		R_{MS} = 0.20	
m/z	Scalar * HOA *m/z*	Scalar * OOA *m/z*	Scalar * HOA *m/z*	Scalar * OOA *m/z*
12	1	1	1	1
13	1	1	1	1
15	0.5	1	0.5	1
16	1	1	1	1
17	1	1	1	1
18	1	1.2	1	1
19	1	1	1	1
20	1	1	1	1
24	1	1	1	1
25	1	1	1	1
26	1	1.1	1	1.1
27	0.2	1	0.3	1.2
29	0.1	1.1	0.3	1.2
30	1	1	1	1
31	1	1	1	1
37	1	1	1	1
38	1	1	1	1
41	1	0.2	1.5	0.7
42	0.3	1	0.5	1
43	1.3	0.1	1.1	0.8
44	1	1.2	1	1
45	1	1	1	1
48	0.3	1	1	1
49	1	1	1	1
50	0.2	1	1	1
51	0.2	1	1	1
52	0.4	1	1	1
53	0.8	1.2	0.8	1.2
54	0.2	1	1	1
55	1	0.2	1.4	0.7
56	1.1	0.4	1.1	1
57	1.5	1	1.3	1
58	0.2	1	1	1
59	1	1	1	1
60	0.2	1	1	1
61	1	1	1	1
62	0.5	1	1	1
63	0.3	1	1	1
64	0.3	1	1	1
65	1	0.2	1	1
66	1	0.4	1	1
67	1.2	0.3	1.2	1
68	1	0.4	1	1
69	1.6	1	1.4	1

	R_{MS} = 0.02	
m/z	Scalar * HOA *m/z*	Scalar * OOA *m/z*
70	1	0.2
71	1.2	0.5
72	1	0.3
73	0.4	1
74	0.5	1
75	1	1
76	0.6	1
77	1	0.4
78	1	0.5
79	1	0.4
80	1	1
81	1.2	0.4
82	0.2	1.2
83	1.4	1
84	1	1
85	1	1
86	1	1
87	0.2	1
88	1	0.3
89	0.4	1
90	0.4	1
91	1.4	0.3
92	1	1
93	1	1
94	1	1
95	1	1
96	1	1
97	1	1
98	1	1
99	1	0.6
100	0.2	1
101	0.3	1
102	1	0.6
103	1	1
104	1	1
105	1	1
106	1	1
107	1	1
108	1	1
109	1	1
110	1	1
111	1	1
112	1	1
113	1	1
114	1	1
115	1	0.3
116-300	1	1

	R_{MS} = 0.20	
m/z	Scalar * HOA *m/z*	Scalar * OOA *m/z*
70	1	1
71	1.2	1
72-300	1	1

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RTS = 0.00
HOA' = HOA
OOA' = -0.415 HOA + OOA

RMS = 0.02
scaled as shown above

RTS = 0.20
HOA' = HOA
OOA' = -0.196 HOA + OOA

RMS = 0.20
scaled as shown above

RTS = 0.36
HOA' = HOA
OOA' = OOA

RMS = 0.35
HOA' = HOA
OOA' = OOA

RTS = 0.60
HOA' = HOA + 0.295 OOA
OOA' = OOA

RMS = 0.60
HOA' = HOA
OOA' = 0.43 HOA + OOA

RTS = 0.80
HOA' = HOA
OOA' = 1.01 HOA + OOA

RMS = 0.80
HOA' = HOA
OOA' = 1.09 HOA + OOA

RTS = 0.95
HOA' = HOA
OOA' = 2.85 HOA + OOA

RMS = 0.95
HOA' = HOA
OOA' = 3.05 HOA + OOA

Table S2. Correlations between PMF factor and selected reference MS from the AMS spectral database.

Reference Spectrum	OOA-II, Real Data 3-factor solution R_{MS}	$R_{MS\ m/z>44}$	OOA-Ia, Real Data 4-factor solution R_{MS}	$R_{MS\ m/z>44}$	"mixed" Factor, 2-factor Synthetic Data 3-factor solution R_{MS}	$R_{MS\ m/z>44}$
HOA Pittsburgh	0.65	0.89	0.63	0.77	0.35	0.98
Diesel Bus Exhaust	0.87	0.92	0.67	0.75	0.57	0.99
Lubricating Oil	0.67	0.92	0.52	0.68	0.29	0.98
OOA Pittsburgh	0.81	0.42	0.87	0.92	1.00	0.46
aged rural	0.83	0.68	0.76	0.96	0.95	0.76
Fulvic Acid	0.75	0.54	0.56	0.86	0.90	0.57
α-pinene ozonolysis SOA	0.69	0.56	0.93	0.93	0.79	0.71
β-caryophyllene ozonolysis SOA	0.73	0.60	0.93	0.88	0.77	0.71
Linalool ozonolysis SOA	0.69	0.52	0.90	0.88	0.77	0.56
α-terpinene ozonolysis SOA	0.76	0.65	0.92	0.93	0.81	0.74
m-xylene photoox. SOA	0.84	0.49	0.81	0.86	0.98	0.50
Diesel Exhaust photoox. 0.25 hr	0.73	0.83	0.79	0.78	0.58	0.85
Diesel Exhaust photoox. 2.25 hr	0.86	0.77	0.90	0.86	0.84	0.81
Diesel Exhaust photoox. 4.25 hr	0.88	0.76	0.90	0.88	0.89	0.81
Ceanothus BBOA	0.80	0.77	0.87	0.83	0.74	0.83
Chamise BBOA	0.88	0.79	0.88	0.88	0.88	0.86
Palmetto BBOA	0.79	0.77	0.92	0.89	0.78	0.84
Juniper BBOA	0.83	0.75	0.89	0.89	0.83	0.87
Manzanita BBOA	0.87	0.79	0.89	0.87	0.87	0.88
Ponderosa Pine Duff BBOA	0.76	0.78	0.90	0.85	0.71	0.84
Ponderosa BBOA	0.71	0.75	0.82	0.82	0.61	0.83
Rice Straw BBOA	0.74	0.77	0.93	0.89	0.78	0.80
Sage and Rabbit Brush BBOA	0.86	0.78	0.86	0.94	0.97	0.85
Wax Myrtle BBOA	0.82	0.76	0.89	0.87	0.79	0.84
Levoglucosan	0.56	0.41	0.74	0.43	0.59	0.42