

1 *Supporting Information for*

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3 **Tracer-based Characterization of Source Variations of PM_{2.5} and Organic**
4 **Carbon in Shanghai Influenced by the COVID-19 Lockdown**

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21 **Contents of this file:**

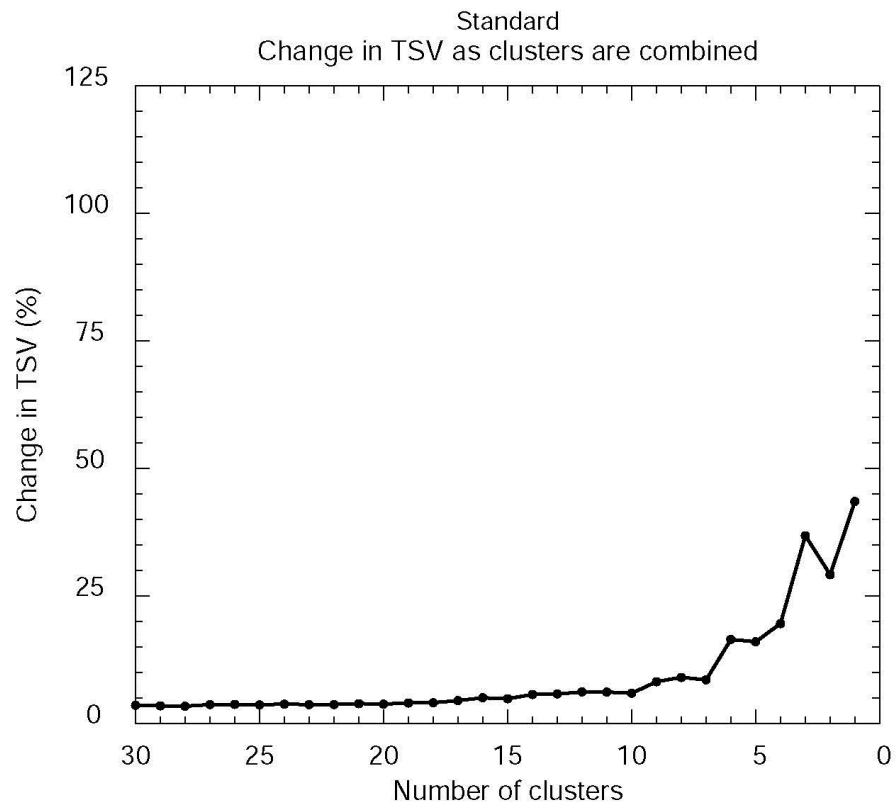
22 Text S1 to S2

23 Figures S1 to S8

24 Table S1 to S5

25 References

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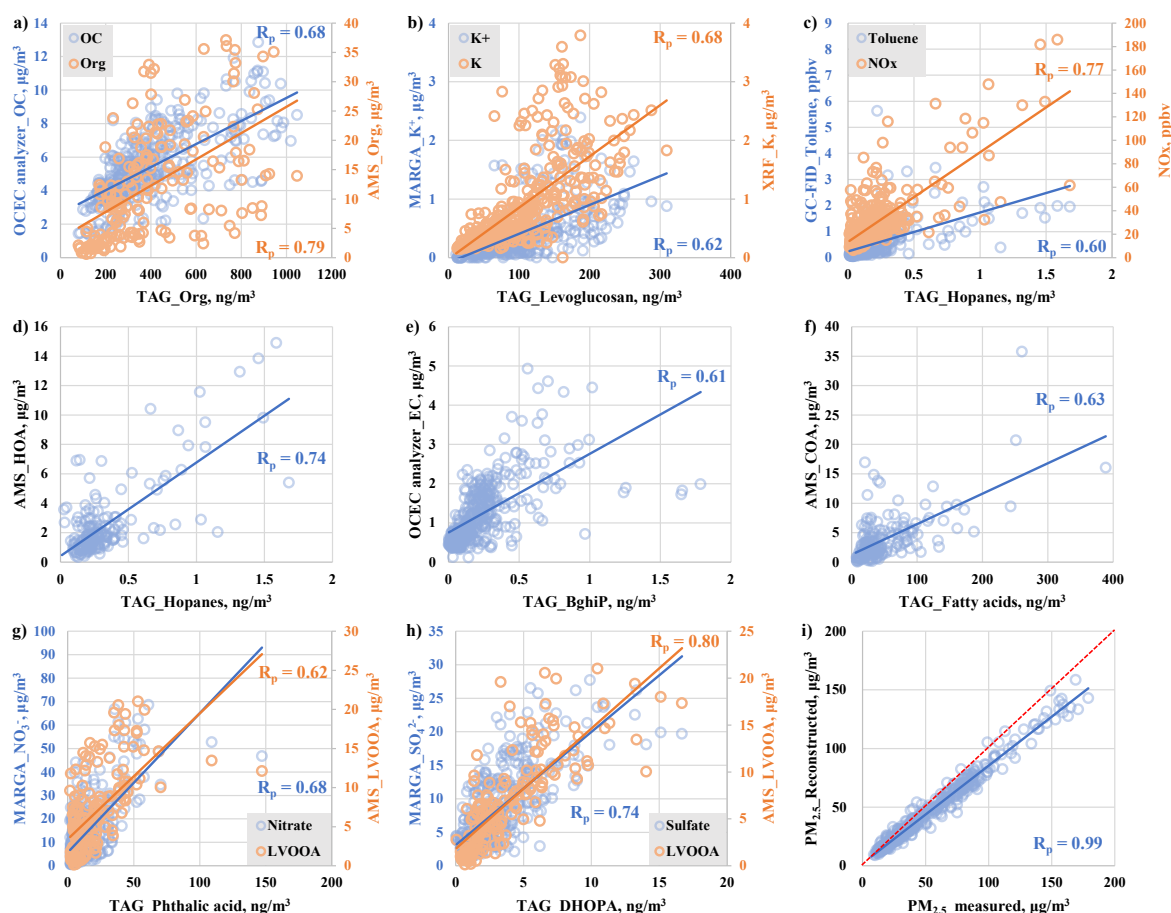
28 **Figure S1.** Change of total spatial variance (TSV) as a function of number of clusters at 100 m arrival
 29 height obtained from the HYSPLIT model.

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31 Text S1. Data checking for TAG-measured organic compounds

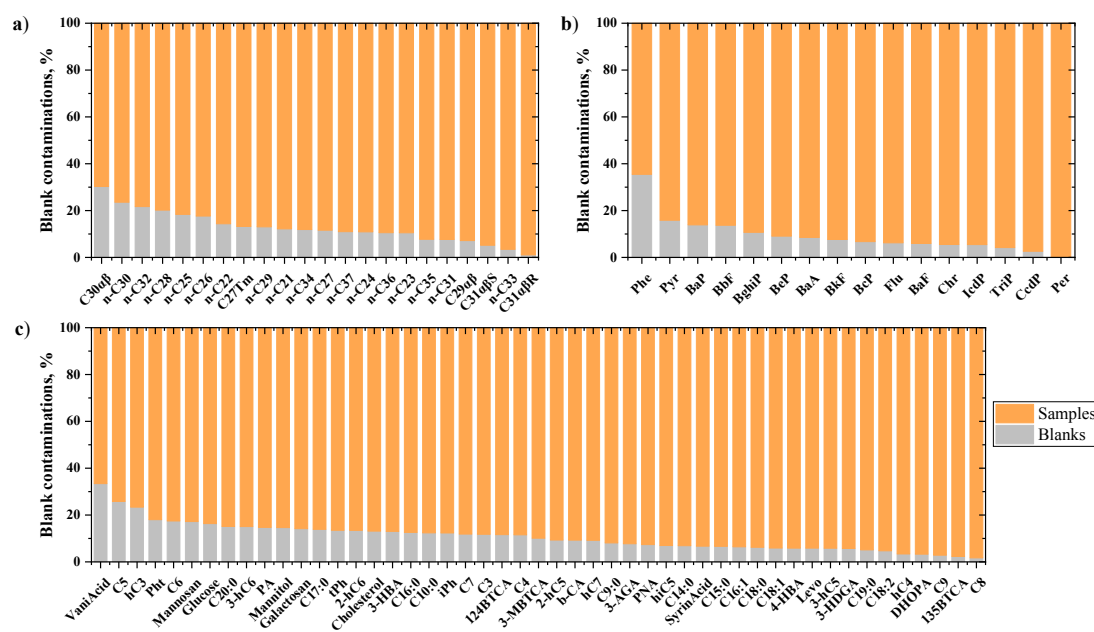
32 Taking advantage of available measurements made by multiple instruments, we carried
33 out several internal data consistency tests between related chemical parameters measured by
34 different instruments. Pairs of parameters are selected based on their known underlying physical
35 relationships. Specifically, the list includes (a) the sum of 87 organic molecules measured by
36 TAG (TAG_Org) versus OC measured by OCEC analyzer and bulk organics in PM₁ measured
37 by AMS; (b) levoglucosan measured by TAG versus K⁺ measured by MARGA and total K
38 measured by XRF; (c) the sum of 5 hopanes measured by TAG versus toluene measured by
39 GC-FID and NO_x measured by the NO_x monitor; (d) the sum of 5 hopanes measured by TAG
40 versus hydrocarbon-like OA (HOA) resolved by PMF analysis of mass spectra data from AMS;
41 (e) BghiP measured by TAG versus EC obtained from OCEC analyzer; (f) the sum of 13 fatty
42 acids measured by TAG versus cooking OA (COA) from AMS data; (g) phthalic acid measured
43 by TAG versus nitrate measured by MARGA and low-volatility OA (LVOOA) from AMS data;
44 (h) DHOPA (mono-aromatic compounds-derived SOA tracer) measured by TAG versus sulfate
45 measured by MARGA and LVOOA by AMS; and (i) reconstructed versus measured PM_{2.5}
46 mass. Scatter correlation plots of the above pairs of parameters are illustrated in Figure S2. In
47 general, moderate to strong correlations were observed, indicating the hourly dataset collected
48 from different instruments are consistent with each other.

49 As part of quality control/quality assurance, blank samples were collected once every five
50 days and a total of 7 blank samples were collected by the TAG system. The presence of the 87
51 target organic compounds in the blank samples were either not detected or lower than 25% of
52 the average concentration level detected in the samples for the majority of target analytes, as
53 shown in Figure S3. Thus, the TAG-measured concentrations were not blank-corrected.



54

55 **Figure S2.** Scatter plots of select pairs of measured parameters with known underlying physical
56 relationships. They serve as internal data consistency check.



57

58 **Figure S3.** Percentage contributions of blank contamination to the average sample
59 concentration for (a) alkanes and hopanes, (b) PAHs, and (c) polar organic compounds.

Table S1. Statistics of hourly concentrations of 87 organic molecules measured by TAG system, among which Abbr represents abbreviations for compound names used in this study, organic molecules shadowed in grey refer to molecules included in PMF model.

Group	Compounds	Abbreviations	Avg ng/m ³	Range ng/m ³	PMF group
C ₃₋₅ DCAs & hDCAs	Malonic acid	C3	11.9	0.76-70.9	LMW- DCAs
	Succinic acid	C4	21.0	1.67-167	
	Glutaric acid	C5	2.74	0.07-29.8	
	Malic_acid	hC4	15.4	BD-97.5	
	Citramalic_acid	hiC5	4.42	0.27-23.4	LMW- hDCAs
	Glyceric_acid	hC3	17.7	1.15-95.2	
	2-hydroxyglutaric acid	2-hC5	0.80	0.01-13.8	
	3-hydroxyglutaric acid	3-hC5	4.07	0.12-43.5	
C ₆₋₉ DCAs & hDCAs	Adipic acid	C6	3.15	0.18-57.8	
	Pimelic acid	C7	1.22	0.05-5.99	
	Suberic acid	C8	4.25	0.06-32.0	
	Azelaic_acid	C9	4.20	0.35-26.4	
	2-hydroxyadipic acid	2-hC6	1.76	0.06-33.5	
	3-Hydroxyadipic acid	3-hC6	2.72	0.16-74.1	
	Hydroxypimelic acid	hC7	1.85	0.03-14.6	
SOA tracers	Pinic acid	PA	2.92	0.13-21.4	aPinT
	Pinonic acid	PNA	0.36	0.03-2.53	
	3-methyl-1,2,3-butanetricarboxylic acid	3-MBTCA	1.07	0.04-7.86	
	3-acetylglutaric acid	3-AGA	3.80	0.10-20.6	
	3-hydroxy-4,4-dimethylglutaric	3-HDGA	2.33	0.07-12.8	bCaryT
	β-caryophyllinic acid	b-CA	1.20	0.03-6.18	
	2,3-dihydroxy-4-oxopentanoic acid	DHOPA	3.03	0.06-16.7	
	Phthalic acid	Pht	13.7	1.81-147	
Aromatic polycarboxylic acids	Isophthalic acid	iPh	0.98	0.10-4.05	BTCAs
	Terephthalic acid	tPh	15.2	0.76-99.2	
	1,2,4-benzentricarboxylic acid	124BTCA	6.24	0.12-80.7	
	1,3,5-benzentricarboxylic acid	135BTCA	0.29	BD-2.84	
Biomass burning tracers	3-hydroxybenzoic acid	3-HBA	0.62	0.10-2.81	VanillicAci d
	4-hydroxybenzoic acid	4-HBA	0.92	0.12-6.07	
	Syringic acid	SyrinAcid	0.17	BD-1.69	
	Vanillic acid	VaniAcid	0.48	0.01-3.97	
	Galactosan	Galactosan	6.50	0.85-26.1	
	Mannosan	Mannosan	6.19	0.39-29.2	
	Levogluconan	Levo	101.1	10.9-309	
	Mannitol	Mannitol	35.0	3.36-332	

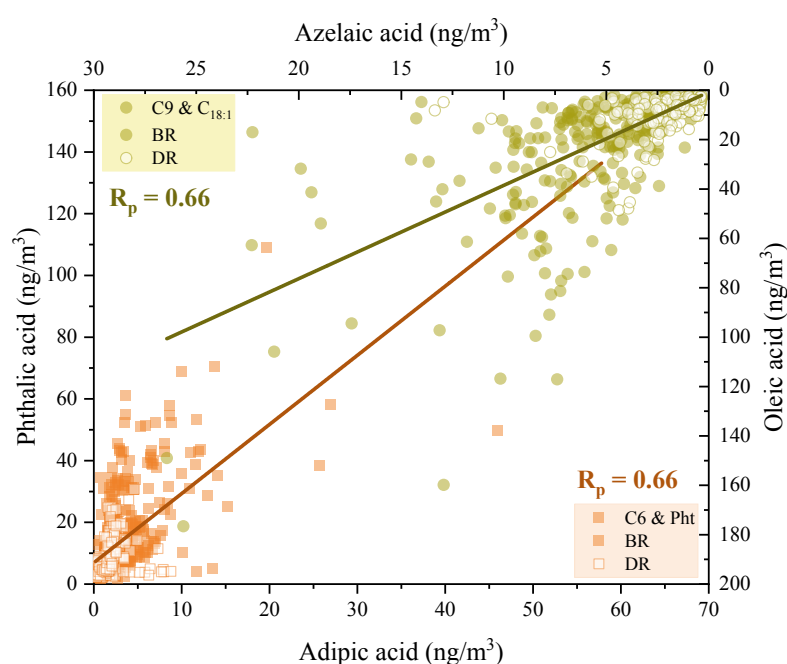
	Glucose	Glucose	4.21	0.58-21.8	
Fatty acids & Cholesterol	Nonanoic acid	C9:0	0.50	0.01-3.33	Saturated fatty acids (sFAs)
	Decanoic acid	C10:0	1.12	BD-7.73	
	Myristic acid	C14:0	0.43	0.07-8.69	
	Pentadecanoic acid	C15:0	0.10	BD-1.57	
	Palmitic acid	C16:0	6.6	1.05-40.3	
	Heptadecanoic acid	C17:0	0.12	BD-2.37	
	Stearic acid	C18:0	8.01	0.79-59.0	
	Nonadecanoic acid	C19:0	0.08	BD-0.58	
	Eicosanoic acid	C20:0	0.24	BD-2.37	Unsaturated fatty acids (usFAs)
	Oleic acid	C18:1	16.6	0.56-177	
	Palmitoleic acid	C16:1	0.03	0.01-0.44	
	Linoleic acid	C18:2	3.36	BD-80.2	
	Cholesterol	Cholesterol	1.22	0.38-5.37	
Alkanes	Heneicosane	n-C21	0.48	0.12-4.60	
	Docosane	n-C22	0.88	0.11-5.86	
	Tricosane	n-C23	1.46	0.27-9.69	
	Tetracosane	n-C24	1.70	0.36-9.16	
	Pentacosane	n-C25	1.75	0.37-10.9	OddAlk
	Hexacosane	n-C26	1.35	0.20-8.78	EvenAlk
	Heptacosane	n-C27	1.31	0.26-9.56	OddAlk
	Octacosane	n-C28	0.76	0.08-7.49	EvenAlk
	Nonacosane	n-C29	1.16	0.03-11.4	OddAlk
	Tracotane	n-C30	0.47	0.01-4.11	EvenAlk
	Hentriacontane	n-C31	0.79	0.01-6.33	OddAlk
	Dotriacontane	n-C32	0.27	0.01-2.63	EvenAlk
	Tritriactotane	n-C33	0.34	BD-3.08	
	Tetratriactotane	n-C34	0.20	0.02-1.46	
	Pentatriactotane	n-C35	0.14	BD-1.08	
	Hexatriactotane	n-C36	0.11	BD-0.95	
	Heptatriactotane	n-C37	0.17	BD-15.7	
Hopanes	22,29,30-trisnorhopane	C27Tm	0.02	BD-0.26	Hopanes
	$\alpha\beta$ -norhopane	C29 $\alpha\beta$	0.06	BD-0.70	
	$\alpha\beta$ -hopane	C30 $\alpha\beta$	0.05	BD-0.52	
	$\alpha\beta$ -22S-homohopane	C31 $\alpha\beta$ S	0.03	BD-0.22	
	$\alpha\beta$ -22R-homohopane	C31 $\alpha\beta$ R	0.02	BD-0.27	
PAHs	Phenanthrene	Phe	0.14	0.03-0.43	
	Fluoranthene	Flu	0.17	0.01-0.74	
	Pyrene	Pyr	0.15	BD-0.56	
	Benzo[c]phenanthrene	BcP	0.05	BD-0.33	
	Cyclopenta[cd]pyrene	CcdP	0.10	BD-0.55	
	Triphenylene	TriP	0.23	BD-2.08	
	Chrysene	Chr	0.42	BD-3.77	
	Benzo[a]anthracene	BaA	0.13	BD-1.00	

Benzo[b]fluoranthene	BbF	0.18	0.01-1.48	PAHs252
Benzo[k]fluoranthene	BkF	0.20	0.01-0.92	
Benzo[a]fluoranthene	BaF	0.10	BD-0.72	
Benzo[e]pyrene	BeP	0.22	BD-1.54	PAHs252
Benzo[a]pyrene	BaP	0.17	BD-2.02	
Perylene	Per	0.03	BD-0.34	PAHs276
Indeno[1,2,3-cd]pyrene	IcdP	0.29	BD-2.64	
Benzo[ghi]perylene	BghiP	0.24	BD-1.78	

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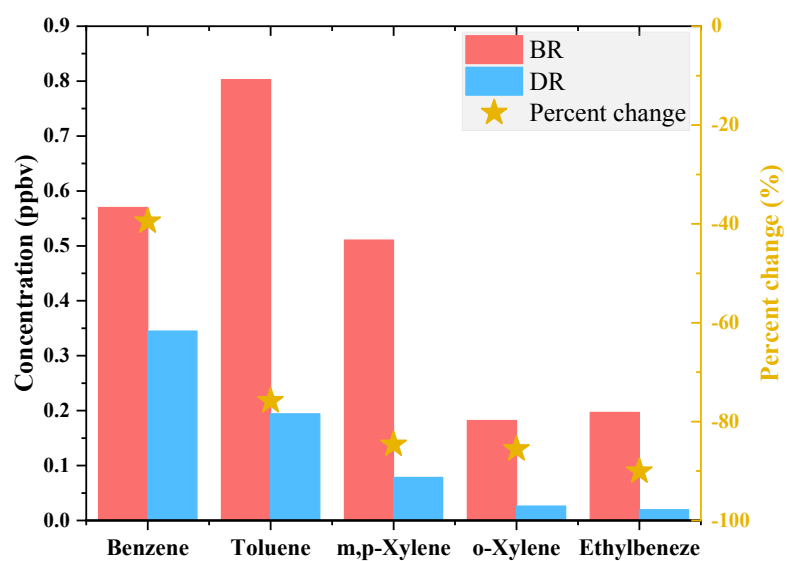
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67 **Figure S4.** Correlation plots of adipic acid (C_6 -DCA) versus phthalic acid (Pht) and azelaic
68 acid (C_9 -DCA) versus oleic acid. The data from BR and DR periods are distinguished in
69 different colors while the correlation coefficient (R_p) values are derived from combined BR
70 and DR data.



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72 **Figure S5.** Stage-wise averaged concentrations of four monoaromatic VOCs and the
73 percentage changes in their concentrations from BR to DR stage.

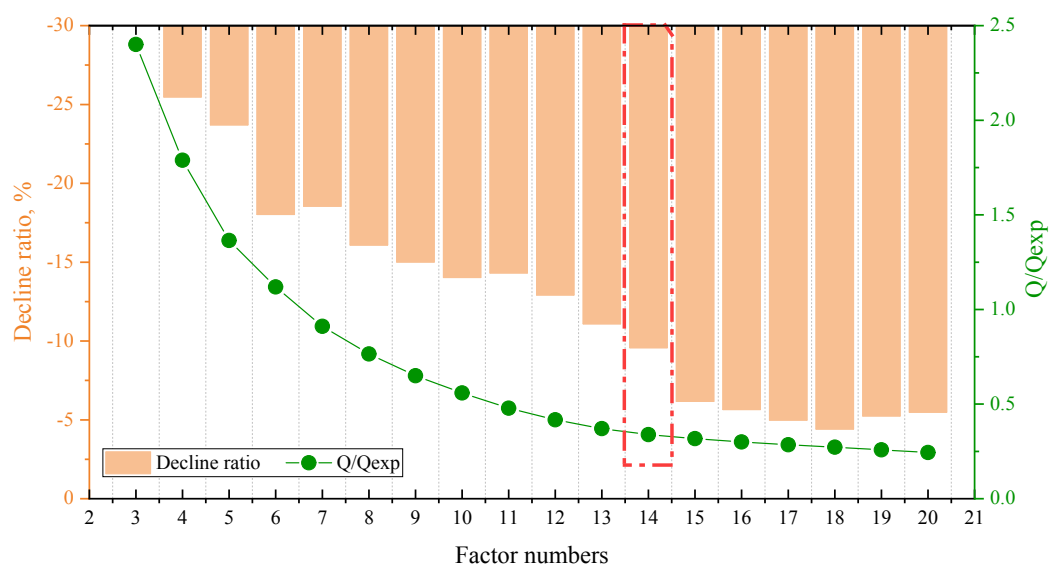
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75 Text S2. PMF modeling diagnostics

76 The input data matrix is a dataset of 480×27 , consisting of 480 hourly samples and 27
77 lumped or individual species in each hourly sample. Three to 20 factors were initially tried in
78 the PMF model. The Q/Q_{exp} ratio, which represents the ratio between the actual sum of the
79 squares of the scaled residuals (Q) (obtained from the PMF least square fit) and the ideal Q
80 (Q_{exp}) (obtained if the fit residuals at each point were equal to the noise specified for each data
81 point),¹ was applied to seek the optimal factor numbers. A PMF solution of a certain factor
82 number with a lower Q/Q_{exp} value normally indicates a more robust result.² Figure S6 shows a
83 diagnostic plot of the Q/Q_{exp} value versus factor number. The Q/Q_{exp} value had a decline trend
84 with the increase of factor number and ranged from 0.24 to 2.40 (Figure S6). The Q/Q_{exp}
85 changed by 6% from the 14- to 15-factor solution, less significant than the 10–25% observed
86 when the number of factors varied from 3 to 13 (Figure S6), suggesting the factor number
87 reaching 14 was needed for explaining the input data. The 14-factor solution also provides
88 explainable source profiles. Thus, it was chosen as the optimal solution.

89 The stability of the 14-factor solution was also assessed by performing two commonly
90 used error estimation methods provided in the PMF model, namely bootstrap (BS) and
91 displacement (DISP). The BS method evaluates effect of random errors by recomputing the
92 model solution with randomly selecting non-overlapping blocks of consecutive samples and
93 comparing the correlation between the BS run factor and the base run factor.³ A robust solution
94 with lower effect from random errors normally demonstrates higher degree of mappings in BS
95 results. In addition to the BS method, the DISP method estimates effect of rotational ambiguity
96 by displacing the fitted value of each species in factors far enough to achieve predetermined
97 increase value for Q (dQ^{max}). Swaps occur when factors change so much that they exchange
98 identities, indicating that the solution is not sufficiently robust to be used due to the significant
99 rotational ambiguity.⁴ The BS and DISP results in this study show that all the 14 source factors
100 resolved in the base run were mapped over 93% of BS runs (Table S2). Neither factor swap or
101 Q change occurred with DISP estimation. Therefore, the 14-factor solution is quite robust.
102 Figure S7 shows an excellent correlation between reconstructed $\text{PM}_{2.5}$ mass concentrations by
103 summing up all resolved 14 source factors and the measured $\text{PM}_{2.5}$ mass concentrations, also
104 confirming that the 14-factor solution appropriately models the measured $\text{PM}_{2.5}$ concentrations.
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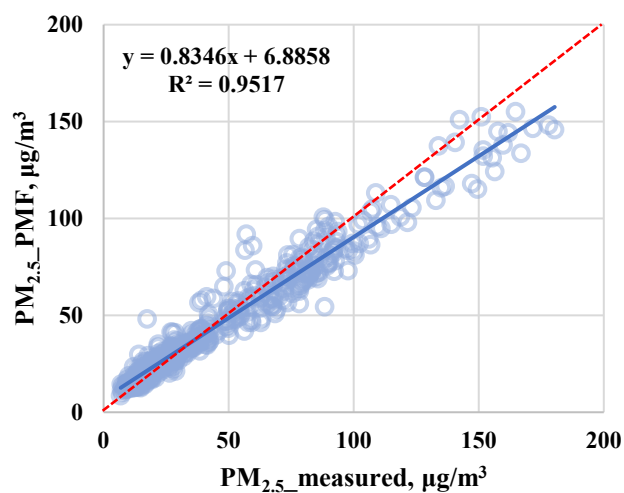


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108 **Figure S6.** The Q/Q_{exp} ratios obtained from PMF solution with a factor number from 3 to 20.
 109 The 14-factor solution is determined to be the optimal solution and highlighted with red dash
 110 rectangle in the figure.

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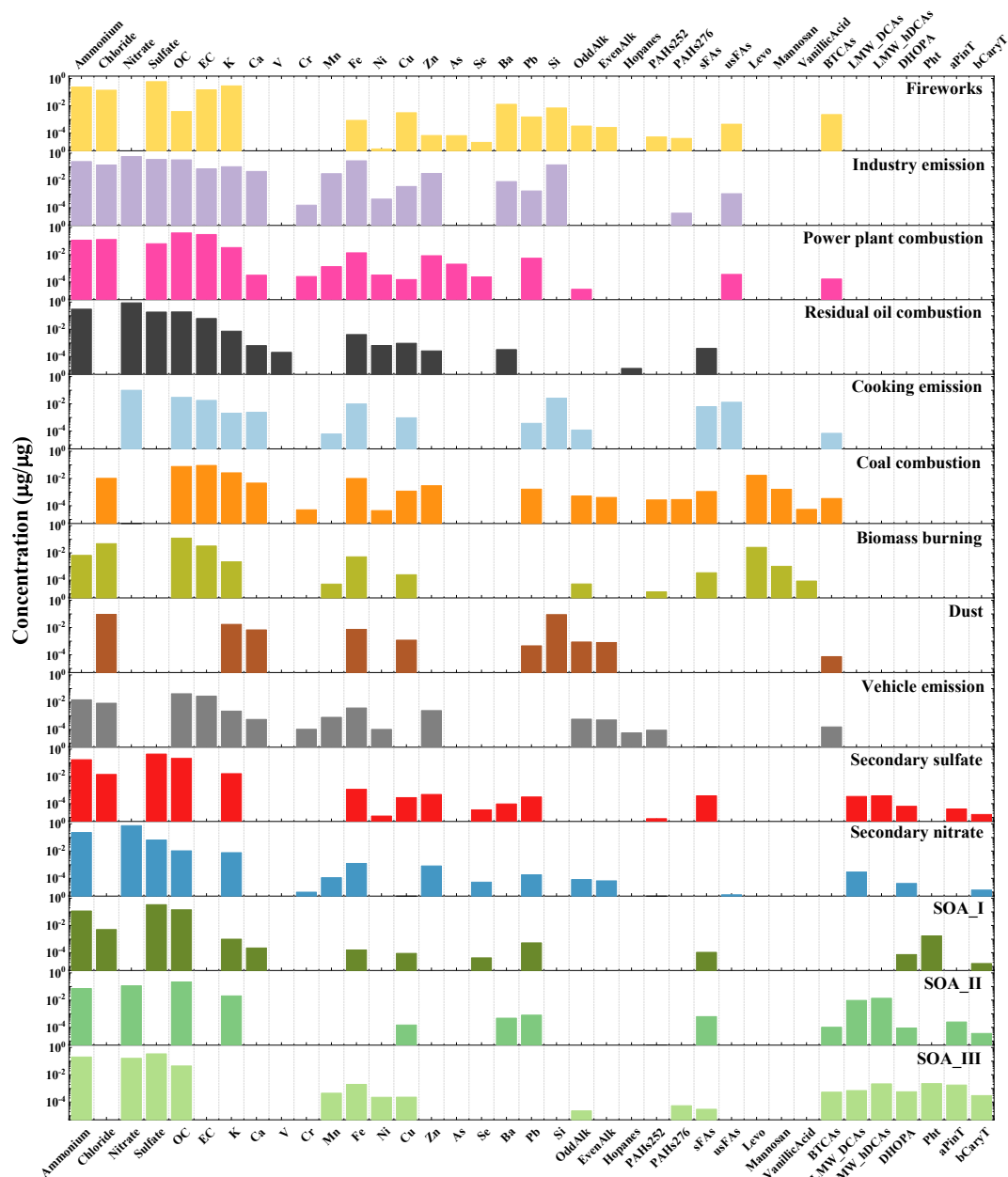


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114 **Figure S7.** Comparison of reconstructed $\text{PM}_{2.5}$ mass obtained from the 14-factor PMF solution
 115 versus measured $\text{PM}_{2.5}$ mass.

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119 **Figure S8.** Source profiles in mass fractions of input species resolved by PMF model.

120

121 **Table S2.** Summary of error estimation diagnostics from BS and DISP for PMF model (F1: fireworks, F2: industry emission, F3: power plant combustion, F4:
122 residual oil combustion, F5: cooking emission, F6: coal combustion, F7: biomass burning, F8: dust, F9: vehicle emission, F10: secondary sulfate, F11: secondary
123 nitrate, F12: SOA_I, F13: SOA_II, F14:SOA_III).

BS mapping	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12	F13	F14	Unmap ped
F1	100	0	0	0	0	0	0	0	0	0	0	0	0	0	0
F2	0	100	0	0	0	0	0	0	0	0	0	0	0	0	0
F3	0	0	100	0	0	0	0	0	0	0	0	0	0	0	0
F4	0	0	0	100	0	0	0	0	0	0	0	0	0	0	0
F5	0	0	0	0	100	0	0	0	0	0	0	0	0	0	0
F6	0	0	0	0	0	100	0	0	0	0	0	0	0	0	0
F7	0	0	0	0	0	2	97	0	0	0	0	0	0	0	1
F8	0	3	0	0	0	2	0	93	1	0	0	0	0	0	1
F9	0	0	0	0	0	0	0	0	100	0	0	0	0	0	0
F10	0	0	0	0	0	0	0	0	0	100	0	0	0	0	0
F11	0	0	0	0	0	0	0	0	0	0	100	0	0	0	0
F12	0	0	0	0	0	0	0	0	0	0	1	97	0	0	2
F13	0	0	0	0	0	0	0	0	0	0	0	0	100	0	0
F14	0	0	0	0	0	0	0	0	0	0	1	0	0	98	1
DISP diagnostics	Error code: 0							Largest decrease in Q: 0							
Swaps by factor	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0

125 **Table S3.** Correlation (Pearson R) coefficients among PMF-resolved factors and regular pollutants, meteorological parameters (F1: fireworks, F2: industry
126 emission, F3: power plant combustion, F4: residual oil combustion, F5: cooking emission, F6: coal combustion, F7: biomass burning, F8: dust, F9: vehicle
127 emission, F10: secondary sulfate, F11: secondary nitrate, F12: SOA_I, F13: SOA_II, F14:SOA_III).

Factors*	F1	F2	F3	F4	F5	F6	F7	F8	F9	F10	F11	F12	F13	F14
CO	0.336	0.211	0.672	-0.418	0.147	0.461	0.495	0.401	0.418	0.403	0.778	0.513	0.137	0.370
NO	-0.055	0.579	0.195	0.005	0.264	0.621	0.049	0.070	0.648	-0.144	0.044	-0.041	-0.058	0.144
NO ₂	-0.182	0.506	0.355	0.067	0.488	0.432	0.222	0.255	0.466	-0.242	0.449	0.298	-0.014	0.472
SO ₂	0.203	0.356	0.509	-0.207	0.052	0.371	0.243	0.393	0.384	0.191	0.610	0.284	-0.038	0.317
O ₃	0.124	-0.401	-0.157	-0.079	-0.345	-0.484	-0.102	-0.044	-0.476	0.268	-0.141	-0.010	0.162	-0.263
Ox	-0.058	0.056	0.211	-0.023	0.112	-0.142	0.127	0.251	-0.092	0.073	0.342	0.347	0.211	0.208
Temperature	-0.226	0.249	-0.040	0.154	0.060	-0.055	-0.068	-0.037	-0.005	-0.238	-0.236	-0.122	0.092	0.087
RH	-0.165	0.039	-0.048	0.286	0.037	0.090	0.041	-0.098	0.114	-0.219	-0.162	-0.189	0.064	0.119
Pressure	-0.087	-0.102	-0.165	0.015	-0.026	-0.112	-0.224	0.023	-0.045	0.130	-0.016	-0.047	0.018	-0.068
Visibility	-0.249	-0.189	-0.555	0.144	-0.056	-0.419	-0.482	-0.230	-0.427	-0.295	-0.625	-0.376	-0.274	-0.437
WS	0.027	-0.104	-0.027	-0.052	-0.209	-0.151	-0.093	-0.025	-0.182	0.014	-0.227	-0.051	-0.179	-0.150
PBL	0.251	-0.128	-0.071	-0.075	-0.224	0.041	-0.033	-0.008	0.029	0.148	0.093	-0.018	-0.042	-0.017
Geological materials	-0.083	0.908	0.492	-0.062	0.187	0.428	0.162	0.505	0.585	-0.070	0.322	0.196	-0.079	0.389
POA	0.292	0.298	0.831	-0.291	0.101	0.472	0.539	0.411	0.533	0.356	0.884	0.563	0.102	0.367
SOA	0.506	-0.113	0.506	-0.516	-0.065	0.140	0.402	0.397	0.094	0.644	0.620	0.446	0.216	0.179
Toluene	-0.064	0.508	0.511	-0.090	0.280	0.500	0.188	0.232	0.521	-0.045	0.346	0.217	-0.036	0.364
HOA**	0.309	0.558	0.307	-0.089	0.361	0.639	0.274	0.107	0.685	-0.043	0.154	-0.028	0.188	0.165
COA**	0.359	0.182	0.245	-0.154	0.628	0.239	0.333	0.226	0.118	-0.027	0.236	0.163	0.265	0.078
LVOOA**	0.292	0.247	0.356	-0.404	0.048	0.380	0.467	0.333	0.367	0.578	0.921	0.545	0.456	0.606

128 *SVOOA obtained from AMS was not included in the table since it did not show strong correlations with PMF-resolved source factors.

129 **Comparisons among AMS-resolved OA factors and PMF-resolved source factors are limited to data for BR stage, as AMS data was not available for the DR period.

130 **Table S4.** Mass contributions of 14-resolved PMF factors to PM_{2.5} under each cluster at both BR and DR stages in units of µg/m³ (F1: fireworks, F2: industry
131 emission, F3: power plant combustion, F4: residual oil combustion, F5: cooking emission, F6: coal combustion, F7: biomass burning, F8: dust, F9: vehicle
132 emission, F10: secondary sulfate, F11: secondary nitrate, F12: SOA_I, F13: SOA_II, F14:SOA_III).

Factors	CL#1		CL#2		CL#3		CL#4		Total	
	BR	DR	BR	DR	BR	DR	BR	DR	BR	DR
F1	0.26	0.46	0.49	3.61	0.54	0.77	1.12	6.04	0.51	1.93
F2	0.69	0.14	0.96	0.30	1.27	0.28	0.48	0.27	0.87	0.21
F3	0.87	0.77	2.68	1.20	1.29	0.28	3.00	1.59	1.75	0.92
F4	1.67	0.86	0.43	0.26	1.32	1.48	0.25	0.05	1.06	0.67
F5	1.09	0.64	1.02	0.72	2.18	0.70	2.62	0.75	1.56	0.68
F6	1.01	0.37	2.56	0.81	1.75	0.40	3.49	0.47	1.95	0.51
F7	2.25	2.05	2.99	3.84	3.37	1.57	4.58	4.98	3.05	2.80
F8	1.62	1.80	3.05	2.32	2.18	1.00	4.92	1.51	2.61	1.84
F9	2.81	0.47	6.53	1.01	4.97	0.15	4.79	0.68	4.59	0.61
F10	4.05	7.62	9.10	18.6	4.07	4.99	5.18	21.4	5.54	11.8
F11	12.4	3.21	36.2	17.7	11.0	14.4	38.1	21.7	22.0	10.2
F12	4.87	2.88	10.4	2.84	4.29	2.22	17.6	7.21	8.00	3.23
F13	1.65	2.71	1.39	2.22	2.15	6.15	2.45	3.28	1.82	2.96
F14	2.40	0.71	3.04	0.91	2.20	0.57	1.49	0.58	2.39	0.74
Combined Primary factors	12.3	7.56	20.7	14.1	18.9	6.63	25.3	16.3	18.0	10.2
Combined Secondary factors	25.3	17.1	60.0	42.3	23.8	28.4	64.8	54.2	39.7	29.0

134 **Table S5.** Mass contributions of 14-resolved PMF factors to OC under each cluster at both BR and DR stages in units of $\mu\text{gC}/\text{m}^3$ (F1: fireworks, F2: industry
135 emission, F3: power plant combustion, F4: residual oil combustion, F5: cooking emission, F6: coal combustion, F7: biomass burning, F8: dust, F9: vehicle
136 emission, F10: secondary sulfate, F11: secondary nitrate, F12: SOA_I, F13: SOA_II, F14:SOA_III).

Factors	CL#1		CL#2		CL#3		CL#4		Total	
	BR	DR	BR	DR	BR	DR	BR	DR	BR	DR
F1	0.00	0.00	0.00	0.01	0.00	0.00	0.00	0.02	0.00	0.01
F2	0.22	0.04	0.31	0.10	0.41	0.09	0.15	0.09	0.28	0.07
F3	0.34	0.30	1.06	0.47	0.51	0.11	1.19	0.63	0.69	0.37
F4	0.32	0.16	0.08	0.05	0.25	0.28	0.05	0.01	0.20	0.13
F5	0.03	0.02	0.03	0.02	0.07	0.02	0.08	0.02	0.05	0.02
F6	0.29	0.11	0.73	0.23	0.50	0.11	0.99	0.13	0.55	0.14
F7	0.27	0.25	0.37	0.47	0.41	0.19	0.56	0.61	0.37	0.34
F8	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
F9	0.45	0.08	1.05	0.16	0.80	0.02	0.77	0.11	0.74	0.10
F10	0.86	1.61	1.92	3.93	0.86	1.05	1.09	4.53	1.17	2.50
F11	0.13	0.03	0.38	0.19	0.12	0.15	0.40	0.23	0.23	0.11
F12	0.70	0.41	1.48	0.41	0.61	0.32	2.52	1.03	1.14	0.46
F13	0.36	0.59	0.30	0.49	0.47	1.35	0.54	0.72	0.40	0.65
F14	0.11	0.03	0.14	0.04	0.10	0.03	0.07	0.03	0.11	0.03
Combined Primary factors	1.92	0.96	3.63	1.51	2.95	0.82	3.79	1.62	2.88	1.18
Combined Secondary factors	2.16	2.67	4.22	5.06	2.16	2.90	4.62	6.54	3.05	3.75

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