Supplementary Information

Measurement report: Underestimated reactive organic gases from residential combustion: insights from a near-complete speciation

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8 figures
5 tables
22 pages

Figure S1. Sampling diagram relates to six solid fuels types, household stoves, sampling port and equipment. n refers to the number of different samples.

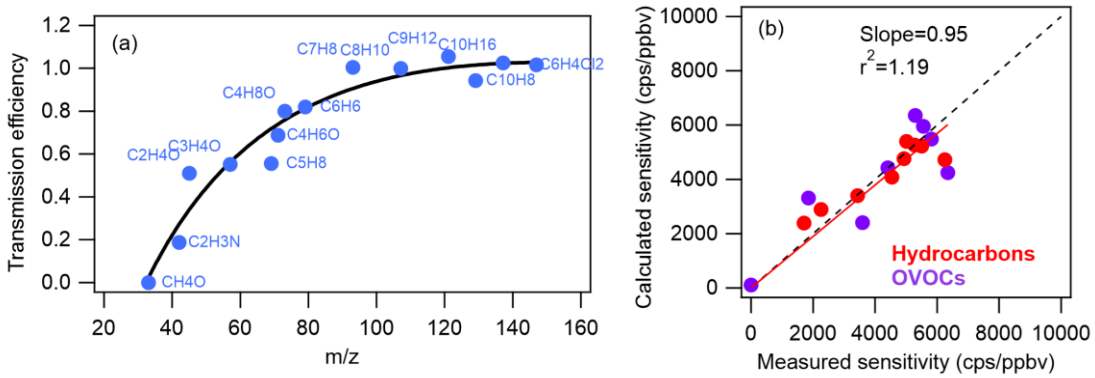

Figure S2. (a) The transmission efficiency of the Vocus PTR-ToF-MS and (b) ccomparison of measured and calculated calibration factors for several ROGs. The black dash line means 1:1.

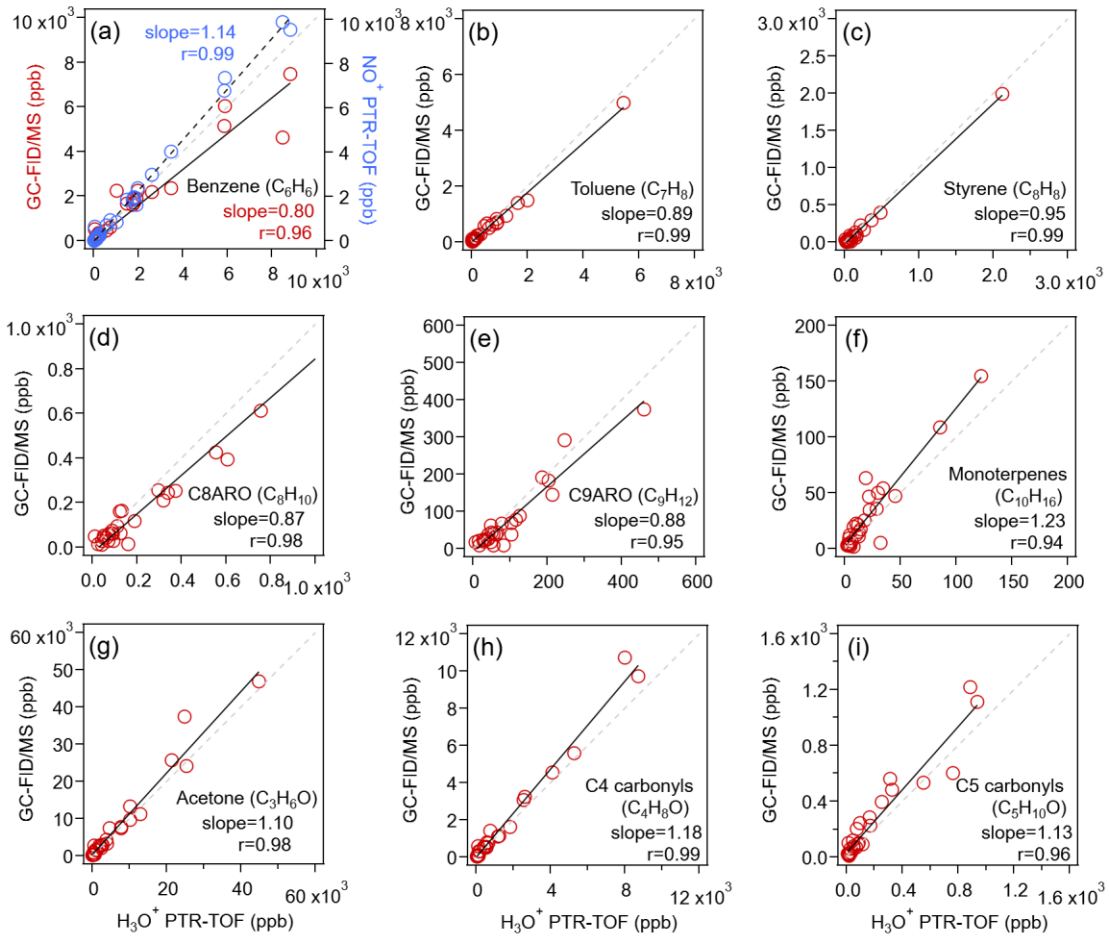

Figure S3. Intercomparisons between species measurement of samples by GC-FID/MS and by H_3O^+/NO^+ Vocus PTR-ToF-MS. C8ARO and C9ARO refer to aromatics containing 8 carbon and 9 carbon atoms, respectively.

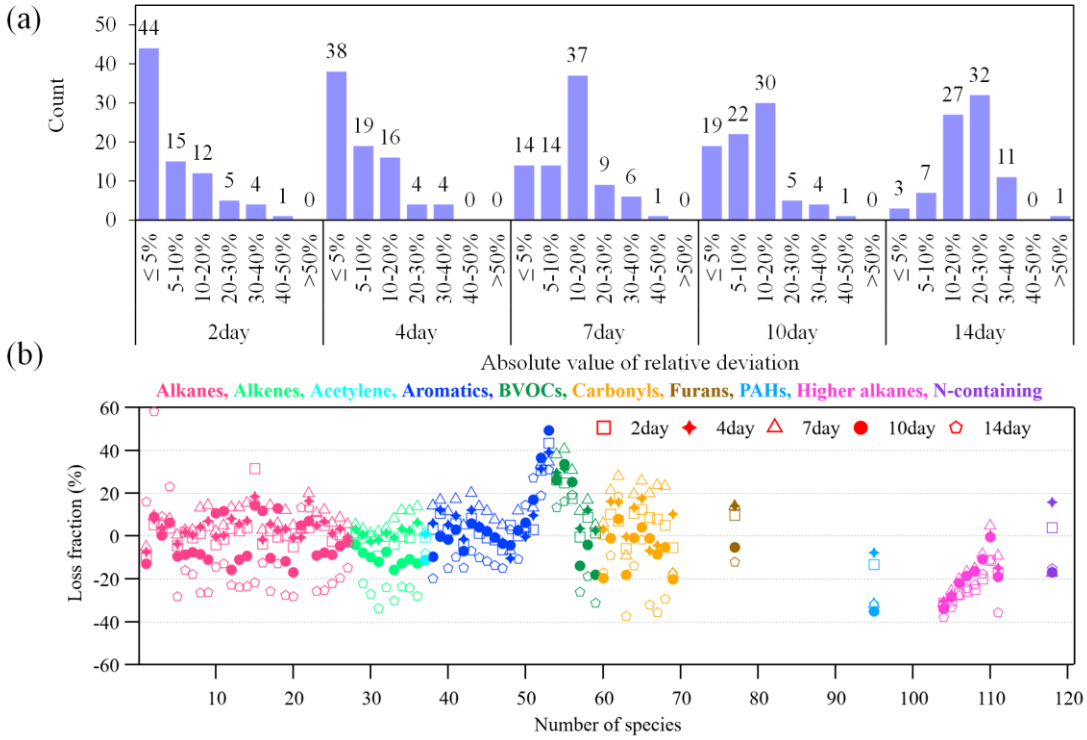

Figure S4. Statistical evaluation on the loss fraction of ROGs in the canisters. (a) Species counts in different loss fraction bins on 2, 4, 7, 10, 14 days (x-axis) of storage in the canisters. (b) The loss fraction of each compound standards on 2, 4, 7, 10, 14 days of storage in the canisters. The measured species corresponding to the numbers of horizontal axis are listed in Table S1.

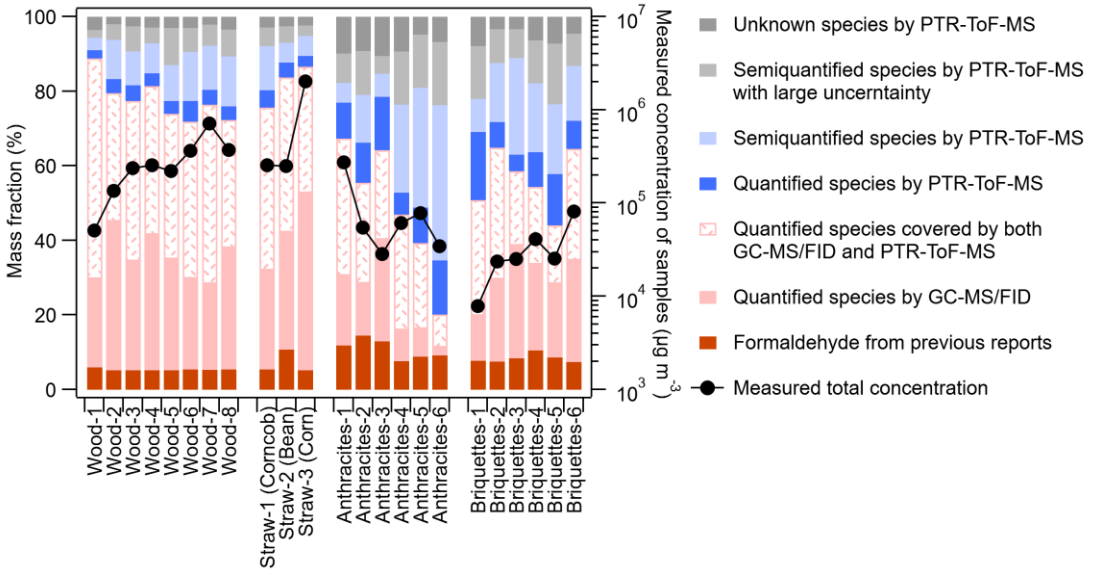

Figure S5. Profile composition of species for different samples measured by GC-MS/FID and Vocus PTR-ToF-MS and the measured total ROG concentration of each sample (black line).

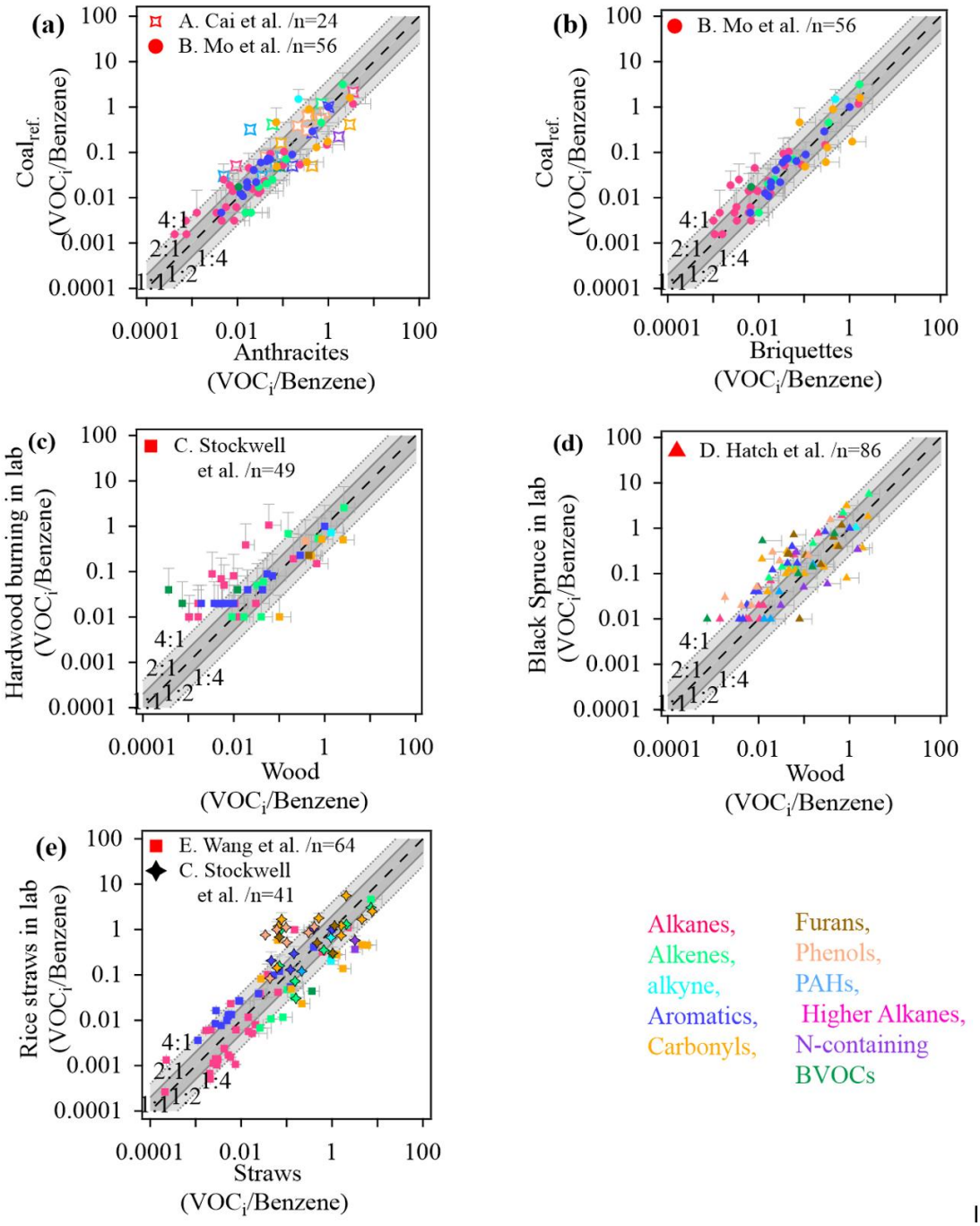

Figure S6. Comparison of emission ratios between this study and the previous studies (Hatch et al., 2017; Mo et al., 2016; Stockwell et al., 2015; Wang et al., 2014; Cai et al., 2019; Stockwell et al., 2016). The black dashed lines indicate the 1:1 relationship, and the gray and light gray areas show agreements within a factor of 2 and 4, respectively. n is the number of compared species with the corresponding reference.

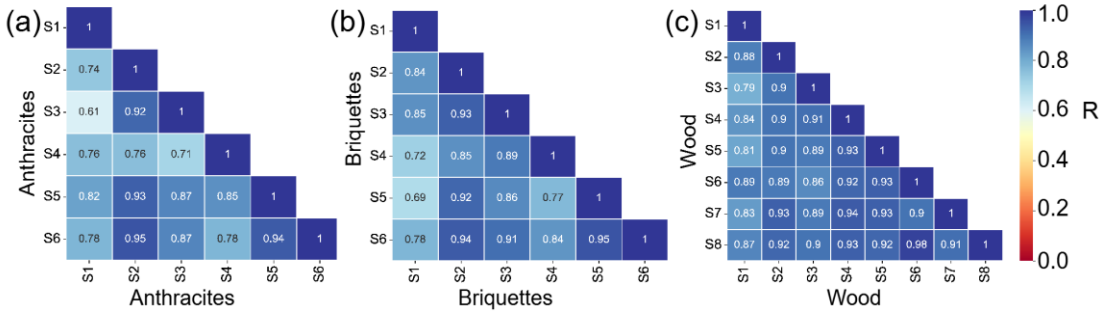

Figure S7. Correlation between ROGs source profile of different samples of the same fuel. The number represents the Spearman correlation coefficient (R).

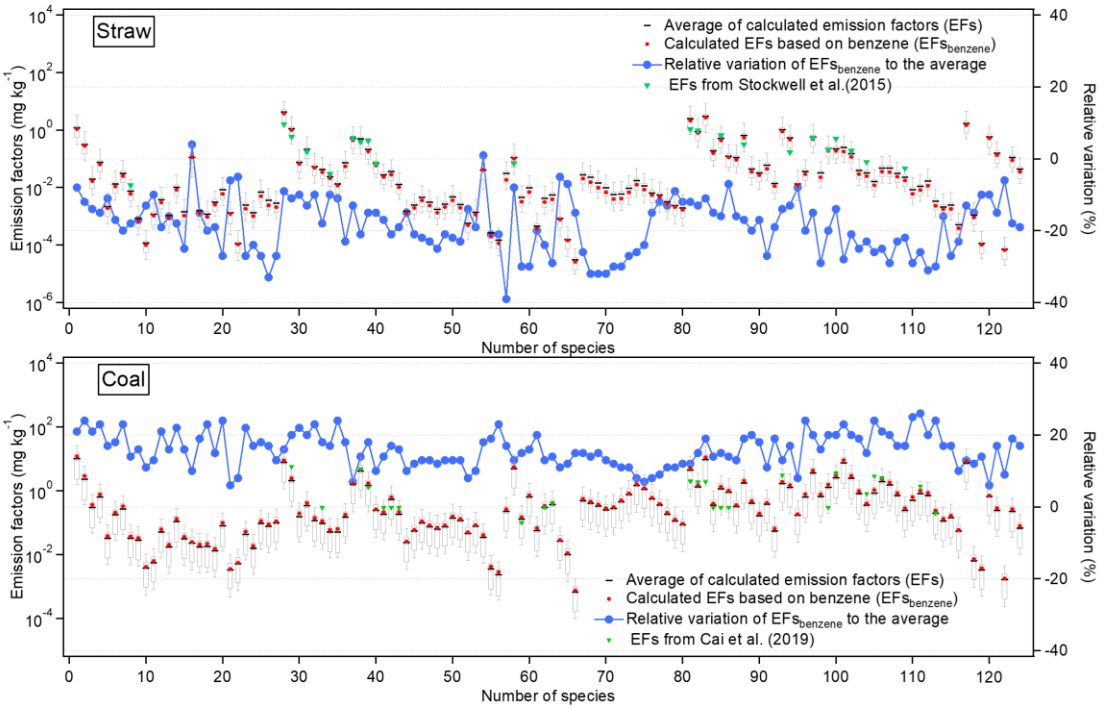

Figure S8. Box plot of estimated emission factors (EFs) of newly identified ROGs based on reported EF of ROGs and the relative variation (blue line) of EFs based on benzene to the average of all tests. The red dot is the calculated EFs based on benzene. The box range is the calculated EFs based on other reported species. The green dot is the EFs from references(Cai et al., 2019; Stockwell et al., 2015) used in calculation.

Table S1 Literature review on residential combustion emissions.

Method	Fuel types	Reference	Numbers of species by GC-MS(/ FID)	Numbers of species by Vocus PTR-ToF-MS	Numbers of species (Other instruments)
Combustion in stove	Residential coals, biomass	This study	71	84 (84-92% of the overall peak mass)	—
	Anthracite, bituminous coal	(Cai et al., 2019)	—	79-89 (90-96% of the overall peak intensities)	—
	Corncob	(Wu et al., 2022)	—	13	—
Combustion simulation in Lab	western US biomass fuels	(Akherati et al., 2020)	—	150	—
	burned fuels characteristic of the western U.S.	(Koss et al., 2018)	—	172 (~95% of the overall peak intensities)	—
	four burns: ponderosa pine boughs, , Chinese rice straw, Indonesian peat, and black spruce boughs	(Hatch et al., 2017)	~27	~71	~13 (FTIR) ~418 (GC×GC)
	Authentic globally significant fuels	(Stockwell et al., 2015)	—	46-92	—
	laboratory biomass burns of 18 fuel types from 3 geographic regions in the US	(Gilman et al., 2015)	187	Unpublished	Unpublished (OP-FTIR)
	Residential coal, rice, maize, and wheat straw	(Mo et al., 2016)	62	—	13 (DNPH-HPLC)
	biomass, residential coal	(Liu et al., 2008)	92	—	—

OP-FTIR: open-path Fourier transform infrared spectroscopy

DNPH-HPLC: 2, 4-Dinitrophenyl hydrazine followed by high performance liquid chromatography (HPLC)

Table S2. Measurement method, loss fraction in canisters, method detection limit (MDL) and uncertainty for individual species in this study.

Number	Formula	Name (recommended species for Vocus PTR-ToF-MS)	GC-MS /FID[a]	Vocus PTR-ToF-MS[b]	Loss ratio on day 10th[d] (avg. ± sd., %)	MDL (ppt)	Uncertainty (%)
			Alkanes (27)				
1	C_2H_6	Ethane	Yes	No	-12.9 ± 3.4	54.3	14
2	C_3H_8	Propane	Yes	No	8.9 ± 13.8	45.9	10
3	C_4H_{10}	Isobutane	Yes	No	0.3 ± 3.8	54.3	4
4	C_4H_{10}	n-Butane	Yes	No	6.2 ± 10.3	56.1	8
5	C_5H_{10}	Cyclopentane	Yes	No	-9.5 ± 7.3	63.4	10
6	C_5H_{12}	Isopentane	Yes	No	-8.7 ± 6.7	55.5	9
7	C_5H_{12}	n-Pentane	Yes	No	-7.6 ± 5.4	67.5	8
8	C_6H_{12}	Methylcyclopentane	Yes	No	-8.6 ± 10.9	46.0	10
9	C_6H_{12}	Cyclohexane	Yes	No	-11.0 ± 11.3	36.4	12
10	C_6H_{14}	2,2-Dimethylbutane	Yes	No	-14.4 ± 8.2	36.7	15
11	C_6H_{14}	2,3-Dimethylbutane	Yes	No	-13.0 ± 9.6	46.7	16
12	C_6H_{14}	2-Methylpentane	Yes	No	-15.8 ± 8.1	26.6	16
13	C_6H_{14}	3-Methylpentane	Yes	No	-11.0 ± 10.2	34.6	11
14	C_6H_{14}	n-Hexane	Yes	No	-9.2 ± 10.2	36.4	10
15	C_7H_{14}	Methylcyclohexane	Yes	No	14.3 ± 14.8	33.0	15
16	C_7H_{16}	2,4-Dimethylpentane	Yes	No	-12.6 ± 10.9	36.6	14
17	C_7H_{16}	2-Methylhexane	Yes	No	-10.2 ± 11.5	38.7	12
18	C_7H_{16}	2,3-Dimethylpentane	Yes	No	-13.0 ± 11.5	36.5	13
19	C_7H_{16}	3-Methylhexane	Yes	No	-11.7 ± 11.8	40.8	14
20	C_7H_{16}	n-Heptane	Yes	No	-17.0 ± 9.6	9.6	21
21	C_8H_{18}	2,2,4-Trimethylpentane	Yes	No	-10.5 ± 12.0	23.8	11
22	C_8H_{18}	2,3,4-Trimethylpentane	Yes	No	-6.4 ± 12.1	6.9	13
23	C_8H_{18}	2-Methylheptane	Yes	No	-9.1 ± 11.9	3.7	15
24	C_8H_{18}	3-Methylheptane	Yes	No	-7.8 ± 12.2	4.0	15
25	C_8H_{18}	n-Octane	Yes	No	-8.7 ± 11.3	13.1	20
26	C_9H_{20}	n-Nonane	Yes	No	-4.7 ± 12.1	13.6	15
27	$C_{10}H_{22}$	n-Decane	Yes	No	-2.8 ± 12.1	26.9	20
			Alkenes (9)/Alkyne (1)				
28	C_2H_4	Ethylene	Yes	No	-4.1 ± 6.7	24.5	7
29	C_3H_6	Propylene	Yes	No	-7.7 ± 8.2	34.3	10
30	C_4H_8	Trans-2-butene	Yes	No	-9.8 ± 7.7	69.2	10
31	C_4H_8	1-Butene	Yes	No	-11.9 ± 13.4	50.6	12
32	C_4H_8	Cis-2-butene	Yes	No	-7.4 ± 7.4	27.6	8
33	C_5H_{10}	1-Pentene	Yes	No	-15.8 ± 9.6	33.3	16
34	C_5H_{10}	Trans-2-pentene	Yes	No	-12.7 ± 9.3	36.8	13
35	C_5H_{10}	Cis-2-pentene	Yes	No	-10.9 ± 13.0	37.1	11
36	C_6H_{12}	1-Hexene	Yes	No	-12.7 ± 9.7	36.4	14
37	C_2H_2	Acetylene	Yes	No	-11.2 ± 6.5	83.1	12
			Aromatics (16)				
38	C_6H_6	Benzene*	Yes	Yes	-9.7 ± 11.8	17.6	11
39	C_7H_8	Toluene*	Yes	Yes	-0.3 ± 10.9	7.8	1
40	C_8H_8	Styrene*	Yes	Yes	-1.6 ± 12.3	45.9	6
41	C_8H_{10}	Ethylbenzene	Yes	Yes	2.9 ± 12.7	16.3	9
42	C_8H_{10}	m/p-Xylene*	Yes	Yes	-6.9 ± 11.2	28.5	16
43	C_8H_{10}	o-Xylene	Yes	Yes	5.8 ± 13.6	15.1	11
44	C_9H_{12}	iso-Propylbenzene	Yes	Yes	4.1 ± 13.5	16.4	6
45	C_9H_{12}	n-Propylbenzene	Yes	Yes	2.2 ± 13.2	21.0	7
46	C_9H_{12}	m-Ethyltoluene	Yes	Yes	-0.7 ± 12.8	28.1	4

47	C_9H_{12}	p-Ethyltoluene	Yes	Yes	-3.5 ± 12.3	47.9	7
48	C_9H_{12}	1,3,5-Trimethylbenzene*	Yes	Yes	-4.5 ± 12.0	30.3	15
49	C_9H_{12}	o-Ethyltoluene	Yes	Yes	2.5 ± 13.2	25.6	7
50	C_9H_{12}	1,2,4-Trimethylbenzene	Yes	Yes	5.8 ± 13.6	61.7	10
51	C_9H_{12}	1,2,3-Trimethylbenzene	Yes	Yes	19.8 ± 12.4	33.4	21
52	$C_{10}H_{14}$	m-Diethylbenzene	Yes	Yes	36.4 ± 16.1	42.9	37
53	$C_{10}H_{14}$	p-Diethylbenzene	Yes	Yes	49.2 ± 17.0	26.8	50
		BVOCs (6)					
54	C_5H_8	Isoprene*	Yes	Yes	-13.8 ± 11.1	27.2	16
55	$C_{10}H_{16}$	alpha-Pinene*	Yes	Yes	26.2 ± 8.2	49.2	28
56	$C_{10}H_{16}$	beta-Pinene	Yes	Yes	33.5 ± 0.2	29.8	35
57	$C_{10}H_{16}$	Cinene (Limonene)	Yes	Yes	25.2 ± 2.6	60.9	30
58	C_4H_6O	Methacrolein	Yes	Yes	-4.2 ± 2.6	28.1	13
59	C_4H_6O	Methyl vinyl ketone*	Yes	Yes	-18.0 ± 14.6	20.2	19
		Carbonyls (15)					
60	C_3H_4O	Acrolein*	Yes	Yes	-19.6 ± 5.1	44.1	20
61	C_3H_6O	Propanal	Yes	Yes	-1.1 ± 6.0	20.2	4
62	C_3H_6O	Acetone*	Yes	Yes	7.9 ± 7.2	29.6	9
63	C_4H_6O	Crotonaldehyde	Yes	Yes	-18.0 ± 4.0	32.5	24
64	C_4H_8O	n-Butanal	Yes	Yes	-0.9 ± 2.5	30.2	5
65	C_4H_8O	Methyl ethyl ketone*	Yes	Yes	4.2 ± 1.6	38.7	5
66	$C_5H_{10}O$	2-Pentanone*	Yes	Yes	-1.0 ± 2.3	26.8	19
67	$C_5H_{10}O$	n-Pentanal	Yes	Yes	-8.6 ± 4.0	29.7	10
68	$C_5H_{10}O$	3-Pentanone	Yes	Yes	-5.2 ± 3.6	37.1	6
69	C_2H_4O	Acetaldehyde*	Yes	Yes	-20.1 ± 11.9	6.5	21
70	CH_2O	Formaldehyde[c]	—	—	—	—	—
71	$C_3H_4O_2$	Methylglyoxal, acrylic acid	No	Yes	—	1.5	12
72	C_5H_4O	Cyclopentadienone	No	Yes	—	0.7	4
73	C_5H_8O	EVK, Dihydromethylfuran, cyclopentanone	No	Yes	—	0.8	11
74	C_7H_6O	Benzaldehyde	No	Yes	—	0.3	16
75	C_8H_6O	benzofuran	No	Yes	—	0.1	27
		Furans (10)					
76	C_4H_4O	Furan*	No	Yes	-5.3 ± 2.2	0.9	10
77	C_4H_8O	Tetrahydrofuran	No	Yes	—	45.5	10
78	C_5H_6O	Methyl furan	No	Yes	—	0.9	19
79	$C_4H_4O_2$	Furanone	No	Yes	—	1.1	27
80	$C_5H_4O_2$	Furfural	No	Yes	—	0.8	27
81	C_6H_8O	Dimethylfuran	No	Yes	—	0.7	27
82	$C_5H_6O_2$	Furfuryl alcohol, PentynoicAcid	No	Yes	—	0.7	27
83	$C_7H_{10}O$	TriMetfuran	No	Yes	—	0.2	27
84	$C_6H_8O_2$	DiMetfuranone	No	Yes	—	0.8	27
85	$C_8H_{12}O$	butylfuran	No	Yes	—	0.1	27
		Phenols (9)					
86	C_6H_6O	Phenol	No	Yes	—	1.1	20
87	C_7H_8O	Cresols	No	Yes	—	0.2	20
88	$C_6H_6O_2$	Benzenediols, methylfurfural	No	Yes	—	0.9	29
89	$C_8H_{10}O$	C2 phenols	No	Yes	—	0.1	27
90	$C_7H_8O_2$	Guaiacol, methyl benzenediols	No	Yes	—	0.2	29
91	$C_9H_{12}O$	Trimethylphenol	No	Yes	—	0.1	27
92	$C_{10}H_8O$	Naphthalenol	No	Yes	—	0.0	19
93	$C_{10}H_{12}O$	methyl chavicol	No	Yes	—	0.0	27
94	$C_8H_{10}O_3$	Syringol	No	Yes	—	0.2	27
		PAHs (9)					
95	$C_{10}H_8$	naphthalene*	No	Yes	-35.2 ± 7.4	0.2	37

96	$C_{10}H_{10}$	dihydroNaphth	No	Yes	—	0.1	40
97	$C_{11}H_{10}$	Methylnaphthalene	No	Yes	—	0.1	40
98	$C_{12}H_8$	Acenaphthalene	No	Yes	—	0.0	40
99	$C_{12}H_{10}$	acenaphthene	No	Yes	—	0.0	40
100	$C_{12}H_{12}$	diMetNap	No	Yes	—	0.0	40
101	$C_{13}H_{10}$	Fluorene	No	Yes	—	0.0	40
102	$C_{14}H_{10}$	Phenanthrene, Anthracene	No	Yes	—	0.0	41
103	$C_{16}H_{10}$	Pyrene, Fluoranthene	No	Yes	—	0.0	41
		Higher alkanes (14)					
104	C_8H_{18}	C8 Alkanes*	No	Yes	-34.0 ± 3.2	12.2	39
105	C_9H_{20}	C9 Alkanes*	No	Yes	-28.4 ± 1.3	7.3	31
106	$C_{10}H_{22}$	C10 Alkanes*	No	Yes	-21.9 ± 1.4	4.2	25
107	$C_{11}H_{24}$	C11 Alkanes*	No	Yes	-18.6 ± 1.3	3.2	23
108	$C_{12}H_{26}$	C12 Alkanes*	No	Yes	-16.4 ± 3.4	3.3	22
109	$C_{13}H_{28}$	C13 Alkanes*	No	Yes	-10.8 ± 15.9	2.4	22
110	$C_{14}H_{30}$	C14 Alkanes*	No	Yes	-0.5 ± 30.8	2.6	17
111	$C_{15}H_{32}$	C15 Alkanes*	No	Yes	-19.0 ± 26.7	2.1	23
112	$C_{16}H_{34}$	C16 Alkanes	No	Yes	—	3.4	27
113	$C_{17}H_{36}$	C17 Alkanes	No	Yes	—	2.3	27
114	$C_{18}H_{38}$	C18 Alkanes	No	Yes	—	2.3	27
115	$C_{19}H_{40}$	C19 Alkanes	No	Yes	—	2.8	27
116	$C_{20}H_{42}$	C20 Alkanes	No	Yes	—	3.5	27
117	$C_{21}H_{44}$	C21 Alkanes	No	Yes	—	4.0	27
		N-containing (8)					
118	C_2H_3N	Acetonitrile*	No	Yes	-17.0 ± 10.5	43.5	23
119	C_2H_5N	Ethenamine	No	Yes	—	1.6	25
120	C_2H_7N	C2 amines	No	Yes	—	1.3	25
121	C_3H_3N	Acrylonitrile	No	Yes	-13.9 ± 1.4	0.7	16
122	C_3H_5N	Propanenitrile	No	Yes	—	0.8	24
123	C_3H_9N	C3 amines	No	Yes	—	0.2	24
124	C_4H_5N	Pyrrole	No	Yes	—	0.4	23
125	C_4H_7N	Dihydropyrrole, butane nitrile, pyrroline	No	Yes	—	0.5	25

[a] GC-FID/MS measured concentrations for overlapped ROG species by both two instruments were used in this study.

[b]The species with star mark was the standard species for Vocus PTR-ToF-MS calibration.

[c]Formaldehyde discussed in this study was estimated from previous studies(Cai et al., 2019; Stockwell et al., 2015).

[d]In total, loss fraction of 81 species were determined.

Table S3. Emission ratio relative to benzene of individual species in different fuels.

Number	Formula	Name	Emission ratio (μg mg^{-1})					
			Anthracites	Briquettes	Wood	Corncob	Corn straw	Bean straw
1	C_2H_6	Ethane	2713.8 ± 1519.3	1708.6 ± 695.7	1049.9 ± 1125.1	1047.5	2168.9	5022.1
2	C_3H_8	Propane	829.2 ± 389.7	356.6 ± 222.4	336.3 ± 390.0	392.9	453.1	1277.8
3	C_4H_{10}	Isobutane	139.3 ± 84.7	65.5 ± 61.4	28.5 ± 26.3	27.4	37.4	61.8
4	C_4H_{10}	n-Butane	265.4 ± 93.6	122.2 ± 77.3	92.4 ± 92.6	117.6	106.7	263.6
5	C_5H_{12}	Cyclopentane	8.7 ± 2.0	8.5 ± 6.7	2.3 ± 2.7	2.6	2.2	9.7
6	C_5H_{12}	Isopentane	79.1 ± 73.4	53.3 ± 64.3	16.1 ± 16.3	22.4	20.3	40.3
7	C_5H_{12}	n-Pentane	94.9 ± 55.0	52.5 ± 37.2	44.4 ± 45.3	63.9	32.7	94.3
8	C_6H_{12}	Methylcyclopentane	19.4 ± 15.7	10.3 ± 4.7	9.4 ± 6.5	12.9	14.6	18.0
9	C_6H_{12}	Cyclohexane	7.1 ± 3.9	6.1 ± 2.5	1.8 ± 1.9	1.5	1.2	2.6
10	C_6H_{14}	2,2-Dimethylbutane	0.9 ± 0.7	0.9 ± 0.3	0.2 ± 0.2	0.2	0.2	0.4
11	C_6H_{14}	2,3-Dimethylbutane	1.3 ± 0.7	1.8 ± 1.5	1.4 ± 2.7	0.8	5.9	1.3
12	C_6H_{14}	2-Methylpentane	15.1 ± 11.1	10.4 ± 6.0	5.1 ± 4.7	7.2	4.9	10.7
13	C_6H_{14}	3-Methylpentane	6.1 ± 3.5	4.8 ± 3.6	1.8 ± 2.1	1.9	0.2	4.6
14	C_6H_{14}	n-Hexane	34.2 ± 24.5	22.0 ± 12.4	17.3 ± 21.6	18.5	14.4	30.7
15	C_7H_{14}	Methylcyclohexane	7.8 ± 3.7	7.0 ± 3.0	2.4 ± 2.3	3.5	1.7	2.7
16	C_7H_{16}	2,4-Dimethylpentane	14.1 ± 14.4	11.7 ± 17.1	46.5 ± 119.1	0.6	16.5	856.5
17	C_7H_{16}	2-Methylhexane	6.1 ± 4.5	4.3 ± 3.4	1.2 ± 0.8	2.4	2.3	5.4
18	C_7H_{16}	2,3-Dimethylpentane	5.0 ± 4.9	3.3 ± 3.2	1.3 ± 1.4	2.5	1.3	3.4
19	C_7H_{16}	3-Methylhexane	3.7 ± 1.9	3.8 ± 3.7	1.7 ± 1.1	4.8	13.0	1.6
20	C_7H_{16}	n-Heptane	27.6 ± 26.0	12.9 ± 12.6	16.5 ± 13.4	22.0	8.3	15.3
21	C_8H_{18}	2,2,4-Trimethylpentane	0.9 ± 0.9	1.5 ± 2.9	0.5 ± 0.8	0.1	9.1	0.2

22	C_8H_{18}	2,3,4-Trimethylpentane	1.9 ± 1.8	2.2 ± 2.8	0.3 ± 0.3	0.1	0.1	0.6
23	C_8H_{18}	2-Methylheptane	12.3 ± 11.0	8.2 ± 6.9	4.9 ± 3.9	6.6	3.1	4.0
24	C_8H_{18}	3-Methylheptane	9.4 ± 7.8	4.6 ± 3.7	3.2 ± 2.1	3.1	2.1	2.5
25	C_8H_{18}	n-Octane	34.7 ± 23.2	25.2 ± 14.6	15.2 ± 11.6	18.2	9.6	10.2
26	C_9H_{20}	n-Nonane	26.8 ± 18.7	21.7 ± 15.4	9.0 ± 8.1	11.4	4.3	2.4
27	$C_{10}H_{22}$	n-Decane	34.0 ± 21.9	35.4 ± 28.3	7.6 ± 6.2	7.5	3.9	4.4
28	C_2H_4	Ethylene	1944.1 ± 957.8	2019.3 ± 1089.0	3019.6 ± 1283.7	2429.3	20434.6	5954.7
29	C_3H_6	Propylene	845.8 ± 567.7	465.8 ± 338.0	993.0 ± 670.6	1052.1	3463.9	3077.6
30	C_4H_8	Trans-2-butene	86.6 ± 68.6	33.3 ± 36.9	72.7 ± 82.1	79.1	126.2	303.6
31	C_4H_8	1-Butene	170.3 ± 131.3	85.6 ± 75.4	221.8 ± 162.6	277.3	513.5	627.0
32	C_4H_8	Cis-2-butene	61.3 ± 46.2	24.2 ± 26.8	52.4 ± 58.0	56.9	93.4	218.9
33	C_5H_{10}	1-Pentene	43.1 ± 35.9	26.0 ± 20.1	60.4 ± 57.0	73.8	76.9	109.5
34	C_5H_{10}	Trans-2-pentene	30.2 ± 25.3	15.3 ± 12.7	25.9 ± 28.8	25.6	42.2	92.1
35	C_5H_{10}	Cis-2-pentene	26.2 ± 19.3	9.7 ± 6.6	14.8 ± 16.4	15.9	20.7	52.8
36	C_6H_{12}	1-Hexene	65.6 ± 71.6	41.0 ± 30.4	92.4 ± 73.3	157.8	149.1	110.2
37	C_2H_2	Acetylene	259.2 ± 181.4	631.5 ± 422.2	1259.7 ± 598.9	590.4	1751.7	1026.2
38	C_6H_6	Benzene	1000.0 ± 0.0	1000.0 ± 0.0	1000.0 ± 0.0	1000.0	1000.0	1000.0
39	C_7H_8	Toluene	567.3 ± 233.2	356.9 ± 146.8	362.3 ± 183.2	267.8	786.0	317.7
40	C_8H_8	Styrene	129.0 ± 123.4	83.8 ± 39.0	80.9 ± 50.7	74.5	355.4	16.7
41	C_8H_{10}	Ethylbenzene	79.3 ± 51.2	58.0 ± 24.5	53.1 ± 26.3	37.3	123.3	16.3
42	C_8H_{10}	m/p-Xylene	238.5 ± 136.0	144.3 ± 72.4	76.8 ± 54.2	68.1	97.0	49.2
43	C_8H_{10}	o-Xylene	82.2 ± 47.5	53.9 ± 26.9	28.9 ± 21.4	21.0	40.7	16.0
44	C_9H_{12}	iso-Propylbenzene (Cumene)	7.1 ± 4.6	9.0 ± 9.1	2.5 ± 1.2	1.7	7.1	1.1
45	C_9H_{12}	n-Propylbenzene	18.9 ± 12.7	19.5 ± 15.4	6.2 ± 4.2	4.8	7.8	2.2
46	C_9H_{12}	m-Ethyltoluene	42.6 ± 31.4	32.8 ± 20.4	11.1 ± 7.6	9.1	12.6	5.3
47	C_9H_{12}	p-Ethyltoluene	30.5 ± 22.5	26.5 ± 20.0	7.4 ± 4.9	6.6	7.1	4.1
48	C_9H_{12}	1,3,5-Trimethylbenzene	23.7 ± 16.6	21.9 ± 16.8	5.3 ± 4.3	4.3	3.0	2.7
49	C_9H_{12}	o-Ethyltoluene	28.1 ± 19.9	25.7 ± 19.7	7.8 ± 5.6	5.0	7.8	3.2
50	C_9H_{12}	1,2,4-Trimethylbenzene	70.0 ± 56.8	48.1 ± 31.8	14.5 ± 11.8	9.9	10.0	7.3

51	C_9H_{12}	1,2,3-Trimethylbenzene	48.4 ± 39.4	41.9 ± 33.2	8.3 ± 6.2	5.9	4.5	4.6
52	$C_{10}H_{114}$	m-Diethylbenzene	12.2 ± 8.5	20.2 ± 26.7	1.5 ± 0.9	0.8	1.0	1.9
53	$C_{10}H_{14}$	p-Diethylbenzene	29.2 ± 23.4	30.6 ± 29.6	4.1 ± 2.9	2.6	2.4	3.7
54	$C_{10}H_{16}$	alpha-Pinene	3.7 ± 4.4	1.0 ± 0.7	1.0 ± 1.3	0.5	0.7	0.3
55	$C_{10}H_{16}$	beta-Pinene	2.8 ± 4.3	0.5 ± 0.5	0.5 ± 0.5	0.3	0.2	0.3
56	$C_{10}H_{16}$	Cinene(Limonene)	193.6 ± 264.8	69.3 ± 58.5	86.2 ± 115.7	119.1	6.9	13.5
57	C_5H_8	Isoprene	24.7 ± 21.0	11.7 ± 17.4	24.5 ± 42.5	7.7	11.5	291.9
58	C_4H_6O	Methacrolein	189.6 ± 162.7	122.8 ± 86.7	220.5 ± 156.1	266.3	525.3	414.1
59	C_4H_6O	Methyl vinyl ketone	933.7 ± 1094.1	377.8 ± 315.3	592.0 ± 304.9	785.5	1469.5	1072.1
60	C_3H_4O	Acrolein	2653.4 ± 2492.5	1664.7 ± 1313.5	2492.8 ± 1229.3	2683.4	7437.6	6116.1
61	C_3H_6O	Propanal	838.9 ± 646.7	464.9 ± 420.5	969.7 ± 502.8	1151.0	1792.8	2980.5
62	C_3H_6O	Acetone	8404.5 ± 8112.2	2526.9 ± 1872.0	3826.5 ± 3651.0	3681.0	4654.4	12189.5
63	C_4H_6O	Crotonaldehyde	676.5 ± 755.0	327.2 ± 324.3	233.7 ± 131.9	61.1	531.1	274.7
64	C_4H_8O	n-Butanal	165.6 ± 121.6	131.8 ± 159.0	136.0 ± 94.9	177.5	229.6	301.0
65	C_4H_8O	Methyl ethyl ketone	1746.3 ± 1795.9	502.6 ± 467.5	762.5 ± 729.0	1086.5	1093.7	1858.9
66	$C_5H_{10}O$	2-Pentanone	164.7 ± 162.1	47.4 ± 44.2	58.5 ± 51.5	53.8	47.9	100.9
67	$C_5H_{10}O$	n-Pentanal	197.1 ± 186.5	170.2 ± 208.4	108.2 ± 53.2	156.3	109.7	74.0
68	$C_5H_{10}O$	3-Pentanone	55.8 ± 53.2	15.7 ± 14.7	22.5 ± 19.0	26.2	21.9	35.7
69	C_2H_4O	Acetaldehyde	942.7 ± 748.7	605.1 ± 389.0	1054.3 ± 569.9	1432.2	1825.6	3554.3
70	CH_2O	Formaldehyde	2125 ± 581.1	2125 ± 581.1	2856± 532.9	2848 ± 555.3	2848 ± 555.3	2848 ± 555.3
71	$C_3H_4O_2$	Methylglyoxal, acrylic acid (AcryAcid_Mgly)	78.9 ± 85.1	70.5 ± 66.7	13.9 ± 8.8	12.3	18.0	62.2
72	C_5H_4O	Cyclopentadienone	1336.1 ± 2106.0	112.3 ± 138.7	66.8 ± 96.9	65.3	121.2	33.0
73	C_5H_8O	EVK, Dihydromethylfuran, cyclopentanone	1839.1 ± 2062.5	330.1 ± 408.8	414.2 ± 357.3	457.6	409.2	550.7
74	C_7H_6O	Benzaldehyde	337.9 ± 380.3	103.4 ± 51.1	71.2 ± 36.1	65.3	113.1	8.8
75	C_8H_6O	benzofuran	231.3 ± 246.8	67.5 ± 54.5	59.1 ± 44.3	41.6	87.8	4.7
76	C_4H_4O	Furan	1489.0 ± 1726.1	451.8 ± 780.5	741.1 ± 835.3	713.8	920.7	1872.7
77	C_4H_8O	Tetrahydrofuran	527.4 ± 640.1	110.4 ± 122.5	124.3 ± 150.8	88.0	77.9	100.2

78	C_5H_6O	Methyl furan	5654.4 ± 7399.9	954.4 ± 1275.5	987.4 ± 1258.0	883.3	763.2	2035.8
79	$C_4H_4O_2$	Furanone	744.7 ± 873.2	176.1 ± 115.8	58.1 ± 50.8	87.4	66.1	17.9
80	$C_5H_4O_2$	Furfural	14120.4 ± 18694.4	1457.6 ± 1830.3	920.7 ± 987.8	662.8	495.6	187.6
81	C_6H_8O	Dimethylfuran	3903.1 ± 5098.9	569.7 ± 513.1	373.3 ± 428.7	312.8	229.0	345.1
82	$C_5H_6O_2$	Furfuryl alcohol, PentynoicAcid	1188.0 ± 1534.8	197.4 ± 133.5	86.8 ± 91.8	90.8	99.9	30.8
83	$C_7H_{10}O$	TriMetfuran	2317.1 ± 3058.2	347.4 ± 284.7	165.2 ± 188.9	134.2	69.8	55.2
84	$C_6H_8O_2$	DiMetfuranone	944.6 ± 1281.7	187.2 ± 132.9	67.7 ± 62.9	65.2	93.2	22.2
85	$C_8H_{12}O$	butylfuran	1083.4 ± 1458.3	167.0 ± 139.4	67.2 ± 74.8	51.7	22.5	13.2
86	C_6H_6O	Phenol	3762.9 ± 5889.4	574.3 ± 526.1	443.5 ± 451.8	258.1	908.1	281.9
87	C_7H_8O	Cresols	2017.8 ± 3924.1	166.0 ± 277.1	76.9 ± 150.0	41.5	24.5	25.3
88	$C_6H_6O_2$	Benzenediols, methylfurfural	3372.0 ± 4703.2	407.2 ± 292.3	175.9 ± 196.4	114.2	118.2	38.5
89	$C_8H_{10}O$	C2 phenols (Dimethylphenol)	1248.1 ± 2563.9	94.9 ± 151.4	35.1 ± 54.5	24.3	12.6	8.5
90	$C_7H_8O_2$	Guaiacol, methyl benzenediols	1995.4 ± 4089.5	128.8 ± 143.4	41.2 ± 43.9	26.3	26.8	8.7
91	$C_9H_{12}O$	Trimethylphenol	432.0 ± 795.3	36.5 ± 42.0	14.6 ± 19.3	10.0	4.8	3.0
92	$C_{10}H_8O$	Naphthalenol	132.5 ± 185.6	32.5 ± 22.6	5.9 ± 7.2	3.5	2.8	7.2
93	$C_{10}H_{12}O$	methyl chavicol	173.9 ± 230.0	40.3 ± 29.1	10.4 ± 11.9	6.7	2.7	4.3
94	$C_8H_{10}O_3$	Syringol	40.7 ± 50.8	21.2 ± 18.8	2.6 ± 2.8	1.1	1.3	0.5
95	$C_{10}H_8$	naphthalene	2325.2 ± 1892.3	1790.4 ± 1896.7	176.4 ± 105.6	107.0	126.8	540.0
96	$C_{10}H_{10}$	dihydroNaphth	94.6 ± 92.4	40.3 ± 39.3	18.0 ± 20.5	12.8	9.0	2.5
97	$C_{11}H_{10}$	Methylnaphthalene	560.8 ± 625.0	188.8 ± 271.0	42.6 ± 49.9	28.8	9.2	14.0
98	$C_{12}H_8$	Acenaphthalene	109.4 ± 217.4	13.2 ± 15.9	2.7 ± 5.2	0.9	0.6	1.3
99	$C_{12}H_{10}$	acenaphthene	250.6 ± 313.4	95.7 ± 74.7	18.9 ± 20.5	9.7	8.4	5.8
100	$C_{12}H_{12}$	diMetNap	308.7 ± 370.9	115.3 ± 178.4	29.5 ± 37.8	15.9	4.1	9.5
101	$C_{13}H_{10}$	Fluorene	20.5 ± 30.7	9.7 ± 13.2	1.6 ± 1.4	0.6	0.6	4.7
102	$C_{14}H_{10}$	Phenanthrene, anthracene (PA_Ant)	6.4 ± 6.6	3.6 ± 3.1	0.6 ± 0.5	0.1	0.3	0.7
103	$C_{16}H_{10}$	Pyrene, Fluoranthene	0.6 ± 0.7	0.2 ± 0.1	0.1 ± 0.1	0.0	0.1	0.0
104	C_8H_{18}	C8 Alkanes	161.2 ± 109.4	169.3 ± 151.2	58.1 ± 39.3	72.0	35.0	48.7
105	C_9H_{20}	C9 Alkanes	134.1 ± 97.6	141.0 ± 128.4	49.4 ± 32.2	70.8	23.0	22.5

106	$C_{10}H_{22}$	C10 Alkanes	106.5 ± 73.9	111.6 ± 101.2	36.3 ± 28.2	45.4	16.2	12.6
107	$C_{11}H_{24}$	C11 Alkanes	84.3 ± 65.3	93.9 ± 91.0	28.2 ± 21.4	31.3	9.6	10.5
108	$C_{12}H_{26}$	C12 Alkanes	96.5 ± 86.3	107.4 ± 95.3	23.0 ± 17.5	16.9	3.4	9.6
109	$C_{13}H_{28}$	C13 Alkanes	164.5 ± 151.8	176.6 ± 153.1	29.0 ± 24.5	18.3	1.3	11.4
110	$C_{14}H_{30}$	C14 Alkanes	298.0 ± 300.5	306.3 ± 288.7	43.0 ± 45.3	26.0	4.6	21.3
111	$C_{15}H_{32}$	C15 Alkanes	497.7 ± 515.5	723.1 ± 933.1	73.1 ± 78.4	46.3	6.7	42.3
112	$C_{16}H_{34}$	C16 Alkanes	354.9 ± 370.6	562.7 ± 783.3	46.3 ± 47.1	28.6	2.9	32.7
113	$C_{17}H_{36}$	C17 Alkanes	216.9 ± 210.3	265.8 ± 327.3	24.1 ± 20.0	10.8	1.5	29.5
114	$C_{18}H_{38}$	C18 Alkanes	161.7 ± 156.8	153.5 ± 147.5	17.9 ± 14.2	7.9	0.9	27.4
115	$C_{19}H_{40}$	C19 Alkanes	96.7 ± 91.4	72.4 ± 55.9	10.8 ± 8.5	4.9	0.5	15.4
116	$C_{20}H_{42}$	C20 Alkanes	57.0 ± 49.4	44.1 ± 44.2	6.4 ± 4.9	2.7	0.2	13.3
117	$C_{21}H_{44}$	C21 Alkanes	41.0 ± 34.3	33.6 ± 38.6	4.2 ± 3.0	2.8	0.1	9.9
118	C_2H_3N	Acetonitrile	3273.2 ± 2921.0	2628.6 ± 1550.5	1879.6 ± 1117.9	2003.1	5377.2	3826.7
119	C_2H_5N	Ethenamine	4.8 ± 5.5	2.3 ± 1.5	1.1 ± 0.6	1.6	2.0	3.3
120	C_2H_7N	Dimethylamine, Ethylamine	2.2 ± 2.2	1.2 ± 0.8	1.5 ± 3.5	0.1	0.4	0.3
121	C_3H_3N	Acrylonitrile	163.7 ± 153.7	315.3 ± 301.7	386.6 ± 344.1	301.1	3491.1	146.9
122	C_3H_5N	Propanenitrile	170.5 ± 232.1	69.9 ± 54.8	144.3 ± 141.0	188.6	685.1	144.0
123	C_3H_9N	Trimethylamine,1-Propanamine, 2-Propanamine, Methylethylamine	1.0 ± 1.2	0.6 ± 0.6	0.1 ± 0.1	0.0	0.2	0.2
124	C_4H_5N	Pyrrole	326.8 ± 425.7	70.4 ± 135.3	104.9 ± 96.0	163.5	474.6	38.7
125	C_4H_7N	Dihydropyrrole, butane nitrile, pyrroline	47.7 ± 62.8	21.2 ± 17.7	47.4 ± 49.6	68.7	168.4	31.8

Table S4. Annual consumption of residential coal and biomass combustion in China mainland.

Year	Residential coal consumption (10^4 t)	Biomass combustion (10^8 t)
2010	9159	3.1
2011	9212	3.1
2012	9253	3.0
2013	9290	2.9
2014	9303	2.8
2015	9627	2.7
2016	9492	2.6
2017	9283	2.2
2018	7714	2.3
2019	6547	2.2

Table S5. Annual consumption of residential coal and biomass combustion by province in 2019 and 2017, respectively.

NO.	Region	Residential coal consumption (10^4 t)	Biomass combustion (10^4 t)
1	Beijing	48.7	5.1
2	Tianjin	38.2	60.1
3	Hebei[a]	1313.3	178.8
4	Shanxi	422.7	288.2
5	Inner Mongolia	333.7	60.1
6	Liaoning[a]	413.6	244.4
7	Jilin	188.5	1242.9
8	Heilongjiang	273.2	2845.7
9	Shanghai	4.1	20.2
10	Jiangsu	-	1470.1
11	Zhejiang	28.2	163.9
12	Anhui	35.0	1480.3
13	Fujian	21.4	104.1
14	Jiangxi	250.1	894.1
15	Shandong	478.7	1600.0
16	Henan	331.6	1700.0
17	Hubei	501.5	1138.1
18	Hunan	408.4	1488.5
19	Guangdong	65.9	862.7
20	Guangxi	0.9	970.0
21	Hainan	-	101.4
22	Chongqing	48.1	208.8
23	Sichuan	72.1	800.0
24	Guizhou	494.0	144.0
25	Yunnan	327.7	500.0
26	Tibet	-	-
27	Shaanxi	284.7	244.1
28	Gansu	327.5	210.2
29	Qinghai	65.0	23.3
30	Ningxia	40.3	78.6
31	Xinjiang	465.9	642.0
32	National	6547.0	22000.0

[a] Consumption from biomass combustion in Hebei and Liaoning are from 2020 statistic data.

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