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Supplement of

Mass spectral characterization of primary emissions and implications in source apportionment of organic aerosol

Weiqi Xu et al.

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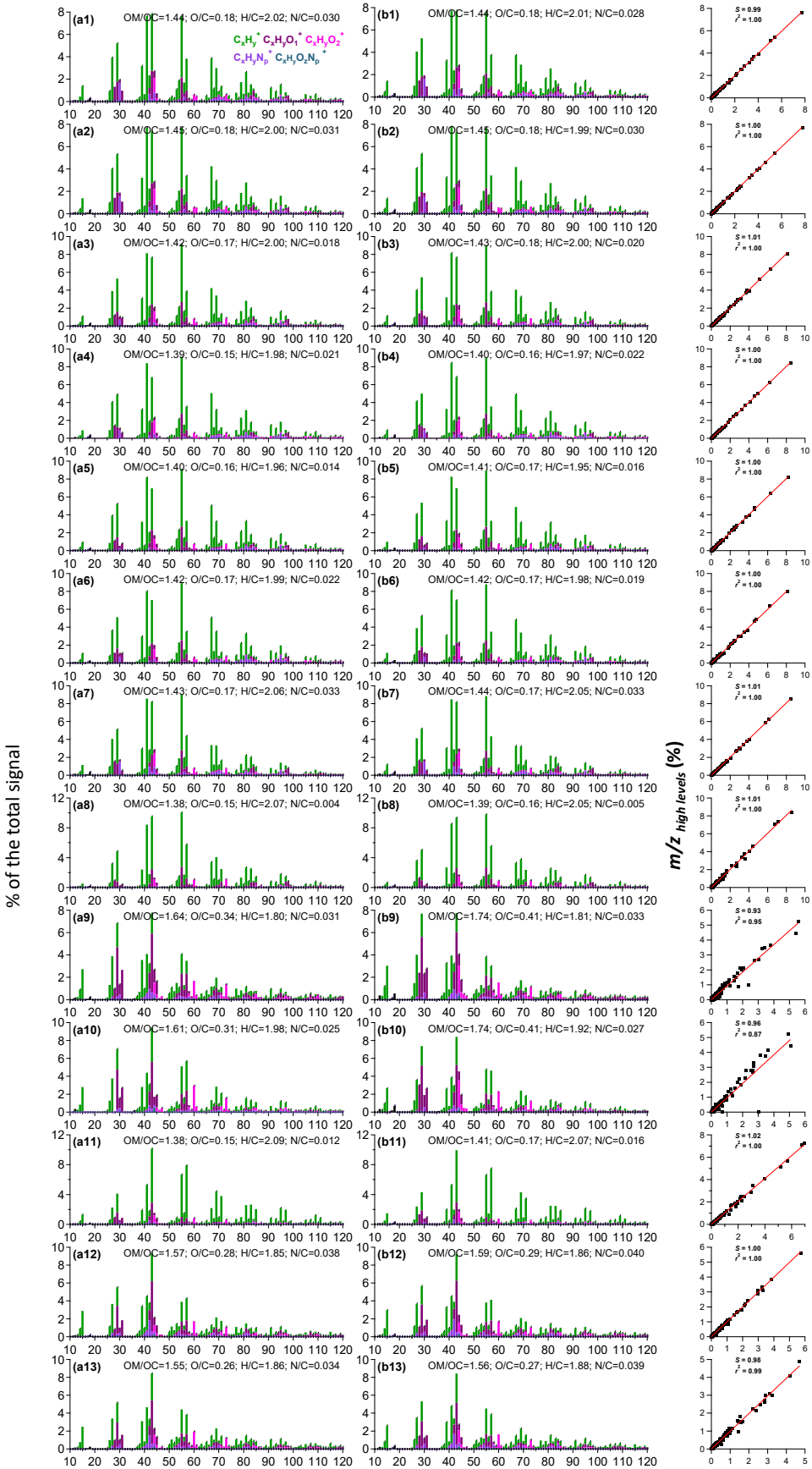

% of the total signal
m/z high levels (%)
(a1) OM/OC=1.44; O/C=0.18; H/C=2.02; N/C=0.030
(b1) OM/OC=1.44; O/C=0.18; H/C=2.01; N/C=0.028
(a2) OM/OC=1.45; O/C=0.18; H/C=2.00; N/C=0.031
(b2) OM/OC=1.45; O/C=0.18; H/C=1.99; N/C=0.030
(a3) OM/OC=1.42; O/C=0.17; H/C=2.00; N/C=0.018
(b3) OM/OC=1.43; O/C=0.18; H/C=2.00; N/C=0.020
(a4) OM/OC=1.39; O/C=0.15; H/C=1.98; N/C=0.021
(b4) OM/OC=1.40; O/C=0.16; H/C=1.97; N/C=0.022
(a5) OM/OC=1.40; O/C=0.16; H/C=1.96; N/C=0.014
(b5) OM/OC=1.41; O/C=0.17; H/C=1.95; N/C=0.016
(a6) OM/OC=1.42; O/C=0.17; H/C=1.99; N/C=0.022
(b6) OM/OC=1.42; O/C=0.17; H/C=1.98; N/C=0.019
(a7) OM/OC=1.43; O/C=0.17; H/C=2.06; N/C=0.033
(b7) OM/OC=1.44; O/C=0.17; H/C=2.05; N/C=0.033
(a8) OM/OC=1.38; O/C=0.15; H/C=2.07; N/C=0.004
(b8) OM/OC=1.39; O/C=0.16; H/C=2.05; N/C=0.005
(a9) OM/OC=1.64; O/C=0.34; H/C=1.80; N/C=0.031
(b9) OM/OC=1.74; O/C=0.41; H/C=1.81; N/C=0.033
(a10) OM/OC=1.61; O/C=0.31; H/C=1.98; N/C=0.025
(b10) OM/OC=1.74; O/C=0.41; H/C=1.92; N/C=0.027
(a11) OM/OC=1.38; O/C=0.15; H/C=2.09; N/C=0.012
(b11) OM/OC=1.41; O/C=0.17; H/C=2.07; N/C=0.016
(a12) OM/OC=1.57; O/C=0.28; H/C=1.85; N/C=0.038
(b12) OM/OC=1.59; O/C=0.29; H/C=1.86; N/C=0.040
(a13) OM/OC=1.55; O/C=0.26; H/C=1.86; N/C=0.034
(b13) OM/OC=1.56; O/C=0.27; H/C=1.88; N/C=0.039
$C_xH_y^+$ $C_xH_yO_1^+$ $C_xH_yO_2^+$
$C_xH_yN_p^+$ $C_xH_yO_2N_p^+$

[continued]

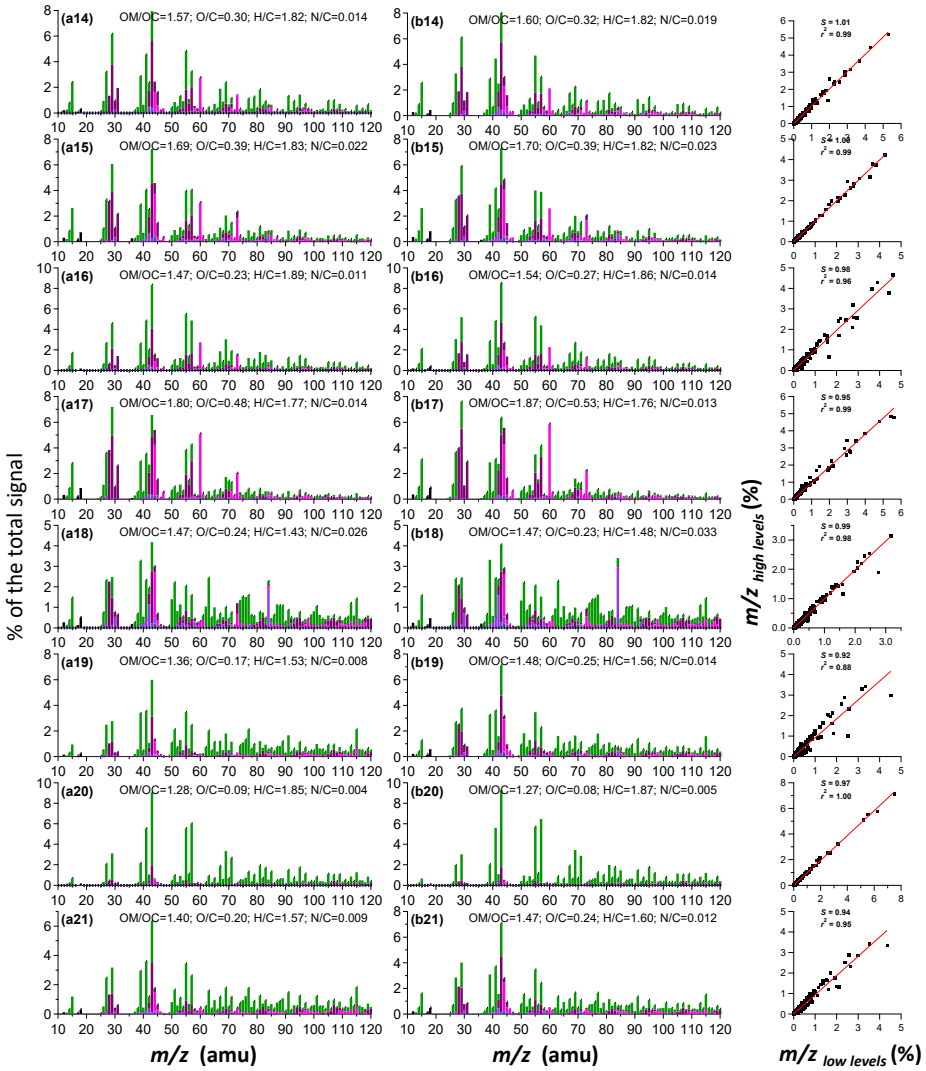
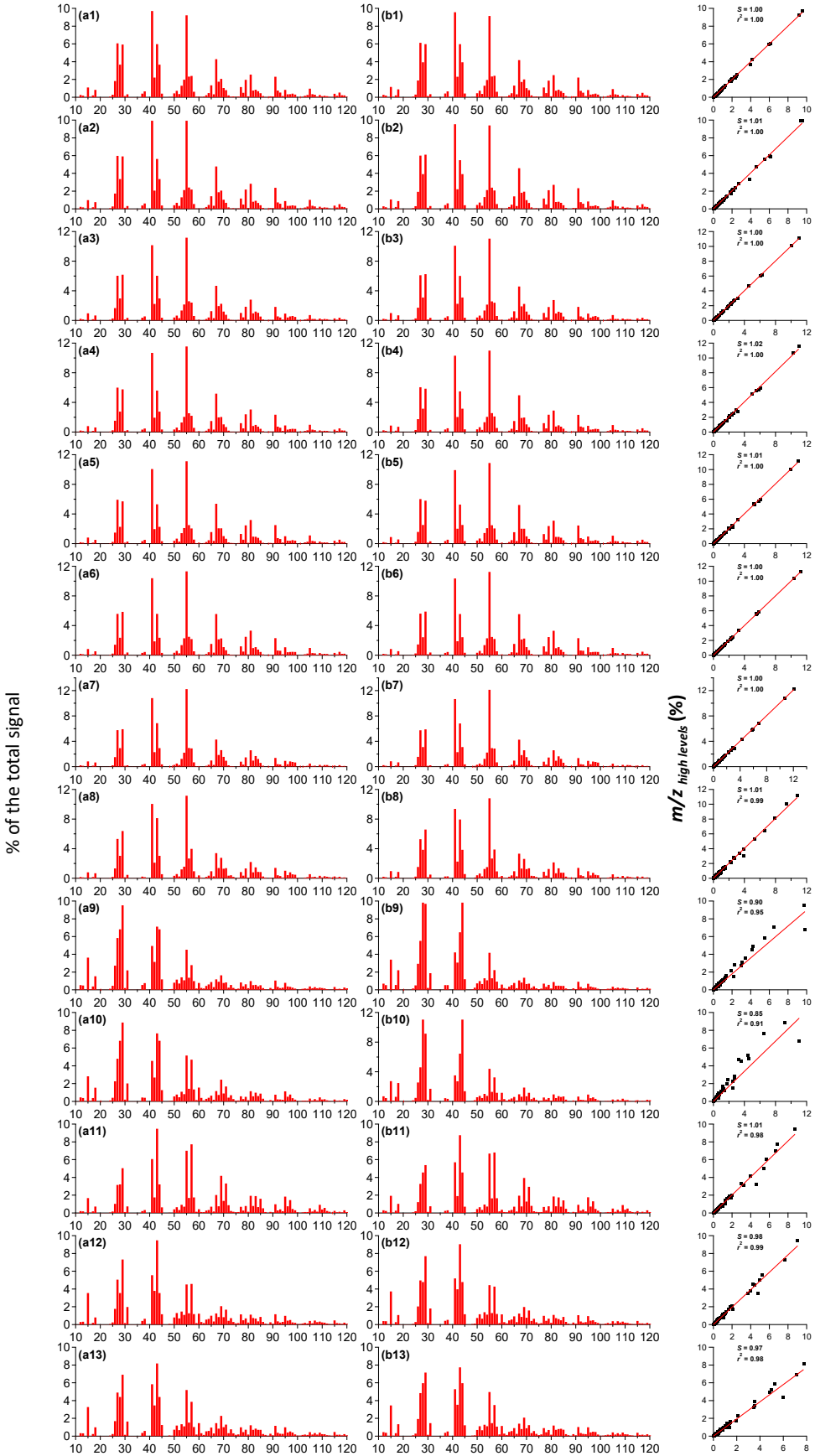


Figure S1. The mass spectral profiles of OA measured by SV-AMS at (a) high and (b) low levels from (1) stir-fried garlic with corn oil, (2) stir-fried celery with corn oil, (3) peanut oil, (4) bean oil, (5) sunflower oil, (6) blend oil, (7) lard oil and (8) barbecue (9) wheat, (10) corn, (11) bean, (12) rape, (13) cotton, (14) birchen, (15) pine tree, (16) poplar, (17) Chinese oak, (18) flaming combustion of brown coal, (19) smoldering combustion of brown coal, (20) flaming combustion of bituminous coal and (21) smoldering combustion of bituminous coal. The comparison of mass spectrum for each experiment is shown. The detailed descriptions of cooking and burning fuels are presented in Table S1.


% of the total signal
m/z high levels (%)
(a1)
(b1)
S = 1.00
r² = 1.00
(a2)
(b2)
S = 1.01
r² = 1.00
(a3)
(b3)
S = 1.00
r² = 1.00
(a4)
(b4)
S = 1.02
r² = 1.00
(a5)
(b5)
S = 1.01
r² = 1.00
(a6)
(b6)
S = 1.00
r² = 1.00
(a7)
(b7)
S = 1.00
r² = 1.00
(a8)
(b8)
S = 1.01
r² = 0.99
(a9)
(b9)
S = 0.90
r² = 0.95
(a10)
(b10)
S = 0.85
r² = 0.91
(a11)
(b11)
S = 1.01
r² = 0.98
(a12)
(b12)
S = 0.98
r² = 0.99
(a13)
(b13)
S = 0.97
r² = 0.98

[continued]

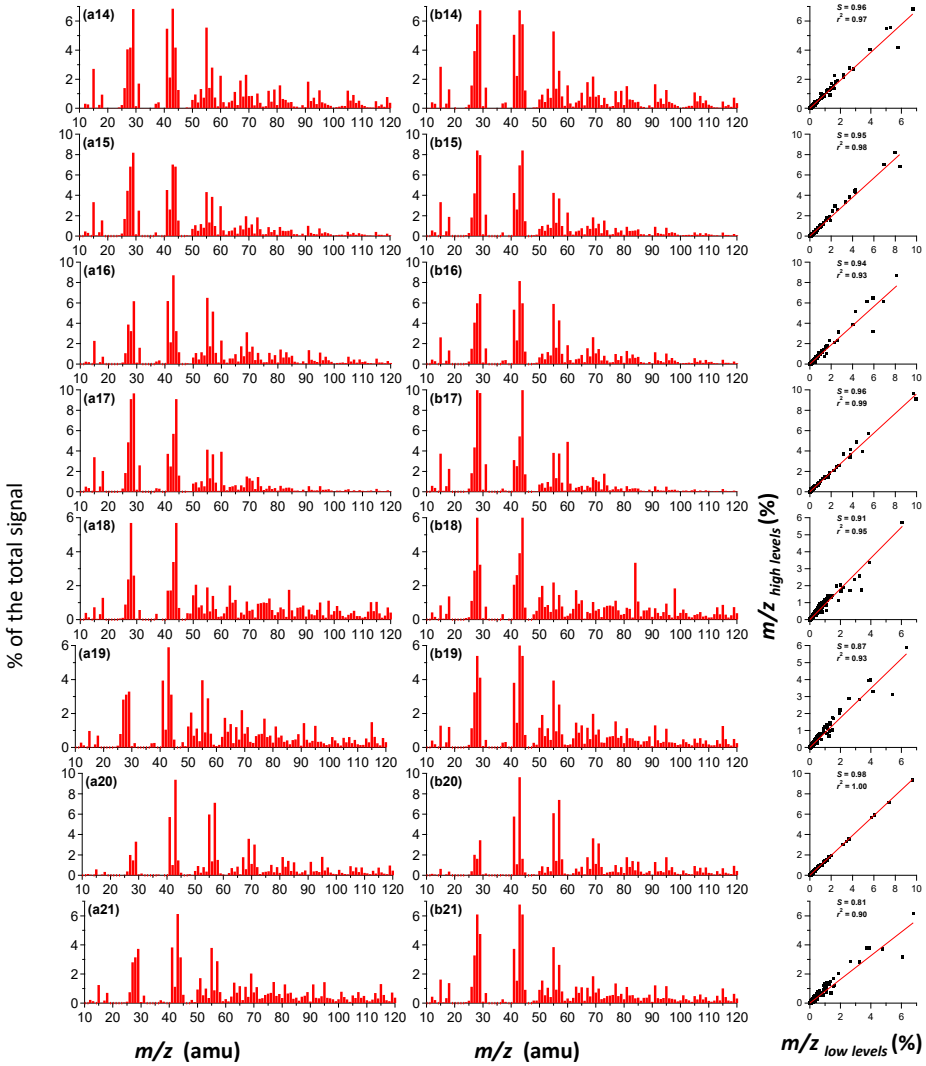
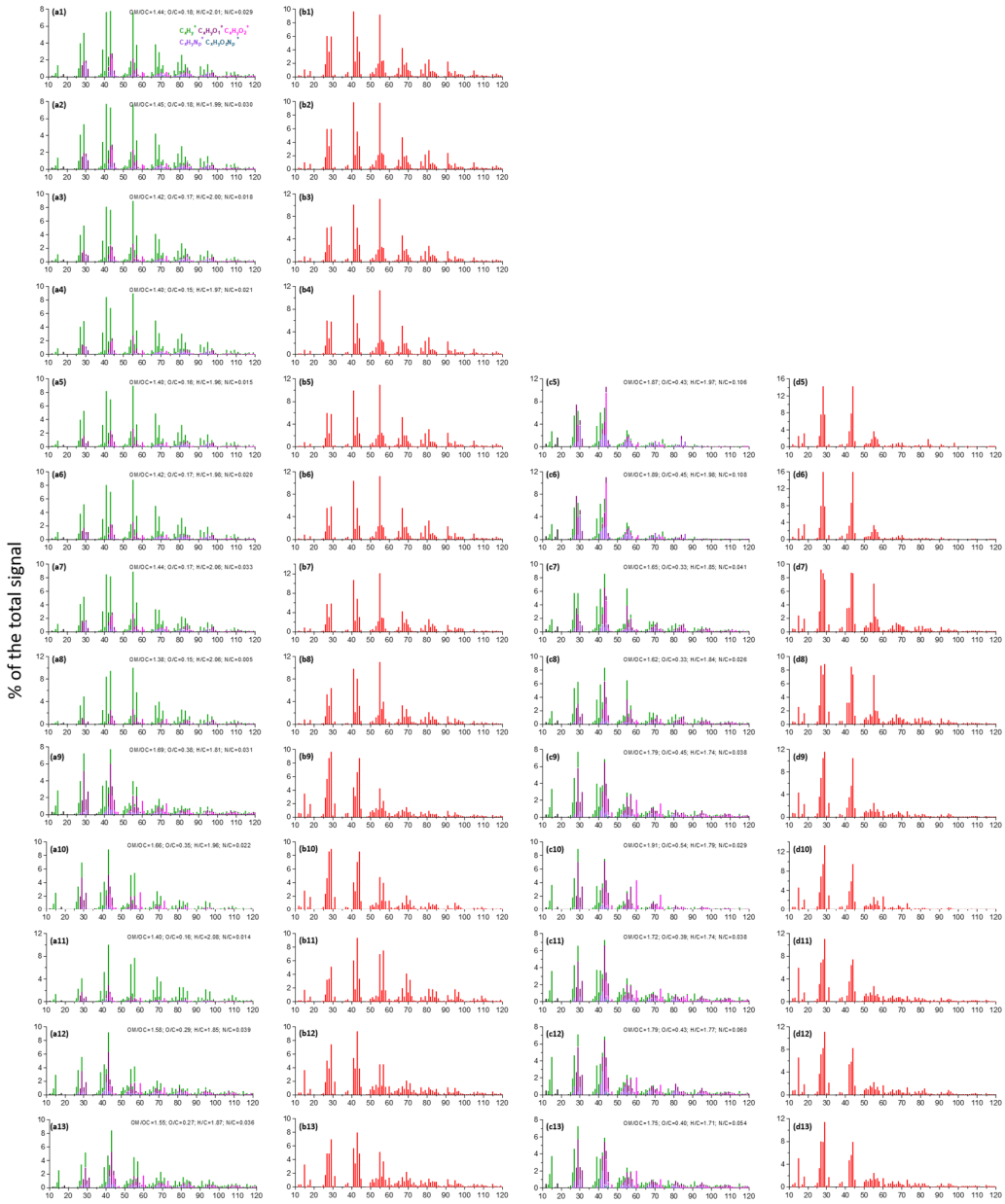


Figure S2. The mass spectral profiles of OA measured by CV-ACSM at (a) high and (b) low levels from (1) stir-fried garlic with corn oil, (2) stir-fried celery with corn oil, (3) peanut oil, (4) bean oil, (5) sunflower oil, (6) blend oil, (7) lard oil and (8) barbecue (9) wheat, (10) corn, (11) bean, (12) rape, (13) cotton, (14) birchen, (15) pine tree, (16) poplar, (17) Chinese oak, (18) flaming combustion of brown coal, (19) smoldering combustion of brown coal, (20) flaming combustion of bituminous coal and (21) smoldering combustion of bituminous coal. The comparison of mass spectrum for each experiment is shown. The detailed descriptions of cooking and burning fuels are presented in Table S2.


% of the total signal
(a1)
OM/OC=1.44; O/C=0.18; H/C=2.01; N/C=0.029
(b1)
(a2)
OM/OC=1.45; O/C=0.18; H/C=1.99; N/C=0.030
(b2)
(a3)
OM/OC=1.42; O/C=0.17; H/C=2.00; N/C=0.018
(b3)
(a4)
OM/OC=1.40; O/C=0.15; H/C=1.97; N/C=0.021
(b4)
(a5)
OM/OC=1.40; O/C=0.16; H/C=1.96; N/C=0.015
(b5)
(c5)
OM/OC=1.87; O/C=0.43; H/C=1.97; N/C=0.106
(d5)
(a6)
OM/OC=1.42; O/C=0.17; H/C=1.98; N/C=0.020
(b6)
(c6)
OM/OC=1.69; O/C=0.45; H/C=1.98; N/C=0.108
(d6)
(a7)
OM/OC=1.44; O/C=0.17; H/C=2.06; N/C=0.033
(b7)
(c7)
OM/OC=1.65; O/C=0.33; H/C=1.85; N/C=0.041
(d7)
(a8)
OM/OC=1.38; O/C=0.15; H/C=2.06; N/C=0.005
(b8)
(c8)
OM/OC=1.62; O/C=0.33; H/C=1.84; N/C=0.026
(d8)
(a9)
OM/OC=1.69; O/C=0.38; H/C=1.81; N/C=0.031
(b9)
(c9)
OM/OC=1.79; O/C=0.45; H/C=1.74; N/C=0.038
(d9)
(a10)
OM/OC=1.66; O/C=0.35; H/C=1.96; N/C=0.022
(b10)
(c10)
OM/OC=1.91; O/C=0.54; H/C=1.79; N/C=0.029
(d10)
(a11)
OM/OC=1.40; O/C=0.16; H/C=2.08; N/C=0.014
(b11)
(c11)
OM/OC=1.72; O/C=0.39; H/C=1.74; N/C=0.038
(d11)
(a12)
OM/OC=1.58; O/C=0.29; H/C=1.85; N/C=0.039
(b12)
(c12)
OM/OC=1.79; O/C=0.43; H/C=1.77; N/C=0.060
(d12)
(a13)
OM/OC=1.55; O/C=0.27; H/C=1.87; N/C=0.036
(b13)
(c13)
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(d13)

[continued]

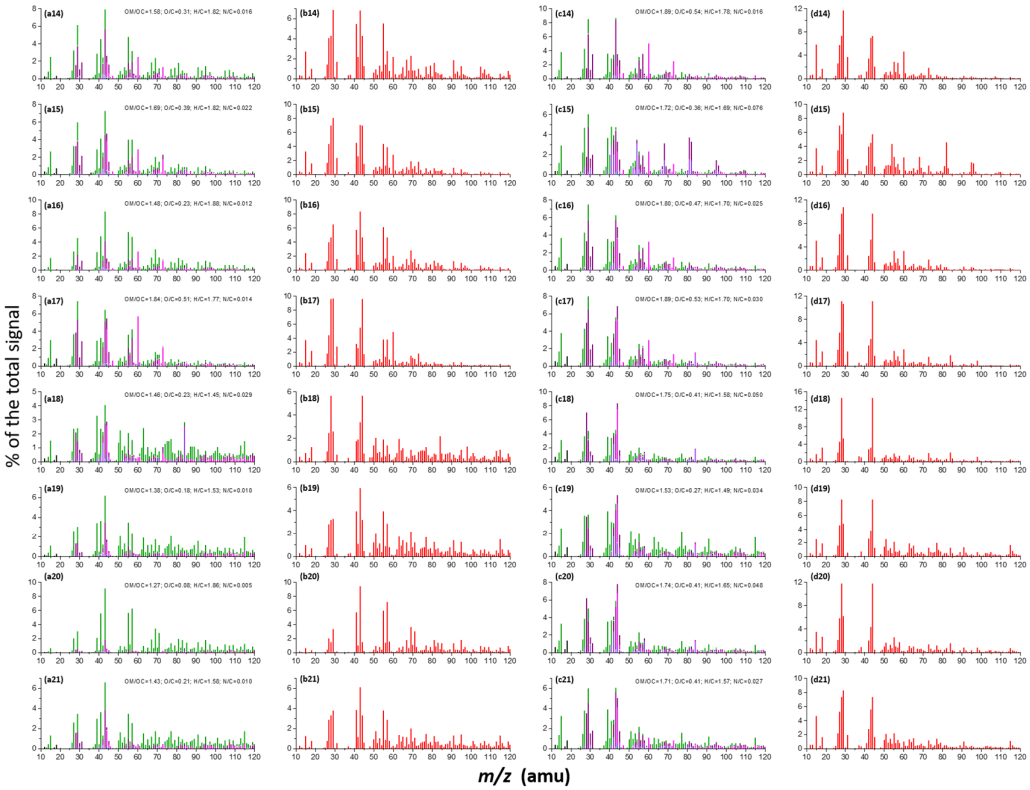

Figure S3. The mass spectral profiles of OA measured by (a) SV-AMS, (b) CV-ACSM and WSOA measured by (c) SV-AMS and (d) CV-ACSM from (1) stir-fried garlic with corn oil, (2) stir-fried celery with corn oil, (3) peanut oil, (4) bean oil, (5) sunflower oil, (6) blend oil, (7) lard oil and (8) barbecue (9) wheat, (10) corn, (11) bean, (12) rape, (13) cotton, (14) birchen, (15) pine tree, (16) poplar, (17) Chinese oak, (18) flaming combustion of brown coal, (19) smoldering combustion of brown coal, (20) flaming combustion of bituminous coal and (21) smoldering combustion of bituminous coal.

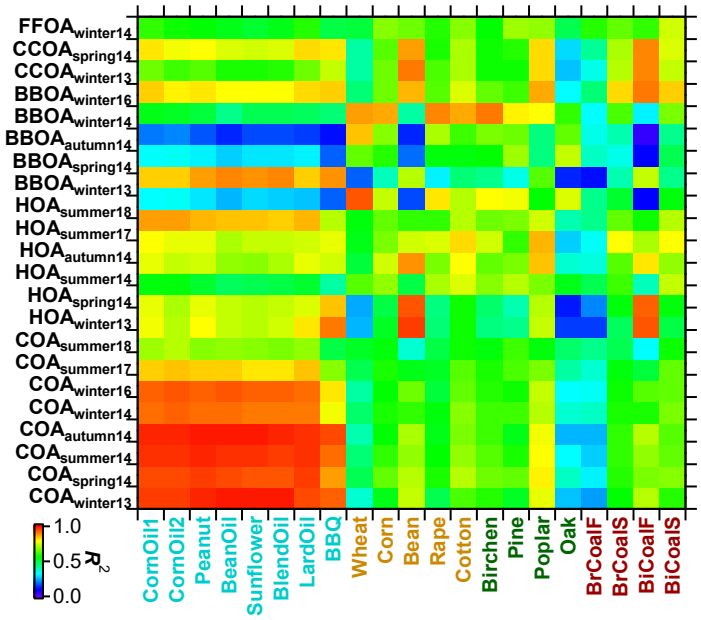

Figure S4. Mass spectral correlations of primary emissions (including cooking, crop straw burning, wood burning and coal combustion) in this study with the previous PMF-resolved OA factors in Beijing (Sun et al., 2016;Xu et al., 2017;Xu et al., 2019).

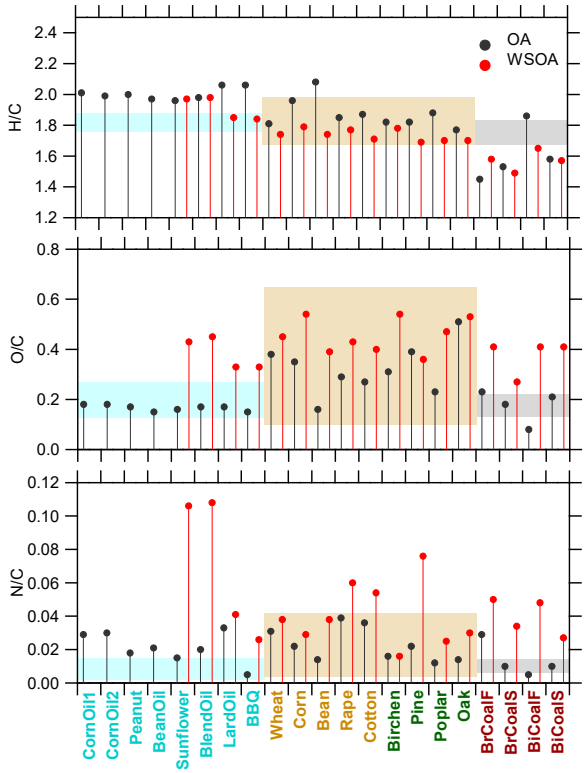

Figure S5. Comparison of H/C, O/C and N/C ratios between OA and WSOA measured by SV-AMS for different primary emissions. The shaded areas indicate the range of elemental ratios that were determined from previous AMS studies in Beijing (Sun et al., 2016;Xu et al., 2017;Xu et al., 2019).

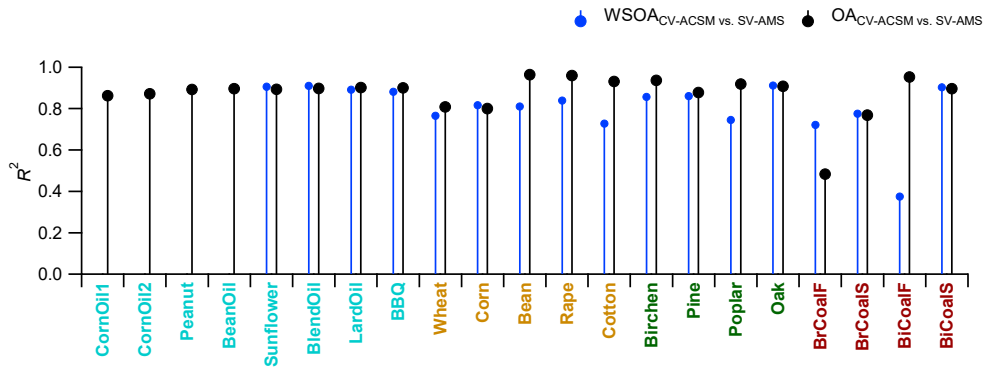

Figure S6. The correlation coefficients between OA and WSOA measured by CV-ACSM and SV-AMS.

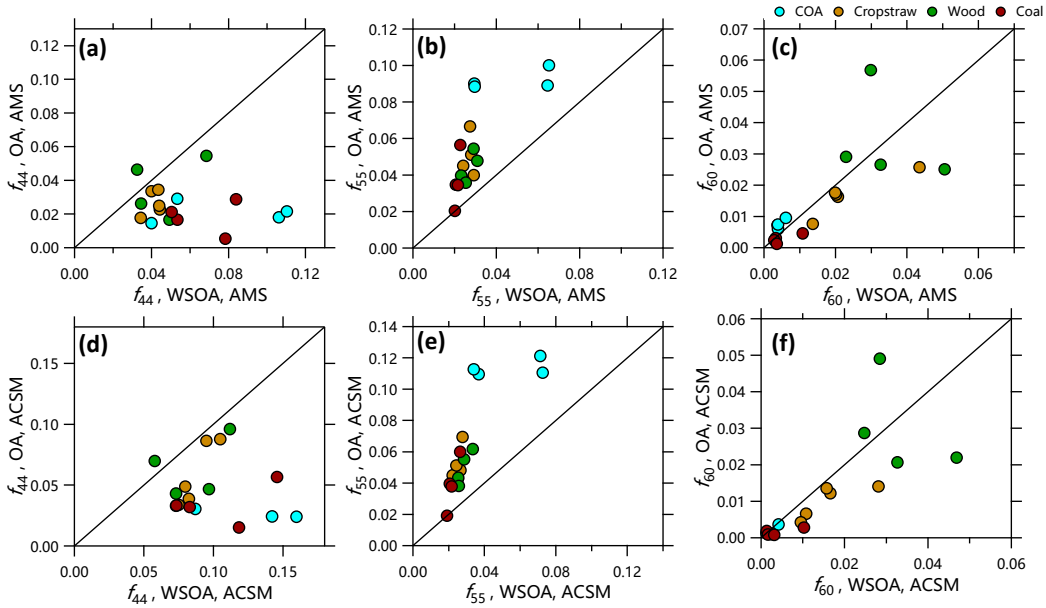

Figure S7. Relationship between OA and WSOA of f_{44}, f_{55} and f_{60} measured by SV-AMS and CV-ACSM.

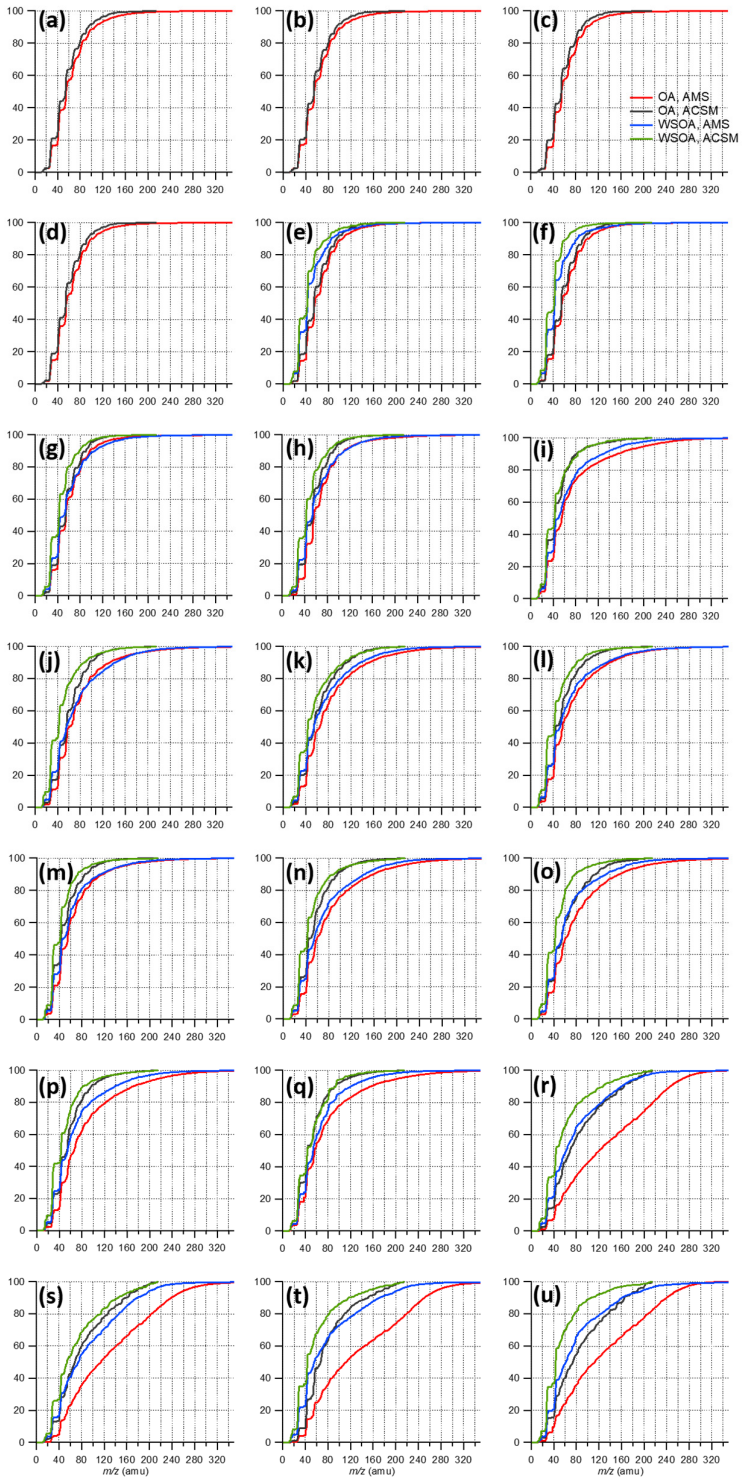

Figure S8. Cumulative mass fraction of mass spectral profiles of OA from (a) stir-fried garlic with corn oil, (b) stir-fried celery with corn oil, (c) peanut oil, (d) bean oil, (e) sunflower oil, (f) blend oil, (g) lard oil and (h) barbecue (i) wheat, (j) corn, (k) bean, (l) rape, (m) cotton, (n) birchen, (o) pine tree, (p) poplar, (q) Chinese oak, (r) flaming combustion of brown coal, (s) smoldering combustion of brown coal, (t) flaming combustion of bituminous coal and (u) smoldering combustion of bituminous coal.

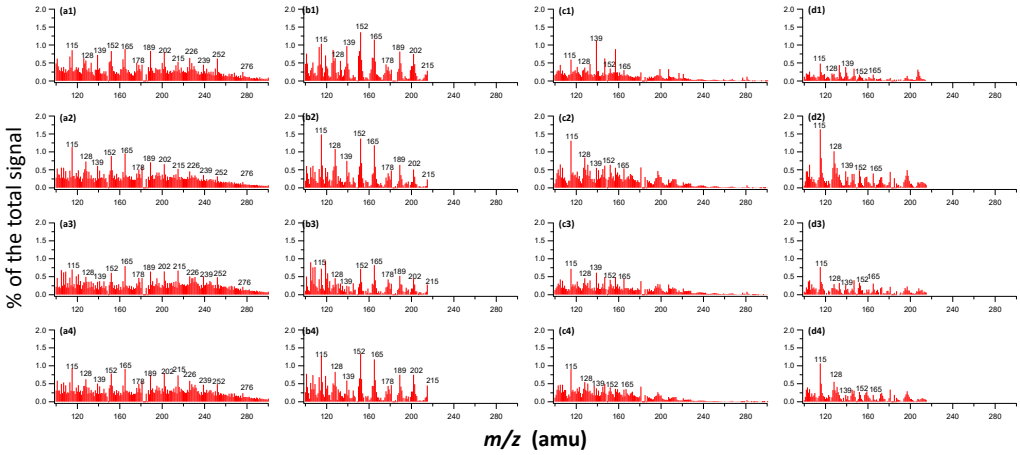

Figure S9. Unit mass resolution spectra (*m/z* 100–350) of OA measured by (a) SV-AMS, (b) CV-ACSM and WSOA measured by (c) SV-AMS and (d) CV-ACSM from (1) flaming combustion of brown coal, (2) smoldering combustion of brown coal, (3) flaming combustion of bituminous coal and (4) smoldering combustion of bituminous coal.

Table S1. A summary of f_{44}, f_{43}, f_{60} and OA concentration (μg m^{-3}) at high and low OA levels measured by SV-AMS in each experiment. The default RIE (1.4) and CE=1 were used.

Fuels	OA	f_{44}	f_{43}	f_{60}	OA	f_{44}	f_{43}	f_{60}
	High Conc.				Low Conc.			
CornOil1	503.9	0.027	0.078	0.006	382.9	0.029	0.077	0.006
CornOil2	507.7	0.029	0.074	0.006	382.6	0.030	0.073	0.006
Peanut	564.3	0.021	0.077	0.008	388.8	0.023	0.077	0.008
BeanOil	485.0	0.023	0.068	0.006	338.3	0.024	0.069	0.006
Sunflower	624.0	0.017	0.070	0.007	388.3	0.019	0.070	0.007
BlendOil	666.9	0.020	0.070	0.006	313.8	0.023	0.070	0.006
LardOil	221.4	0.029	0.082	0.008	162.2	0.030	0.082	0.007
BBQ	421.7	0.014	0.095	0.010	150.4	0.018	0.094	0.009
Wheat	862.7	0.027	0.077	0.017	79.4	0.041	0.077	0.015
Corn	548.2	0.031	0.102	0.032	151.0	0.047	0.084	0.023
Bean	849.2	0.016	0.101	0.008	364.0	0.021	0.099	0.007
Rape	642.1	0.021	0.093	0.017	241.5	0.025	0.092	0.017
Cotton	742.0	0.023	0.084	0.019	264.9	0.028	0.084	0.016
Birchen	338.4	0.025	0.079	0.028	150.4	0.031	0.080	0.021
Pine	361.0	0.047	0.072	0.031	173.8	0.050	0.073	0.026
Poplar	1369.6	0.016	0.084	0.027	185.6	0.028	0.085	0.023
Oak	513.5	0.055	0.066	0.051	201.5	0.056	0.063	0.059
BrCoalF	154.2	0.029	0.042	0.003	154.4	0.029	0.041	0.003
BrCoalS	269.8	0.014	0.060	0.002	103.1	0.034	0.071	0.003
BiCoalF	376.4	0.006	0.091	0.001	339.4	0.005	0.092	0.001
BiCoalS	275.8	0.018	0.064	0.004	120.6	0.029	0.071	0.005

Note: CornOil1= stir-fried garlic with corn oil; CornOil2= stir-fried celery with corn oil; Peanut= stir-fried celery with peanut oil; Sunflower= stir-fried celery with sunflower oil; BeanOil= stir-fried celery with bean oil; BlendOil= stir-fried celery with blend oil; LardOil= stir-fried celery with lard oil; BBQ= barbecue; Wheat= dry wheat stalk burning; Corn= dry corn stalk burning; Bean= dry bean stalk burning; Rape= dry rape stalk burning; Cotton= dry cotton stalk burning; Birchen= dry birchen burning; Pine= dry pine tree burning; Poplar= dry poplar burning; Oak= dry Chinese oak burning; BrCoalF= brown coal combustion under flaming conditions; BrCoalS= brown coal combustion under smoldering conditions; BiCoalF= bituminous coal combustion under flaming conditions; BiCoalS= bituminous coal combustion under smoldering conditions.

Table S2. A summary of f_{44}, f_{43}, f_{60} and OA concentration (μg m^{-3}) at high and low OA levels measured by CV-ACSM in each experiment. The default RIE (1.4) and CE=1 were used.

Fuels	OA	f_{44}	f_{43}	f_{60}	OA	f_{44}	f_{43}	f_{60}
	High Conc.				Low Conc.			
CornOil1	715.3	0.037	0.060	0.001	517.0	0.039	0.060	0.001
CornOil2	714.4	0.033	0.056	0.001	265.3	0.039	0.055	0.000
Peanut	799.2	0.030	0.060	0.001	676.5	0.031	0.060	0.001
BeanOil	613.9	0.028	0.056	0.001	286.7	0.032	0.055	0.001
Sunflower	1064.2	0.023	0.053	0.001	730.2	0.025	0.053	0.001
BlendOil	927.0	0.024	0.056	0.001	829.7	0.024	0.056	0.001
LardOil	518.7	0.029	0.069	0.001	366.6	0.031	0.068	0.001
BBQ	290.4	0.030	0.081	0.004	102.5	0.038	0.079	0.003
Wheat	294.8	0.068	0.071	0.008	83.3	0.098	0.065	0.006
Corn	523.5	0.068	0.077	0.016	119.8	0.110	0.064	0.012
Bean	893.0	0.032	0.095	0.004	279.7	0.046	0.088	0.004
Rape	683.8	0.035	0.095	0.012	172.8	0.048	0.090	0.011
Cotton	615.2	0.044	0.082	0.015	188.1	0.060	0.077	0.012
Birchen	558.3	0.042	0.068	0.022	206.8	0.058	0.067	0.016
Pine	402.8	0.068	0.070	0.029	107.1	0.084	0.069	0.023
Poplar	616.4	0.032	0.087	0.023	104.8	0.060	0.081	0.018
Oak	485.9	0.091	0.057	0.039	133.4	0.100	0.054	0.049
BrCoalF	121.6	0.057	0.034	0.002	82.1	0.061	0.039	0.002
BrCoalS	269.4	0.031	0.059	0.001	104.8	0.054	0.063	0.001
BiCoalF	334.9	0.015	0.094	0.001	241.4	0.016	0.096	0.001
BiCoalS	276.8	0.031	0.061	0.003	101.4	0.061	0.068	0.003

Note: CornOil1= stir-fried garlic with corn oil; CornOil2= stir-fried celery with corn oil; Peanut= stir-fried celery with peanut oil; Sunflower= stir-fried celery with sunflower oil; BeanOil= stir-fried celery with bean oil; BlendOil= stir-fried celery with blend oil; LardOil= stir-fried celery with lard oil; BBQ= barbecue; Wheat= dry wheat stalk burning; Corn= dry corn stalk burning; Bean= dry bean stalk burning; Rape= dry rape stalk burning; Cotton= dry cotton stalk burning; Birchen= dry birchen burning; Pine= dry pine tree burning; Poplar= dry poplar burning; Oak= dry Chinese oak burning; BrCoalF= brown coal combustion under flaming conditions; BrCoalS= brown coal combustion under smoldering conditions; BiCoalF= bituminous coal combustion under flaming conditions; BiCoalS= bituminous coal combustion under smoldering conditions.

Table S3. A summary of elemental ratios and f_{44}, f_{43}, f_{60}, f_{73}, f_{55}, f_{57} of OA and WSOA measured by SV-AMS and CV-ACSM.

Fuels	O/C	H/C	f_{44}	f_{43}	f_{60}	f_{73}	f_{55}	f_{57}	f_{44}	f_{43}	f_{60}	f_{73}	f_{55}	f_{57}
	OA measure by SV-AMS								OA measured by CV-ACSM					
CornOil1	0.18	2.01	0.028	0.078	0.006	0.006	0.076	0.038	0.037	0.060	0.001	0.001	0.092	0.024
CornOil2	0.18	1.99	0.029	0.073	0.006	0.007	0.077	0.034	0.034	0.056	0.001	0.001	0.099	0.022
Peanut	0.17	2.00	0.022	0.077	0.008	0.009	0.090	0.039	0.030	0.060	0.001	0.001	0.111	0.024
BeanOil	0.15	1.97	0.024	0.068	0.006	0.006	0.090	0.035	0.029	0.056	0.001	0.001	0.114	0.022
Sunflower	0.16	1.96	0.018	0.070	0.007	0.008	0.090	0.033	0.024	0.053	0.001	0.001	0.110	0.020
BlendOil	0.17	1.98	0.022	0.070	0.006	0.007	0.088	0.035	0.024	0.056	0.001	0.001	0.113	0.022
LardOil	0.17	2.06	0.029	0.082	0.007	0.008	0.089	0.044	0.030	0.068	0.001	0.001	0.121	0.029
BBQ	0.15	2.06	0.015	0.095	0.010	0.011	0.100	0.057	0.033	0.080	0.004	0.004	0.111	0.040
Wheat	0.38	1.81	0.034	0.078	0.016	0.013	0.040	0.033	0.088	0.067	0.007	0.005	0.043	0.024
Corn	0.35	1.96	0.035	0.090	0.026	0.014	0.051	0.055	0.086	0.071	0.014	0.006	0.048	0.040
Bean	0.16	2.08	0.018	0.100	0.008	0.006	0.067	0.077	0.034	0.094	0.004	0.002	0.070	0.075
Rape	0.29	1.85	0.023	0.092	0.017	0.011	0.038	0.042	0.039	0.093	0.012	0.007	0.045	0.045
Cotton	0.27	1.87	0.025	0.085	0.018	0.011	0.045	0.039	0.049	0.080	0.014	0.007	0.051	0.038
Birchen	0.31	1.82	0.026	0.080	0.025	0.013	0.048	0.032	0.043	0.068	0.022	0.010	0.055	0.028
Pine	0.39	1.82	0.046	0.072	0.029	0.023	0.040	0.040	0.070	0.071	0.029	0.018	0.043	0.039
Poplar	0.23	1.88	0.017	0.083	0.027	0.015	0.054	0.048	0.047	0.084	0.021	0.009	0.062	0.047
Oak	0.51	1.77	0.055	0.065	0.057	0.022	0.036	0.042	0.096	0.055	0.049	0.018	0.038	0.038
BrCoalF	0.23	1.45	0.029	0.041	0.003	0.011	0.020	0.015	0.057	0.034	0.002	0.009	0.019	0.014
BrCoalS	0.18	1.53	0.017	0.062	0.002	0.003	0.035	0.024	0.032	0.059	0.001	0.003	0.040	0.029
BiCoalF	0.08	1.86	0.005	0.092	0.001	0.002	0.057	0.063	0.015	0.095	0.001	0.001	0.060	0.072
BiCoalS	0.21	1.58	0.021	0.066	0.005	0.005	0.035	0.026	0.033	0.062	0.003	0.004	0.038	0.029
	WSOA measure by SV-AMS								WSOA measured by CV-ACSM					
Sunflower	0.43	1.97	0.106	0.069	0.004	0.004	0.029	0.015	0.142	0.079	0.001	0.001	0.037	0.018
BlendOil	0.45	1.98	0.110	0.073	0.004	0.004	0.030	0.016	0.160	0.086	0.002	0.001	0.034	0.018
LardOil	0.33	1.85	0.053	0.086	0.004	0.004	0.065	0.026	0.087	0.088	0.003	0.003	0.071	0.019
BBQ	0.33	1.84	0.040	0.084	0.006	0.008	0.065	0.028	0.073	0.085	0.004	0.004	0.073	0.020
Wheat	0.45	1.74	0.040	0.069	0.021	0.016	0.029	0.028	0.105	0.056	0.011	0.010	0.025	0.014
Corn	0.54	1.79	0.044	0.075	0.044	0.022	0.028	0.035	0.095	0.059	0.028	0.014	0.027	0.019
Bean	0.39	1.74	0.034	0.072	0.014	0.015	0.027	0.020	0.075	0.065	0.010	0.010	0.028	0.013
Rape	0.43	1.77	0.044	0.069	0.020	0.012	0.024	0.020	0.082	0.059	0.017	0.013	0.022	0.014
Cotton	0.40	1.71	0.044	0.059	0.020	0.010	0.024	0.020	0.080	0.056	0.016	0.013	0.024	0.015
Birchen	0.54	1.78	0.035	0.087	0.051	0.024	0.031	0.036	0.073	0.070	0.047	0.019	0.029	0.027
Pine	0.36	1.69	0.033	0.048	0.023	0.011	0.023	0.019	0.058	0.045	0.025	0.013	0.025	0.016
Poplar	0.47	1.70	0.049	0.063	0.033	0.015	0.029	0.026	0.097	0.053	0.033	0.019	0.034	0.020
Oak	0.53	1.70	0.069	0.056	0.030	0.014	0.025	0.023	0.112	0.047	0.028	0.016	0.026	0.017
BrCoalF	0.41	1.58	0.084	0.046	0.003	0.001	0.020	0.010	0.146	0.032	0.001	0.019	0.019	0.008
BrCoalS	0.27	1.49	0.054	0.046	0.003	0.001	0.021	0.009	0.083	0.038	0.002	0.012	0.021	0.006
BiCoalF	0.41	1.65	0.078	0.059	0.004	0.002	0.023	0.011	0.118	0.044	0.003	0.014	0.026	0.008
BiCoalS	0.41	1.57	0.050	0.061	0.011	0.008	0.022	0.015	0.073	0.055	0.010	0.012	0.022	0.012

Note: CornOil1= stir-fried garlic with corn oil; CornOil2= stir-fried celery with corn oil; Peanut= stir-fried celery with peanut oil; Sunflower= stir-fried celery with sunflower oil; BeanOil= stir-fried celery with bean oil; BlendOil= stir-fried celery with blend oil; LardOil= stir-fried celery with lard oil; BBQ= barbecue; Wheat= dry wheat stalk burning; Corn= dry corn stalk burning; Bean= dry bean stalk burning; Rape= dry rape stalk burning; Cotton= dry cotton stalk burning; Birchen= dry birchen burning; Pine= dry pine tree burning; Poplar= dry poplar burning; Oak= dry Chinese oak burning; BrCoalF= brown coal combustion under flaming conditions; BrCoalS= brown coal combustion under smoldering conditions; BiCoalF= bituminous coal combustion under flaming conditions; BiCoalS= bituminous coal combustion under smoldering conditions.

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