Characterization the properties of VOCs and submicron organic aerosol at a street canyon environment

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Supplemental material

Table S1. Detection limits (DL), average (± stdev) concentrations and reaction rate coefficients of studied VOCs.

VOC species	DL ng m^{-3}	Conc ng m^{-3} (ave ± stdev)	kOH (298K) cm^{-3} s^{-1}	kO_3 (298K) cm^{-3} s^{-1}	kNO_3 (298K) cm^{-3} s^{-1}
Benzene	5.3	340 ± 220	1.2E-12	-	n.a.
Toluene	18	1630 ± 1340	5.6E-12	-	n.a.
Ethylbenzene	2.7	370 ± 360	7.0E-12	-	1.2E-16
p/m-xylene	4.1	1070 ± 1060	3.7E-11 (avg)	-	2.8E-16 (avg)
styrene	11	65 ± 78	5.8E-11	-	1.5E-12
o-xylene	1.6	400 ± 410	1.4E-11	-	4.1E-16
3-ethyltoluene	0.4	190 ± 2020	1.9E-11	-	4.5E-16
4-ethyltoluene	0.6	83 ± 110	1.2E-11	-	8.6E-16
1,3,5-trimethylbenzene	0.7	93 ± 130	5.7E-11	-	8.8E-16
2-ethyltoluene	1.6	110 ± 150	1.2E-11	-	7.1E-16
1,2,4-trimethylbenzene	0.9	390 ± 560	3.3E-11	-	1.8E-15
1,2,3-trimethylbenzene	0.4	83 ± 140	3.3E-11	-	1.9E-15
aVOCs sum		4820 ± 4390			
isoprene	14	38 ± 35	1.0E-10	1.3E-17	6.5E-13
α-pinene	9	200 ± 310	5.3E-11	9.4E-17	6.2E-12
camphene	1.9	13 ± 20	7.8E-11	6.8E-19	6.2E-13
β-pinene	1.1	78 ± 142	7.4E-11	1.9E-17	2.5E-12
Δ3-carene	4.5	92 ± 194	8.8E-11	4.8E-17	9.1E-12
p-cymene	3.3	27 ± 27	1.5E-11	5.0E-20	n.a.
1,8-cineol	4.6	33 ± 27	1.1E-11	1.5E-19	n.a.
limonene	5.6	54 ± 63	1.6E-10	2.1E-16	1.2E-11
terpinolene	6.3	15 ± 21	2.3E-10	1.6E-15	9.7E-11
longicyclene	2.5	0.1 ± 1.1	9.4E-12	-	n.a.
iso-longifolene	7	0.13 ± 1.1	9.6E-11	1.1E-17	3.9E-12
β-caryophyllene	6.7	3.7 ± 7.5	2.0E-10	1.2E-14	1.9E-11
α-humulene	7	0.04 ± 0.63	2.6E-10	1.2E-16	3.5E-11
nopinone	4.5	32 ± 25	1.4E-11	-	n.a.
bVOCs sum		570 ± 770			

'-': irrelevant, 'n.a.': reaction rate not available

Table S2. Time periods and selection criteria for the air quality cases.

Source/ Case	Traffic	Coffee roastery	LRT	Biogenic organics
Time periods	28 August 2019 6:35–9:05; 29 August 2019 6:35–9:05; 3 September 2019 5:40–7:10; 3 September 2019 8:40–9:10; 6 September 2019 8:50–9:20; 7 September 2019 7:50–8:20; 11 September 2019 9:30–10:00	7 September 2019 08:10–13:40	9 September 2019 09:40 – 11 September 2019 05:20	29 August 2019 10:35–14:05; 29 August 2019 15:35–17:05; 2 September 2019 11:40–13:10; 2 September 2019 14:40–16:10; 10 September 2019 12:30–13:00; 10 September 2019 14:30–16:00
Selection criteria	NO_x > 160 µg m^{-3}; NO > 70 µg m^{-3}	CoOA elevated	LV-OOA-LRT elevated; back trajectories indicate LRT	Ambient temperature > 20 °C; Aromatics < 3000 ng m^{-3}

Table S3. Average meteorological parameters and particle and gas concentrations during the air quality cases.

Source / Case		Traffic	Coffee roastery	LRT	Biogenic organics
Temperature (°C)		16.4	16.4	17.9	21
Mixing layer height (m)		207	326	225	764
Ratio toluene/benzene		6.7	4.3	3.1	3.8
VOCs (ng m^{-3})	aromatic	13278	2450	2730	2320
	isoprene	75	20.8	27.9	33
	monoterpene	1849	222	374	235
	sesquiterpene	19.7	0	3.49	0.5
	nopinone	9.8	16.1	25.9	40
Organic aerosol (µg m^{-3})	HOA-1	1.74	0.69	0.38	0.35
	HOA-2	0.57	0.92	0.48	0.25
	CoOA	0.39	6.63	0.42	0.01
	SV-OOA	1.82	0.43	3.46	2.80
	LV-OOA	0.29	0.05	0.14	0.22
	LV-OOA-LRT	0.55	0.26	2.22	1.52
Oxidation state		-1.00	-1.32	0.59	-0.52
Inorganic species (µg m^{-3})	Nitrate	0.15	0.059	0.28	0.075
	Sulfate	0.42	0.16	1.1	0.68
	Ammonium	0.15	0.051	0.33	0.17
	BC_{ff}	2.71	0.69	1.06	1.06
	BC_{wb}	1.33	0.49	0.61	0.42
Gases (µg m^{-3})	O_3	12.3	42.5	34.8	52
	NO	98	14.5	18.1	14
	NO_x	221	49.0	56.3	47
	CO	0.30	0.20	0.217	0.2
	NO_2	70	26.8	28.6	25
Particle number concentration (# cm^{-3})	>10 nm	23100	20700	8150	5840
	10–25 nm	12700	6040	3190	1840

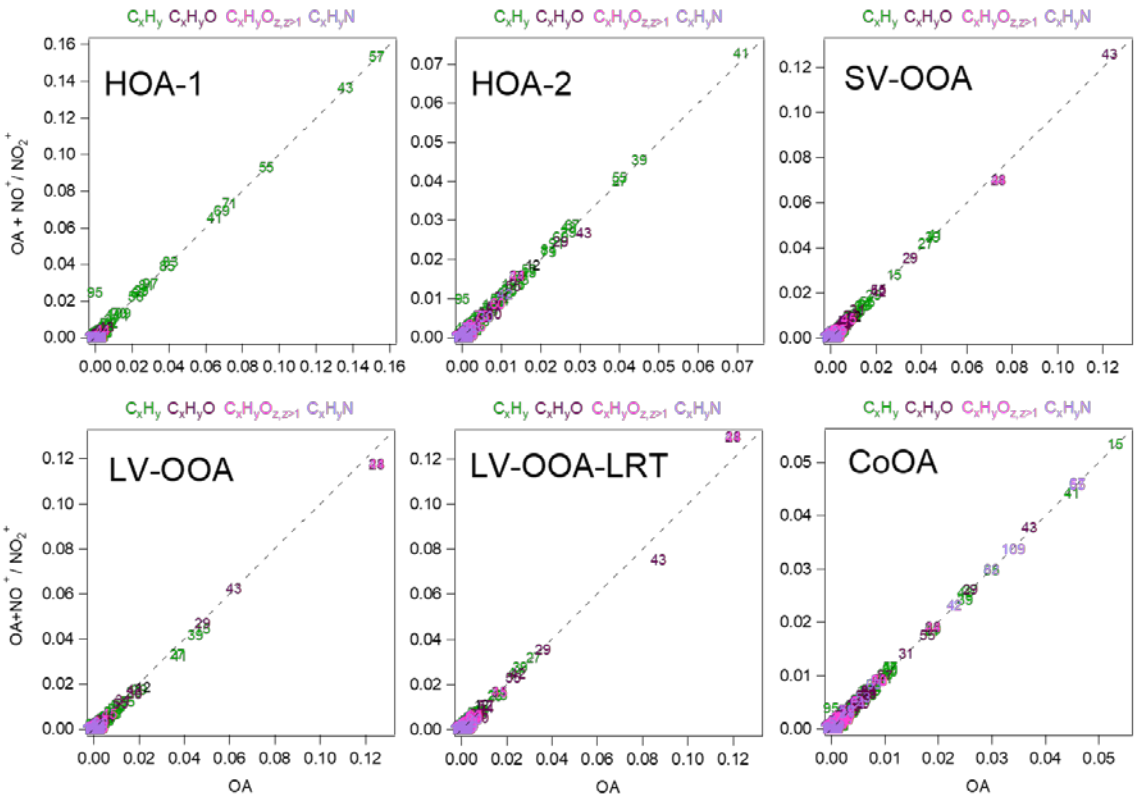

Figure S1. Comparison of the mass spectra for the PMF factors calculated with OA and OA + NO^+/NO_2^+ ions. Units are fraction in OA.

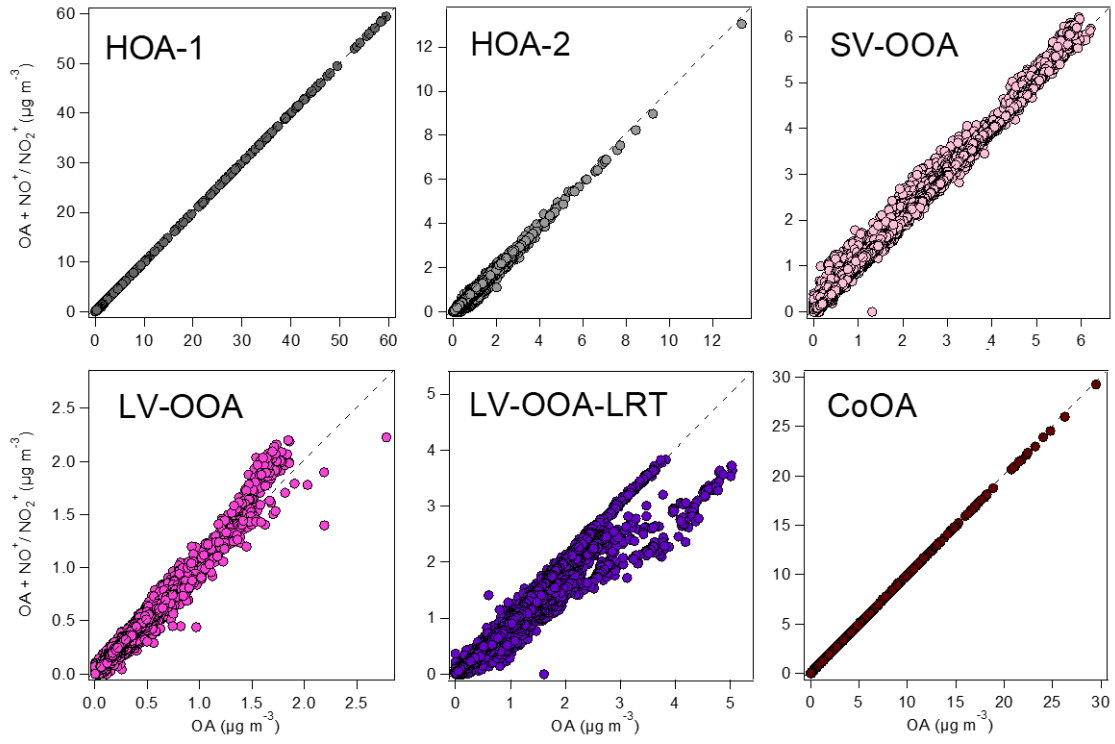

Figure S2. Comparison of the mass concentrations for the PMF factors calculated with OA and OA + NO^+/NO_2^+ ions.

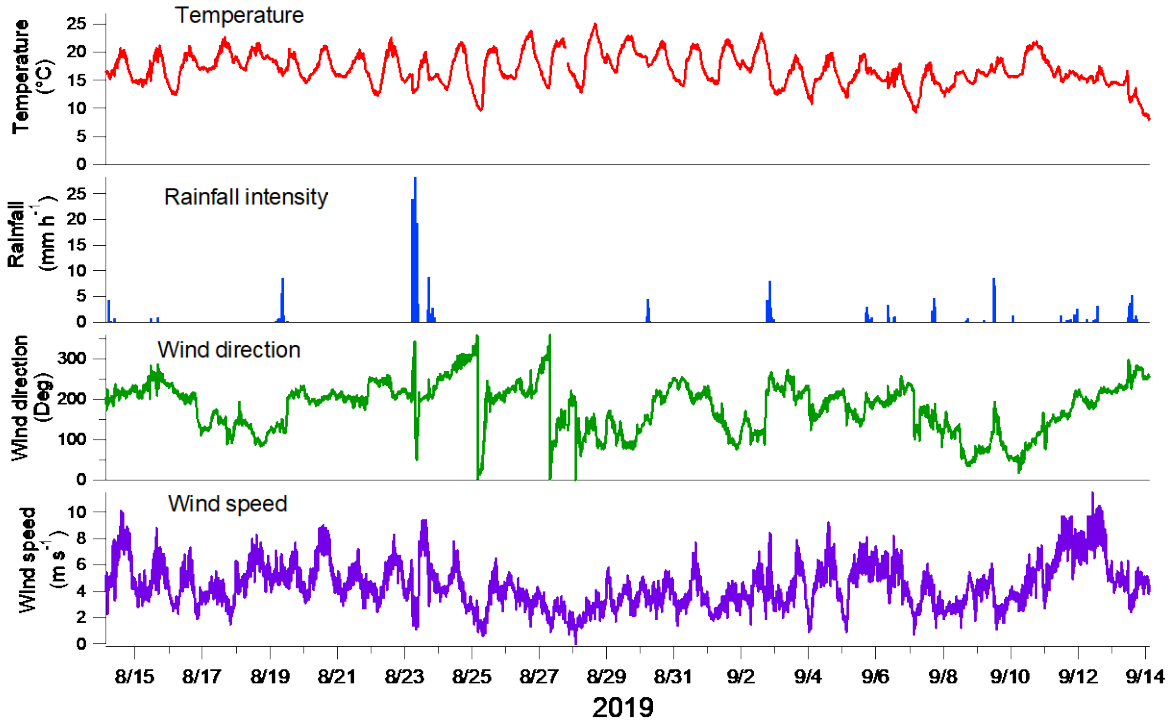

Figure S3. Meteorological parameters during the measurement period. Observations were done every 10 minutes.

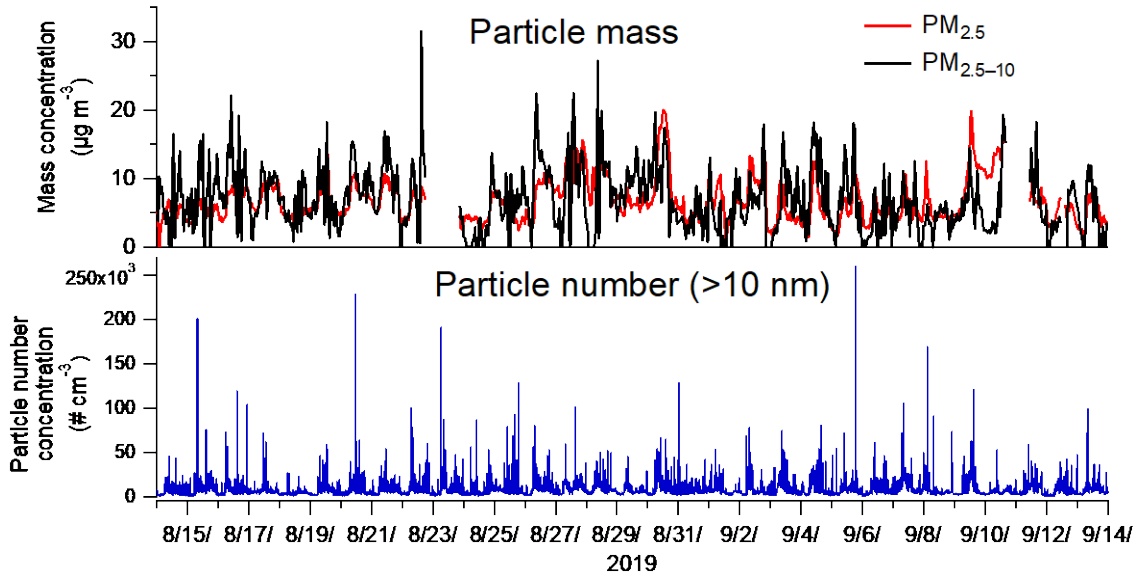

Figure S4. $PM_{2.5}$, $PM_{2.5–10}$ and particle number (> 10 nm) concentrations during the measurement period. $PM_{2.5}$ and $PM_{2.5–10}$ concentrations are presented as 1-hour averages and the number concentration with 9 minutes time-resolution.

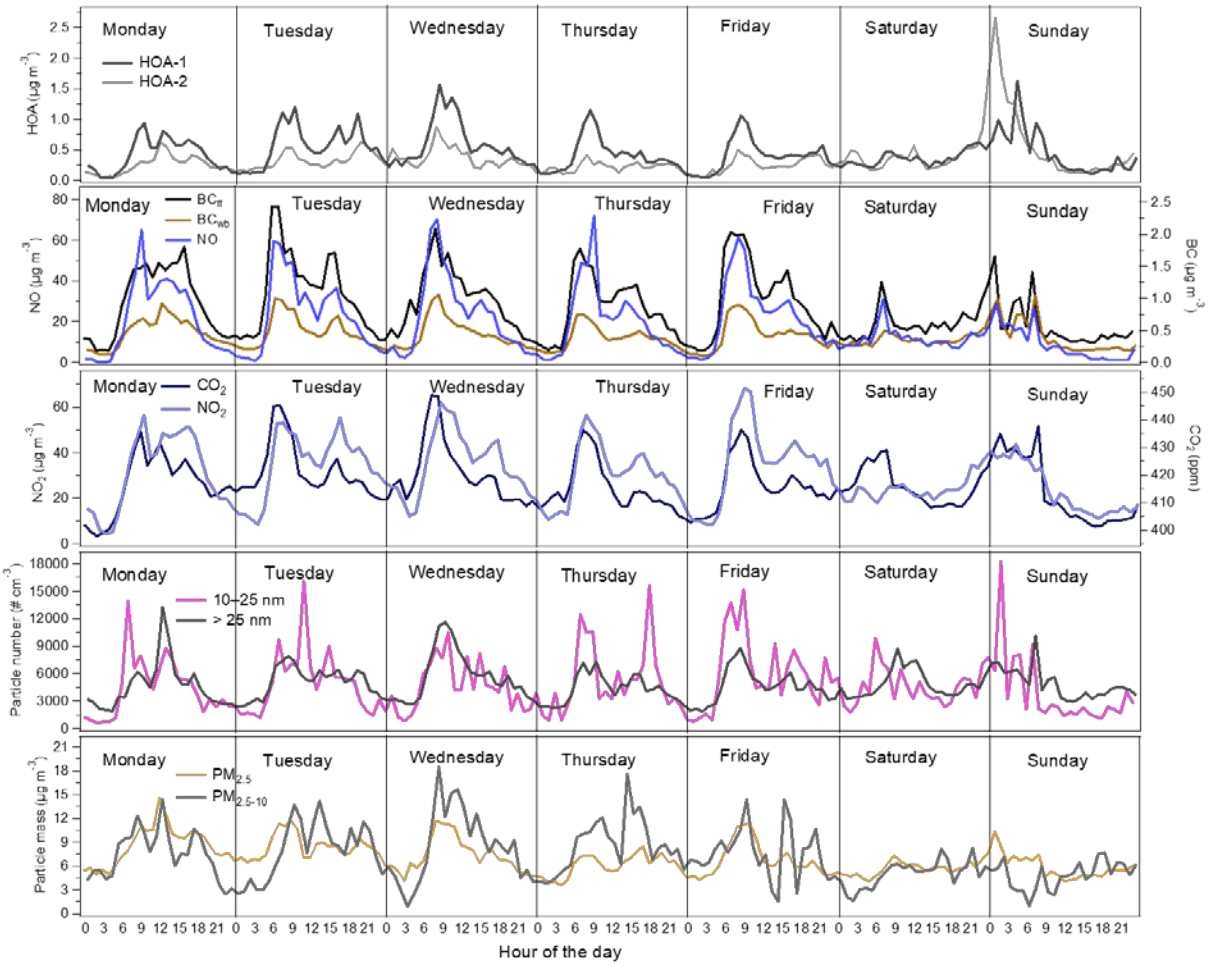

Figure S5. Average diurnal trends of HOA-1, HOA-2, BC_{ff}, BC_{wb} NO, CO_2, NO_2, particle number and particle mass at different days of the week.

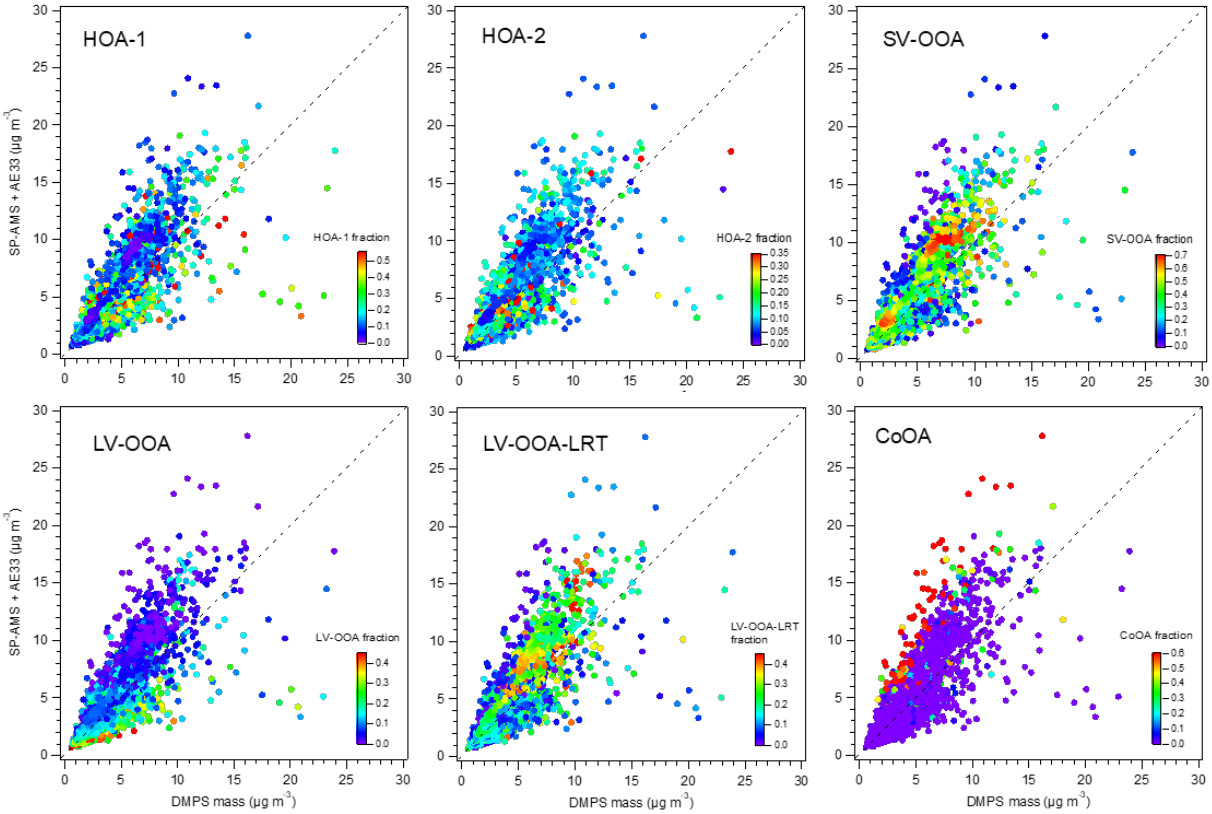

Figure S6. The comparison of PM_1 from the SP-AMS and AE33 against PM_1 from the DMPS in terms of the PMF factor contributions. DMPS number size distributions were converted to PM_1 by using the constant density of 1.42 g cm^{-3}.

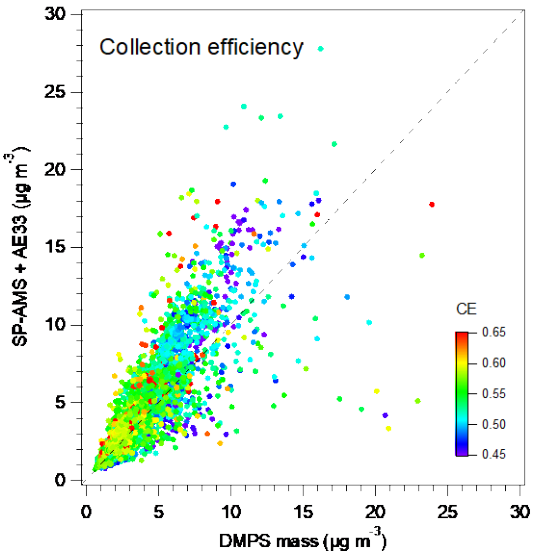

Figure S7. The comparison of PM_1 from the SP-AMS and AE33 against PM_1 from the DMPS for the collection efficiency (CE). DMPS number size distributions were converted to PM_1 by using the constant density of 1.42 g cm^{-3}.

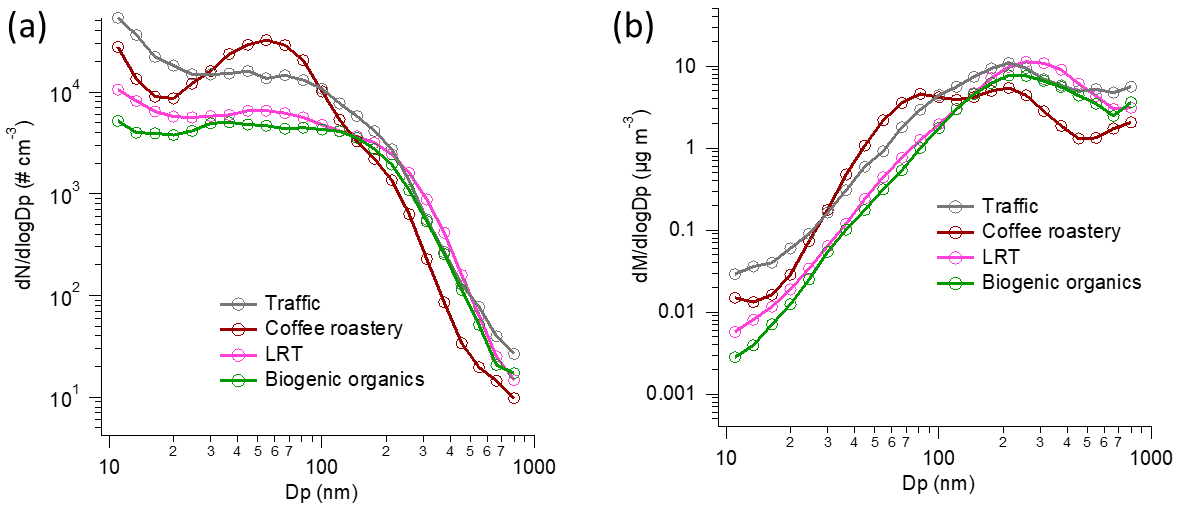

Figure S8. Average number (a) and mass (b) size distributions during four air quality cases measured by the DMPS. D_p denotes mobility diameter.

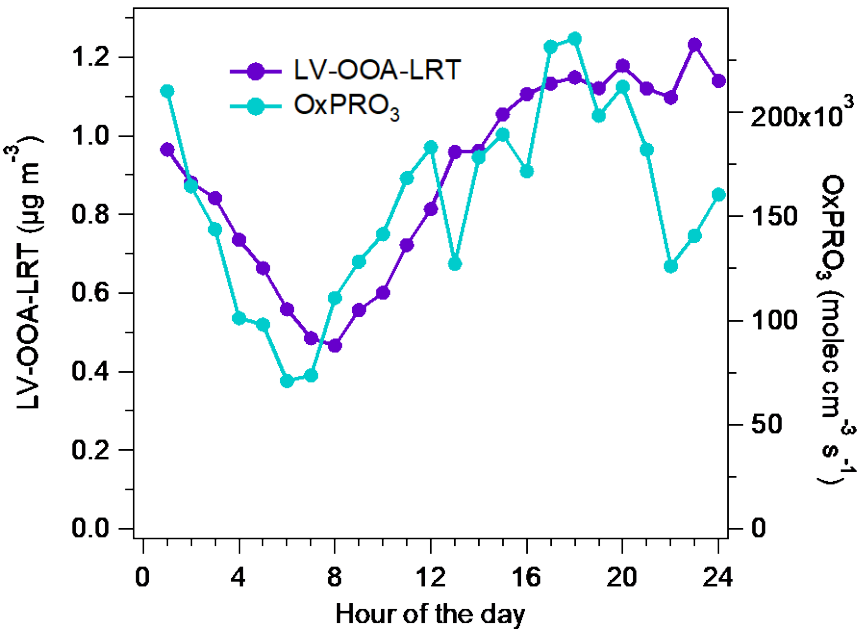

Figure S9. Average diurnal trends for LV-OOA-LRT and $OxPRO_3$.

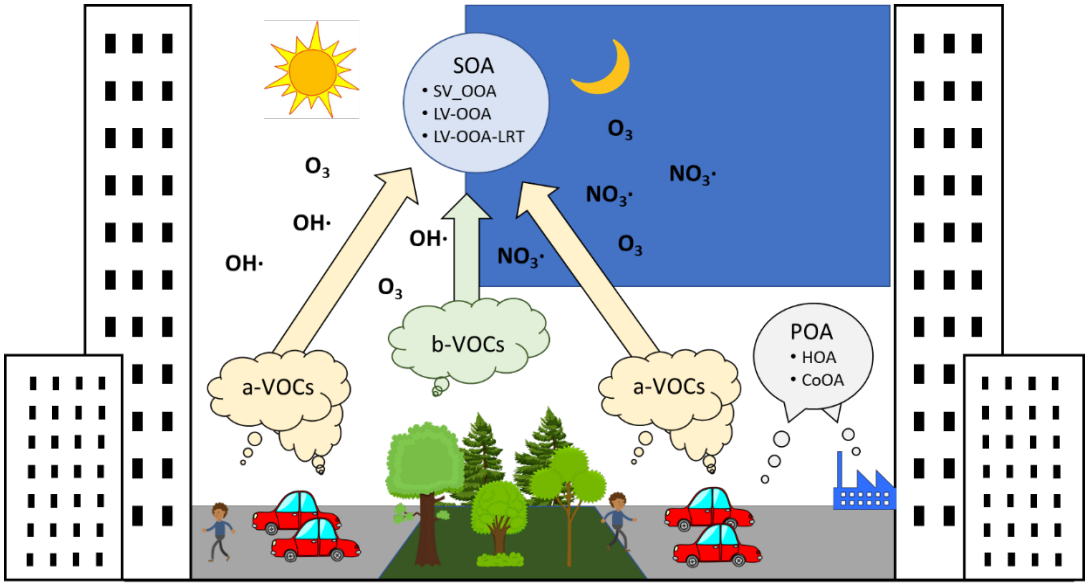

Figure S10. Schematic diagram of the sources and processing of VOCs and OA at the street canyon.