Supplement for:

Variation in chemical composition and volatility of oxygenated organic aerosol in different rural, urban, and remote environments

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Table S1. Campaign-average (average ± 1 standard deviation) parameters for meteorology, trace gases, equivalent black carbon (eBC), total organics and total $PM_{2.5}$, double bond equivalent (DBE) values, and number of carbon atoms (nC) and oxygen atoms (nO) at different locations and different seasons.

Name	*T* (°C)	RH (%)	O_3 (ppbv)	NO_2 (ppbv)	SO_2 (ppbv)	eBC (μg m^{-3})	Org[a] (μg m^{-3})	$PM_{2.5}$[a] (μg m^{-3})	DBE	nC	nO
MCC-t	0.3±2.1	53.0±22.4	/	/	/	0.2±0.4	0.3±0.5	1.0±1.8	3.1±0.2	8.4±0.8	6.2±0.3
MCC-d	-0.4±1.9	52.2±18.8	/	/	/	0.3±0.4	0.5±0.5	1.6±1.4	3.2±0.1	7.7±0.7	5.8±0.3
REL	19.9±3.9	76.1±15.2	22.7±12.4	11.3±5.2	1.4±1.0	0.7±0.4	3.7±2.1	6.6±4.2	3.1±0.1	9.2±0.8	6.6±0.5
RAB	24.2±3.2	83.1±15.2	25.0±12.5	0.6±0.6	0.2±0.4	/	4.1±2.5	6.0±3.2	2.9±0.1	8.0±0.4	5.7±0.2
RHT	8.1±6.1	66.0±23.7	36.1±10.1	0.4±0.6	0.2±0.2	0.1±0.2	1.6±2.0	2.3±2.3	3.1±0.1	9.1±0.6	5.7±0.3
UST-s	24.6±4.0	55.1±12.8	29.6±7.5	9.7±4.1	3.9±2.8	1.0±0.3	5.1±3.2	7.1±3.3	3.4±0.1	8.8±0.4	6.4±0.2
UST-w	2.0±3.7	61.4±10.1	17.1±8.7	15.8±3.9	1.4±0.8	1.2±0.1	8.4±5.6	27.0±11.9	3.4±0.1	8.7±0.9	6.7±0.2
UKA-s	25.9±6.6	49.8±21.0	37.4±19.8	9.6±6.4	/	0.7±0.4	3.9±2.4	5.9±2.8	3.6±0.2	10.7±0.8	7.0±0.4
UKA-w	13.2±3.3	56.4±13.4	27.8±10.0	9.2±7.1	0.6±1.0	0.5±0.5	1.9±1.6	3.9±3.6	3.5±0.1	11.2±0.8	7.1±0.4
UDL	16.8±4.1	73.3±16.7	11.1±13.3	34.6±22.0	/	16.1±13.3	86.4±66.7	172.7±103.8	4.0±0.2	9.4±0.4	4.9±0.1

[a]Data were total non-refractory mass concentration from a high-resolution time-of-flight aerosol mass spectrometer (HR-ToF-AMS, Aerodyne Research Inc.) or an aerosol chemical speciation monitor (ACSM, Aerodyne Research Inc.).

Table S2. Deposition parameters and instrumental parameters at different locations and different seasons.

Name	Total inlet flow (L/min)/ Residence time (s)	Deposition time (min)	Mass loading (μg)[c]	FIGAERO type/ Sample mode	IMR body T (°C)	IMR pressure (mbar)	Ion source	Ratio of sample flow : ionizer flow	Ramp rate (°C/min)
MCC-t	7.0/1.4	120	0.3±0.3	Aerodyne/online	45	100	Corona discharge	2:1.3	13.3
MCC-d	7.0/1.4	120	0.4±0.4	Aerodyne/online	45	480	X-ray	2:1.3	13.3
REL	8.6/1.2	30	1.0±0.7	Aerodyne/online	45	100	Po-210	2:2	13.3
RAB	22/3.6	20	1.8±1.3	UW/online[d]	25	100	Po-210	2:2	10.0
RHT	11/4.2	30	0.5±0.8	UW/online[d]	25	100	Po-210	2:2	10.0
UST-s	8.7/0.8	112±43[b]	3.5±1.4	Aerodyne/offline	45	100	Po-210	2:2	13.3
UST-w	10.0/0.7	86±70[b]	4.0±1.0	Aerodyne/offline	45	100	Po-210	2:2	13.3
UKA-s	6.4/0.8	128±99[b]	3.2±2.1	Aerodyne/offline	45	100	Po-210	2:2	13.3
UKA-w	6.4/0.8	245±124[b]	3.0±1.5	Aerodyne/offline	45	100	Po-210	2:2	13.3
UDL	2.4[a]/2.8	3±1	0.6±0.5	Aerodyne/online	25	250	X-ray	2:1.5	6.7

[a]Average inlet flow of 3.5 L/min for the 1st week and 2 L/min for the next 2.5 weeks.

[b]Deposition time was average ± 1 standard deviation from offline filters.

[c]Mass loadings were calculated based on concurrent HR-ToF-AMS or ACSM measurements.

[d]FIGAERO inlet from the University of Washington, U.S., designed by Lopez-Hilfiker et al. (2014).

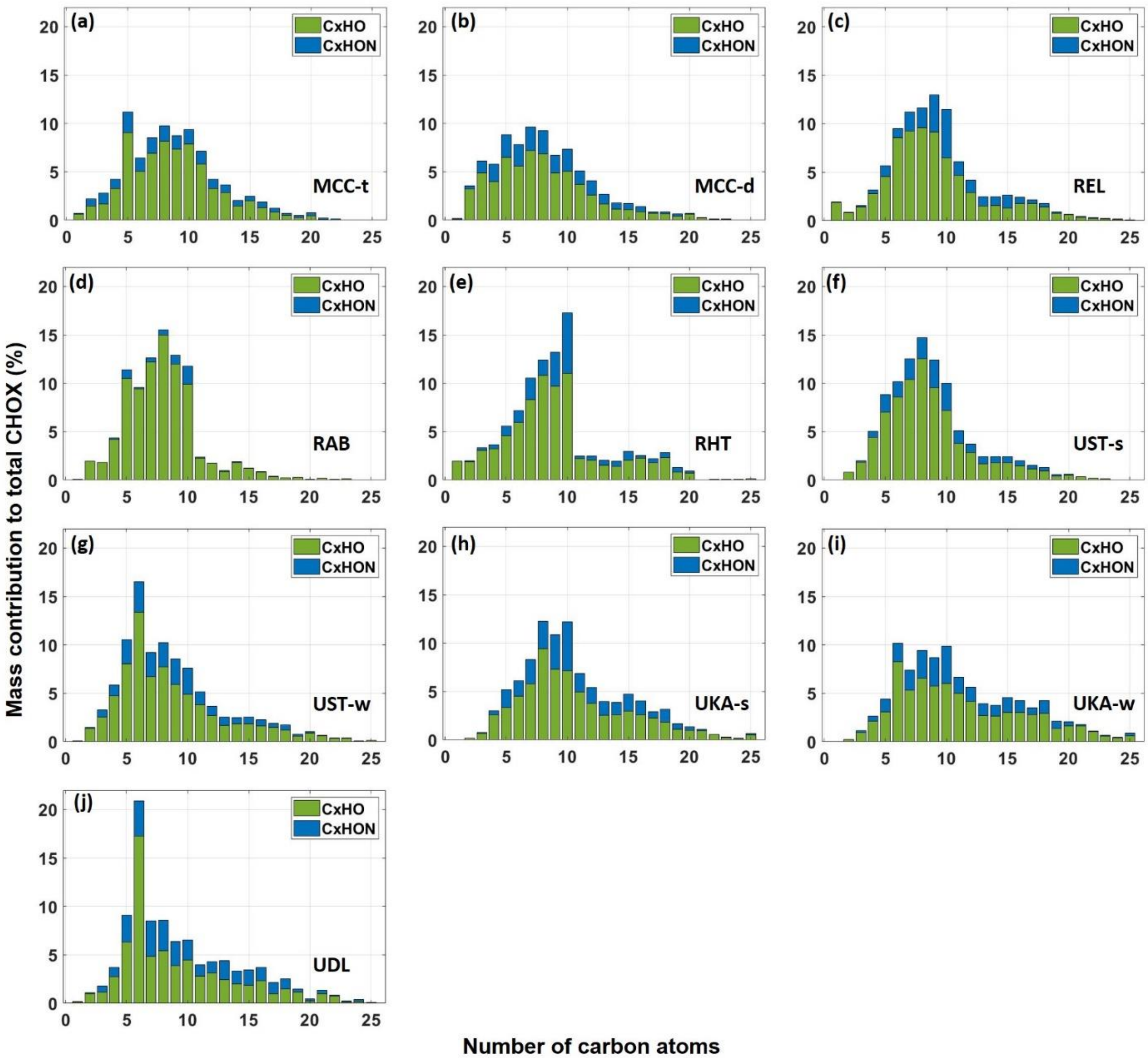

Figure S1. Mass contributions of CHO and CHON compounds to total CHOX compounds as a function of the number of carbon atoms for MCC-t (a), MCC-d (b), REL (c), RAB (d), RHT (e), UST-s (f), UST-w (g), UKA-s (h), UKA-w (i), and UDL (j).

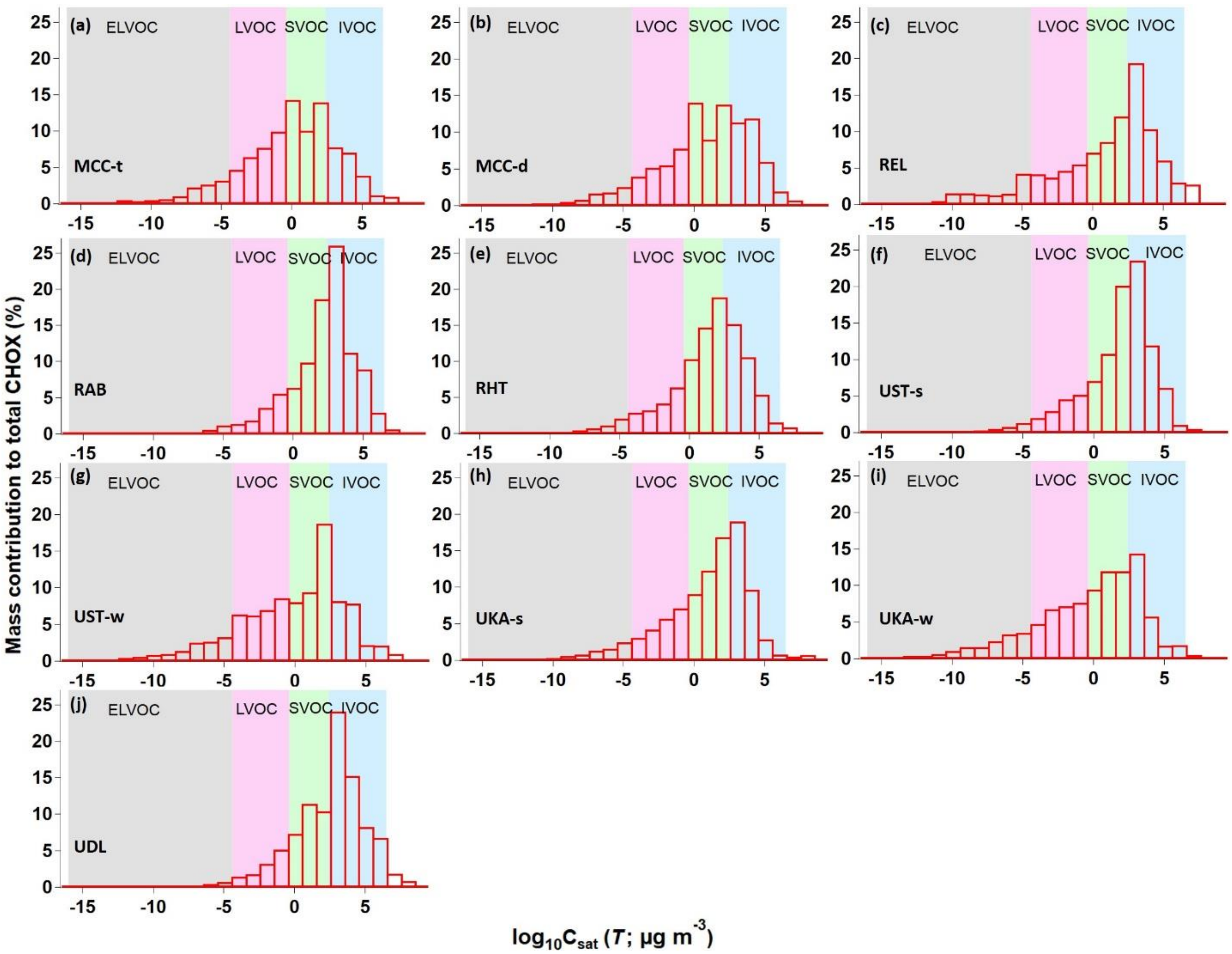

Figure S2. Volatility distribution for MCC-t (a), MCC-d (b), REL (c), RAB (d), RHT (e), UST-s (f), UST-w (g), UKA-s (h), UKA-w (i), and UDL (j) with the modified Li et al. (2016) parameterization method (Daumit et al., 2013;Isaacman-VanWertz and Aumont, 2021).

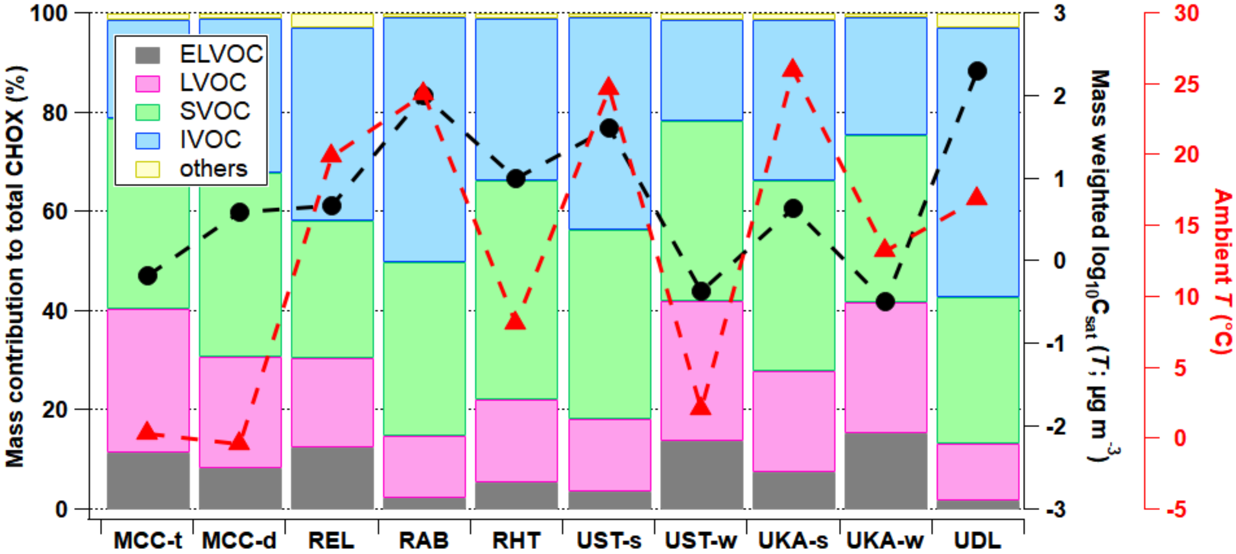

Figure S3. Comparison between ambient temperature (*T*) and campaign-average contribution (%) of different volatility groups resulting from VBS calculations to total organics (colored in bars) and campaign-average mass weighted $\log_{10}C_{sat}$ (*T*) values (in black markers) for different campaigns with the modified Li et al. (2016) parameterization method (Daumit et al., 2013;Isaacman-VanWertz and Aumont, 2021) (same as Figure 2). Compounds more volatile than IVOC with C_{sat} higher than $10^{6.5}$ μg m^{-3} (labelled as "others") contributed negligibly (0.8−2.9 %).

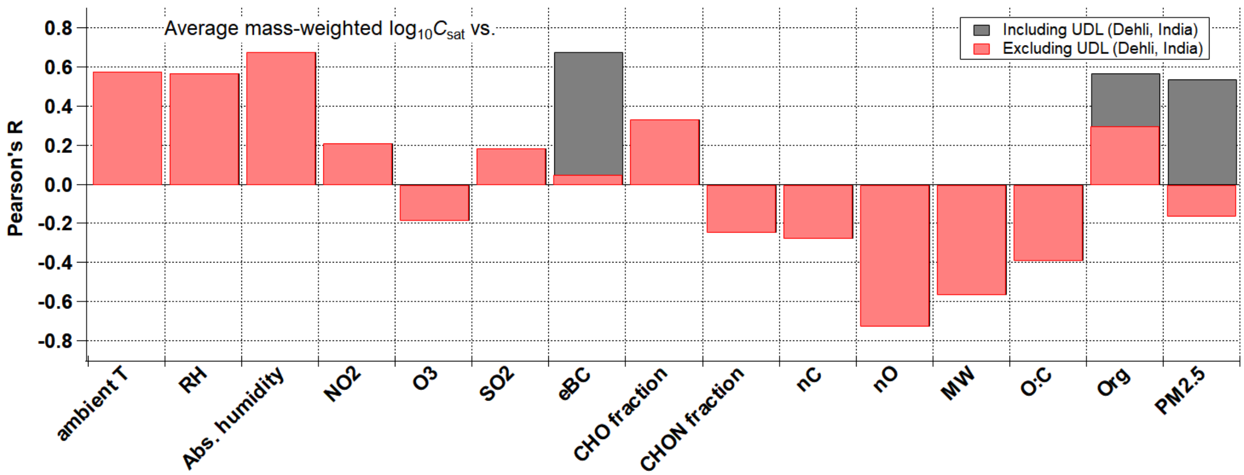

Figure S4. Correlations of campaign-average mass weighted $\log_{10}C_{sat}$ values vs. other parameters. Pearson's R values including and excluding UDL (Dehli, India) data point for eBC, Org, and $PM_{2.5}$ are in gray bars and red bars, respectively, due to their extremely high levels at UDL (see Table S1).

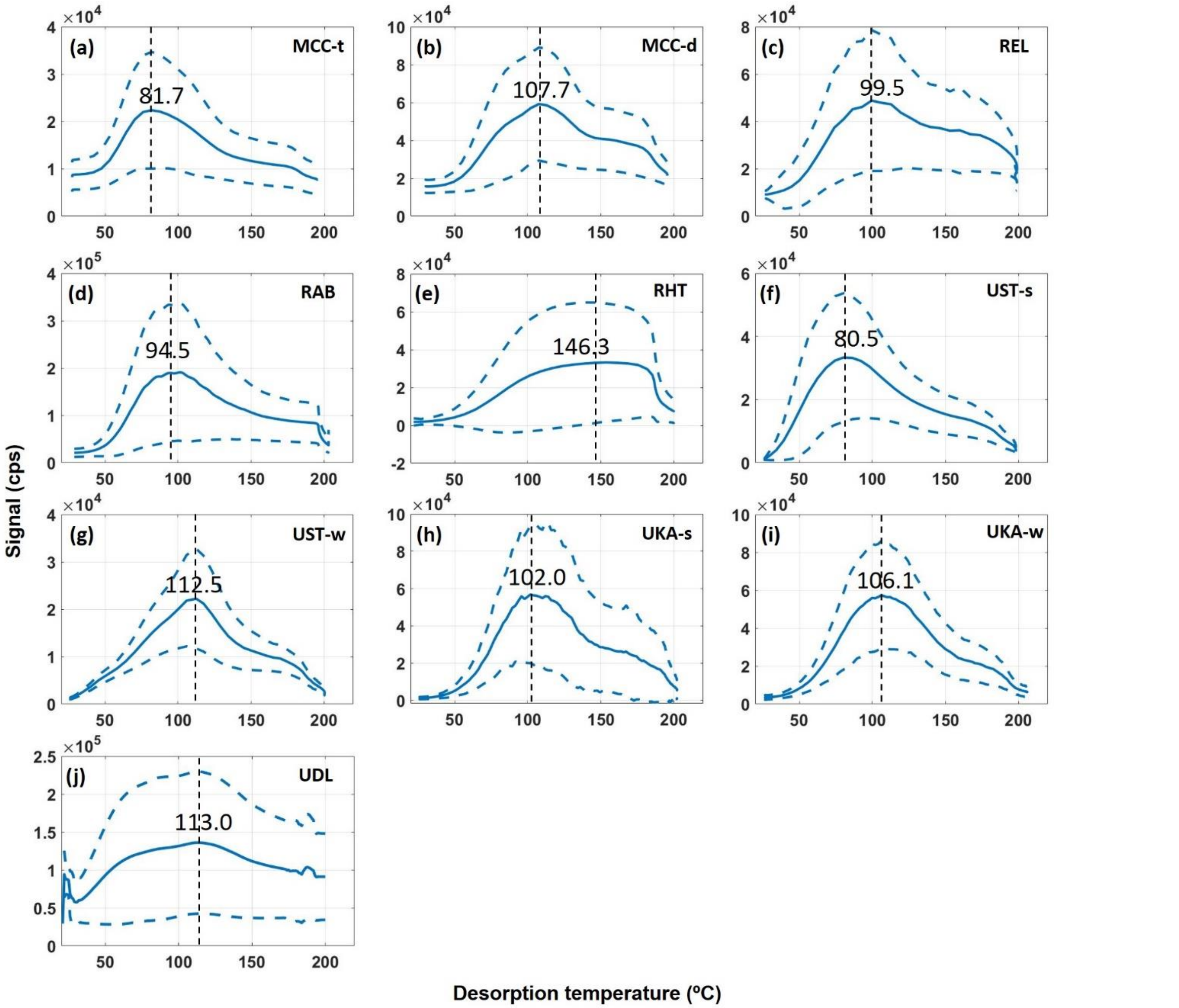

Figure S5. Campaign-average sum thermograms of CHOX compounds for MCC-t (a), MCC-d (b), REL (c), RAB (d), RHT (e), UST-s (f), UST-w (g), UKA-s (h), UKA-w (i), and UDL (j). Dashed blue lines represent ±1 standard deviation and dashed black lines indicate the sumT_{max} values.

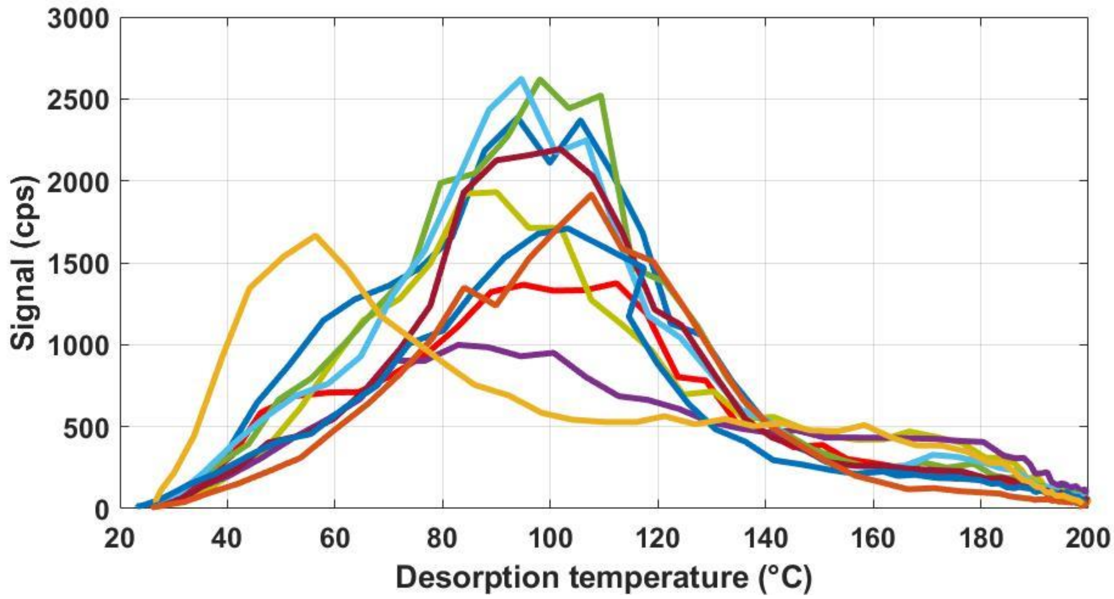

Figure S6. Thermograms of $C_6H_{10}O_5$ compound during the whole campaign in winter Stuttgart (UST-w).

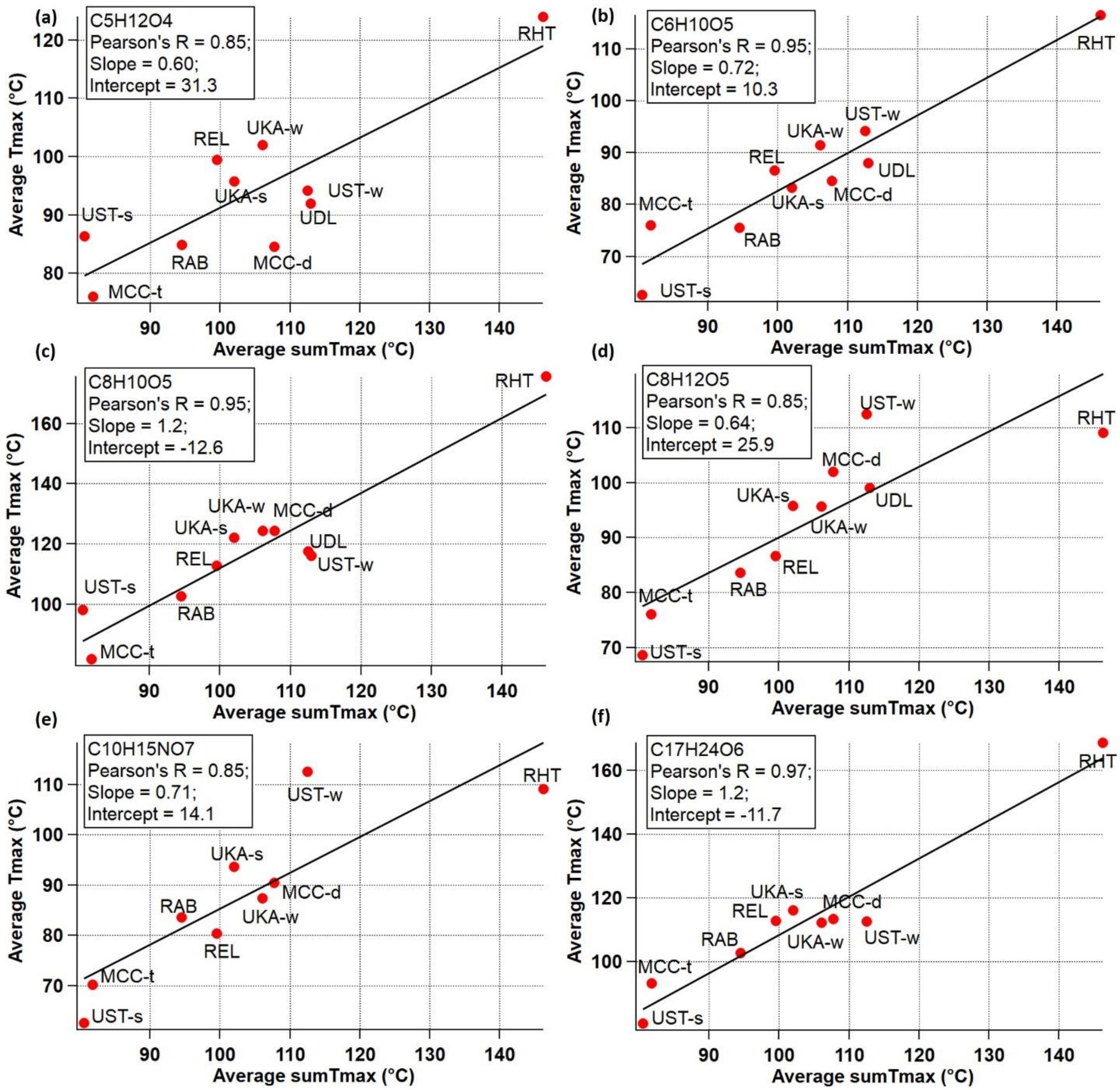

Figure S7. Campaign-average T_{max} values for $C_5H_{12}O_4$ (a), $C_6H_{10}O_5$ (b), $C_8H_{10}O_5$ (c), $C_8H_{12}O_5$ (d), $C_{10}H_{15}NO_7$ (e), and $C_{17}H_{24}O_6$ (f) vs. the corresponding campaign-average $sumT_{max}$ values.

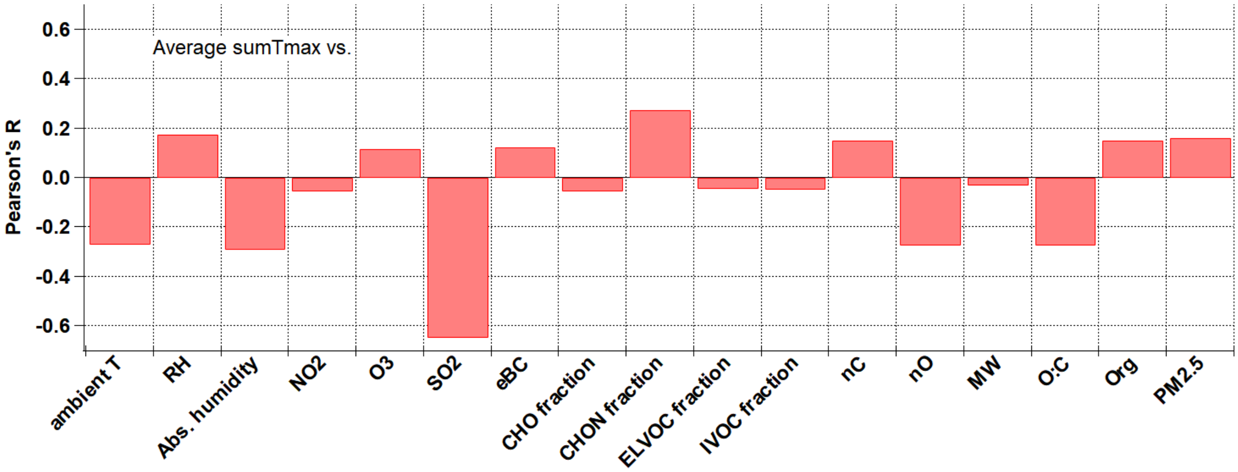

Figure S8. Correlations of campaign-average sumT_{max} values vs. other parameters.

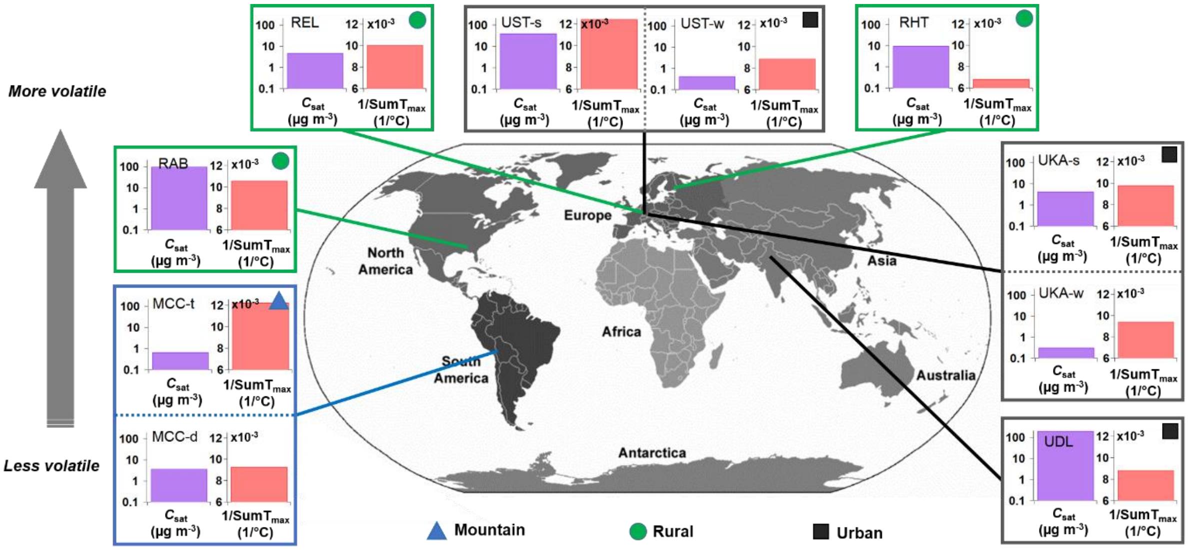

Figure S9. Overview of the comparison of the average C_{sat} (T) (i.e, molecular composition-derived volatility) with the sumT_{max} (i.e., thermal desorption-derived volatility) for different locations and seasons (Mountain sites in triangles, Rural sites in circles, and Urban sites in squares).

References

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