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Seasonal characteristics of organic aerosol chemical composition and volatility in Stuttgart, Germany

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Table S1. Instruments installed in the measurement container.

Measured parameter	Instrument	Data period	
		Summer 2017	**Winter 2018**
Ambient temperature	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Container temperature	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Dew point temperature	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
RH	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Pressure	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Wind speed	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Wind vertical	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Wind direction	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Rain	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Rain type	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Rain rate	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Radiation	WS700 (Lufft GmbH)	July 7–August 17	February 5–March 5
Particle number concentration (>7 nm)	CPC3022 (TSI Inc.)	July 5–August 17	February 5–March 5
Particle number concentration (>2.5 nm)	CPC3776 (TSI Inc.)	July 5–August 17	February 5–March 5
O_3	O341M (Environment SA)	July 5–August 17	February 5–March 5
CO_2	NGA2000 (Rosemount Inc.)	July 5–August 17	February 5–March 5
SO_2	AF22M (Environment SA)	July 5–August 17	February 5–March 5
NO_2	AS32M (Environment SA)	July 5–August 17	February 5–March 5
Particle optical diameter (0.18–18 µm)	OPC FIDAS200 (Palas GmbH)	July 5–August 17	February 5–March 5
Particle size (10–410 nm, d_m)	NanoScan-SMPS (TSI Inc.)	July 5–July 26	/
Black carbon (BC)	AE51 Aethalometer (Aethlabs Inc.)	July 5–August 17	February 5–March 5
Single particle composition and size (0.2–2.5 µm, d_{va})	LAAPTOF (AeroMegt GmbH)	July 5–August 17	February 5–March 5
Particle mass and size (0.07–2.5 µm, d_{va})	AMS (Aerodyne Research Inc.)	July 5–August 17	February 5–March 5
Particle-phase oxygenated organic molecules (offline filters)	FIGAERO-CIMS (Aerodyne Research Inc.)	July 5–August 14	February 8–March 5

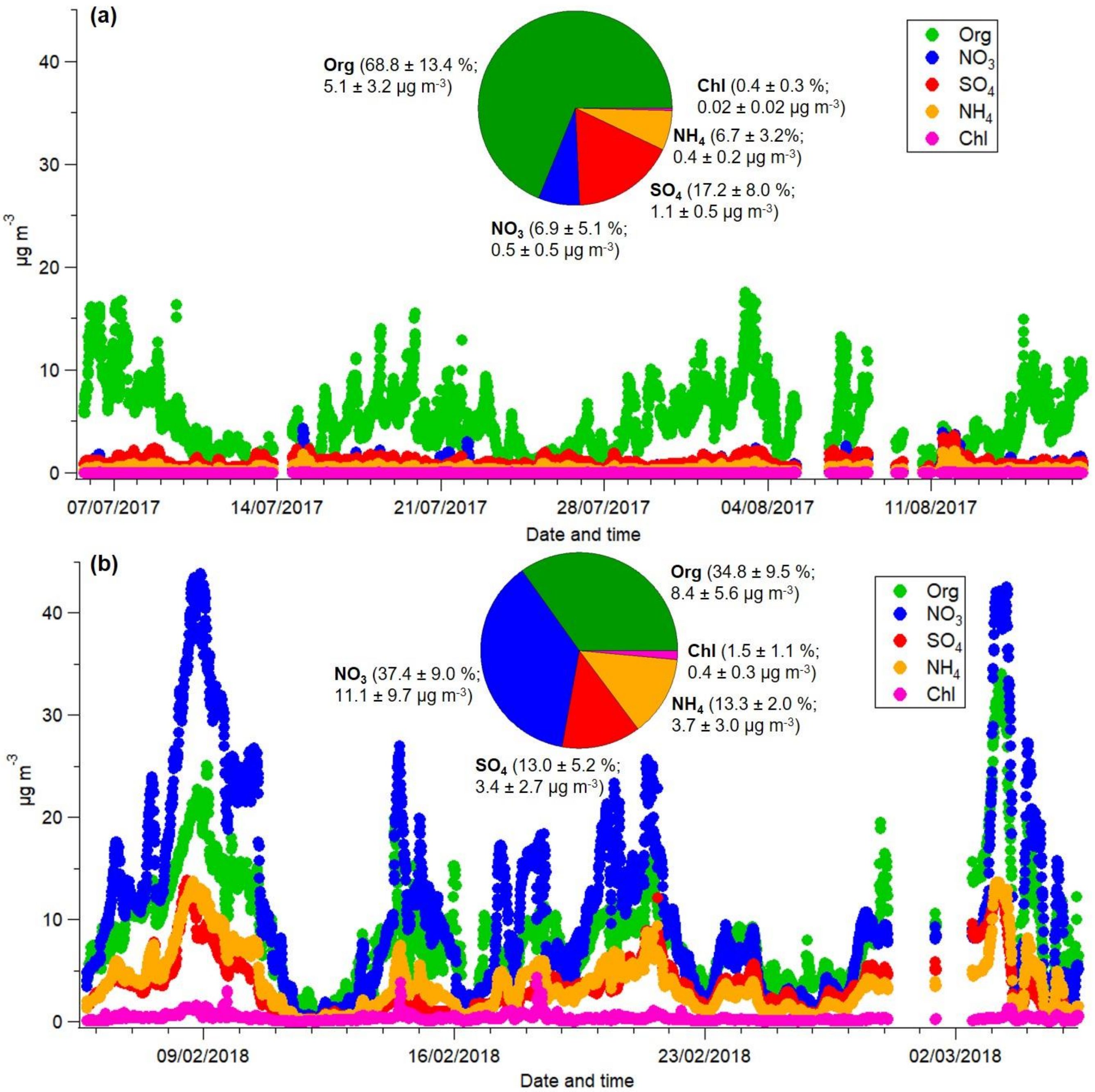


Figure S1. Time series of aerosol composition measured by AMS (Organics (Org), Nitrate (NO_3), Sulfate (SO_4), Ammonium (NH_4), and Chloride (Chl)) in the summer (a) and winter (b) periods.

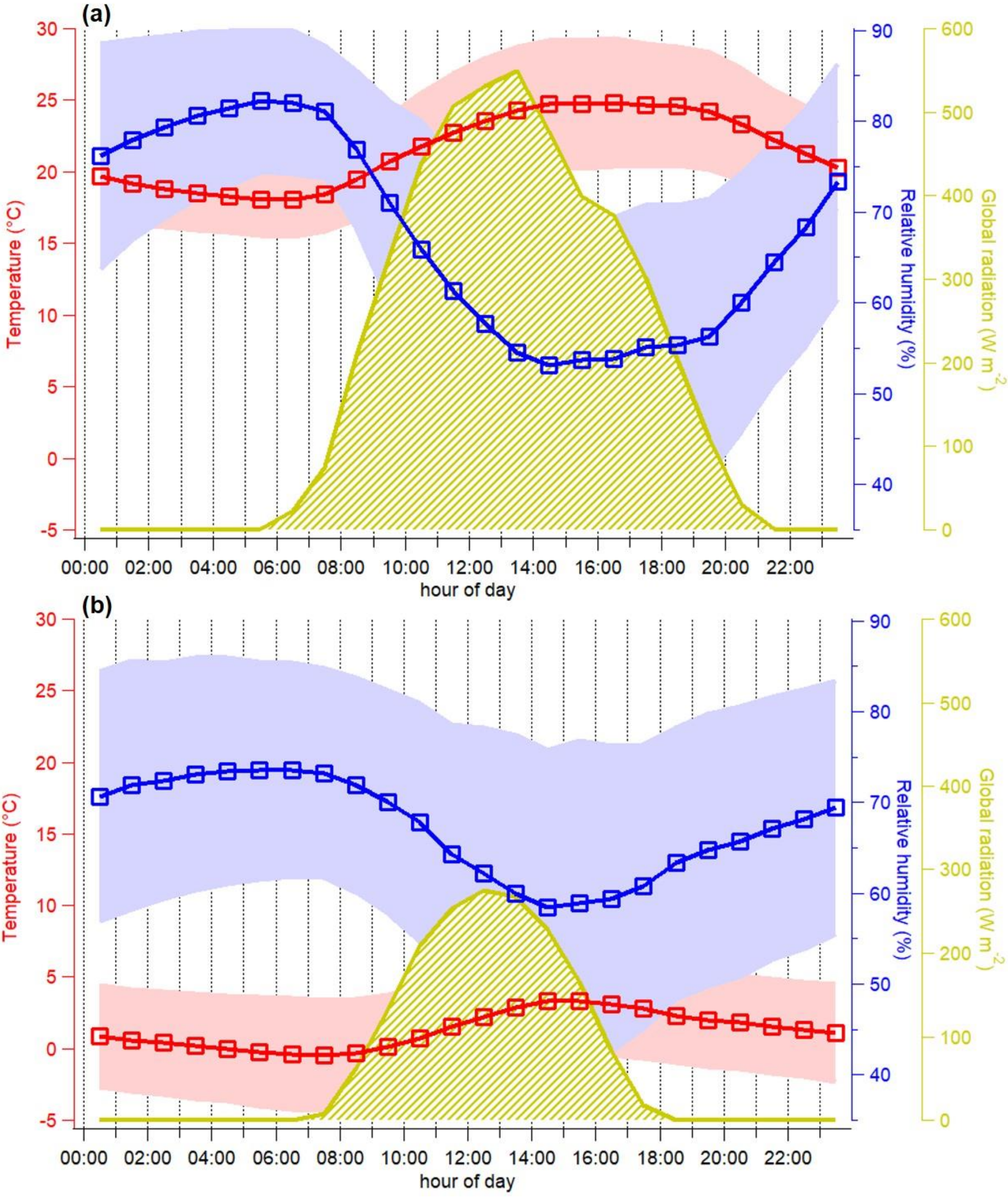


Figure S2. Mean diel patterns of ambient temperature, relative humidity, and global radiation in the summer (a) and winter (b) periods. The shaded areas represent ±1 standard deviation.

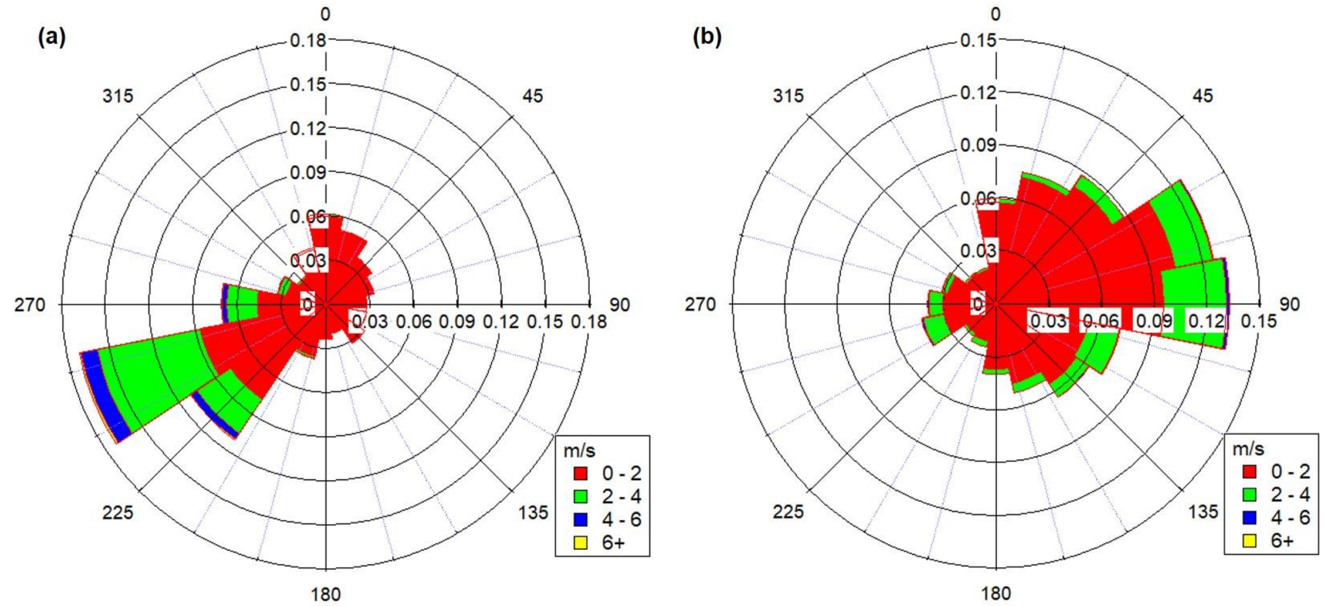


Figure S3. Wind speeds and directions for the summer (a) and winter (b) periods.

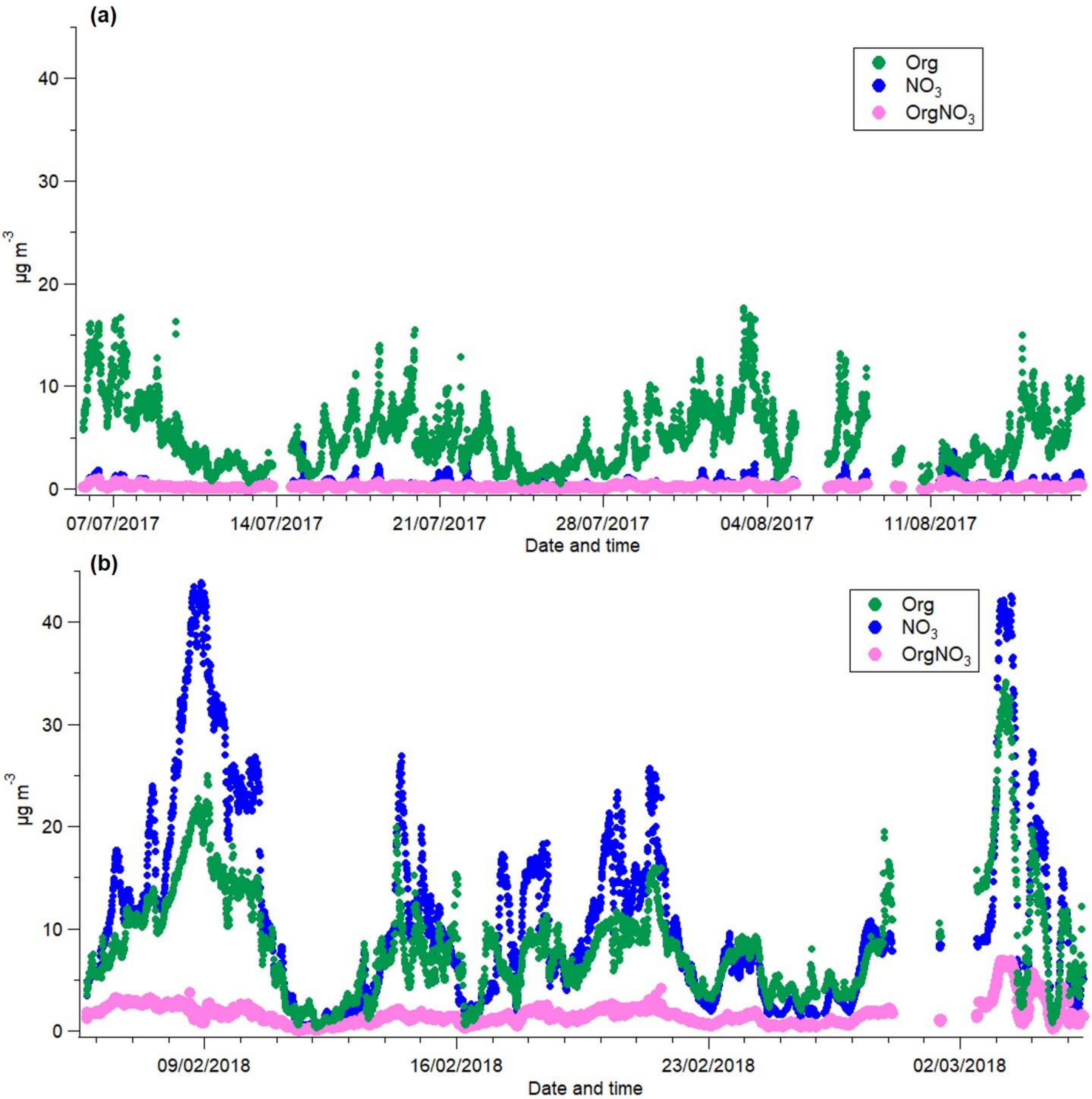


Figure S4. Comparison of time series of Organonitrates ($OrgNO_3$) with Organics (Org) and Nitrate (NO_3) by AMS for the summer (a) and winter (b) periods. $OrgNO_3$ concentrations were estimated based on the NO_2^+/NO^+ ion ratio measured by AMS and assuming a ratio of 0.1 for $OrgNO_3$ (Farmer et al., 2010; Kiendler-Scharr et al., 2016).

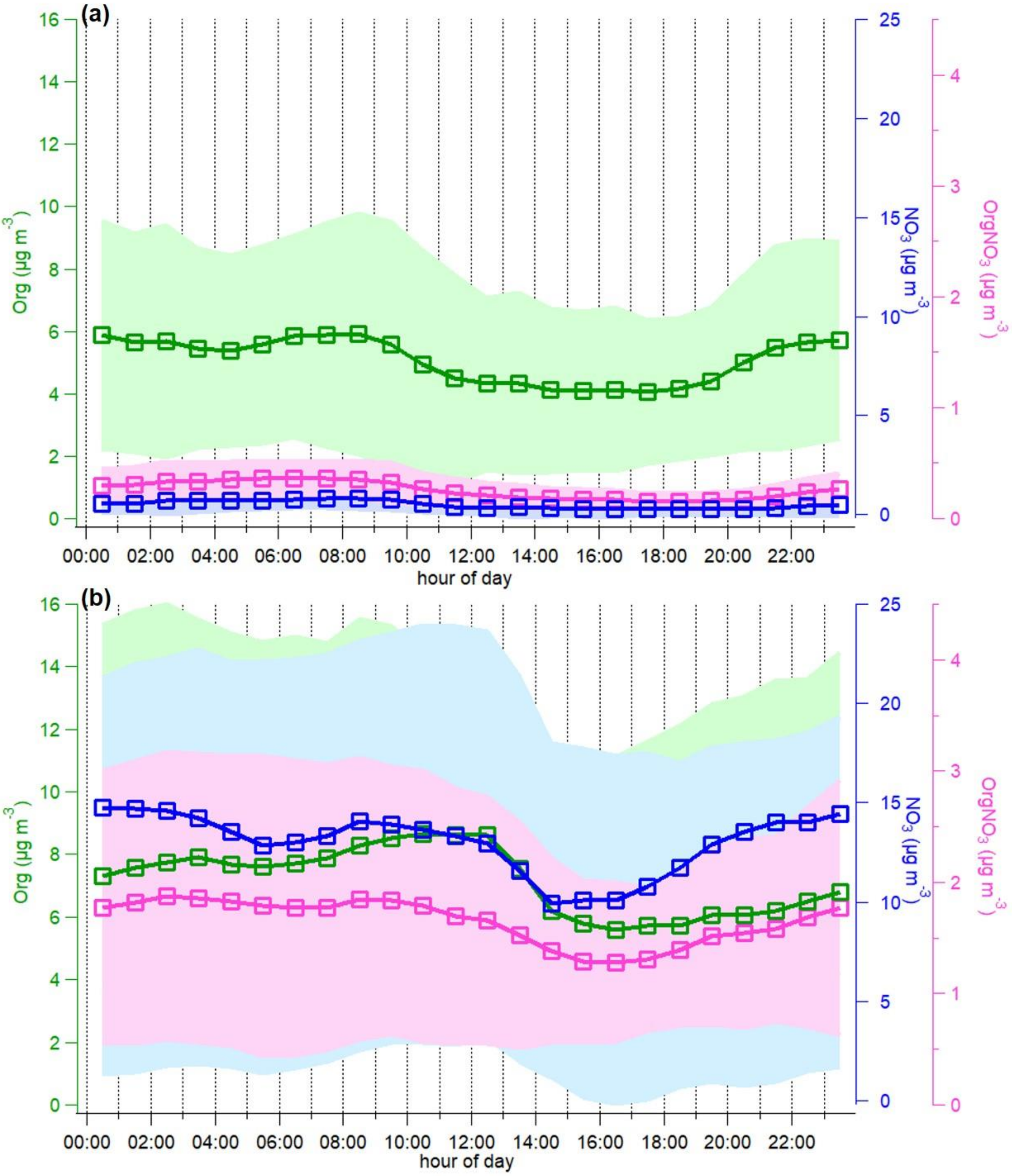


Figure S5. Mean diel patterns of Organics (Org), Nitrate (NO_3), and Organonitrates ($OrgNO_3$) by AMS for the summer (a) and winter (b) periods. The shaded areas represent ±1 standard deviation.

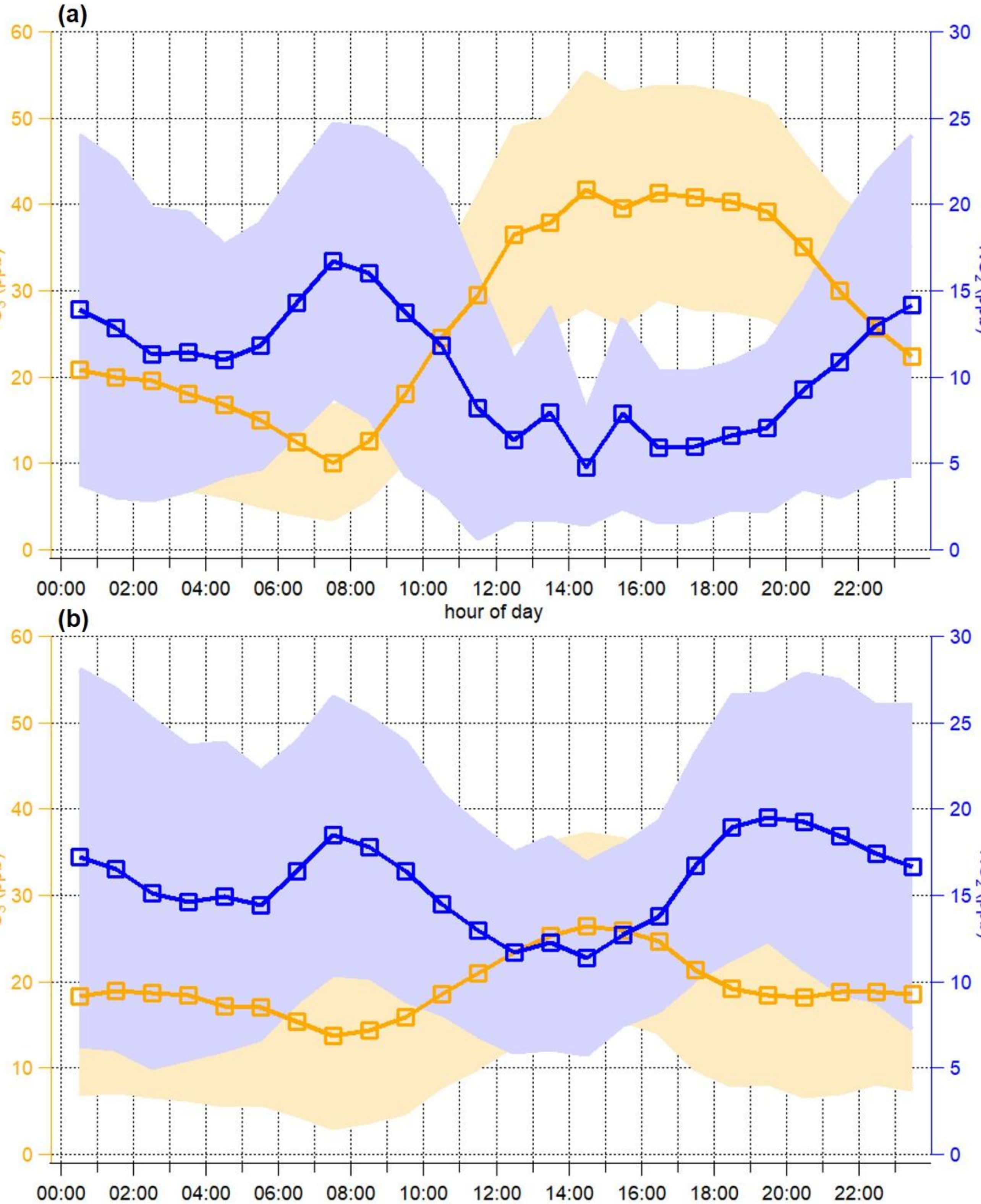


Figure S6. Mean diel patterns of O_3 and NO_2 mixing ratios for the summer (a) and winter (b) periods. The shaded areas represent ±1 standard deviation.

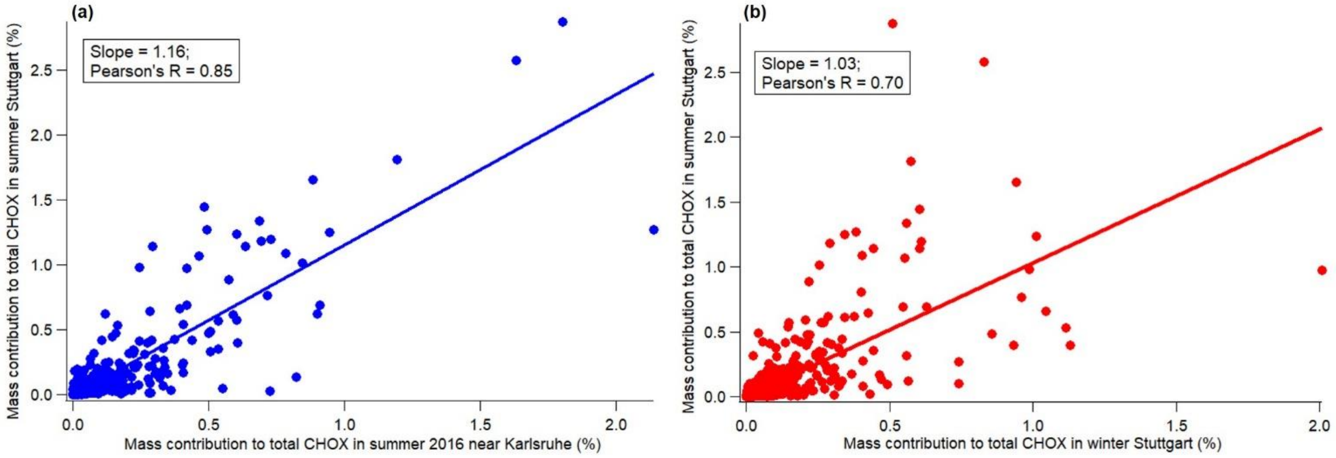


Figure S7. Correlations of CHOX compounds in summer 2017 in Stuttgart (a) with CHOX compounds in summer 2016 near Karlsruhe (Huang et al., 2019) and (b) with CHOX compounds in winter 2018 in Stuttgart after removing five prominent biomass burning tracer compounds ($C_6H_{10}O_5$, $C_6H_5O_3N$, $C_7H_7O_3N$, $C_6H_5O_4N$, and $C_7H_7O_4N$).

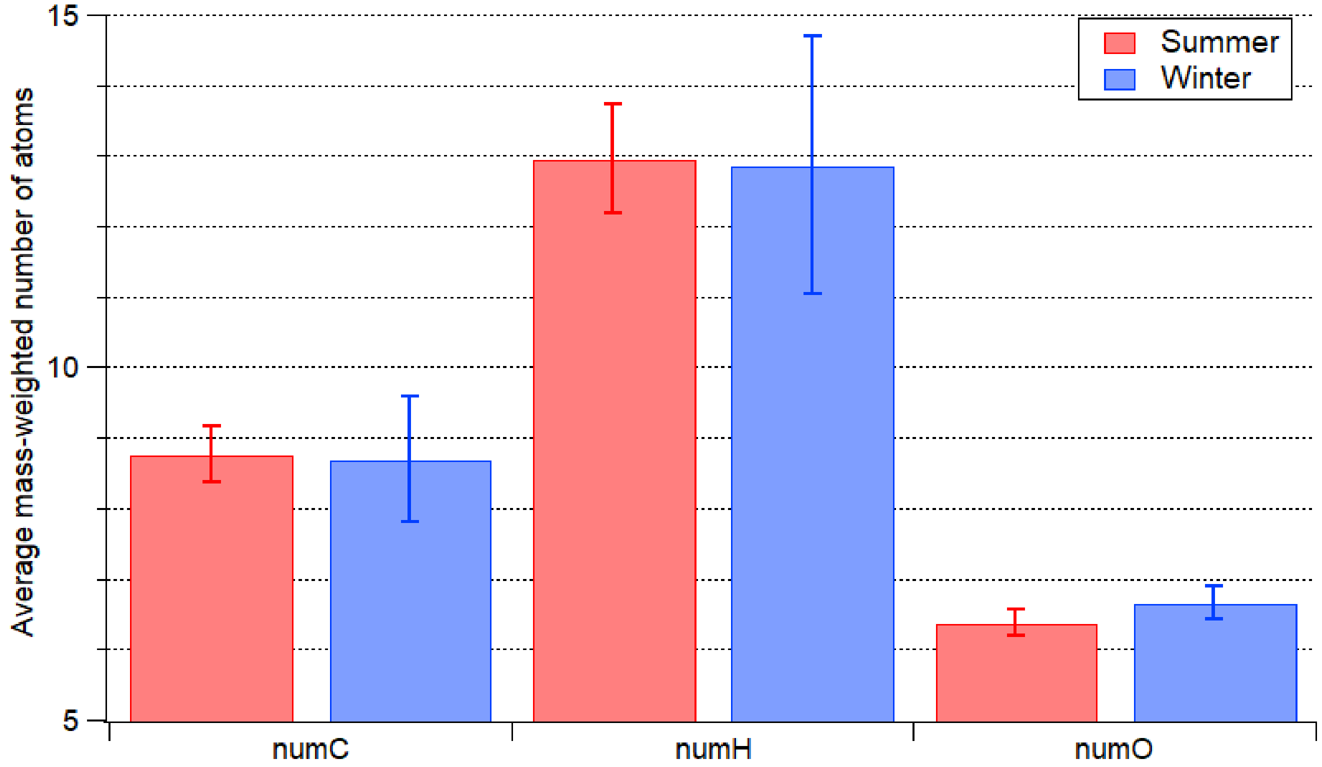
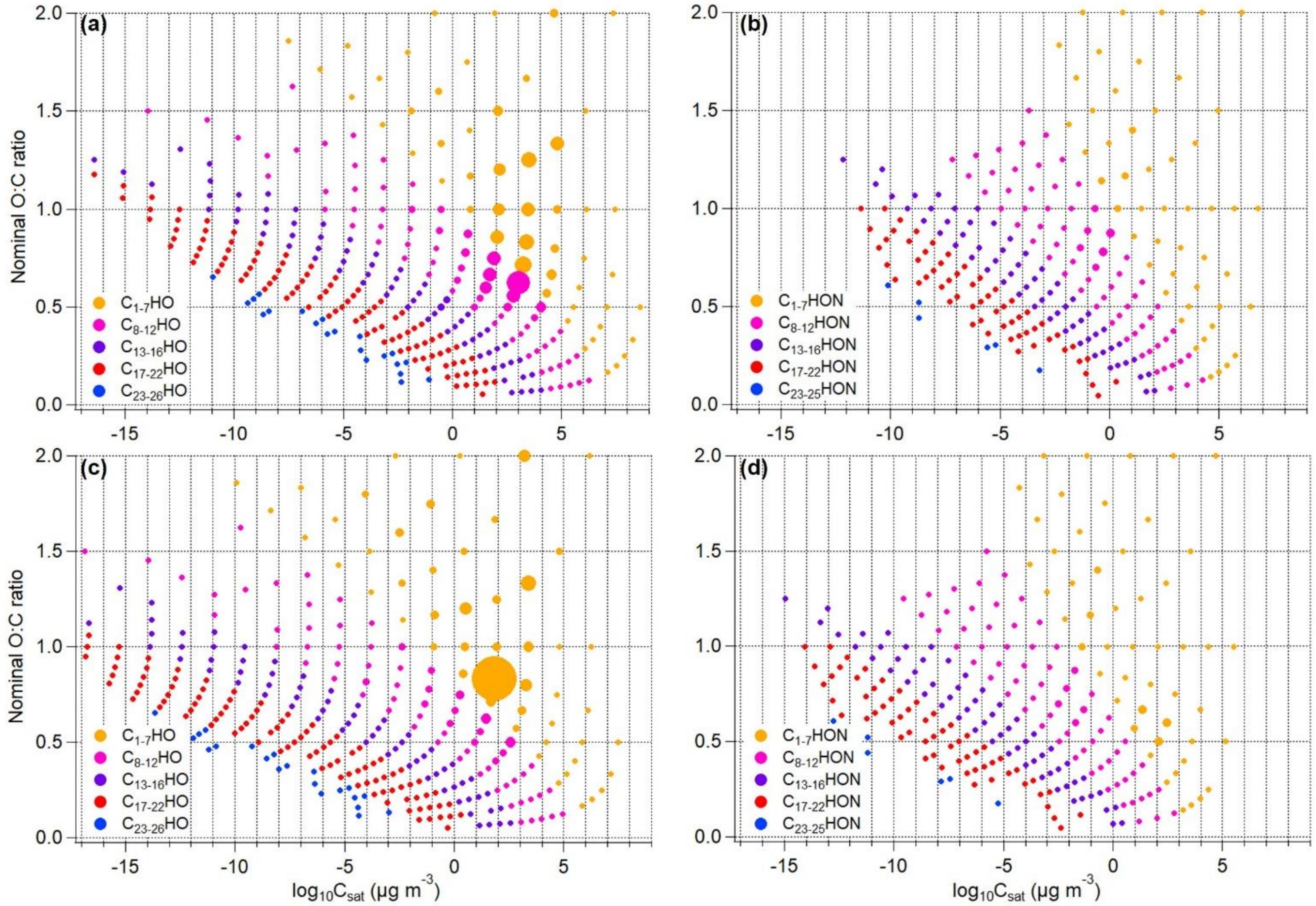


Figure S8. Average mass-weighted number of carbon atoms (numC), hydrogen atoms (numH), and oxygen atoms (numO) of the CHOX compounds for the summer and winter periods.



30 **Figure S9.** Volatility distribution of CHO compounds (a) and CHON compounds (b) in the summer period (24 °C), CHO compounds (c) and CHON compounds (d) in the winter period (2 °C) vs their corresponding nominal O:C ratio. Markers were colored by different number of carbon atoms and sized by their corresponding mass contributions to total CHOX compounds.

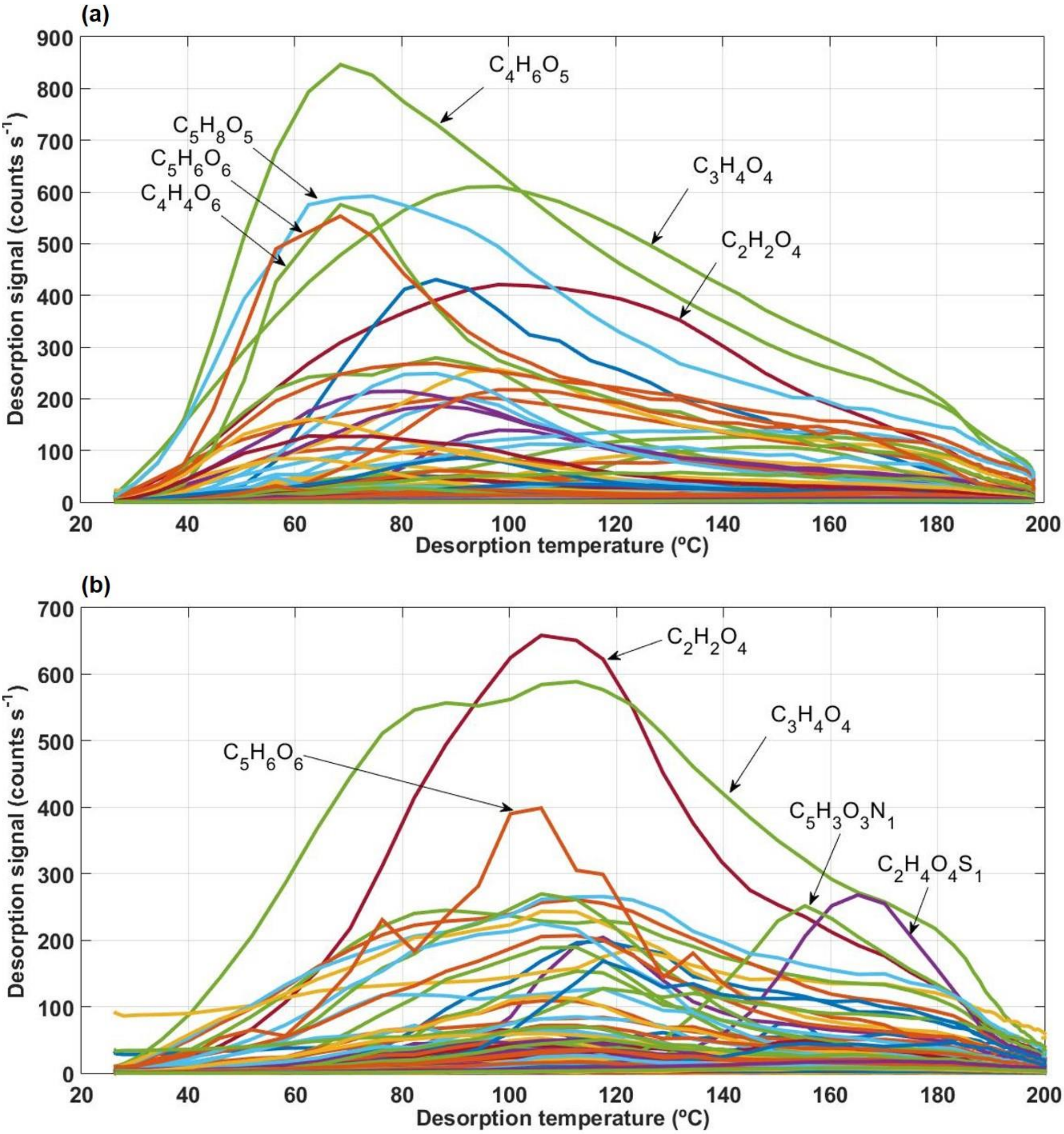


Figure S10. Thermograms of CHOX compounds with 1–5 carbon atoms for the summer (a) and winter (b) periods.

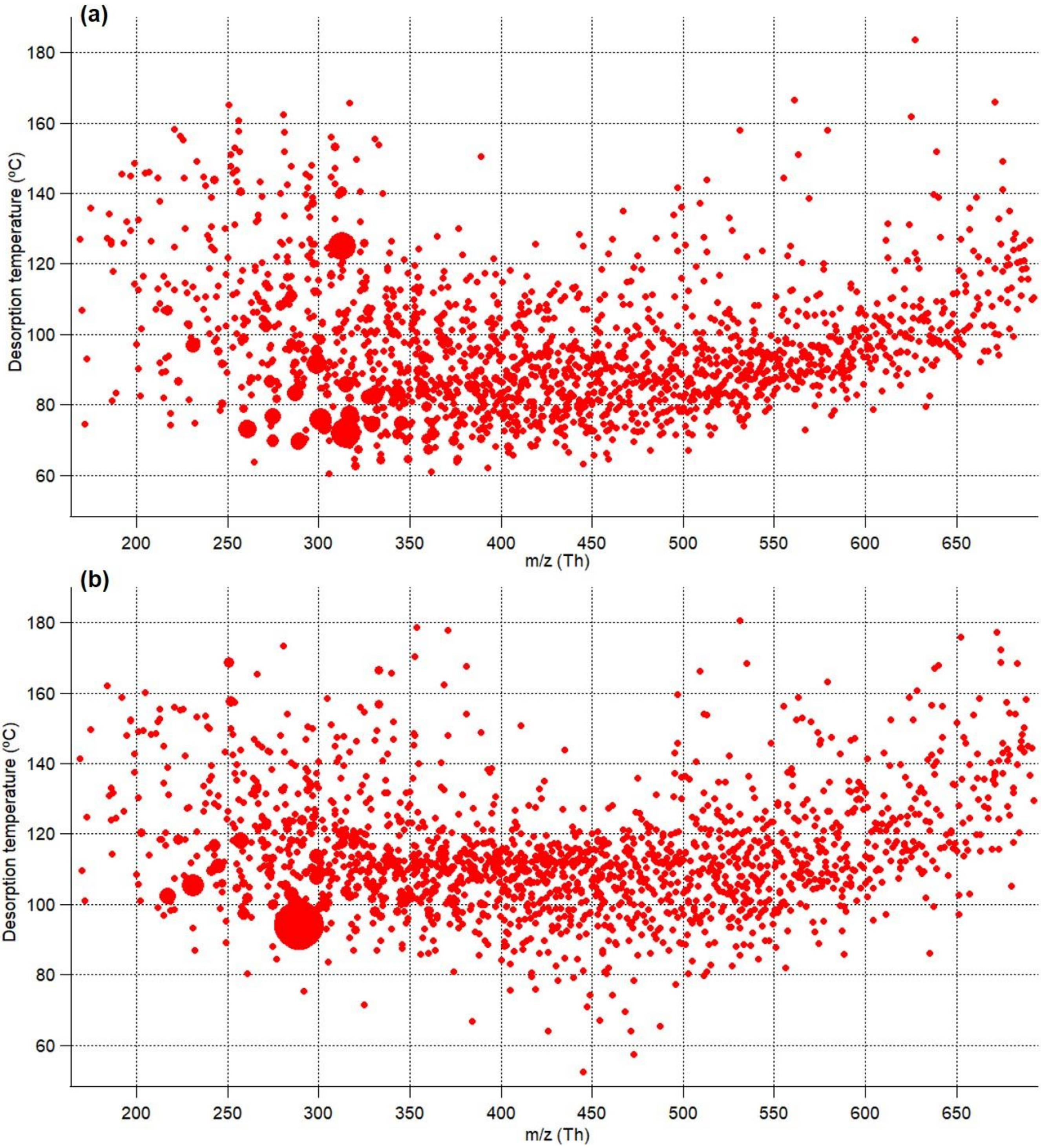


Figure S11. Mean T_{max} distribution of CHOX compounds as a function of *m/z* (includes mass of I^- ion; *m/z* 126.9050 Th) for the summer (a) and winter (b) periods. Markers were sized by their corresponding mass contributions to total CHOX compounds. Mean T_{max} were calculated as the campaign-average of the T_{max} for each CHOX compound.

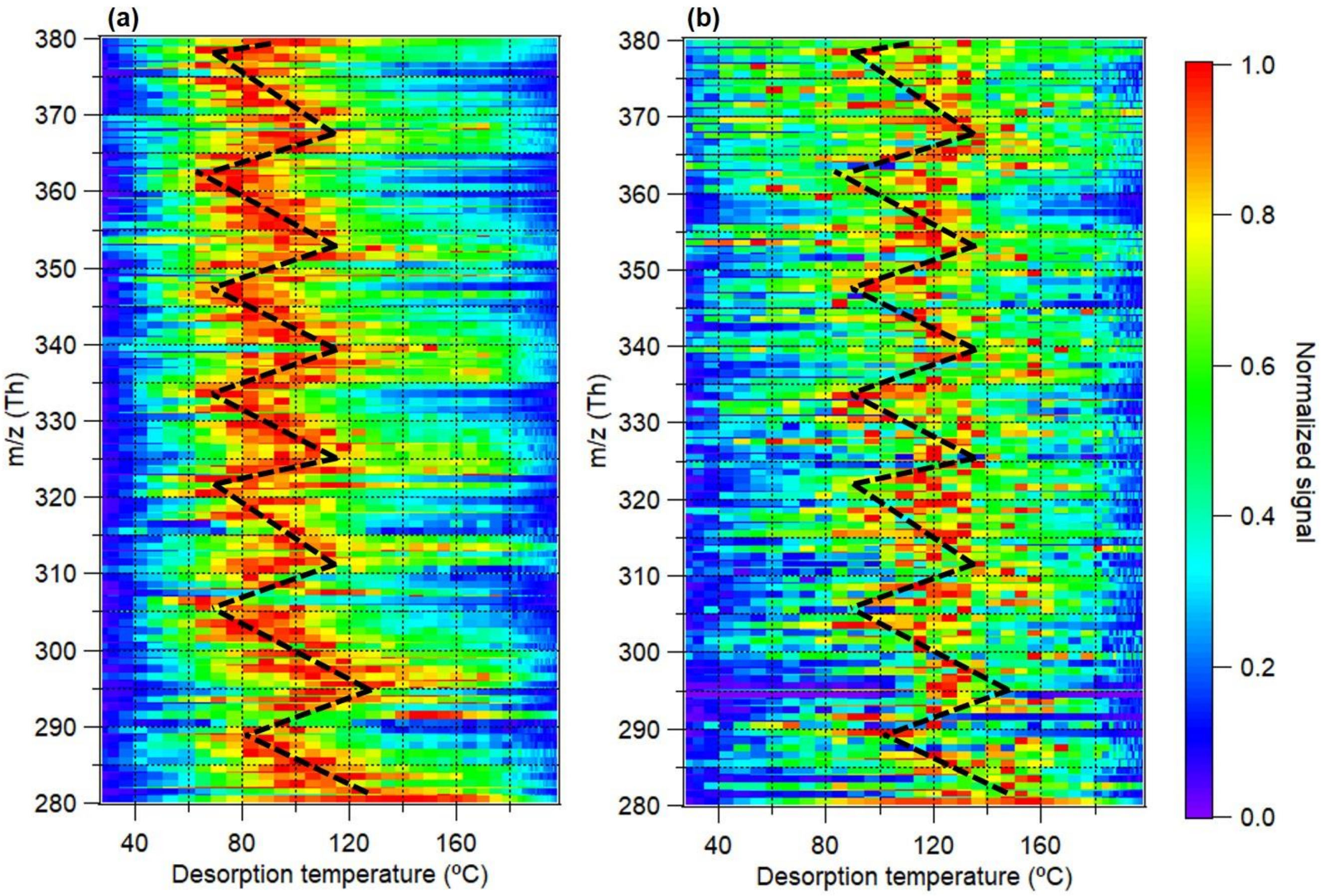


Figure S12. Comparison of high resolution 2D thermograms of CHOX compounds for mass range 280–380 Th of Figure 4 for the summer (a) and winter (b) periods. The 2D thermograms were normalized to their maximum values. A black dotted line was plotted by hand to guide the eye.

References

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