Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts.

Supporting Information for

Aqueous processing of water-soluble organic compounds in the eastern United States during winter

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Introduction

This supporting information is composed of twenty-three pages, twenty figures and one table. Table S1 contains a comparison of daytime and nighttime meteorological data in Baltimore during the winter.

Figure S1 represents a scatterplot of OA concentrations measured at Essex and HU-Beltsville over several years. Figure S2 is a diurnal profile of the percent contribution of primary (in red) and secondary (in blue) aerosol in the winter of 2015 in Baltimore using an EC-tracer method. Figures S3 and S4 present scatterplots of wintertime $WSOC_p$ concentrations versus EC and CO concentrations, respectively at night for data (a) < 0 ^oC, (b) 0 – 10 ^oC and (c) > 10 ^oC. Figure S5 represents average diurnal profiles for $WSOC_g$ and $WSOC_p$ concentrations as a function of temperature. Figure S6 shows average diurnal profiles for $WSOC_g$, $WSOC_p$, CO, and EC concentrations. Figure S7 represents scatter plots of CO and EC concentrations at (a) < 0 ^oC, (b) 0 – 10 ^oC and (c) > 10 ^oC. Figure S8 shows scatter and boxplots of the particulate WSOC fraction, F_p, as a function of OC at (a) daytime and (b) nighttime periods. Figure S9 illustrates wintertime 72-h back trajectories for four days with daily average temperatures below 0 ^oC using HYSPLIT model. Figure S10 is a scatter plot of $PM_{2.5}$ concentrations as a function of temperature during the months of November through March in Baltimore over 2011 – 2015. Figure S11 depicts scatter and boxplots of the particulate WSOC fraction, F_p, as a function of RH at (a) daytime and (b) nighttime periods. Figure S12 is a scatter and box plots of the particulate WSOC fraction, F_p, as a function of RH at daytime (08:00 to 18:00, local time) for different temperature ranges: (a) < 0 °C (b) 0 – 10 °C, and (c) >10 °C. Figure S13 shows a time series of F_p, temperature, and RH levels on (a) 2/7/2015, and (b) 2/20/2015. Figure S14 shows diurnal profiles of $\Delta WSOC_p/\Delta CO$ at three different temperatures, namely < 0 °C, 0 – 10 °C, and > 10°C with error bars. Figure S15 depicts scatter plots of $WSOC_{p,dry}$ versus $WSOC_p$ for winter (a) daytime and (b) nighttime periods. Figure S16 presents average values of the $WSOC_{p,dry}/WSOC_p$ ratio as a function of ambient RH. Figure S17 is a representation of the daily average (a) $WSOC_p$ and (b) $WSOC_g$ concentrations as a function of their corresponding potassium (K^+) concentrations. Figures S18 and S19 are scatterplots of $WSOC_g$ concentrations versus CO and EC concentrations, respectively for data (a) < 0 ^oC, (b) 0 – 10 ^oC and (c) > 10 ^oC. Finally, Figure S20 represents scatter and boxplots for (a) $WSOC_g$ and (b) $WSOC_p$ concentrations as a function of wind speed.

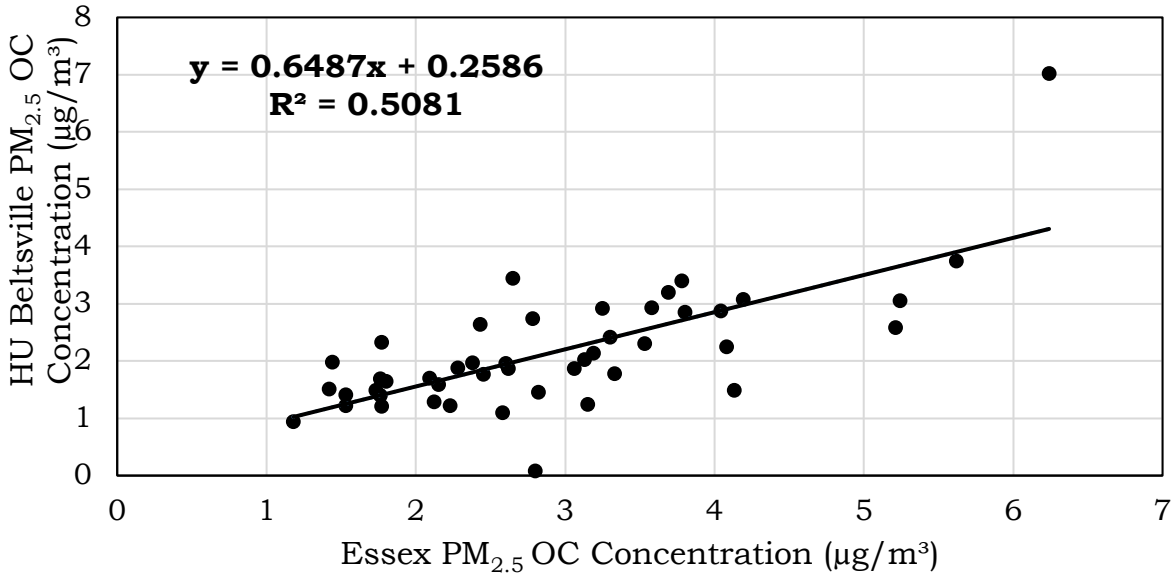

Figure S1. Scatter plot of $PM_{2.5}$ OC Concentrations from HU Beltsville vs. Essex in the winter months of 2014 and 2015.

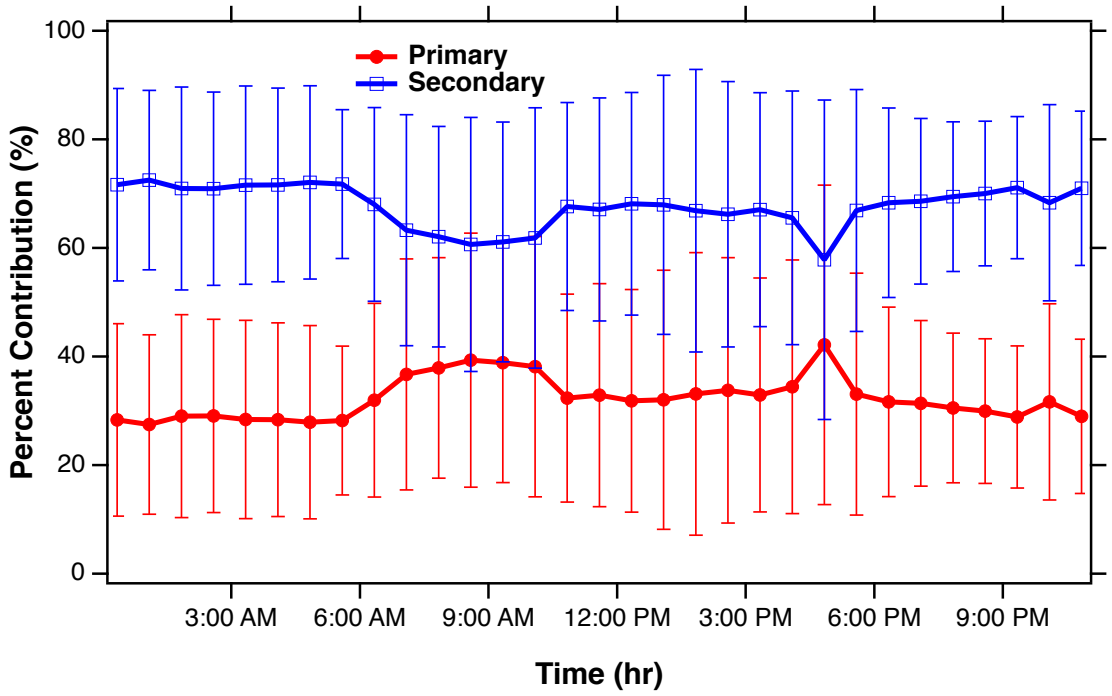

Figure S2. Diurnal profile of the percent contribution of primary (in red) and secondary (in blue) aerosol in the winter of 2015 in Baltimore using an EC-tracer method.

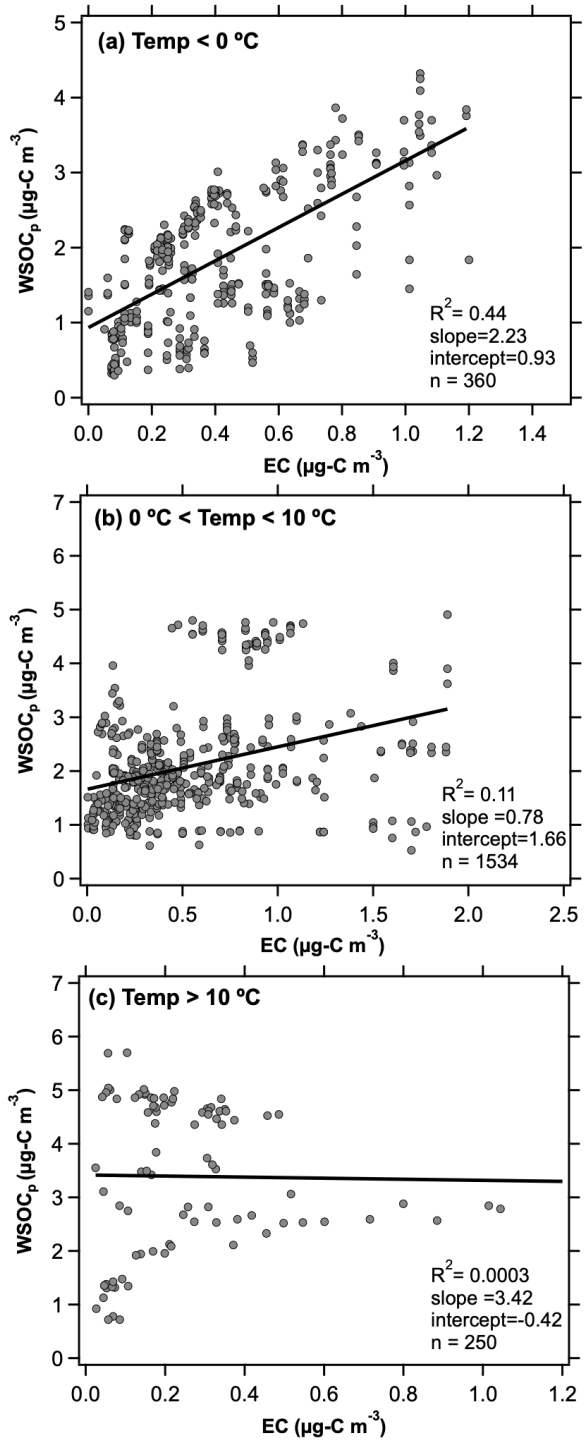

Figure S3. Scatter plots of wintertime $WSOC_p$ concentrations versus EC concentrations for data (a) < 0 ^oC, (b) 0 – 10 ^oC and (c) > 10 ^oC. Solid black lines represent linear fits for data in each panel.

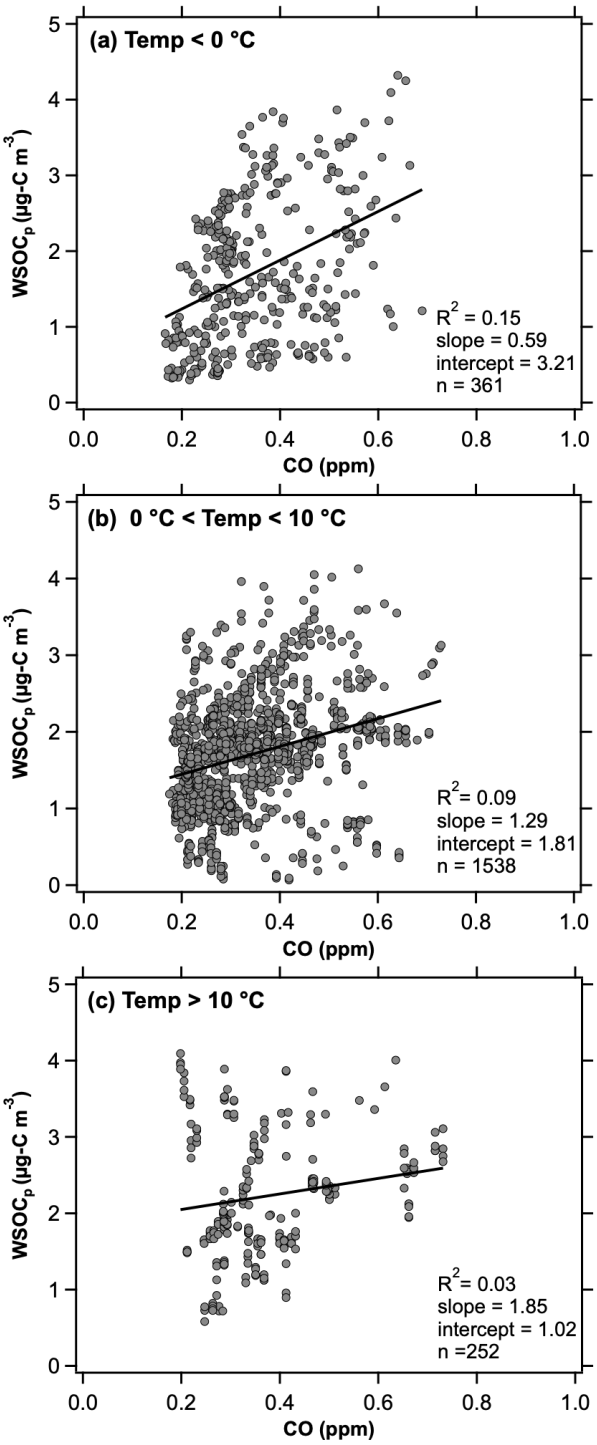

Figure S4. Scatter plots of $WSOC_p$ concentrations versus CO concentrations for data (a) < 0 ^oC, (b) 0 – 10 ^oC and (c) > 10 ^oC. Solid black lines represent linear fits for data in each panel.

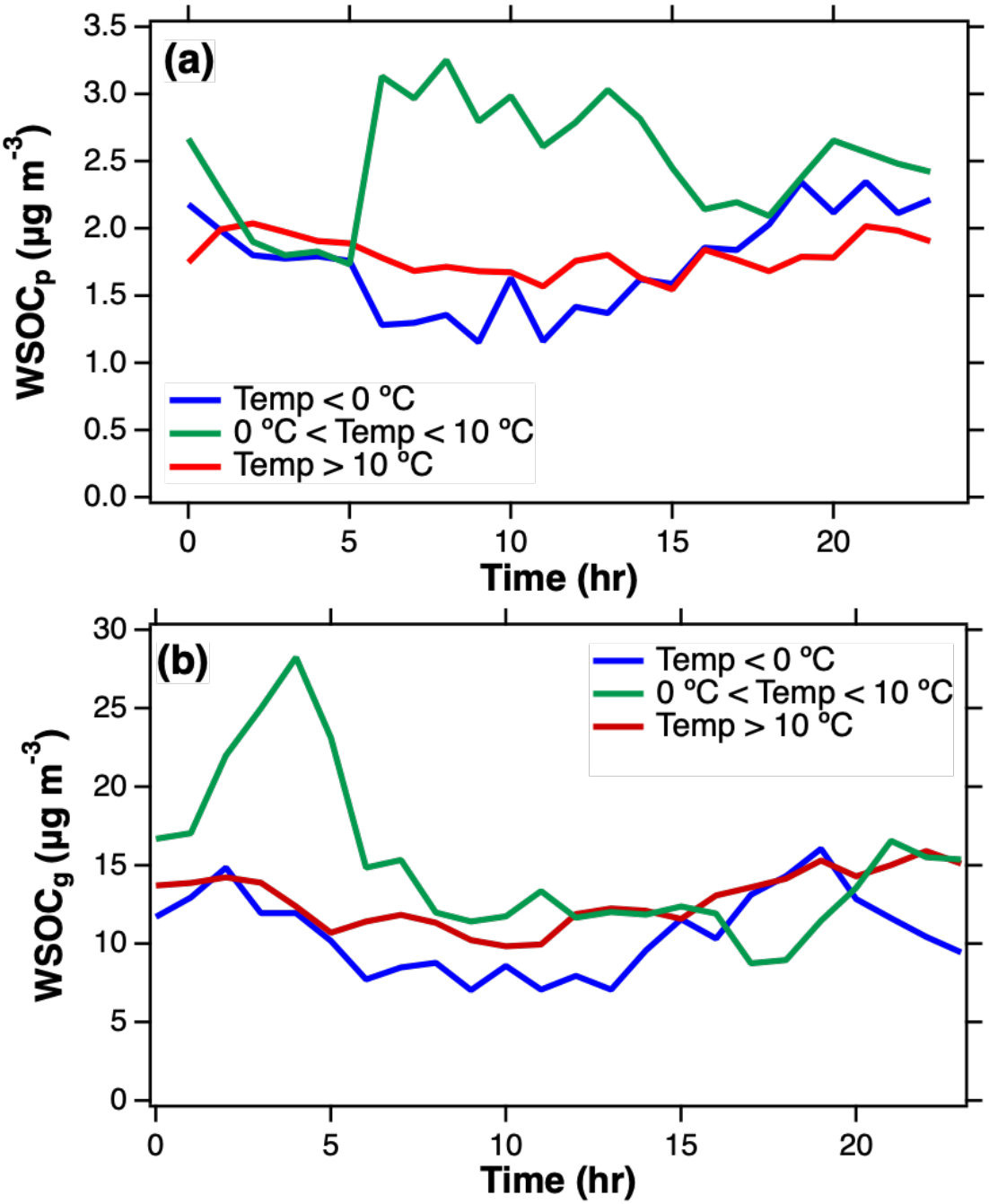

Figure S5. Average diurnal profiles for $WSOC_g$ and $WSOC_p$ concentrations as a function of temperature.

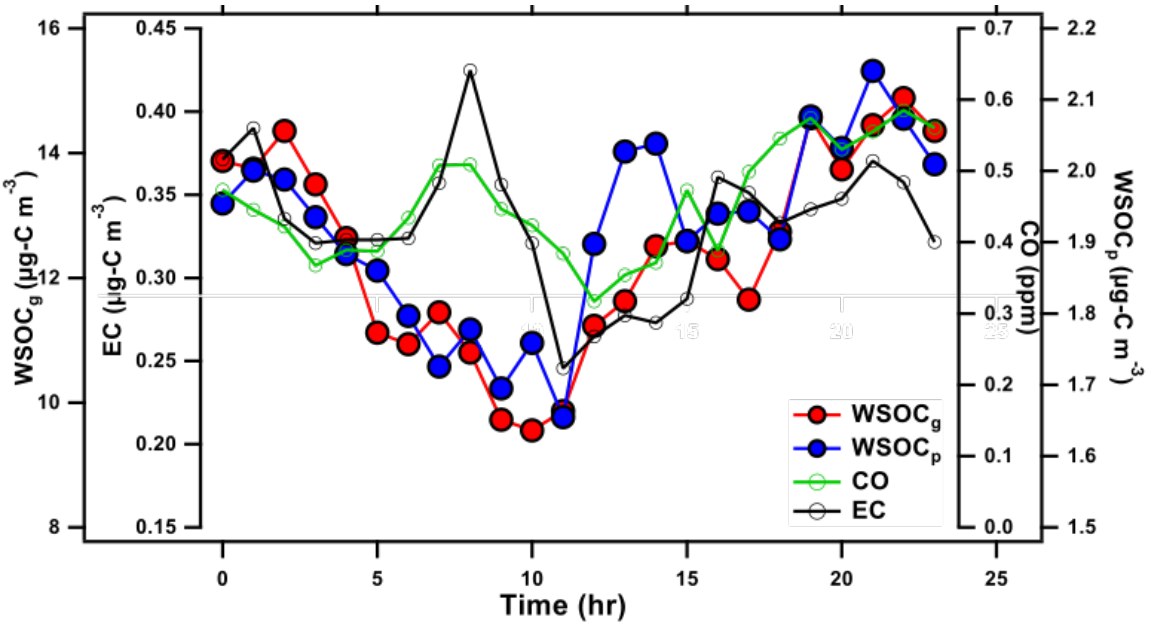

Figure S6. Average diurnal profiles for $WSOC_g$, $WSOC_p$, CO, and EC concentrations.

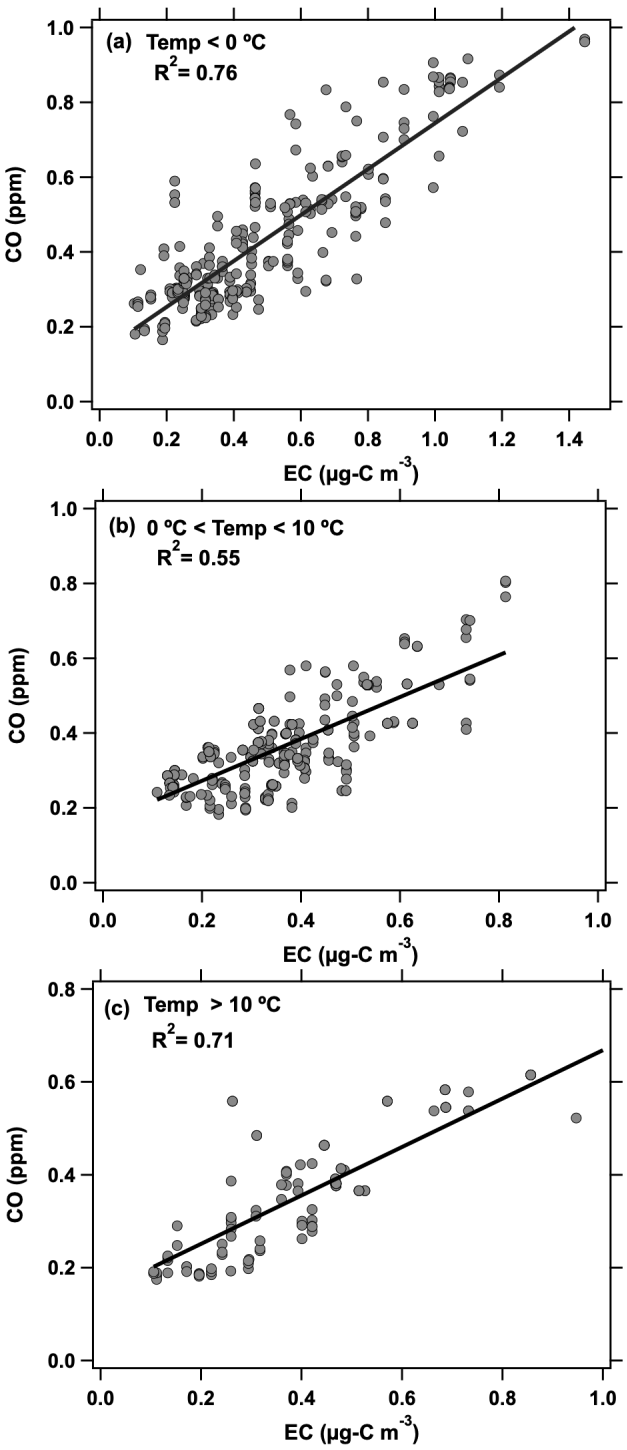

Figure S7. Scatter plots of nighttime CO and EC concentrations at (a) < 0 ^{o}C, (b) 0 – 10 ^{o}C and (c) > 10 ^{o}C.

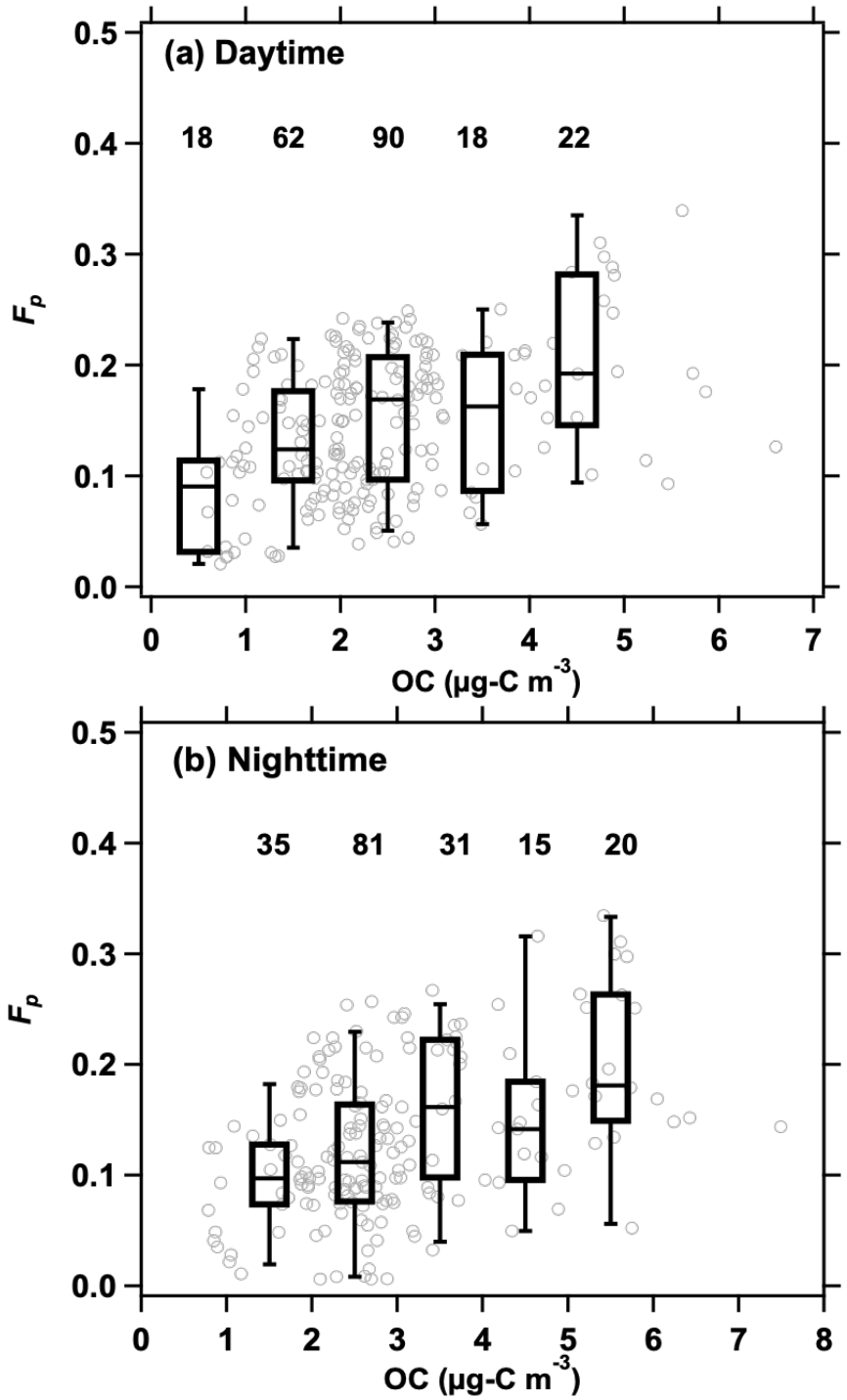

Figure S8. Scatter and boxplots of the hourly particulate WSOC fraction, F_p, as a function of OC at (a) daytime (08:00 to 18:00, local time) and (b) nighttime (20:00 to 07:00, local time) periods. Data were binned based on OC concentrations. (a) Bins were defined as < 1, 1 – 2, 2 – 3, 3 – 4, and > 4 µg m^{-3}. (b) Bins were defined as < 2, 2 – 3, 3 – 4, 4 – 5, and > 5 µg m^{-3}. For each bin, median values (horizontal line), 25th and 75th percentiles (lower and upper box values), as well as 5th and 95th percentiles (vertical lines) are shown.

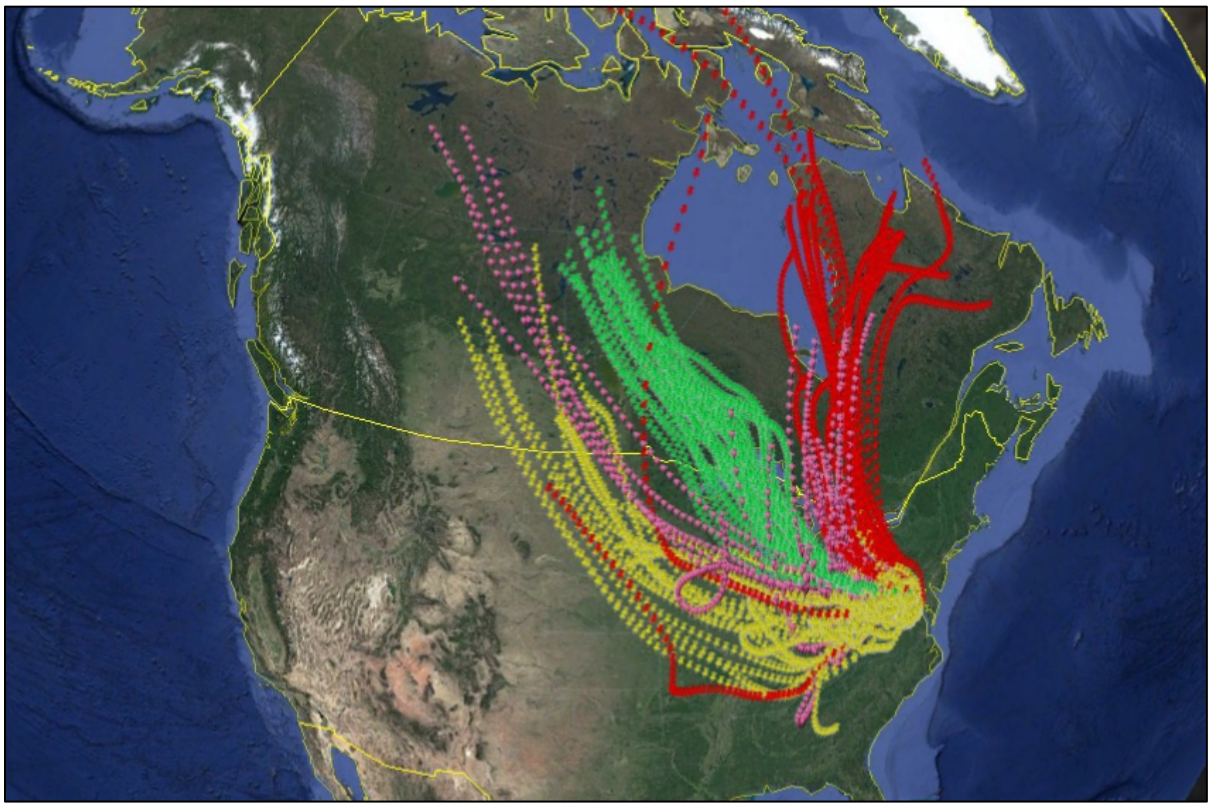

Figure S9. Wintertime 72-h back trajectories for four days with daily average temperatures below 0 ^{o}C using HYSPLIT model. Red: February 17th, 2015, purple: February 18th, 2015, green: February 19th, 2015, and yellow: February 20th, 2015.

Back trajectories were examined by running HYbrid Single-Particle Lagrangian Integrated Trajectory (HYSPLIT) model (Stein et al., 2015), (http://www.arl.noaa.gov/ready/hysplit4.html). The web-based version of HYSPLIT was used to calculate the past trajectories of air masses reaching the UMBC site through 72-h trajectories using archived meteorological data from the NOAA's AIR Resources Laboratory (ARL) using the Global data assimilation system (GDAS) dataset of 0.5 degree horizontal resolution at a latitude of 39.2556^{o} N and a longitude of 76.7110^{o} W.

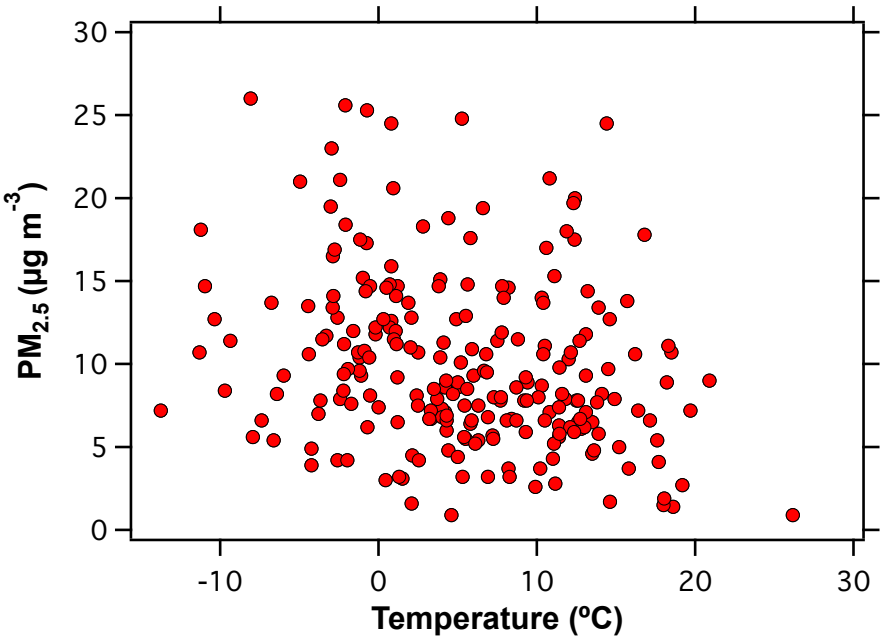

Figure S10. Scatter plot of $PM_{2.5}$ concentrations as a function of temperature during the months of November through March in Baltimore over 2011 – 2015.

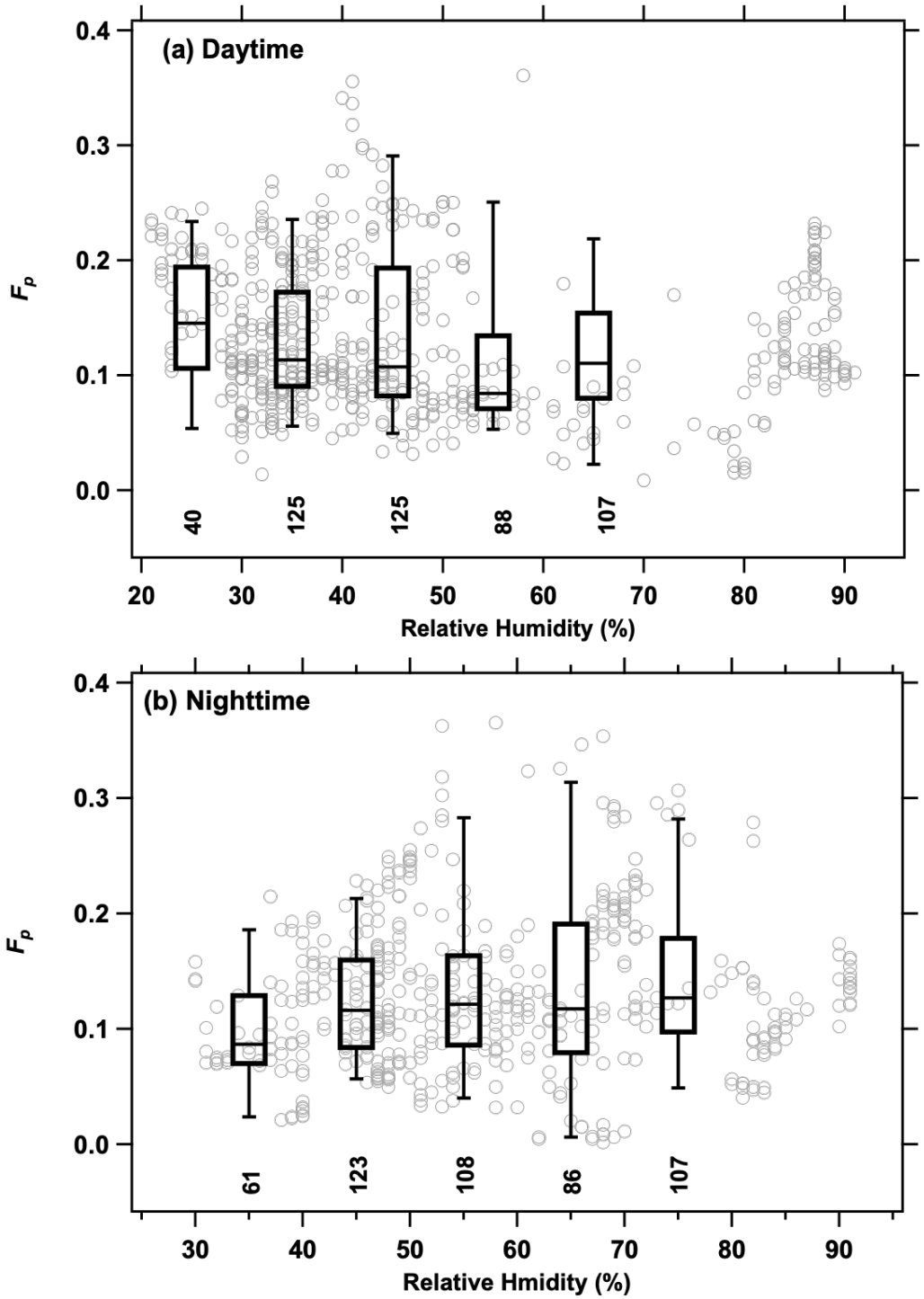

Figure S11. Scatter and boxplots of the particulate WSOC fraction, F_p, as a function of RH at (a) daytime (08:00 to 18:00, local time) and (b) nighttime (20:00 to 07:00, local time) periods. Data were binned based on RH concentrations. (a) Bins were defined as < 40, 40 – 50, 50 – 60, 60 – 70, and > 70%. (b) Bins were defined as < 40, 40 – 50, 50 – 60, 60 – 70 and > 70%. For each bin, median values (horizontal line), 25th and 75th percentiles (lower and upper box values), as well as 5th and 95th percentiles (vertical lines) are shown.

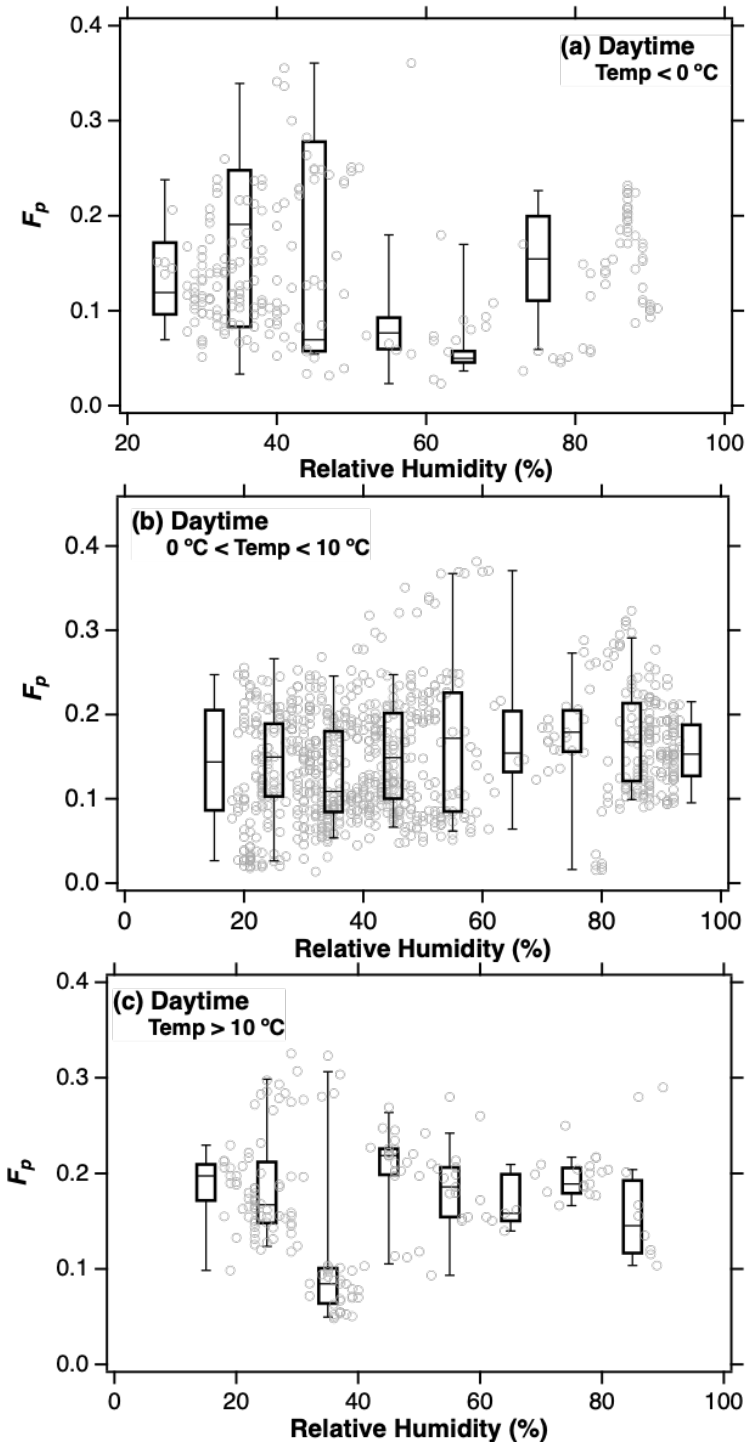

Figure S12. Scatter and box plots of the particulate WSOC fraction, F_p, as a function of RH at daytime (08:00 to 18:00, local time) for different temperature ranges: (a) < 0 °C (b) 0 – 10 °C, and (c) > 10 °C. For each bin, mean (red circles, median (horizontal line), quartiles (lower and upper box values), as well as 5th and 95th percentiles (vertical lines) are shown.

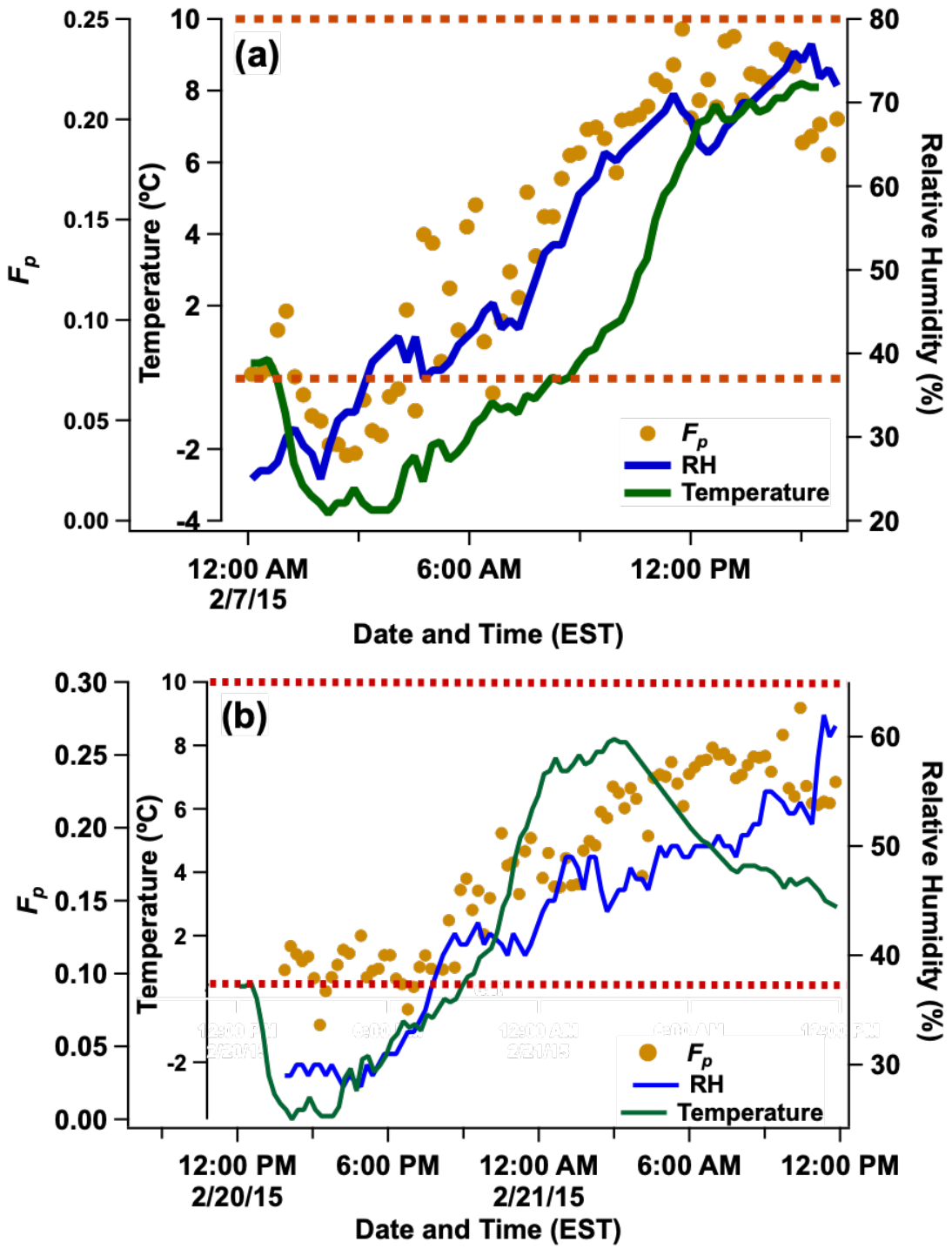

Figure S13. Time series of F_p, temperature, and RH levels on (a) 2/7/2015, and (b) 2/20/2015. The red dotted horizontal lines represent the 0 – 10 °C temperature range.

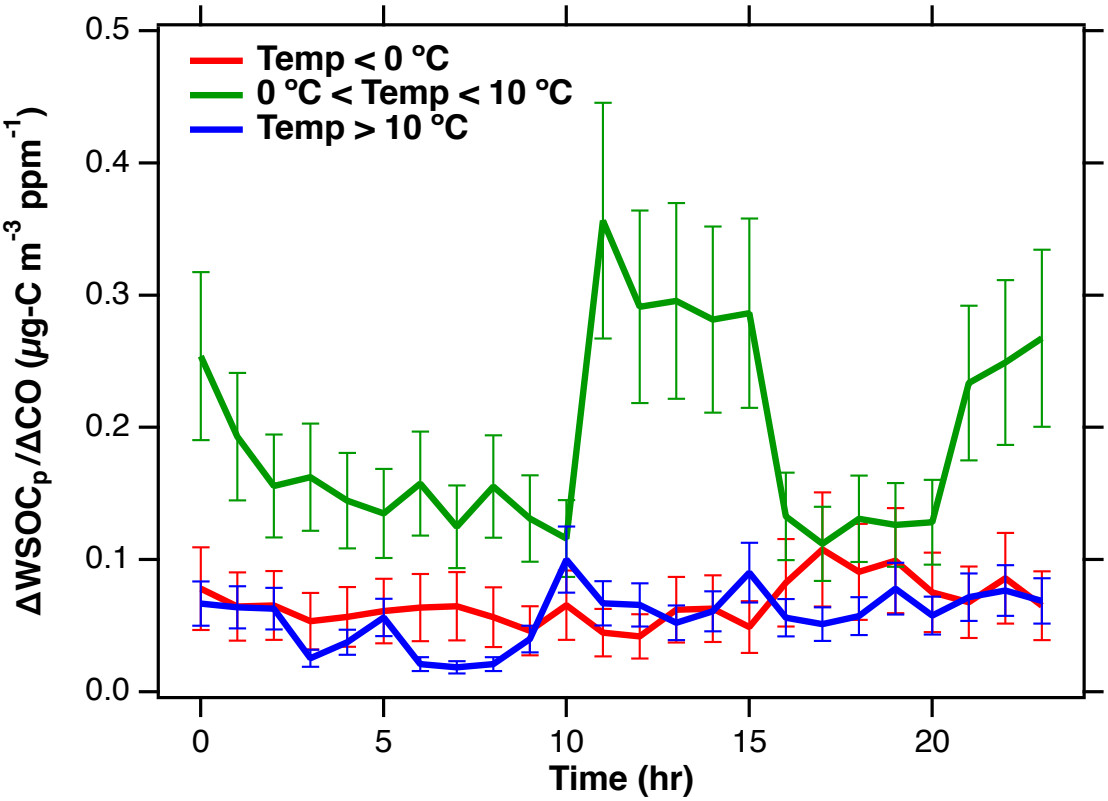

Figure S14. Diurnal profiles of $\Delta WSOC_p/\Delta CO$ at three different temperatures, namely < 0 °C, 0 – 10 °C, and > 10°C with error bars.

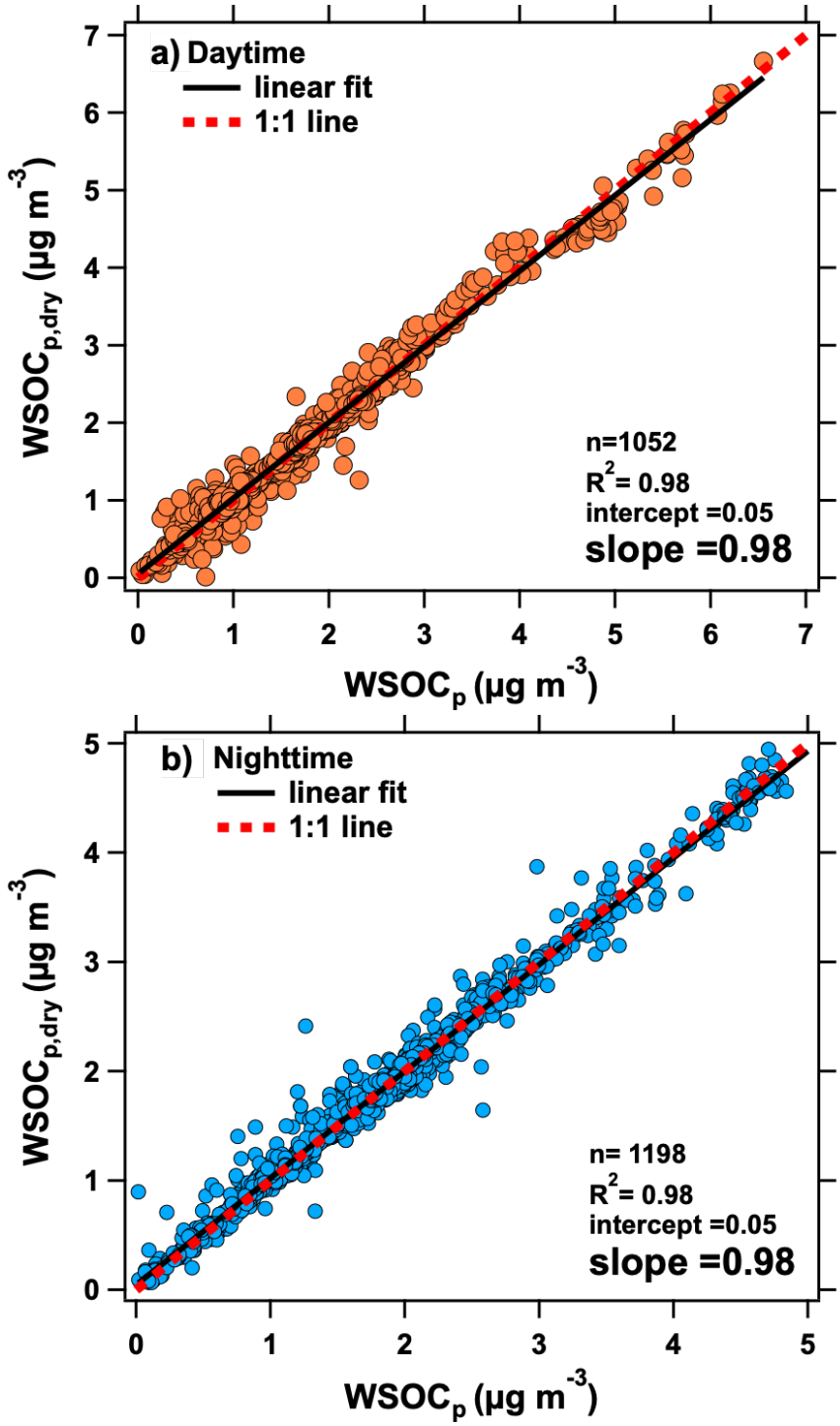

Figure S15. Scatter plots of $WSOC_{p,dry}$ versus $WSOC_p$ for winter (a) daytime (08:00 to 18:00, local time) and (b) nighttime (20:00 to 07:00, local time) periods. The solid black lines in (a) and (b) represent the linear fits to the data using least squares regression analysis; the fit parameters are given in each panel. The red dotted lines in (a) and (b) are the 1:1 lines as visual reference.

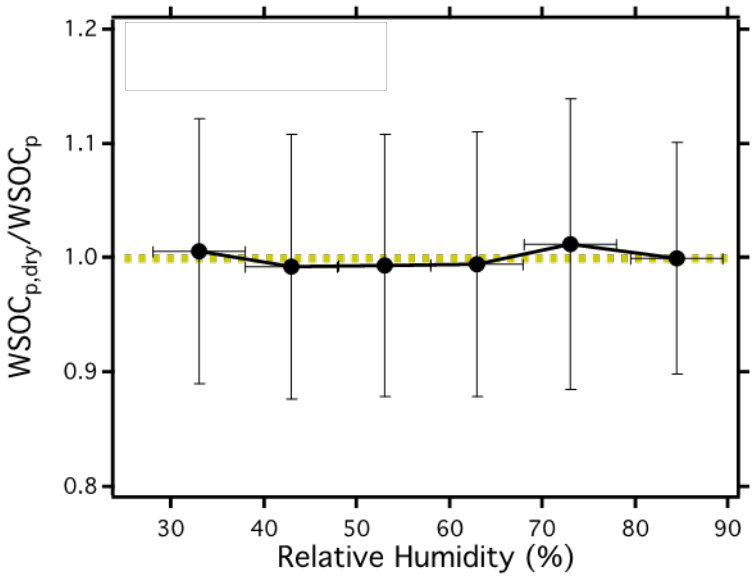

Figure S16. Average values of the $WSOC_{p,dry}/WSOC_p$ ratio as a function of ambient RH. The yellow dotted line at unity is provided for clarification. Vertical error bars represent the standard deviation of the $WSOC_{p,dry}/WSOC_p$ ratio at different RH bins.

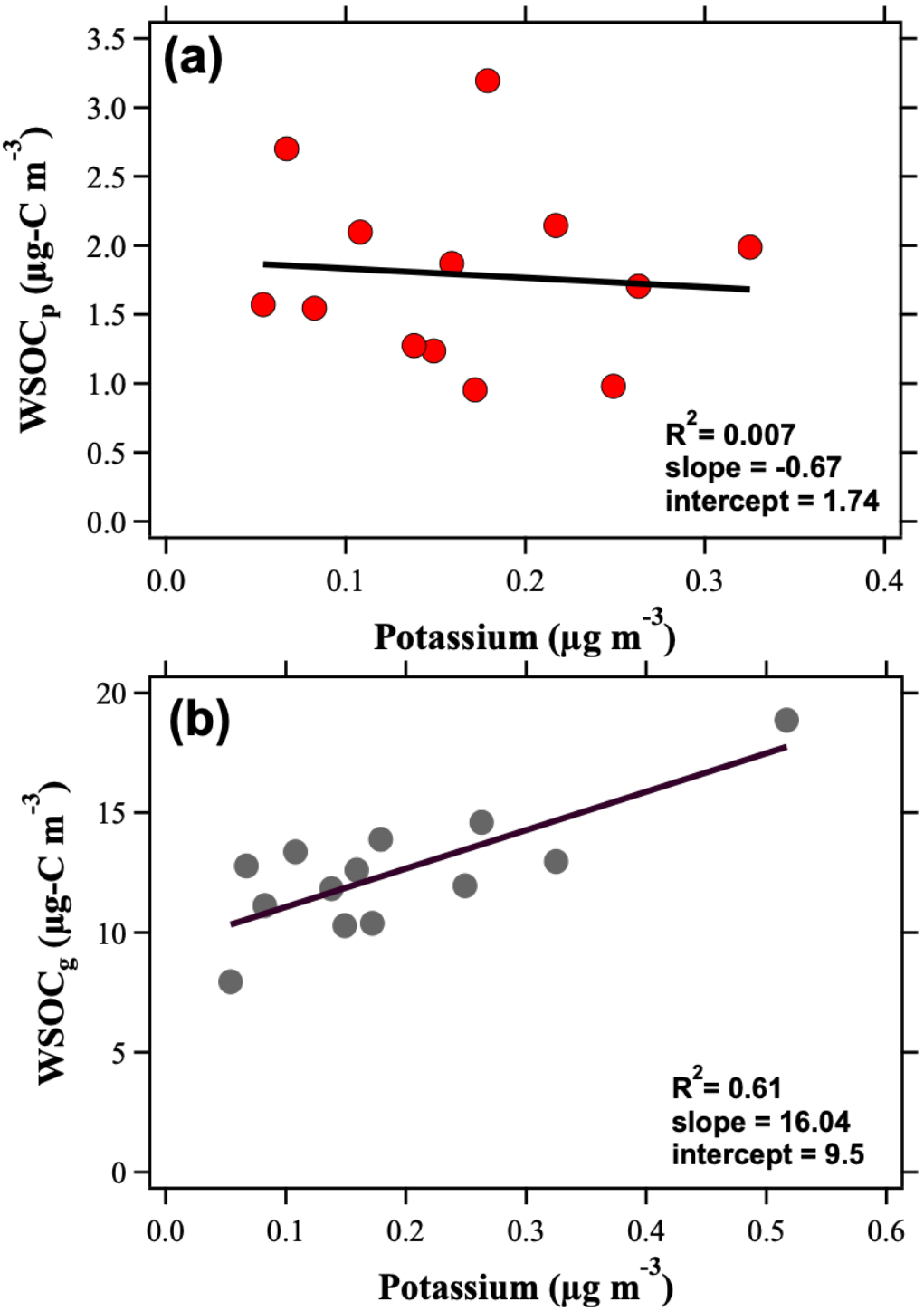

Figure S17. Scatter plot and linear correlation of $WSOC_g$ and potassium (K^+) concentrations during the study period.

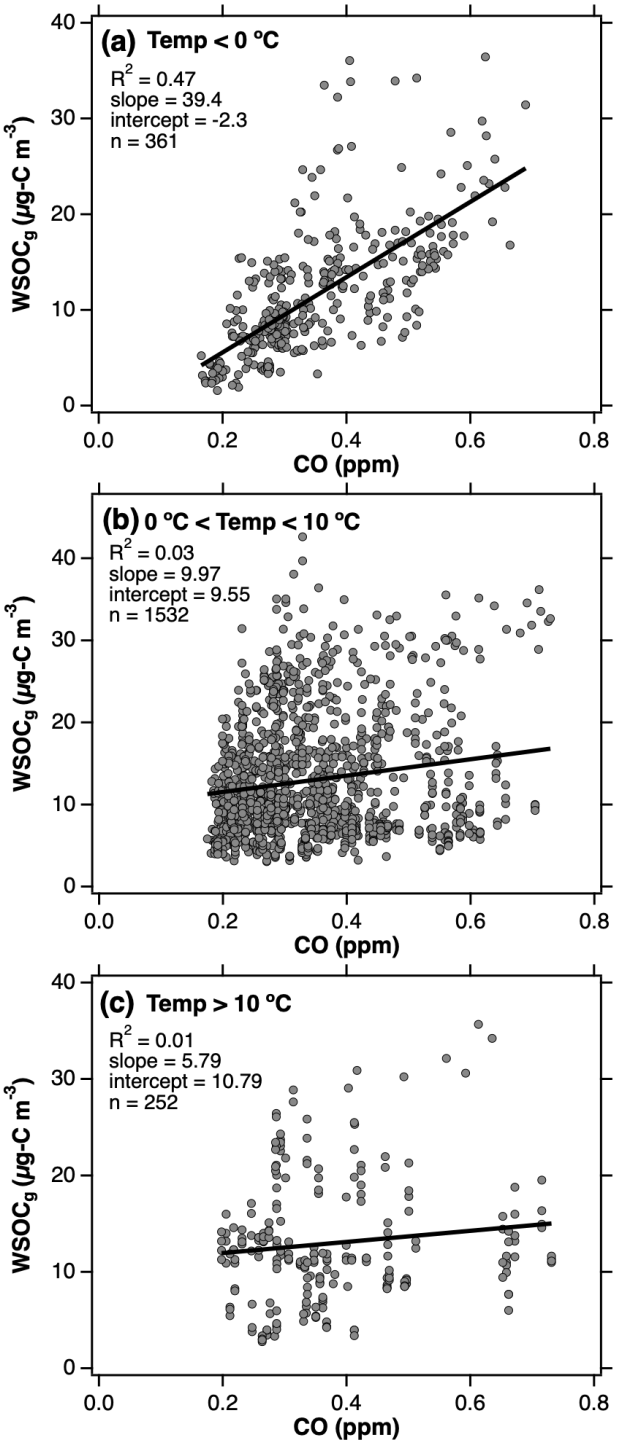

Figure S18. Scatterplots of $WSOC_g$ concentrations versus CO concentrations for data (a) < 0 ^oC, (b) 0 – 10 ^oC and (c) > 10 ^oC.

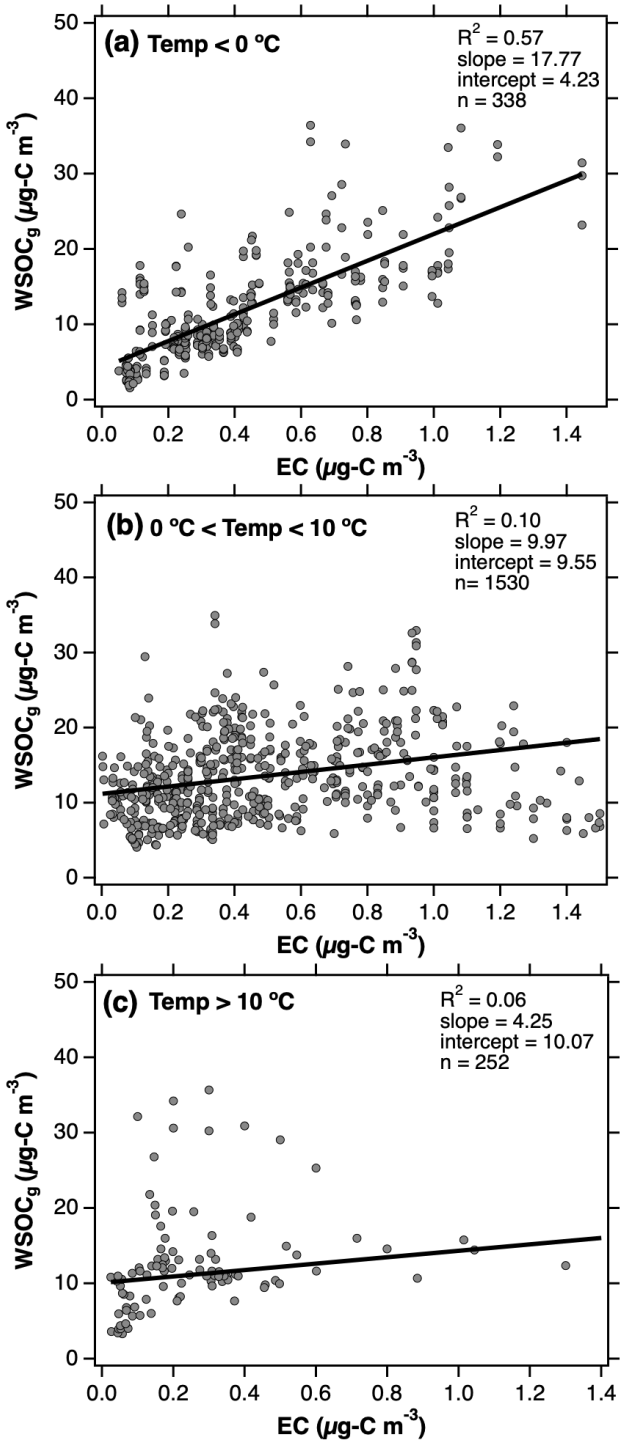

Figure S19. Scatterplots of $WSOC_g$ concentrations versus EC concentrations for data (a) < 0 ^oC, (b) 0 – 10 ^oC and (c) > 10 ^oC.

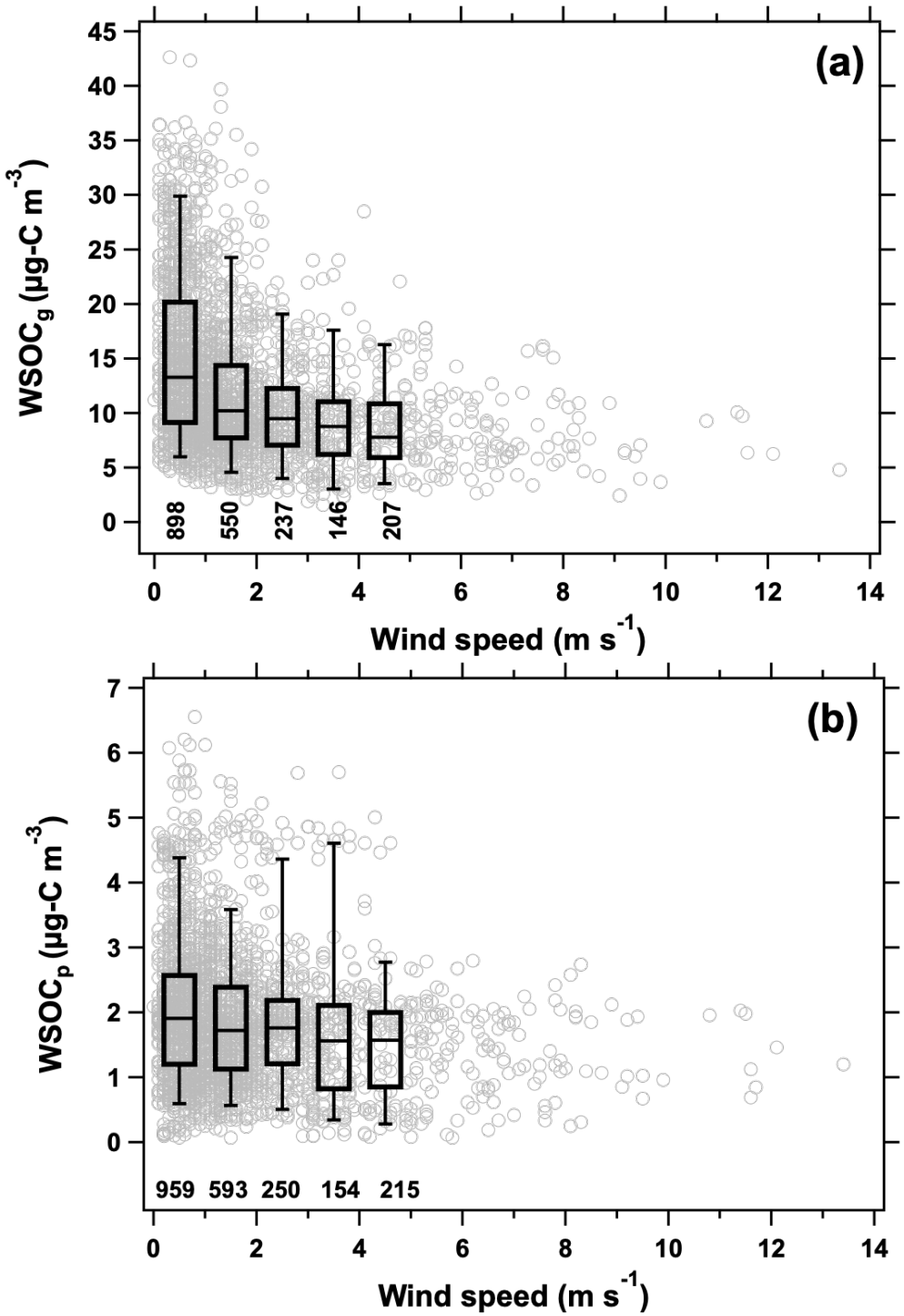

Figure S20. Scatter and boxplots for (a) $WSOC_g$ and (b) $WSOC_p$ concentrations as a function of wind speed. For each bin, median values (horizontal line), 25th and 75th percentiles (lower and upper box values), as well as 5th and 95th percentiles (vertical lines) are shown. Numbers at the bottom represent the number of points within each bin.

Table S1. Daytime and nighttime meteorological data in Baltimore during the winter.

	Daytime		Nighttime	
Winter	**Relative Humidity (%)**	**Temperature** (°C)	**Relative Humidity (%)**	**Temperature** (°C)
Median	44.4	4.5	58.9	1.1
Mean	46.8	4.1	58.0	1.9
Standard deviation	19.4	6.71	14.4	5.9
Range	21.0 – 91.0	-11.1 – 20.1	30.0 – 91.0	-15.9 – 13.7

References

Stein, A. F., Draxler, R. R., Rolph, G. D., Stunder, B. J. B., Cohen, M. D. and Ngan, F. (**2015**) 'NOAA's HYSPLIT Atmospheric Transport and Dispersion Modeling System', *Bulletin of the American Meteorological Society,* 96(12), pp. 2059-2077.