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Evaluation of Pandora HCHO and NO_2 with airborne in situ observations

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S1. Pandora Data Filtering

Figure S1 and S2 present the results for the filtering method for HCHO and NO_2 as described in sect. 2.2.1 The first column shows the agreement between DS total column and MAX DOAS tropospheric column (climatological stratospheric NO_2 has been subtracted from the total NO_2 column), averaged over 30 minute intervals. The slope is calculated using the Theil Sen estimator, a useful method that limits the impact of outliers by determining the slope based on the median slope found through all pairs of points. The second column displays the data after applying the filtering procedure. The colors of the markers indicate the median data quality flag of the scans.

These results illustrate the limitations of the automatic flagging algorithm, particularly its tendency to produce false negatives. Instances where one or both Pandora scans are designated 'low' quality are the points with the worst agreement between DS and MAX DOAS, yet not all such cases show this discrepancy. Consequently, removing all low quality data would unnecessarily eliminate a large portion of the dataset, more than is done by this filtering method (Fig. 1). Data where both DS and MAXDOAS are high quality exhibit much stronger correlations. However, a systematic pattern remains in which DS columns are generally greater than MAX DOAS due to the longer path integration.

The third and fourth columns highlight how the measurement uncertainty is largely correlated with the SZA where, for MAX DOAS, uncertainty tends to increase when the sun is low in the sky and the DS uncertainty increases when the sun is at its peak. Columns 3 and 4 are restricted to data taken on the 5 days analyzed in this study (06/26/23; 07/26/23; 07/28/23; 08/09/23; 08/16/23).

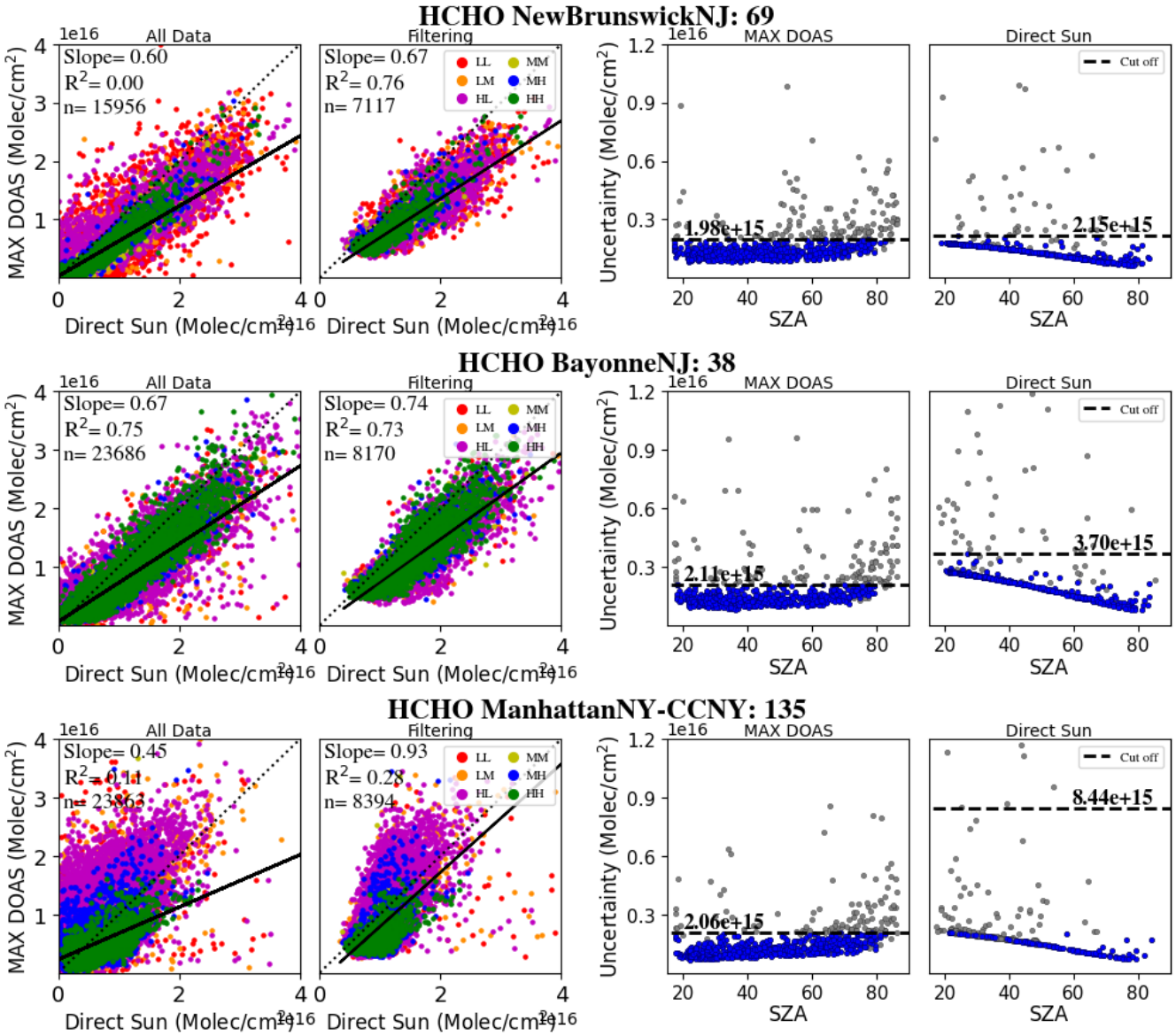


Figure S1. Data quality assessment of the Pandoras used in this study. The first column compares the total column DS HCHO to the tropospheric column MAX DOAS HCHO, each averaged to 30 min. The second column is the same but after the filtering method (Section 2.2.1) has been applied. The six different colors represent the data quality flag based on the automatic detection algorithm for both DS and MAX DOAS. Green are points with median high quality for both scan modes (HH); blue is where one mode is 'high' and another is 'medium' (HM); yellow points are 'medium' quality for both scan modes (MM) etc. The third and fourth columns show only data taken on the 5 days included in this study for MAX DOAS and DS, respectively. The gray points are all data from these days and the blue points are data that passed the filtering checks and are included in analysis

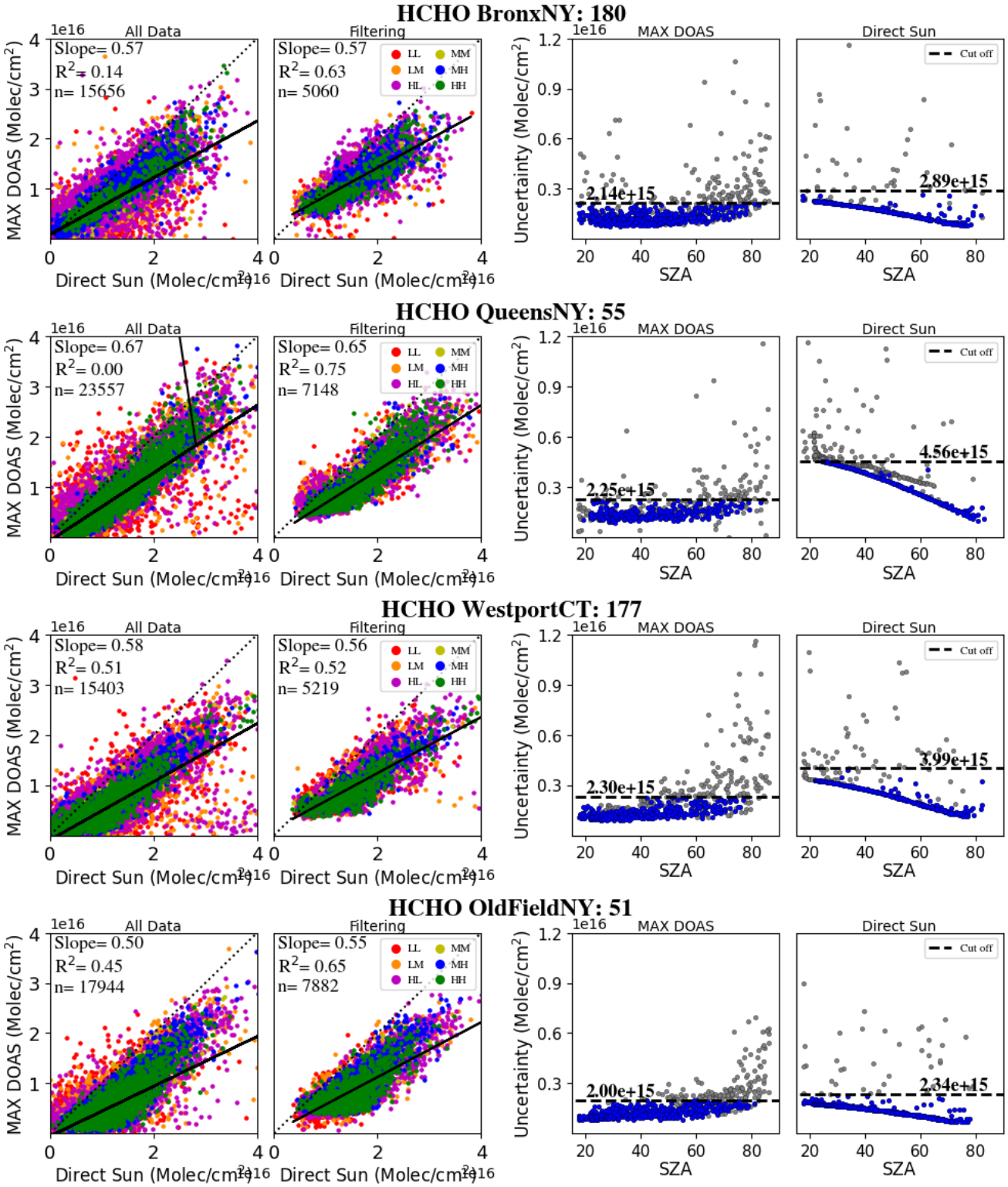


Figure. S1. Cont.

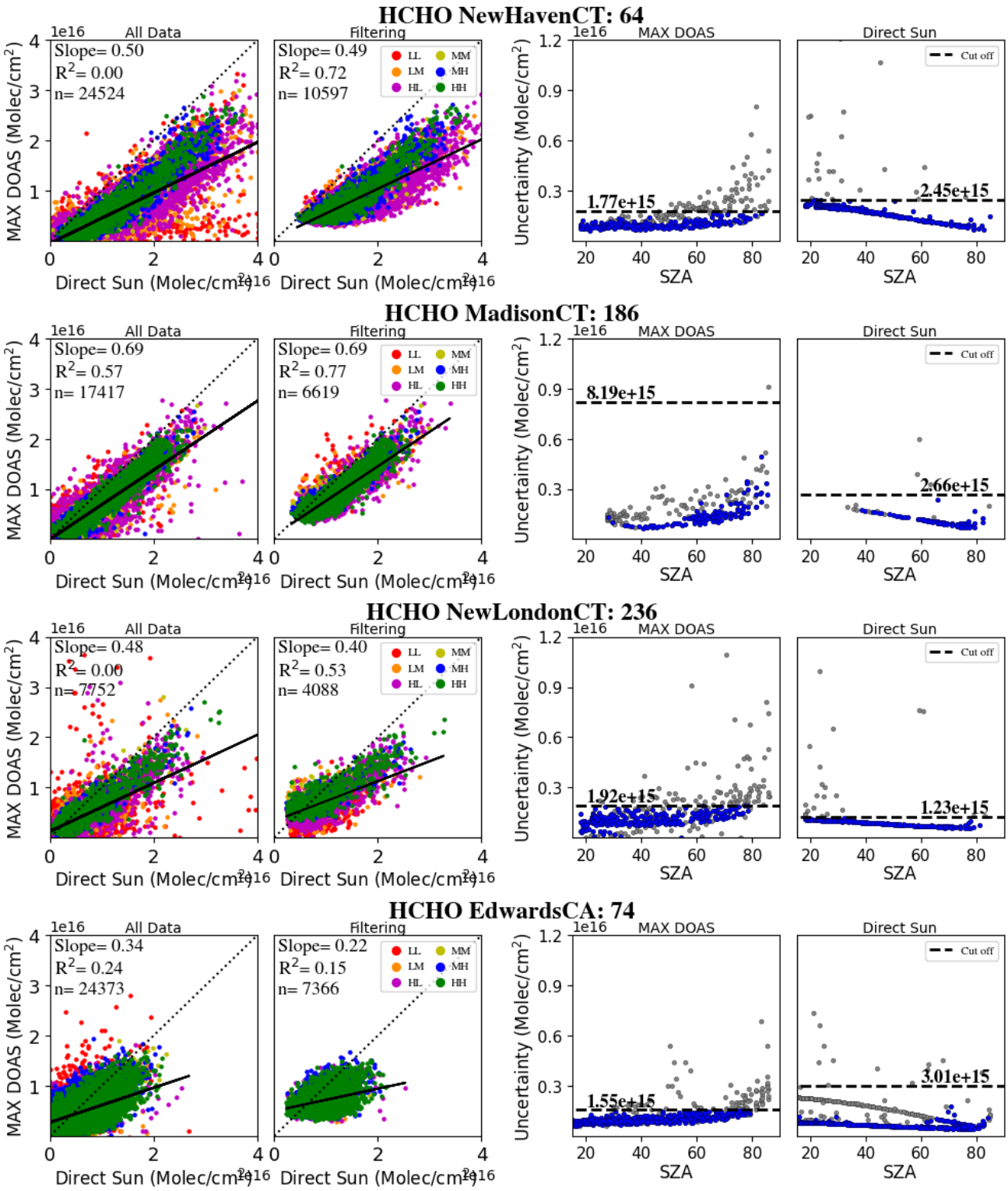


Figure. S1. Cont.

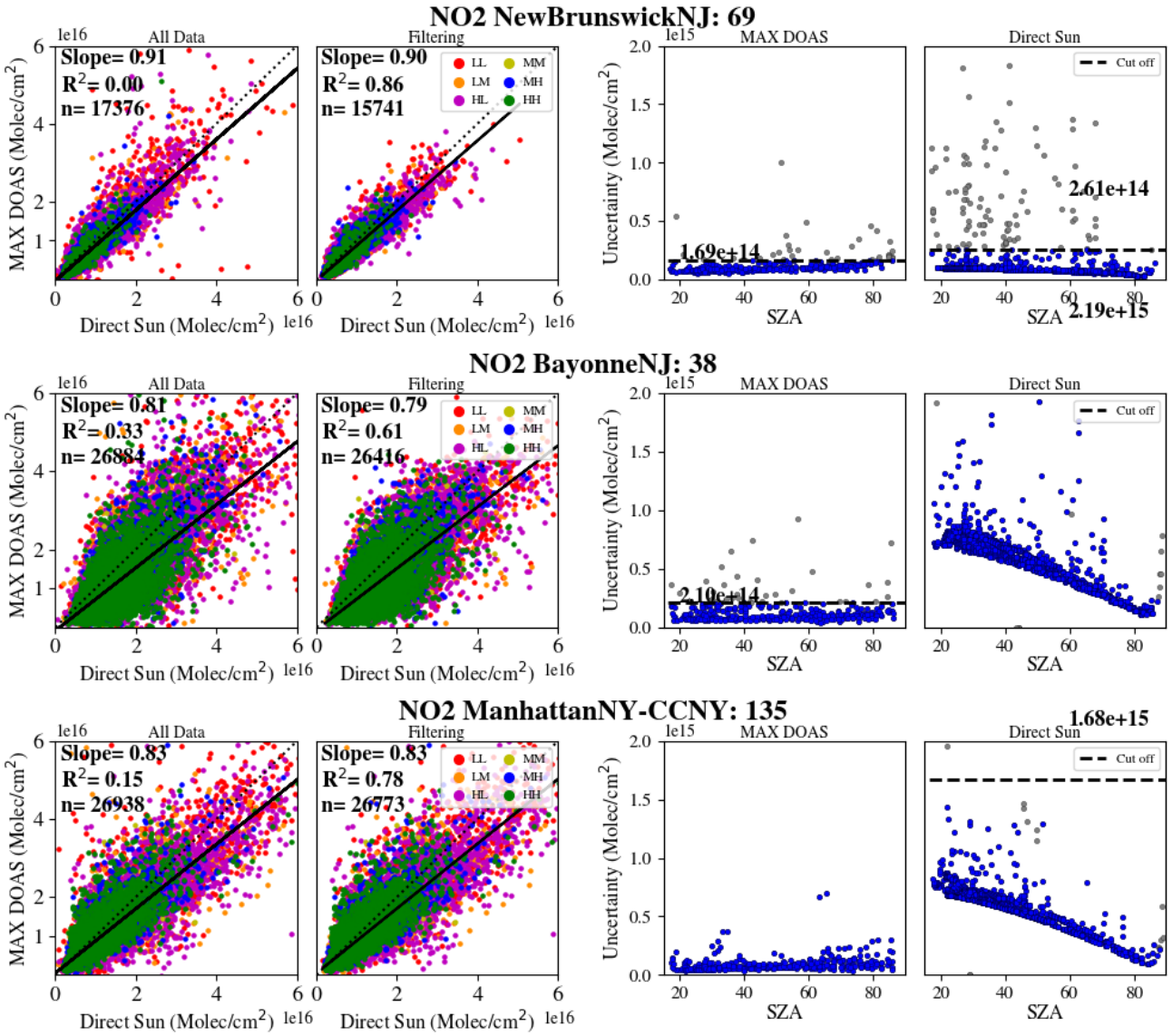


Figure S2: Same as Figure. S1, but for NO_2.

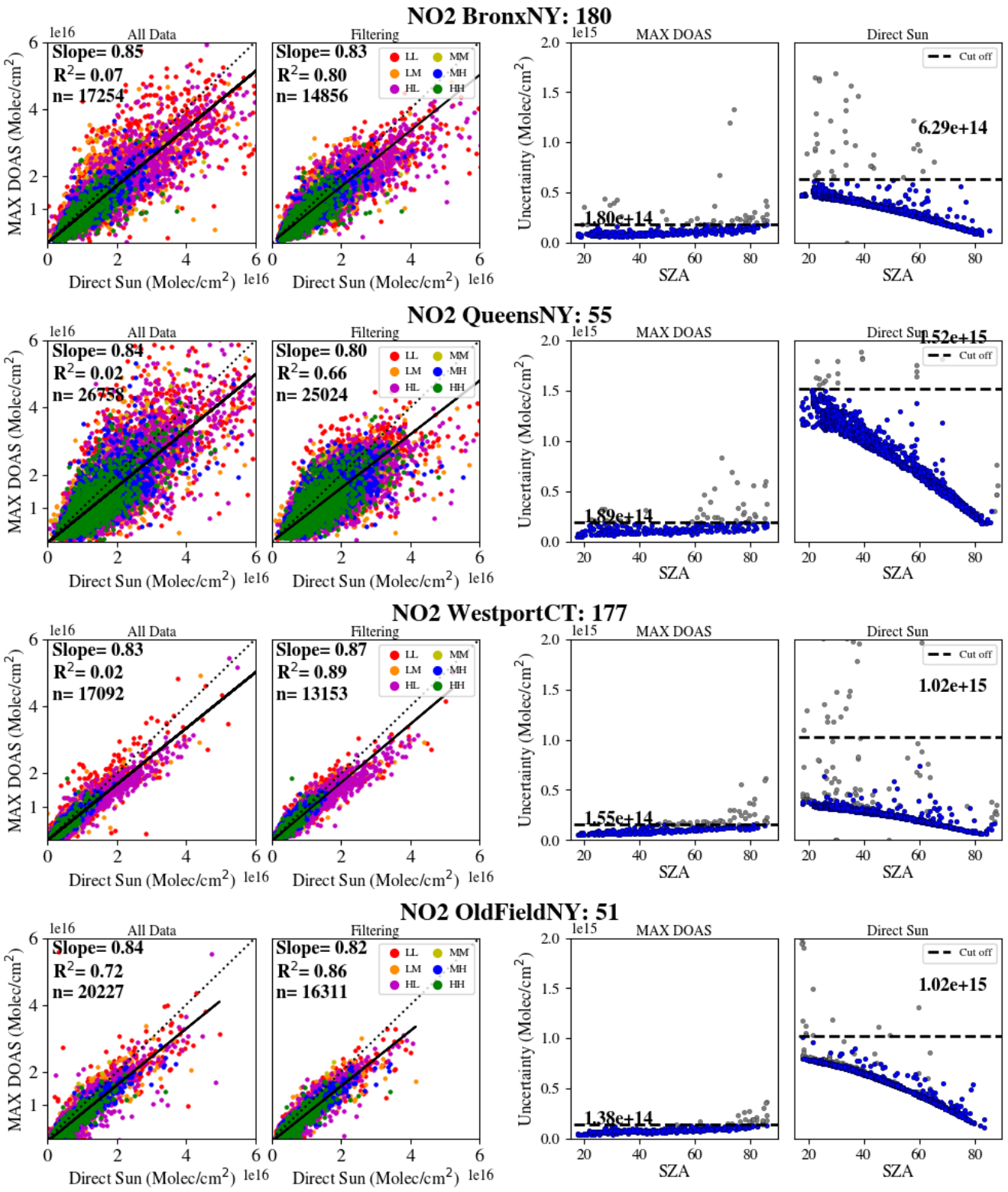


Figure. S2. Cont.

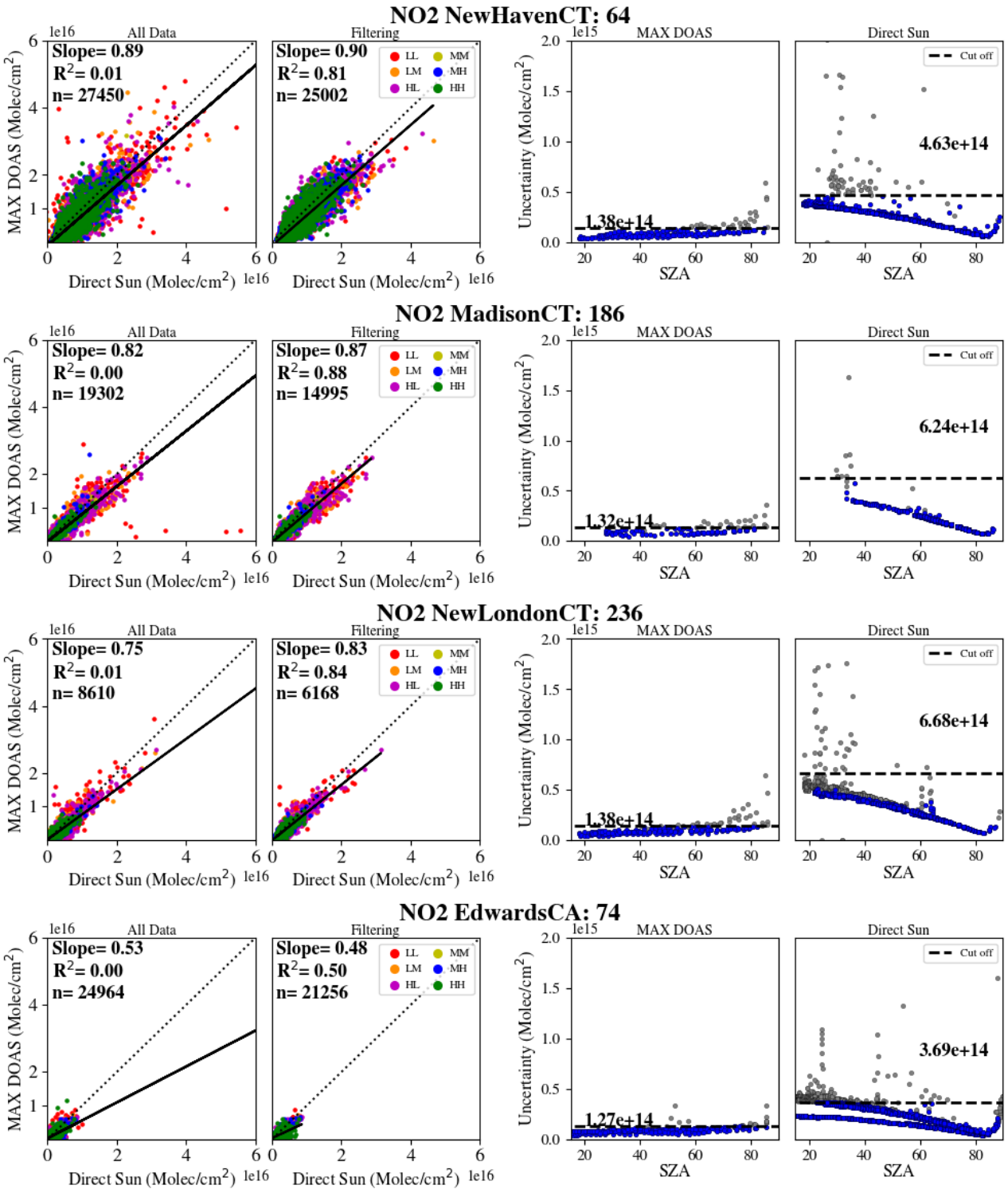


Figure. S2. Cont.

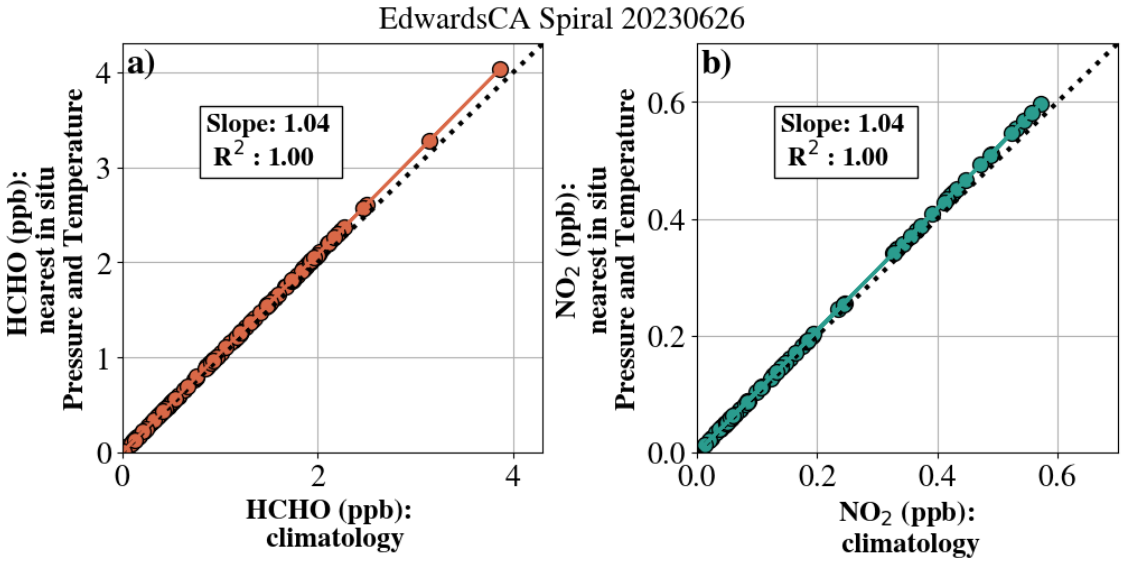
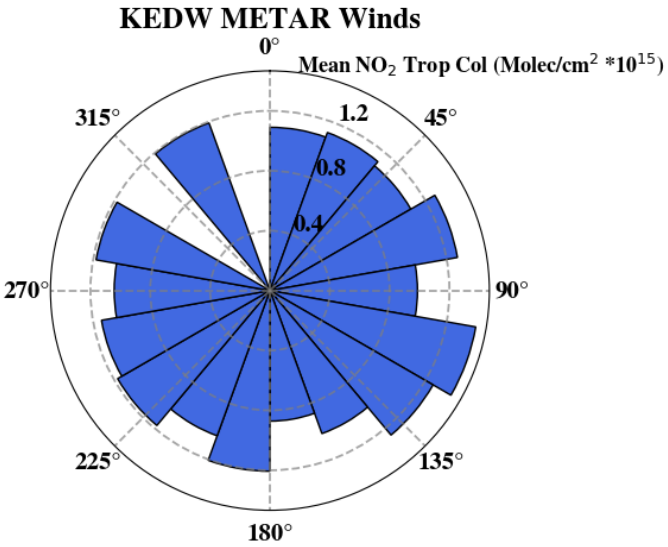


Figure S3. A comparison of Pandora (a) HCHO and (b) NO_2 concentrations, converted from moles/m^2 to ppb during the EdwardsCA spiral. The conversion is performed using both climatological temperature and pressure, and the nearest observed temperature and pressure values during the flight.

S2. Pandora Unit Conversion

Converting moles/m^2 relies on the assumption that the conversion is not sensitive to small variations in temperature and pressure used in calculating air density. Using the case study over EdwardsCA Pandora we can compare the climatology method with the nearest temperature and pressure observed on the aircraft during the spiral. The two methods vary by less than 5% (Figure. S3). Given that we do not often have nearby aircraft measurements to use for the profile conversions, we proceed with using the station's climatological temperature and pressure for this study. We use the provided climatological temperature and pressure throughout the profile as under a standard lapse rate the changes in temperature and pressure do not materially alter the final mixing ratio.



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75 Figure S4: Wind rose of the mean NO_2 Tropospheric Column (molec/cm^2 x10^{15}) from the
76 EdwardsCA Pandora for June 2023 using winds reported from the EdwardsAFB airport (KEDW)
77 Meteorological Aerodrome Report (METAR).

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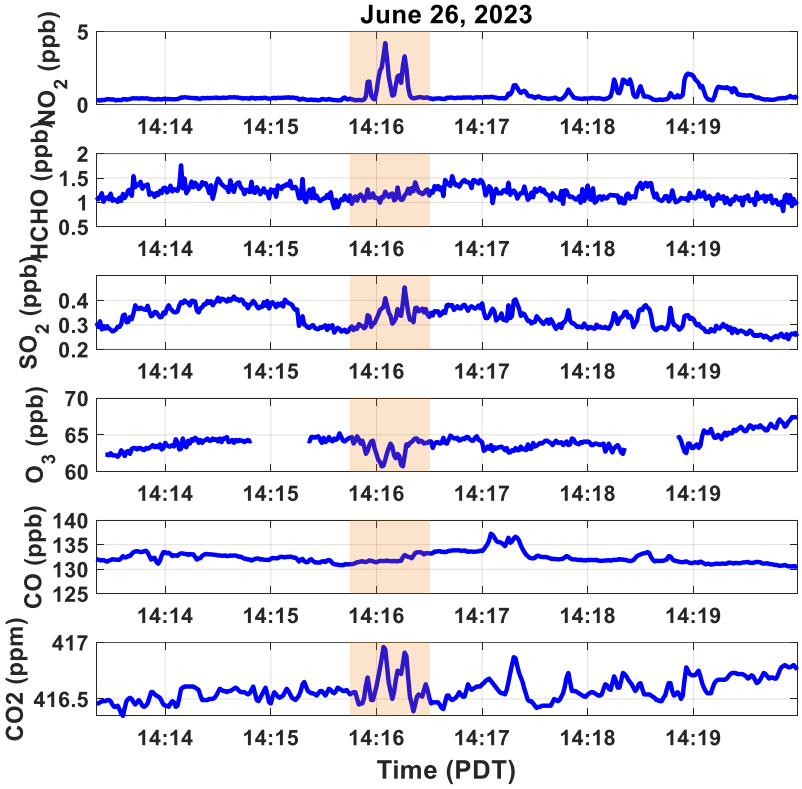

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80 Figure S5: Aircraft observations on June 26th, 2023 during the Edwards AFB spiral of NO_2
81 (Rollins), HCHO (Wolfe), SO_2 (Rollins), O_3 (Chace), CO (Peischl), and CO_2 (Peischl). The time
82 of the NO_2 surface enhancement in the southeastern quadrant of the spiral is highlighted.

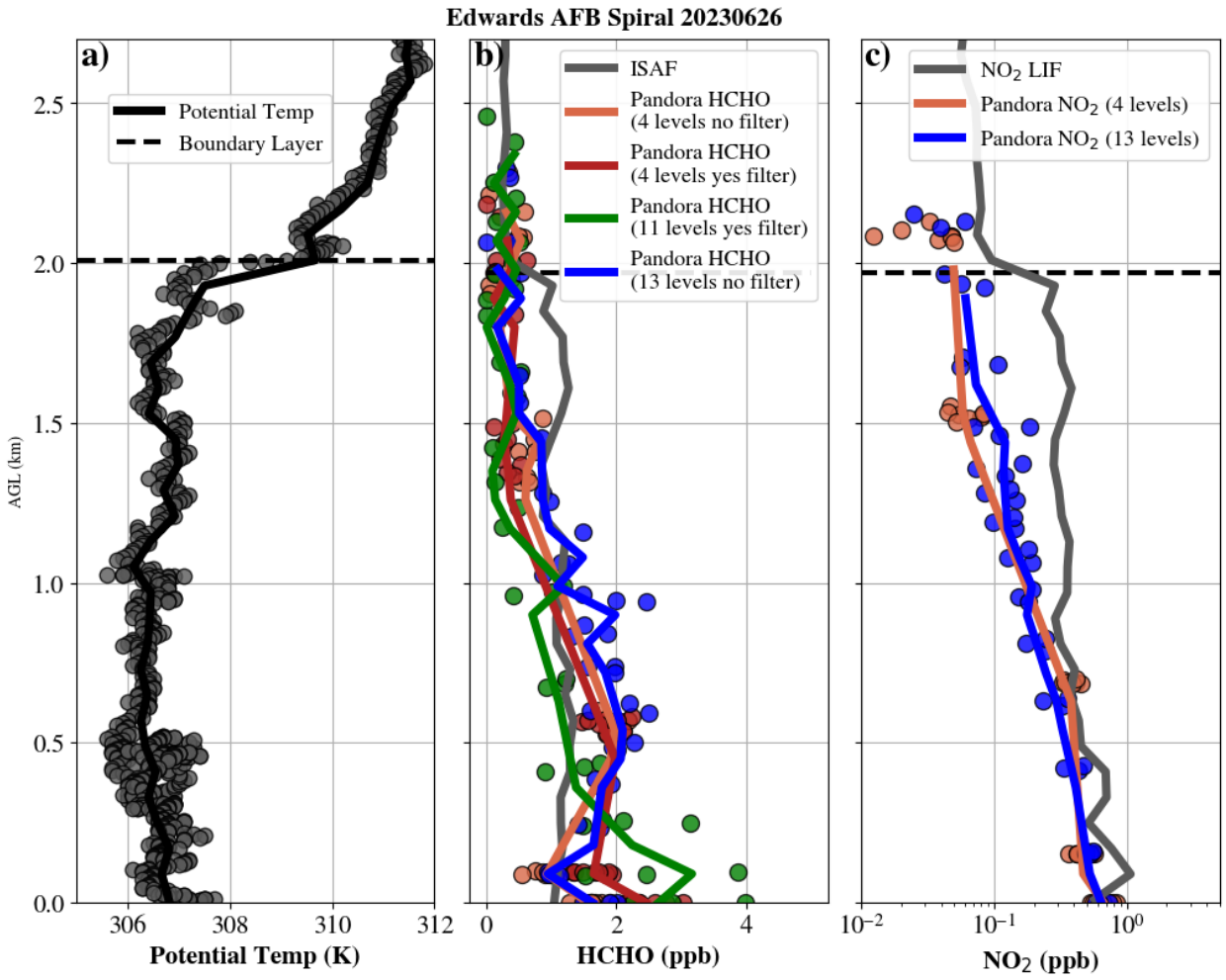

Figure S6: Figure 3 but Pandora data has been separated into the four scan modes: long (11 or 13 levels) or short (4 levels), and with the U340 filter (yes filter) or without the U340 filter (no filter).

S3. Pandora Scan Modes

The MAX DOAS scans have four modes of operation: long or short scans each alternating between using or not using a U340 filter. The short scans find the slant columns at four different elevation angles (0, 60, 75, and 88 degrees) taking about five minutes to complete. The long scans perform either 11 (with filter) or 13 (without filter) elevation levels with the 13 level scans prioritizing more angles near the surface. Each long scan takes approximately ten minutes. The U340 filter determines whether both NO_2 and HCHO can be obtained (no filter lets both UV and visible light through) or only HCHO (with the filter in use only UV light can pass through). The general schedule for the Pandoras is to do eight short scans and two long scans (always alternating

with and without the filter), taking about one hour to complete the cycle. However, the Pandora's operator can decide to change the schedule depending on their needs. These differences in elevation scans do not appear to influence the overall agreement of either HCHO or NO_2 with the in situ data over EdwardsCA for this period. More scans would be needed to investigate these modes individually.

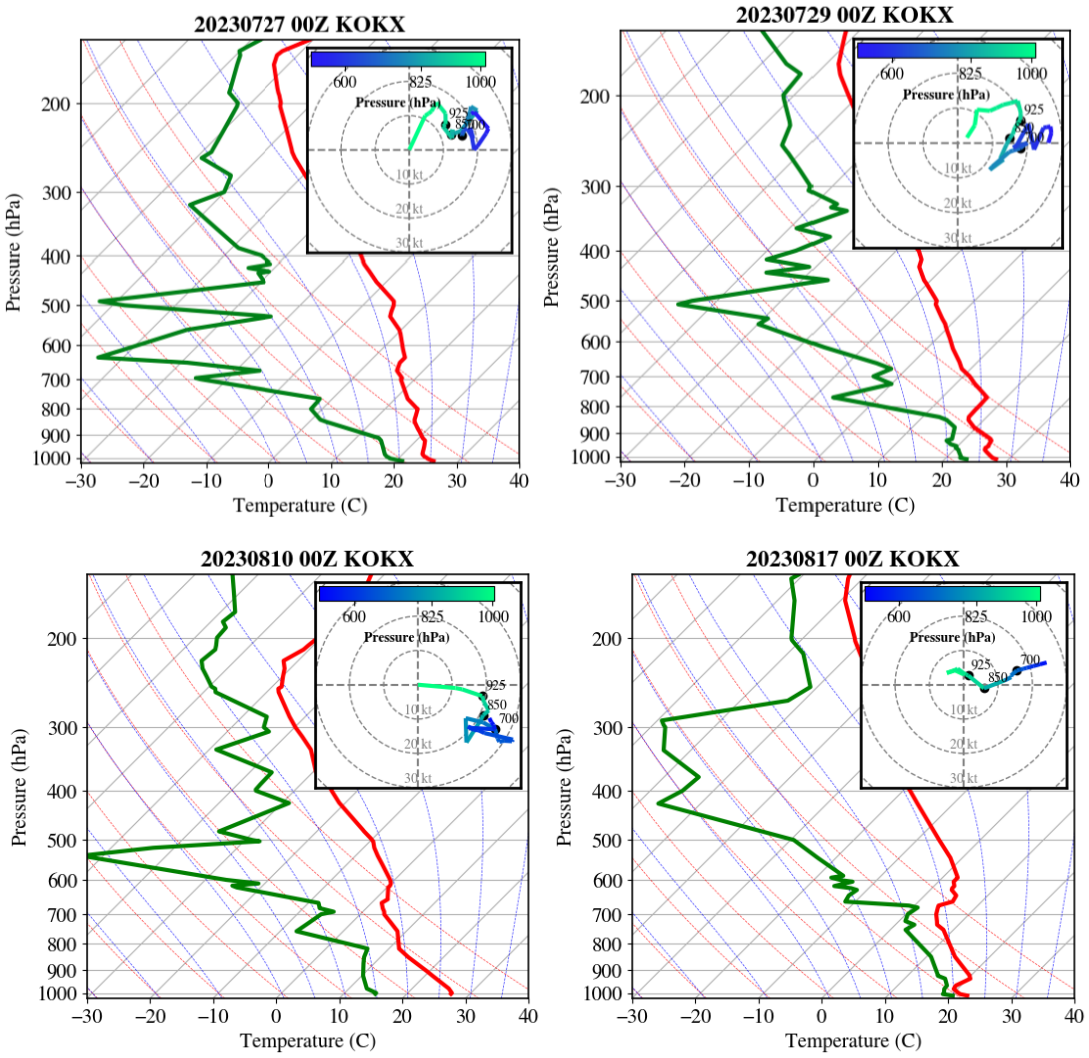

Figure S7. Skew T and hodograph on (top left) July 27th 00Z KOKX, (top right) July 29th 00Z KOKX, (bottom left) August 10th 00Z KOKX, and (bottom right) August 17th 00Z KOKX. The red lines are Temperature (Celsius) and the green lines are the dewpoint (Celsius). There was a deep and well mixed BL on NYC3 and calm surface winds. NYC4 has a shallow BL with a saturated surface and mild winds.

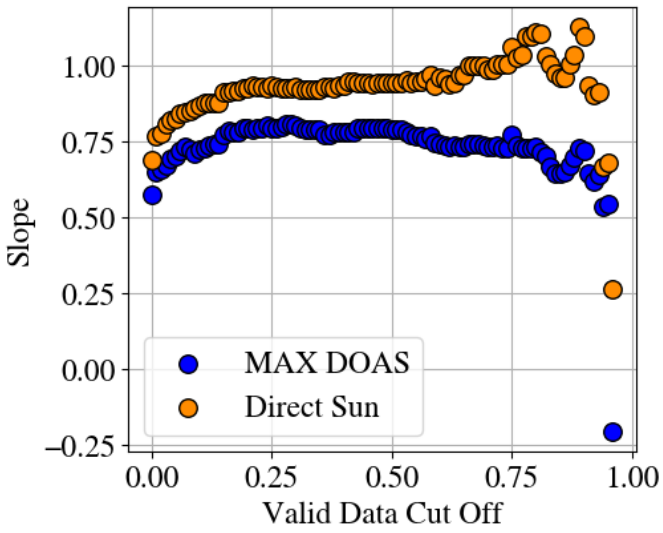

Figure S8. Slopes comparing Pandora HCHO MAX DOAS (blue) and DS (orange) to mean TEMPO HCHO in August 2023 for varying levels of valid data thresholds.

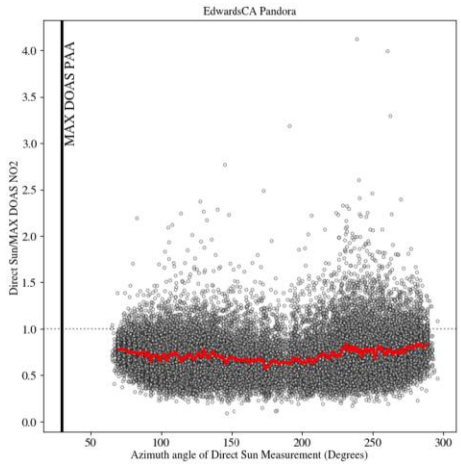

Figure S9. Ratio of contemporaneous DS NO_2 with MAX DOAS NO_2 as a function of Solar Azimuth Angle used in the DS NO_2 measurement for the EdwardsCA Pandora. Data have been averaged to 30 minutes and screened using the previously described filtering method. The horizontal dotted line indicates a 1:1 ratio between the two products. The vertical solid line shows the PAA of the MAX DOAS measurements. The red line is a running mean to show the changes in agreement as a function of viewing angle. In this Pandora the agreement between DS and MAX DOAS NO_2 is not dependent on the azimuth angles.