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ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study

Network Intercomparison Campaign Report

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Acronyms and Abbreviations

AOD	Aerosol optical depth
CC	Pearson product-moment correlation coefficient
CINDI2	Cabauw intercomparison of nitrogen dioxide measuring instruments 2
HorEA	Elevation angle of the horizon
ICC	Intercomparison campaign
KNMI	Royal Netherlands meteorological institute
MLE	Minimum Amount Langley extrapolation
ND	Neutral density filter
NRelInt	Normalized relative intensities
PAN1S	Pandora instrument equipped with 1 spectrometer (UV)
PAN2S	Pandora instrument equipped with 2 spectrometers (UV and VIS)
Pandonia	ESA Ground-Based Air-Quality Spectrometer Validation Network
RelGAS	Relative differential slant column amount
SC	Slant column amount
SLP	Slope of linear regression
SyntRef	Synthetic reference spectrum
TotHCHO	Total column formaldehyde
TotNO2	Total column nitrogen dioxide
TotO3	Total column ozone
VEA	Viewing elevation angle
VZA	Viewing zenith angle

1 Introduction

This report is deliverable D19 of the Pandonia project [1, 2]. The Pandonia network is being established in order to validate satellite trace gas retrievals with ground based remote sensing measurements. Beside the already agreed direct sun gas products, it is planned to have gas products based on scattered sun (equivalent to sky radiance) measurements and aerosol optical depth at a future stage also. This study serves as groundwork to evaluate the possibilities to establish the new data products in Pandonia. An intercomparison campaign (ICC), employing a subgroup of 4 Pandora instruments, was conducted to achieve this goal.

We want to start this report with a summary of the key points and the conclusions out of it (section 2), followed by some details about the ICC itself (section 3). The main parts of this report comprise the results of the four segments

- **Direct sun gas data comparison** (section 4)
- **Scattered sun gas data comparison** (section 5)
- **Direct sun relative intensity comparison** (section 6)
- **Instrument pointing comparison** (section 7).

For each segment, the way how the data is analyzed and detailed results are outlined.

1.1 Applicable Documents

- [1] Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study [Proposal], LuftBlick Proposal 201309A, Issue 2, 2013.
- [2] ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study [Statement of Work], ENVI-SPPA-EOPG-SW-13-0003, Issue 1, Revision 3, 2013.
- [3] A. Cede. *Manual for Blink Software Suite Version 6*, 2017. URL http://pandonia.net/docs/manuals_reports_notes/BlickSoftwareSuite_Manual_v6.pdf.

1.2 Reference Documents

- [4] CINDI-2 campaign. URL <http://www.tropomi.eu/science/cindi-2>.
- [5] A. Cede and M. Tiefengraber. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2017001: Network Calibration and Data Quality Report, 2017.
- [6] J. Herman, A. Cede, E. Spinei, G. Mount, M. Tzortziou, and N. Abuhassan. NO₂ column amounts from ground-based Pandora and MFDOAS spectrometers using the direct-sun DOAS technique: Intercomparisons and application to OMI validation. *Journal of Geophysical Research (Atmospheres)*, 114:D13307, July 2009. doi: 10.1029/2009JD011848.
- [7] M. Tiefengraber and A. Cede. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2014009: Laboratory report, 2014.
- [8] M. Tiefengraber and A. Cede. ESA Ground-Based Air-Quality Spectrometer Validation Network and Uncertainties Study, LuftBlick Report 2016001: Report on Feasibility to Retrieve Trace Gases other than O₃ and NO₂ with Pandora, 2016.

2 Summary and Conclusion

This report gives an overview about the outcome of the ICC that has been conducted to evaluate the agreement between Pandora instrument on four segments: Direct sun gas data, scattered sun gas data, direct sun relative intensities and instrument pointing. Whereas direct sun gas data have been compared already within the Pandonia framework [8], it is the first time for the other segments.

Pandonia direct sun data will be the primary source for satellite validation. Hence accessing the homogeneity of this data within the network is obvious. Using scattered sun data, vertical partitioning of the atmosphere is possible to further support the validation of tropospheric columns and surface concentrations. We do not have a clear image about the homogeneity in this segment right now. Looking also into relative intensities is a mandatory groundwork to assess the possibility for aerosol optical depth retrievals. All mentioned data segments finally stand and fall with the ability of accurate instrument pointing. It is in particular important for scattered sun data, where data quality gives almost no hint on the pointing quality (in contrast to direct sun data).

We choose the framework of the “Cabauw intercomparison of nitrogen dioxide measuring instrument 2” campaign [4] held in Cabauw in September 2016 for this ICC. 4 Pandora instrument were participating the ICC: 2 regular Pandoras, equipped with 1 UV spectrometer (PAN1S) and 2 next generation Pandoras, equipped with 2 spectrometers for UV and VIS spectral range (PAN2S). The latter has been developed within the framework of this project. Please note, when we refer to an individual spectrometer of a PAN1S or PAN2S Pandora, its spectrometer ID is given. That is S1 for spectrometer 1 (covering the UV spectral range) and S2 for spectrometer 2 (covering the VIS spectral range). The name of a Pandora instrument always includes the spectrometer ID in addition to the Pandora ID: e.g. Pandora 129s1.

2.1 Intercomparison Results

For the statistical analysis of all segments, except for the instrument pointing comparison, Pandora 129s1 is selected to be the reference instrument for data based on the UV spectral range and Pandora 129s2 for the VIS spectral range. Further, the gas product comparisons are based on slant column amounts, rather than vertical columns.

Direct sun gas data

The compared data products are total column NO_2 (TotNO₂), total column O_3 (TotO₃) and total column HCHO (TotHCHO). The statistical analysis is summarized in Table 1. The top part gives the Pearson product-moment correlation coefficient (CC) and the bottom part the slope of a linear regression (SLP).

The agreement for TotNO₂ and TotO₃ is excellent. For TotO₃ we have the objection that one instrument (Pandora 118s1) has a higher SLP than the others. We argue that this is a consequence of spectral stray light, which has a stronger impact on this instrument. The disagreement is larger for TotHCHO. The main driver for this is the so-called “unwanted” spectral signal [8], an interference effect impacting each Pandora slightly differently.

	Pan 32s1	Pan 118s1	Pan 128s1	Pan 128s2	Pan 129s2
	CC				
TotNO₂	1.00	0.99	1.00	1.00	1.00
TotO₃	1.00	1.00	1.00	-	-
TotHCHO	0.78	0.94	0.84	-	-
	SLP				
TotNO₂	0.99	1.05	0.98	-	-
TotO₃	1.01	1.09	1.02	-	-
TotHCHO	0.41	1.54	0.84	-	-

Table 1: Overview of the statistical analysis of the direct sun gas comparison for TotNO₂, TotO₃ and TotHCHO. Depicted are the parameters CC in the top part and SLP in the bottom part (parameters explained in the text). Note that TotO₃ and TotHCHO is not covered by S2 spectrometers.

Scattered sun gas data

The compared data products are relative differential slant column amounts (RelGAS) of NO₂, O₃ and HCHO. The statistical analysis is summarized in Table 2. Each CC value (top part in table) and SLP value (bottom part in table) is the median value of the analysis for the viewing zenith angles (VZA) 60, 70, 88 and 89°.

Excellent agreement is given for RelNO₂ and RelO₃. RelHCHO accord significantly better amongst the Pandoras than for direct sun retrievals. This improvement is driven by the use of daily references in the spectral fitting instead of one reference as it is done for direct sun retrievals.

	Pan 32s1	Pan 118s1	Pan 128s1	Pan 128s2	Pan 129s2
CC					
RelNO₂	1.00	1.00	1.00	1.00	1.00
RelO₃	1.00	1.00	1.00	-	-
RelHCHO	0.90	0.93	0.93	-	-
SLP					
RelNO₂	1.00	1.00	1.00	-	-
RelO₃	1.01	1.06	1.02	-	-
RelHCHO	0.89	1.00	0.98	-	-

Table 2: Overview of the statistical analysis of the scattered sun gas comparison for RelNO₂, RelO₃ and RelHCHO. CC and SLP are the median values of the analysis for elevation angles 60, 70, 88 and 89°. Note that RelO₃ and RelHCHO is not covered by S2 spectrometers.

Direct sun relative intensities

Compared are relative intensities at nominal wavelengths 340, 400, 500 and 870 nm (a subgroup of Aeronet standard wavelengths). Table 3 lists the standard deviation σ_{RelInt} of the ratio to the reference. This measure can be translated to spectral stability.

A hardware issue on Pandora 118s1, leading to strong data scatter, is responsible for the absurd σ_{RelInt} for this instrument. Apart from this, the main driver for enhanced σ_{RelInt} turned out to be insufficient filter characterization for S2 spectrometers. For now we have no explanation for this behavior.

	Pan 32s1	Pan 118s1	Pan 128s1	Pan 128s2	Pan 129s2
σ_{RelInt} [%]					
340 nm	1.75	21.68	1.54	-	-
440 nm	1.77	2614.05	1.33	2.46	4.33
500 nm	2.02	2278.14	1.34	2.39	1.02
870 nm	-	-	-	6.04	-

Table 3: Overview of the standard deviation σ_{RelInt} of the relative intensities at 340, 400, 500 and 870 nm. Note that only S2 spectrometers cover 870 nm. For this case, the reference instrument is Pandora 129s2 instead of 129s1.

Instrument pointing

The instrument pointing is analyzed by comparing the calculated elevation angle of the horizon (HorEA) for each Pandora. Based on this analysis we claim that the Pandora pointing accuracy is 0.10° on a 2- σ level.

2.2 Conclusion

Based on this study we come to the following conclusions:

- **Direct sun data comparison**

Spectral stray light and the unwanted spectral signal are still the major limitations in direct sun data precision.

- **Scattered sun data comparison**

The excellent comparison results for retrievals based on measurements on high viewing zenith angles confirms our pursue of implementing scattered sun products.

- **Direct sun relative intensity comparison**

Neutral density filter characterization needs improvement for S2 spectrometers. The spectral stability turned out to be well suitable for meaningful spectral aerosol optical depth (AOD) retrievals. However, longer time series have to be evaluated first. Using a so-called fiber guide [5], which fixes the first meter of the fiber (in photon direction), will potentially further boost the spectral stability of the instrument.

- **Instrument pointing comparison**

Instrument pointing is proven to be a strength for Pandonia instruments.

3 Intercomparison Details

3.1 Campaign

The ICC was held in Cabauw, Netherlands, within the framework of the “Cabauw intercomparison of nitrogen dioxide measuring instrument 2” campaign (CINDI2). Cabauw is a rural location surrounded by the cities Rotterdam, Amsterdam and Utrecht.

From August 26th to 28th we set up the instruments at Cabauw and run the instrument alignment procedures (warm up phase, highlighted as gray region in Figure 1). The CINDI2 core-phase was conducted from September 12th to September 28th (region highlighted in brown in the figure) with an extension period up to October 6th (region highlighted in green in the figure). Thus, the ICC comprises 6 weeks.

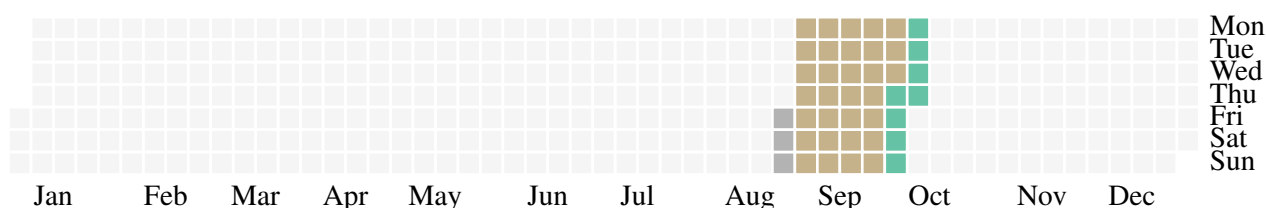


Figure 1: The ICC took place between August 26th and October 6th 2016 (colored region) in Cabauw, Netherlands. The instruments have been set up on August 26th and aligned until August 29th (days colored gray). The CINDI2 core-phase started on September 12th and finished on September 28th (days colored brown). A backup phase until October 6th was used for individual measurement schedules (days colored green).

3.2 Data Acquisition

During the 6 weeks of the ICC two different data acquisition schedules have been exerted: one, tailored for the CINDI2 campaign and the standard Pandonia schedule. The CINDI2 schedule has a stronger focus on scattered sun data (routines starting with E in Table 4), while the Pandonia schedule favors direct sun measurements (routines starting with S in Table 4).

Typical timing for each schedule is illustrated in Figure 2, with the Pandonia (CINDI2) schedule show on the left (right) figure panel. Brief explanations for each measurement routine is listed in Table 4 (further details can be found in the Blick Software Suite manual [3]).

Only a subset of all routines, considered to be most suitable for this intercomparison task, is employed for the ICC. For direct sun gas data intercomparison, routines SO and SU are evaluated. These routines are also used to intercompare direct sun relative intensities (colored in purple in Figure 2). Scattered sun gas data is intercompared based on routines E1 and Z1 (colored in green in Figure 2). The instrument alignment is best assessable by means of the horizon scanning routine EH (colored in red in Figure 2).

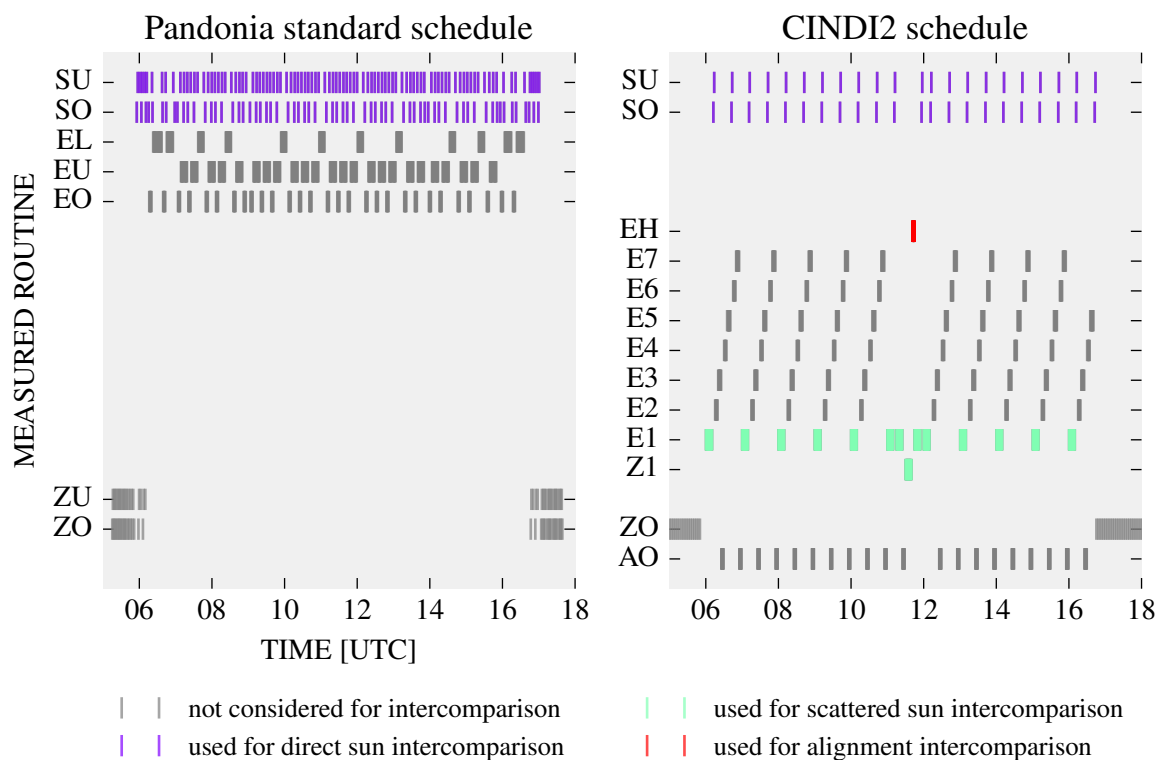


Figure 2: Typical timing of the two measurement schedules during the ICC. The standard Pandonia schedule (left panel) covers direct sun (S^*) and scattered sun measurements (E^*) about equally. The CINDI2 semi-blind comparison schedule (right panel) focuses on scattered sun measurements. Routines colored purple are used in the direct sun gas and intensity comparison, green routines in the scattered sun gas data comparison. The routine colored red (EH) is a horizon scan, suitable to access the instrument pointing quality. Routines highlighted gray are not further considered in the ICC (further explanation about the routines can be found in Table 4).

Routine ID	Pointing	Filter
SO	sun	OPEN
SU	sun	U340
EO	VAA 287; VZA 0,60,75,88,89	OPEN
EU	VAA 287; VZA 0,60,75,88,89	U340
EL	VAA 287; VZA 0,40,50,60,70,75,80,82,85,87,88,89	U340
EH	VAA 287; VZA 95,94,...,90.4,90.2,90,89.8,89.6,89.4,...,86,85	OPEN and U340
E1	VAA 287; VZA 0,60,75,82,84,85,86,87,88,89	OPEN and U340
E2	VAA 355; VZA 75,85,87,89	OPEN and U340
E3	VAA 45; VZA 0,75,85,87,89	OPEN and U340
E4	VAA 95; VZA 75,85,87,89	OPEN and U340
E5	VAA 145; VZA 0,40,50,60,70,75,80,82,85,87,88,89	U340
E6	VAA 195; VZA 75,85,87,89	OPEN and U340
E7	VAA 245; VZA 0,40,50,60,70,75,80,82,85,87,88,89	U340
Z1	zenith	OPEN and U340
ZO	zenith	OPEN
ZA	zenith	U340
AO	almucantar	U340

Table 4: The measurement routines used for the standard Pandonia and the CINDI2 schedule. Routine IDs printed bold are actually used in this ICC. A further explanation about the measurement routines can be found in the Blick Software Suite manual [3]. Filter OPEN means no filter is equipped and filter U340 denotes a bandpass filter with peak transmission at 340 nm.

3.3 Participating Pandora Instruments

Table 5 lists all Pandora instruments participating in the ICC. It is a representative subgroup of all available Pandoras. E.g. Pandora 32s1 and 118s1 are PAN1S instruments, with Pandora 32s1 to be part of an older production series and Pandora 118s1 from a newer one. Pandoras 128 and 129 are the new generation PAN2S instruments, equipped with a UV and a VIS spectrometer. PAN2S Pandoras have been developed within the framework of the Pandonia project.

Pandora ID	Spec ID	Approx. spectral range [nm]	Responsible organization
32	s1	280 to 530	NASA
118	s1	280 to 530	KNMI
128	s1	280 to 530	LuftBlick
128	s2	380 to 910	LuftBlick
129	s1	280 to 530	LuftBlick
129	s2	380 to 910	LuftBlick

Table 5: Pandora instruments participating the ICC. Both PAN1S (only UV) and the next generation PAN2S (UV and VIS) Pandoras are represented.

In the forefront of the ICC, all participating Pandora instruments have been homogeneously calibrated in the laboratory in Innsbruck, Austria, (Pandora 128s1, 128s2, 129s1, 129s2) or at Godard Space Flight Center, USA, (Pandora 32s1, 118s1) in the usual way [7].

Pandora 28s1 (NASA) was also participating in the ICC, but due to frequent instrumental issues during the CINDI2 campaign it is not further considered in this intercomparison.

4 Direct Sun Gas Data Comparison

We perform direct sun data intercomparison for the already agreed satellite validation products TotNO₂, TotO₃ and the most promising expansion [8], TotHCHO. All base on level 2 data (vertical column amounts) [3]. The retrievals of TotNO₂ is based on SO routines and TotO₃ and TotHCHO are retrieved from SU routines (compare routines highlighted in purple in Figure 2).

4.1 Data Preparation

The Pandora standard spectral fitting algorithm for e.g. TotNO₂ applies a reference spectrum which is compiled from measured spectra. In a next step, this reference spectrum is corrected for the estimated gas slant column amount at an estimated effective temperature. With this correction, absolute rather than relative slant columns can be retrieved when this reference is used in the spectral fitting. We assess the slant column amount in the reference spectrum using the Minimum Amount Langley extrapolation (MLE) [6]. This kind of corrected reference spectrum is called “synthetic reference” (SyntRef).

For this study we retrieve all three products using a synthetic reference spectrum. Note, the Pandonia standard TotO₃ applies a theoretical extraterrestrial spectrum as reference. For all participating instruments the reference spectrum is build from the same time period: all measurements taken below 70° solar zenith angle at September 12th. Depending on the measurement timing this embraces approximately 12 single spectra, which are eventually averaged. All direct sun retrievals are hence based on one single reference spectrum applied for the entire comparison period.

To calculate the SyntRefs for all Pandoras (that is to estimate the slant column in the reference spectrum of a wanted gas), one Pandora is selected to be the reference (here Pandora 129s1). For the reference Pandora, SyntRef is based on the MLE. The SyntRefs of the other Pandoras are calculated by comparing to this reference Pandora¹.

The statistical analysis applies slant column amounts (SC) rather than vertical column amounts ($\equiv$ Tot-GAS). Pandora 129s1 serves as reference for all calculations.

The setup used for the spectral fitting is taken from *Tiefengraber and Cede* [8] and is summarized in Table 6.

Gas	Additionally fitted	λ start [nm]	λ end [nm]	Background	Offset	Wvl corr.
NO ₂	O ₃	400	440	1	0	1
O ₃	HCHO, NO ₂ , SO ₂	310	330	1	0	1
HCHO	NO ₂ , O ₂ O ₂ , O ₃	332	359	4	1	1

Table 6: Setup for the spectral fitting of TotNO₂, TotO₃ and TotHCHO. The last three columns designate the order of the polynomial used in the spectral fitting.

Data Filtering

For data included in the ICC, selected parameters have to be below defined thresholds (given in Table 7).

Parameter	TotNO ₂	TotO ₃	TotHCHO
Vertical column uncertainty [DU]	4.0×10^{-2}	1	2.0×10^{-1}
Normalized rms of spectral fitting residual	1.0×10^{-3}	8.0×10^{-3}	1.0×10^{-3}
Wavelength shift [nm]	2.0×10^{-2}	2.0×10^{-2}	2.0×10^{-2}
Direct sun air mass factor	8	5	8

Table 7: Filter criteria for direct sun gas data retrievals. Details about the filter parameters can be found in *Cede* [3].

¹This comparison is based on a linear regression in both slant column data sets. Only the intercept is considered in the regression (hence a 1 parameter calibration). For this calibration step the dataset from August 26th to September 14th was used.

4.2 Intercomparison Results

The direct sun gas data intercomparison results are summarized in 3 figures. Figure 3 illustrates typical time series during the ICC (the full time series is shown in Figure 16 in the appendix). Correlation plots, with Pandora 129s1 as reference, are given in Figure 4. For better orientation the 1:1 line is drawn in the background. Figure 5 condenses the statistical analysis, displaying SLP on the x-axis and CC on the y-axis. Both axes intersect at $SLP = 1$ and $CC = 1$, meaning the closer the data points are at the intercept the better the agreement between the datasets. The axes limits are restricted to 0.7 to 1.0 for CC and 0.75 to 1.25 for SLP. Data points outside this range are marked by an arrow and the actual value is displayed as text.

TotNO₂ The agreement for TotNO₂ amongst the Pandoras is very high. This confirms the results in e.g. *Tiefengraber and Cede* [8].

TotO₃ The agreement for TotO₃ for all but Pandora 118s1 is also very high. For Pandora 118s one can see an artificial diurnal cycle (compare Figure 3) and a SLP of almost 1.1. This behavior is traced back to the SC calibration towards the reference Pandora (explanation in section 4.1). To avoid this pattern, one would have to allow a 2 parameter rather than a 1 parameter correction for the calibration towards the reference. A 2 parameter correction, however, would mean to apply an AMF dependent correction factor, which is physically not correct (it would mean to apply for each AMF an individual SyntRef). What causes this behavior is not fully understood yet. Due to its AMF dependence we see this is in close relation to the presence of spectral stray light.

TotHCHO The agreement amongst the Pandoras is somewhat weaker for TotHCHO. As already pointed out by *Tiefengraber and Cede* [8], TotHCHO suffers from the so-called “unwanted spectral signal” (an interference effect caused by the direct beam in the optical system [8]). This leads to slight differences in the diurnal variation of TotHCHO for each instrument, resulting in a wide range of SLP values. CCs are all above 0.8, which is adequate. It is notable that Pandora 128s1 and 129s1 agree much better compared to the other Pandoras. Also the diurnal variation is very alike. We assume, since both instruments have been constructed in a row, the alignment and quality of the optics is comparable resulting in comparable interference effects.

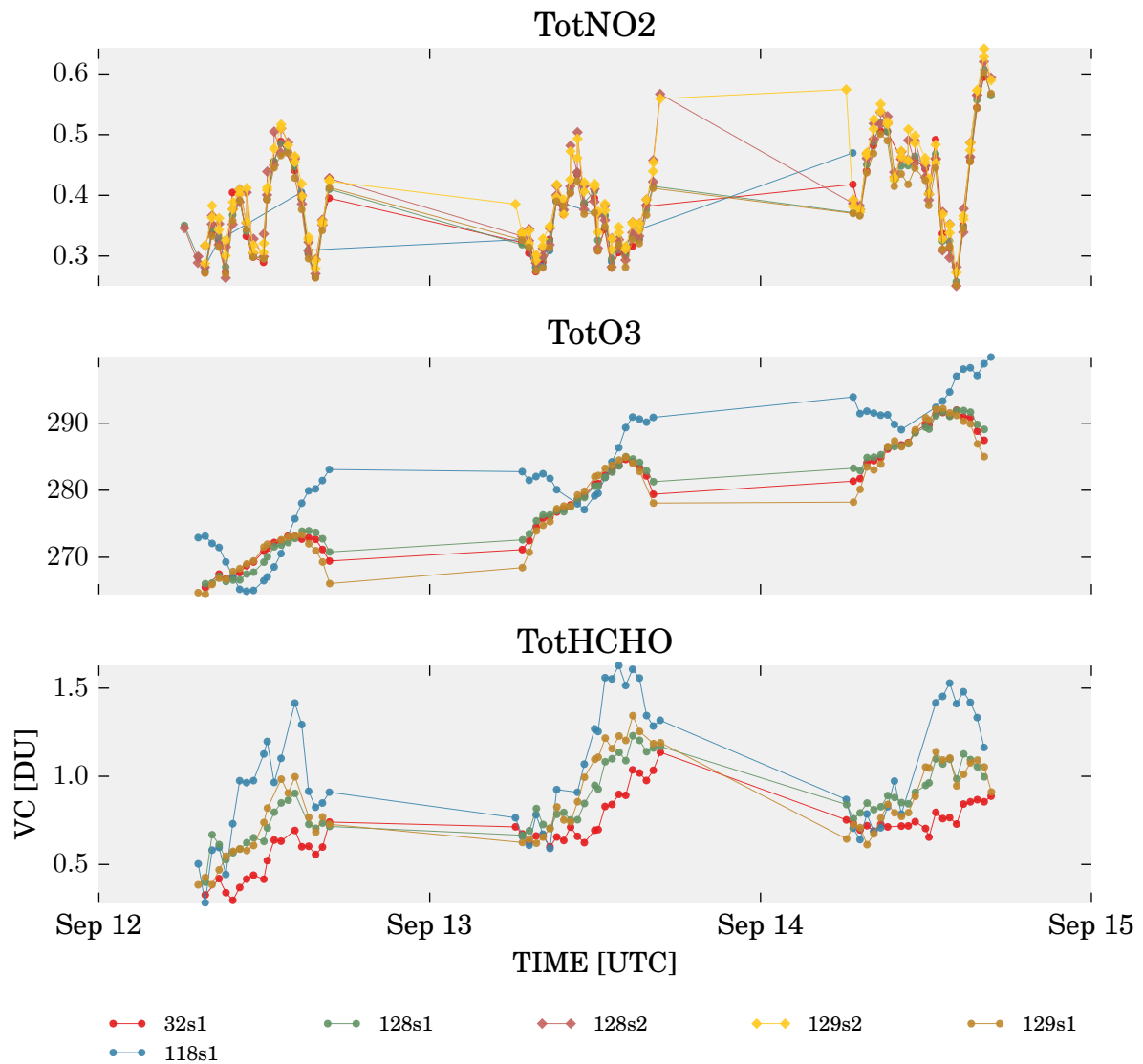


Figure 3: Typical time series during the ICC for direct sun TotNO₂ (top panel), TotO₃ (middle panel) and TotHCHO (bottom panel) for all Pandora instruments. Datasets are filtered as listed in Table 7.

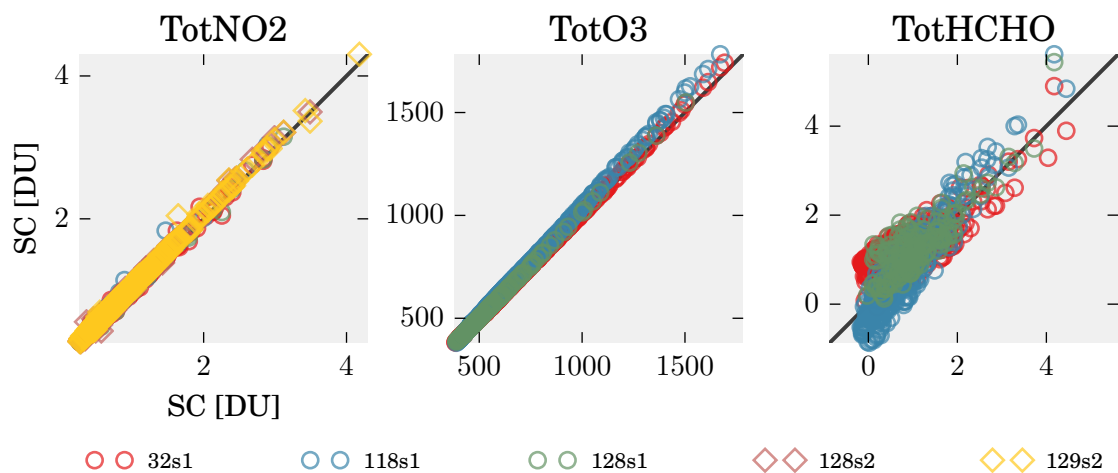


Figure 4: Correlation plots with Pandora 129s1 as reference for TotNO₂ (left panel), TotO₃ (middle panel) and TotHCHO (right panel) SCs. For better orientation, the 1:1 line is drawn in black in the background.

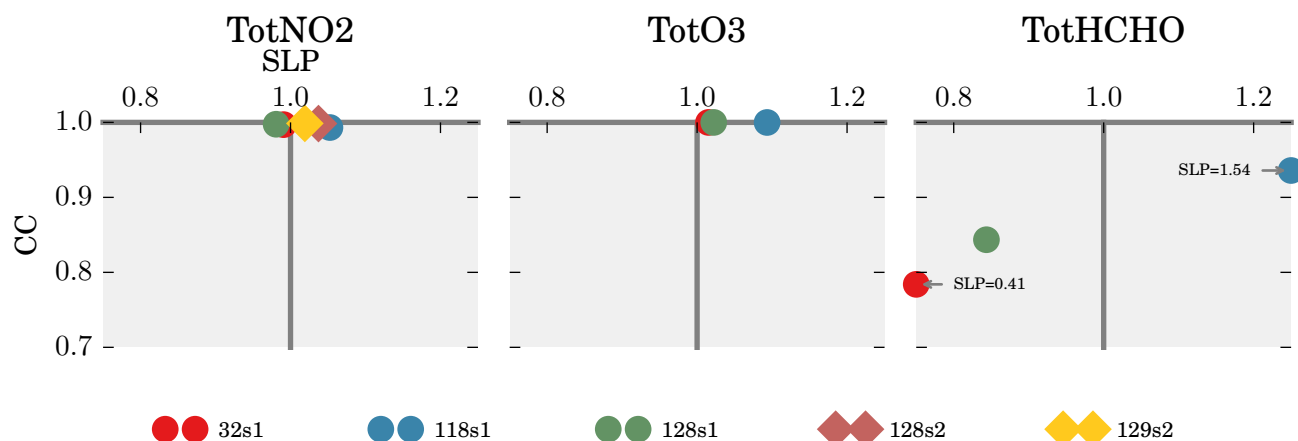


Figure 5: Statistical analysis for TotNO₂ (left panel), TotO₃ (middle panel) and TotHCHO (right panel). The x-axis shows the slope of the linear regression SLP and the y-axis the Pearson product-moment correlation coefficient CC. SLP and CC intersect at 1. The closer the data points are to the intercept the better the agreement. Data points outside the limits are marked by an arrow and the actual value is given as text.

5 Scattered Sun Gas Data Comparison

For comparison of scattered sun data we picked the same gases as for the direct sun comparison. That is NO_2 , O_3 and HCHO . The retrievals base on level 2Fit data (slant column amounts) [3], which are calculated from E1 routines (compare routines highlighted in green in Figure 2). E1 routines feature the densest population of high VZAs, where tropospheric gases like NO_2 are most sensitive to. In particular, we want to emphasize VZAs 88 and 89, which are the essential VZAs for the upcoming gas surface concentration product for Pandonia [3].

5.1 Data Preparation

For direct sun data, a constant reference is used in the spectral fitting for the entire period. For scattered sun data, a new reference is calculated from an average of near noon zenith routines Z1 (see routines highlighted in green in Figure 2) every day. This reference is applied in the spectral fitting to all VZAs part of routine E1. No further post processing is applied meaning that all scattered sun retrievals yield relative differential slant column amounts RelGAS rather than absolute slant columns.

As spectral fitting setup we choose the setup suggested for the CINDI2 campaign. It is summarized in Table 8.

Gas	Additionally fitted	λ start [nm]	λ end [nm]	Background	Offset	Wvl corr.
NO_2	H_2O , O_2O_2 , O_3 , Ring	425	490	5	0	1
O_3	HCHO , NO_2 , Ring	320	340	3	1	1
HCHO	BrO , NO_2 , O_2O_2 , O_3 , Ring	336.5	359	5	1	1

Table 8: Setup for the spectral fitting of RelNO2, RelO3 and RelHCHO. The last three columns designate the order of the polynomial used in the spectral fitting.

Data Filtering

For data included in the ICC, selected parameters have to be below defined thresholds (given in Table 9).

Parameter	TotNO2	TotO3	TotHCHO
Slant column uncertainty [DU]	4.0×10^{-2}	3	3.0×10^{-1}
normalized rms of spectral fitting residual	1.0×10^{-3}	2.0×10^{-3}	1.0×10^{-3}
wavelength shift [nm]	2.0×10^{-2}	2.0×10^{-2}	2.0×10^{-2}
direct sun air mass factor	8	5	8

Table 9: Filter criteria for scattered sun gas data retrievals. Details about the filter parameters can be found in Cede [3].

5.2 Intercomparison Results

The scattered sun gas data intercomparison results are again condensed into 3 figures. Figure 6 shows typical time series for clear sky conditions for all VZAs (the full time series is shown in Figure 17 in the appendix). Correlation plots, with Pandora 129s1 as reference, are shown in Figure 7. The corresponding results of the statistical analysis are displayed in Figure 8. The figures are to read as explained in section 4.2.

RelNO2 Very high agreement amongst all Pandoras is given for all VZAs. The accordance increases for larger VZAs, since the reference spectrum is build from VZA 0 measurements and therefore larger VZAs have larger SCs.

RelO3 Very high agreement amongst all Pandoras is given for all VZAs.

RelHCHO The accordance increases for higher VZAs (same reason as for RelNO₂), but the overall agreement is less than for RelNO₂ and RelO₃. HCHO is a rather weak absorber compared to e.g. NO₂. This, in combination with a relatively short measurement time (≈ 20 seconds per angle²), makes RelHCHO probably noise limited. However, the use of daily references instead of one reference for the entire period (this is done for direct sun retrievals), makes RelHCHO agreeing better amongst the Pandoras than TotHCHO.

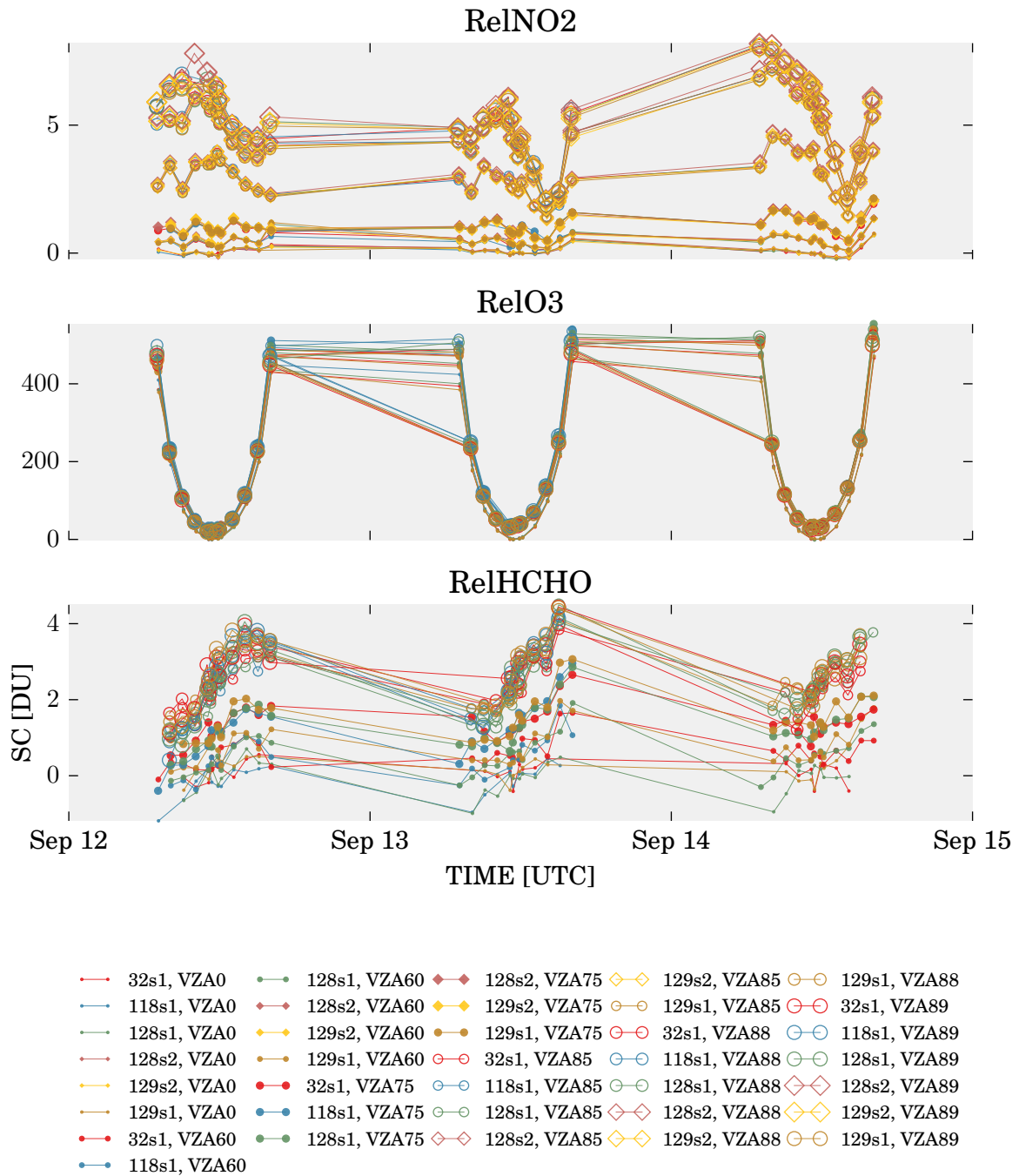


Figure 6: Typical time series for scattered sun RelNO₂ (top panel), RelO₃ (middle panel) and RelHCHO (bottom panel) for all Pandora instruments and VZAs. Datasets are filtered as listed in Table 9.

²For comparison, individual angles in the Pandonia standard schedule are measured 30 seconds. Direct sun routines measure 40 seconds.

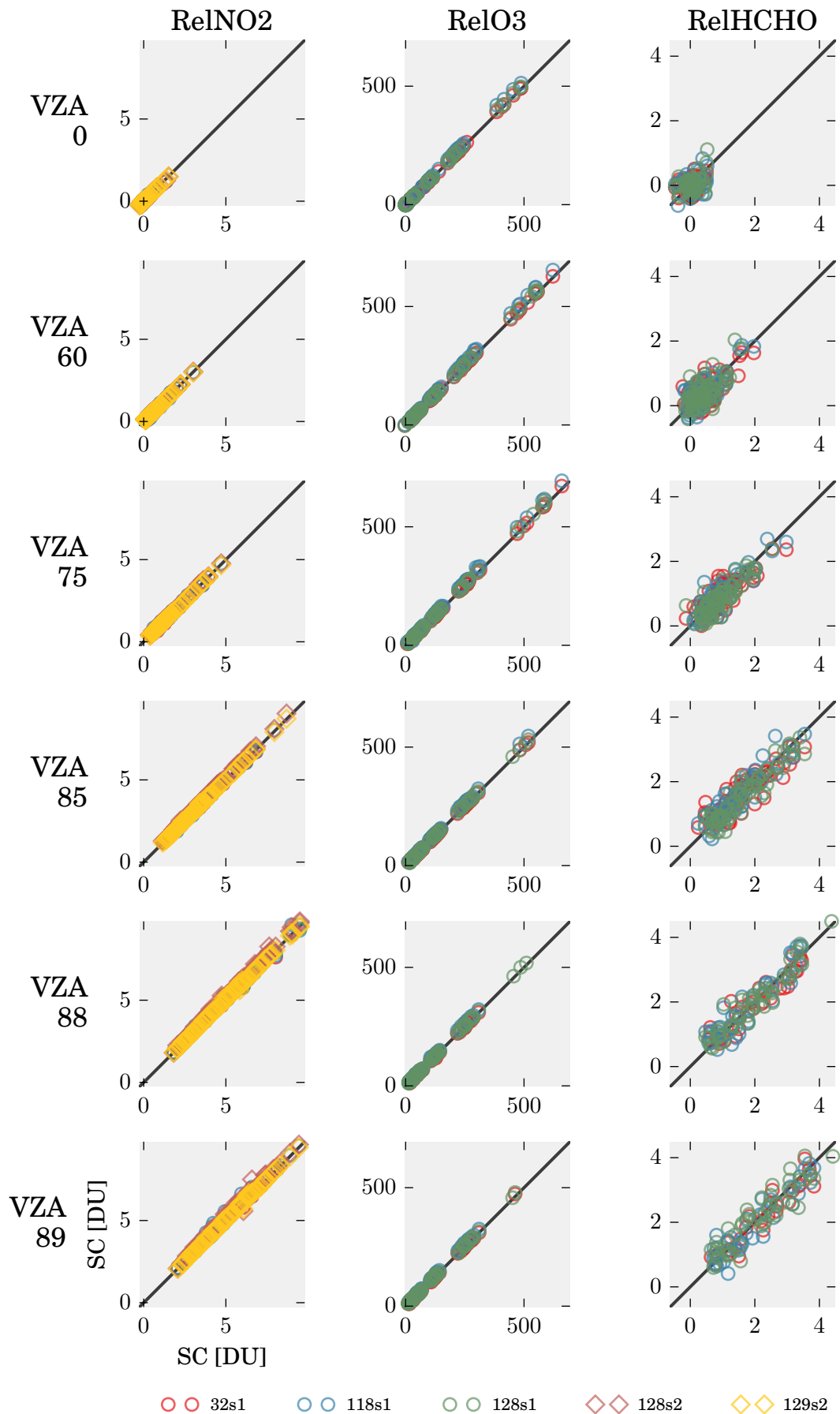


Figure 7: Correlation plots with Pandora 129s1 as reference for RelNO₂ (left column), RelO₃ (middle column) and RelHCHO (right column) SCs for all VZAs (rows). For better orientation, the 1:1 line is drawn in black in the background.

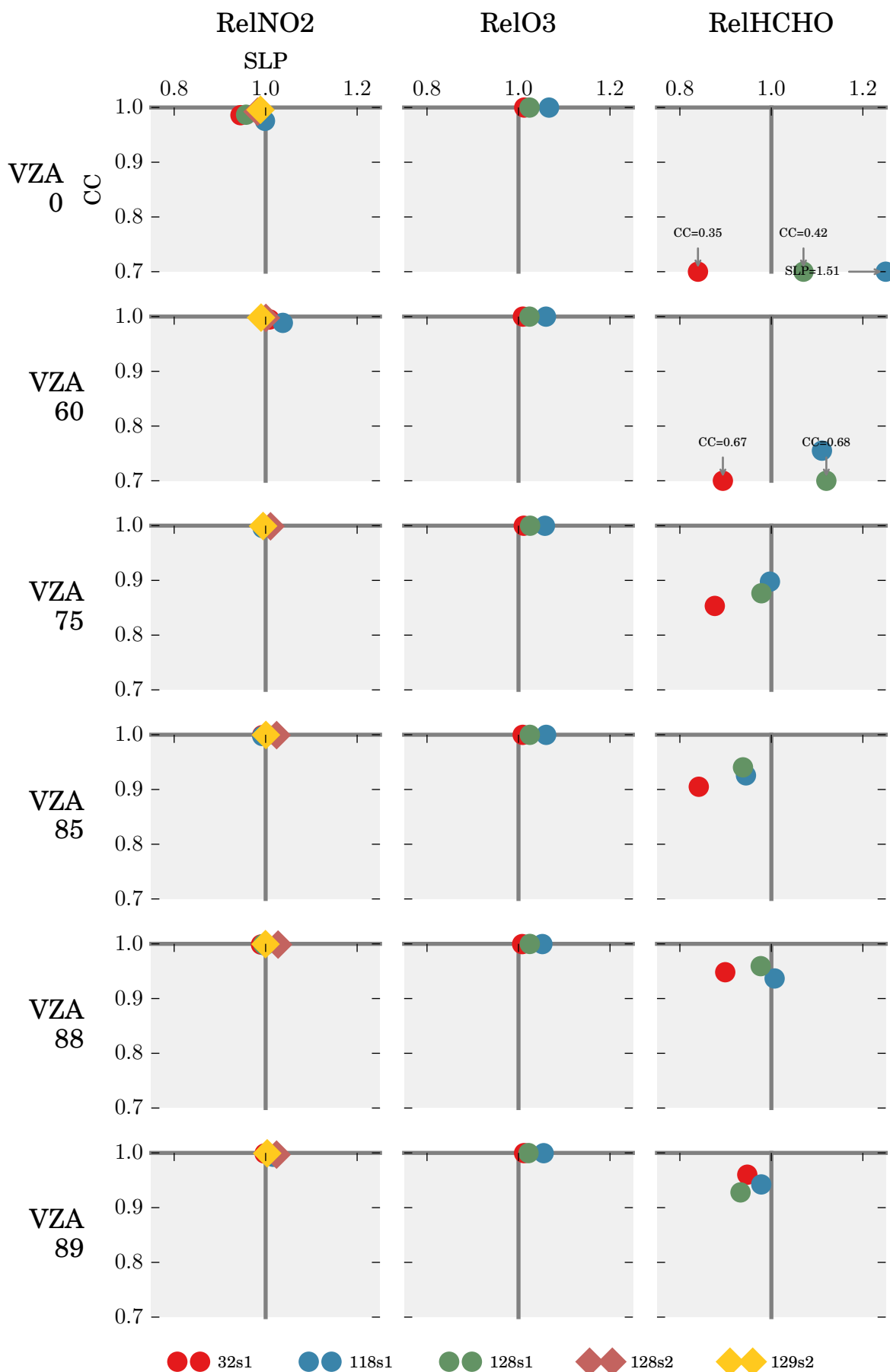


Figure 8: Statistical analysis for RelNO2 (left column), RelO3 (middle column) and RelHCHO (right column). The x-axis shows the slope of the linear regression SLP and the y-axis the Pearson product-moment correlation coefficient CC. SLP and CC intersect at 1. The closer the data points are to the intercept the better the agreement. Data points outside the limits are marked by an arrow and the actual value is given as text.

6 Direct Sun Relative Intensity Comparison

Level 1 data [3], retrieved from direct sun SO and SU routines (compare routines highlighted in purple in Figure 2), comprise the corrected spectra³ for the wavelength ranges mention in Table 5. From these level 1 data the intensities for the nominal wavelengths 340, 440, 500 and 870 nm are extracted (a subgroup of the Aeronet standard wavelengths). 440 and 500 nm are measured by all Pandoras, 340 only by the S1 spectrometers and 870 only by the S2 spectrometers. The UV wavelength 340 nm is analyzed by means of SU measurements since they are less prone to spectral stray light.

Drifts in the intensity does not significantly affect common spectral fitting algorithms for gas retrievals (it is obliterated by the use of higher order background polynomials), but it is a game changer for spectral AOD retrievals. For example, Aeronet claims a standard deviation in intensity of 1 %, yielding a standard deviation of 0.01 in AOD (for AMF 1). At this stage we estimate the spectral stability by comparing the Pandoras against a selected reference Pandora. A comparison to an external reference, like a sun photometer, is not part of this ICC.

6.1 Data Preparation

The current Pandonia level 1 data is given in units of counts per second. Hence the spectra are given as relative intensities rather than absolute intensities in units of e.g. $\text{mW m}^{-2} \text{nm}^{-1}$. Absolute radiometric calibration will be implemented in the operational level 1 processing soon. Since the spectral response is different for each Pandora we picked a reference period where each dataset is normalized to (from 7 to 9 UTC on September 14th). This period exhibits perfect clear sky conditions and no Pandora has an attenuation filter equipped (neutral density filter ND). Thus the actual values which are compared are normalized relative intensities (NRelInt) at the nominal wavelengths [the spectra are averaged around ± 1 nm for S1 and ± 2 nm for S2 spectrometers (approximately 16 pixels)].

For the statistical analysis, Pandora 129s1 is selected to be the reference for 340, 440 and 550 nm and Pandora 129s2 for 870 nm.

Data Filtering

Data filtering is applied in two ways. First, the total uncertainty (including atmospheric as well as instrumental uncertainty) is limited to 0.1 % of the measured signal. Second, the relative difference between the instrumental uncertainty and the total uncertainty must not exceed 9 % (instrumental uncertainty is explained in chapter 6 in Cede [3]).

Figure 9 illustrates the data filtering for an almost perfect clear sky day. The total uncertainty is shown as purple line, the instrumental uncertainty as green line. Only data points marked with filled circles are used for the comparison. Data points marked with a thick circle accomplished to stay below 0.1 % total uncertainty only. Data point exceeding both filter thresholds are shown as thin circles.

³Corrected spectra are raw level 0 data freed from individual instrumental characteristics. E.g. non-linearity, pixel response non uniformity, ... Details can be found in Cede [3]

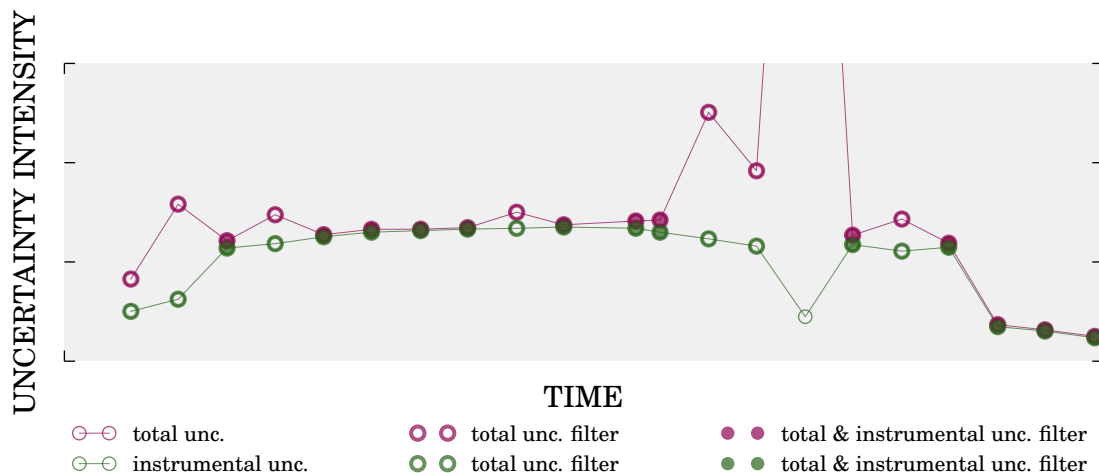


Figure 9: Illustration of the diurnal variation of the total uncertainty (in purple) and the instrumental uncertainty (in green) for a clear sky day. To filter data with atmospheric uncertainty (noise) the instrumental uncertainty has to stay below 9 % of the total uncertainty and the total uncertainty has to be below 0.1 % of the measured signal. Data points fulfilling these requirements are indicated by a filled circle and are included in the comparison. If only the latter criteria is fulfilled, data points are given as thick circle. When neither of the two criteria are accomplished, a thin circle is shown.

6.2 Intercomparison Results

The direct sun relative comparison is summarized by 3 figures. Figure 10 gives a typical variation in intensity for the nominal wavelengths (the full time series is shown in Figure 18 in the appendix). Correlation plots for NRelInts, with Pandora 129s1 (for 340, 440 and 500 nm) and Pandora 129s2 (for 870 nm) as reference, are shown in Figure 11. The respective histograms for the ratio to the reference ($\text{NRelInt}_{\text{Pan}} / \text{NRelInt}_{\text{Ref}}$) is shown in Figure 12. The histograms are limited to the range 0.7 to 1.3. If data points lie outside this range they are mentioned in the text.

We can distinguish three groups of problems affecting the intensity comparison:

Pointing is completely off Pandora 128 (s1, s2) appears to be totally off in the alignment in the period from September 30th to October 5th. It was measuring sky radiance rather the direct sun irradiance, leading to a strong underestimation with respect to the reference. This can be clearly seen in the correlation plot (Figure 11), but is clipped in the histogram. A time series covering this period is shown in Figure 18 in the appendix.

Data scattering Pandora 129s2 and 118s1 suffer from enhanced data scattering. The strong data scattering for Pandora 118s1 (clearly visible in Figure 11) is a consequence of a hardware issue. One filter wheel in the sensor head of Pandora 118s1 was malfunctioning, making the filter wheel to stuck from time to time. Thus the actual filter wheel position was differing from the position the operation software was thinking to have. As a consequence the processing software applies the wrong transmission correction for these cases. Pandora 118s1 is currently under repair. The enhanced scattering for Pandora 129s2 is probably also related to an alignment issue. The last one and a half days of the ICC the signal is biased low (see Figure 18 in the appendix).

Neutral density filter characterization At high solar elevations a ND filter becomes necessary to avoid signal saturation. We see two cases where the characterization of this filter was not successful. Pandora 128s2 is showing a double peak (the second at roughly 0.9) in the histogram plot (Figure 12) and a group of data points parallel below to the 1:1 line (Figure 11). These features stem from measurements using a ND filter, where the filter transmission calculated from lab measurements is obviously overestimated. For Pandora 129s2 the ND characterization is also not as good as required. This explains the broadened histogram (Figure 12) and the “jumps” in the time series for 870 nm. Surprisingly only S2 spectrometers show insufficient ND filter characterization.

Note, since no ND filter is necessary when measuring with U340 bandpass filter, intercomparisons at 340 nm are not affected.

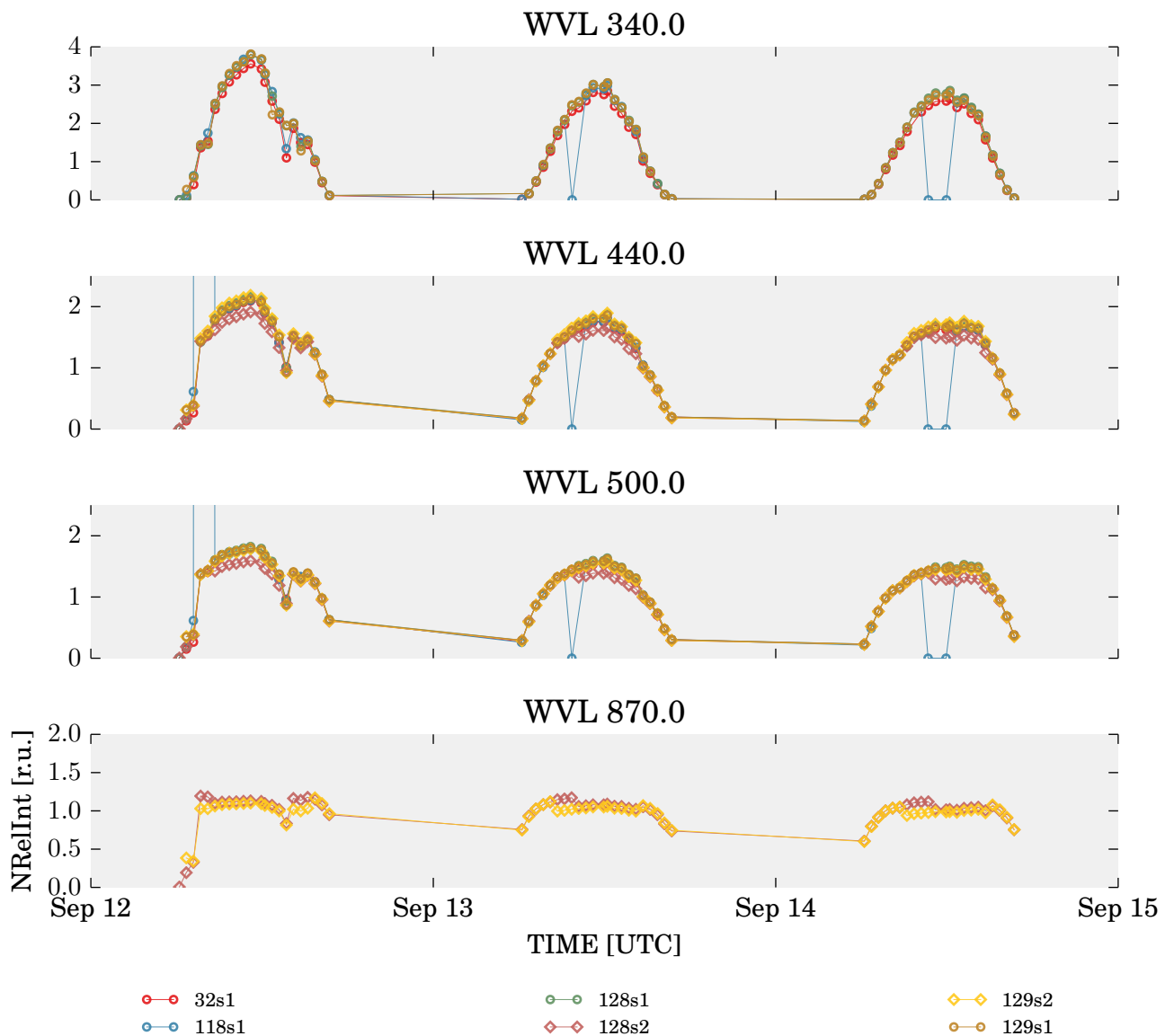


Figure 10: Typical time series during the ICC for direct sun normalized relative intensities NRelInt for nominal wavelengths 340 (top panel), 440 (second panel), 500 (third panel) and 870 nm (bottom panel).

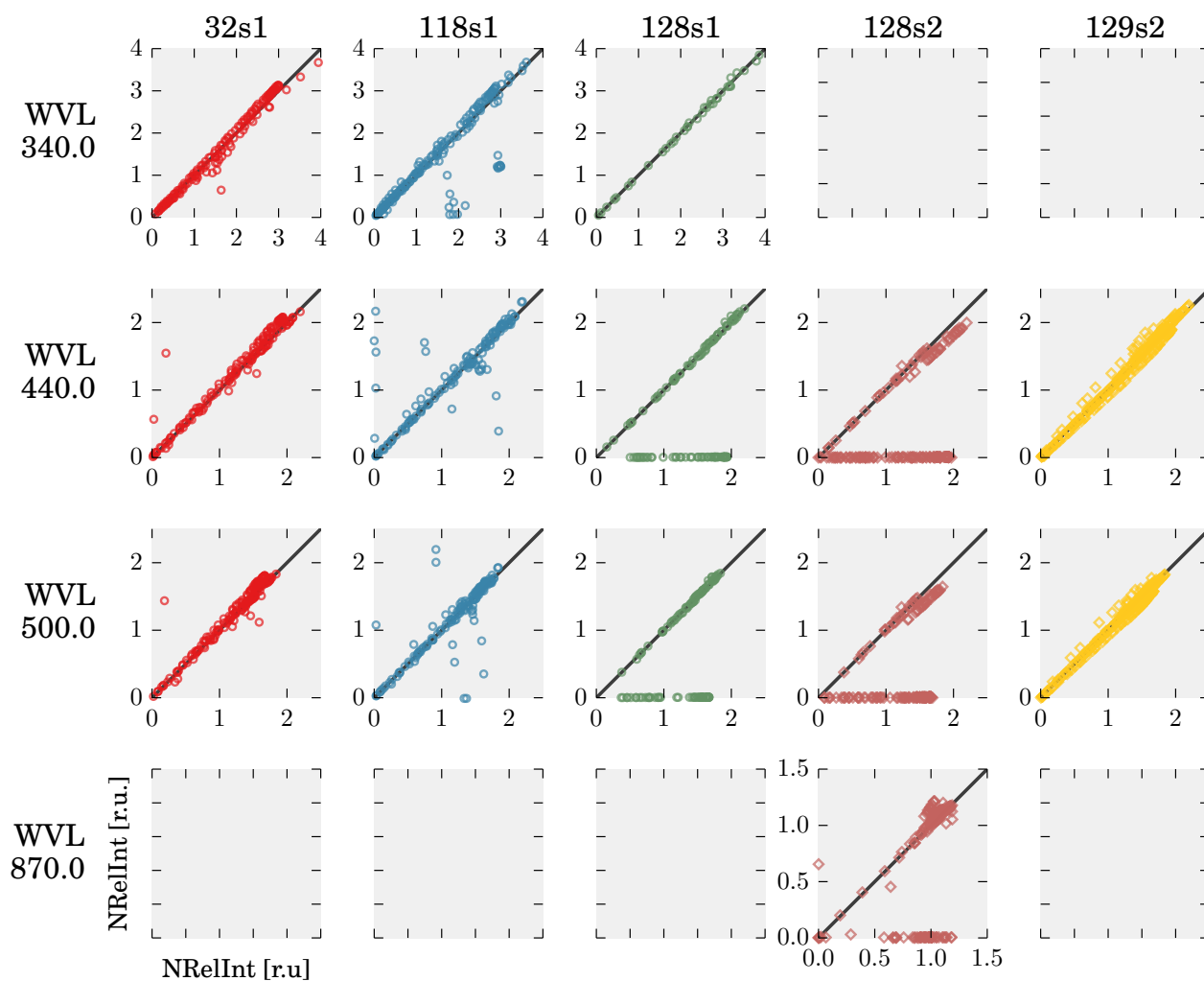


Figure 11: Correlation plots for NRelInt with Pandora 129s1 as reference for nominal wavelengths 340 (top panel), 440 (second panel) and 500 nm (third panel) as well as Pandora 129s2 as reference for 870 nm (bottom panel). For better orientation, the 1:1 line is drawn in black in the background.

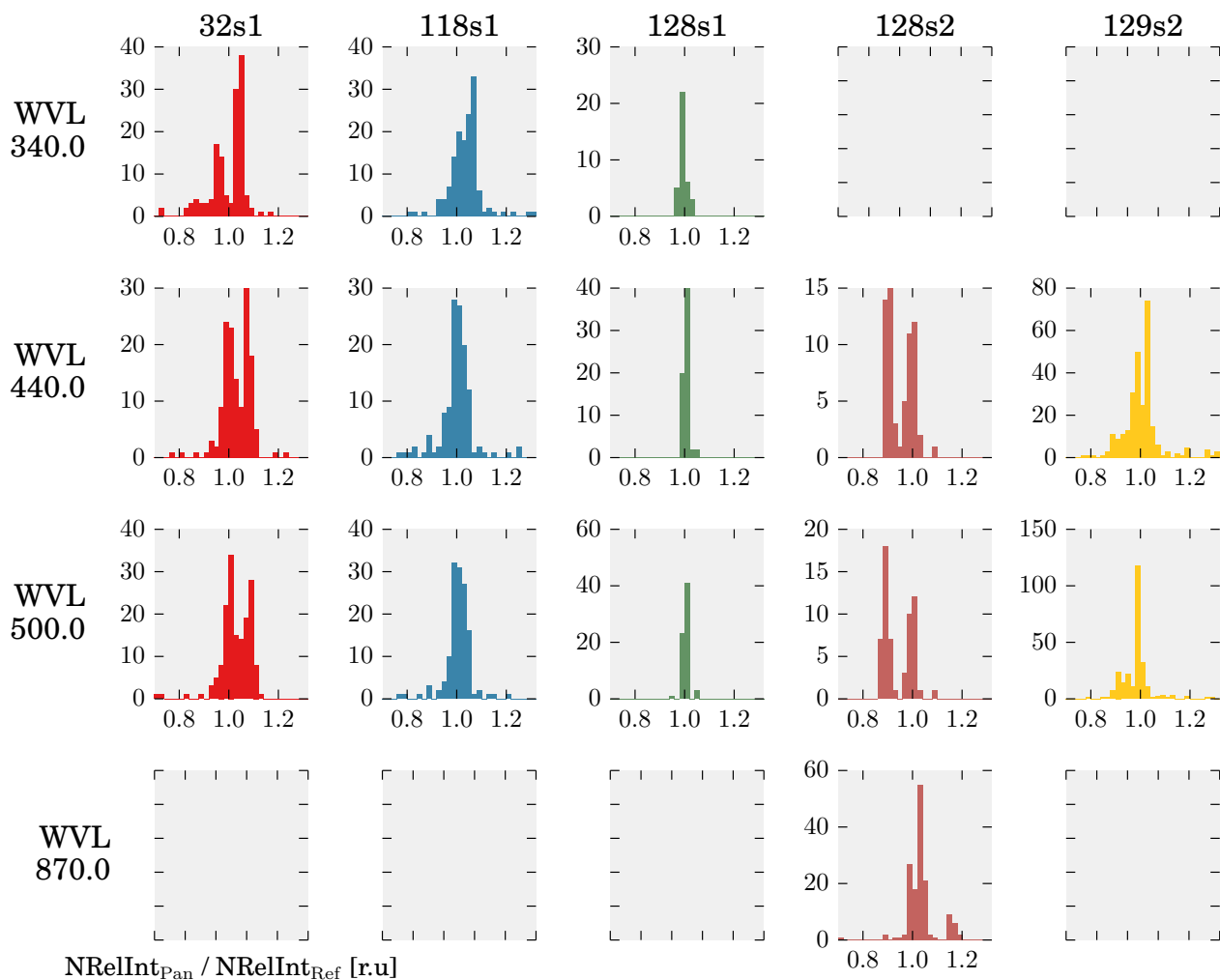


Figure 12: Histogram plots for the ratio $NRelInt_{Pan} / NRelInt_{Ref}$ for nominal wavelengths 340 (top panel), 440 (second panel), 500 (third panel) with Pandora 129s1 as reference and 870 nm (bottom panel) with Pandora 129s2 as reference.

If we exclude all questionable data points, meaning

- to restrict the evaluation period from August 29th to September 29th (that is excluding the warm up phase and the CINDI2 backup week),
- to not allow measurements where a ND was in a filter wheel for Pandora 128s2 and 129s2,
- to skip Pandora 118s1 at all,

the standard deviation σ_{RelInt} for all refined histograms, which can be interpreted as spectral stability, would give an average spectral drift of about 2%. If only S1 spectrometers are considered even about 1.7%. The individual histograms are depicted in Figure 19 in the appendix.

7 Instrument Pointing Comparison

Accurate pointing is a big challenge for direct sun as well as scattered sun measurements. This is why Pandora instruments employ a sophisticated pointing algorithm which makes use of three leveling angles. These leveling angles basically give the difference between the mechanical instrument alignment and the actual optical alignment and are calculated based on sun search routines (see *Cede* [3]). Whereas bad pointing can be recognized in direct sun data, data quality for scattered sun data does not necessarily give a hint on bad pointing due to its relative apathy to pointing inaccuracies.

The measured routines EH (compare routine highlighted in red in Figure 2), which scan from 5° above the horizon to 5° below the horizon in high resolution, give the opportunity to compare the elevation angle of the horizon HorEA retrieved from EH level 1 data for all Pandora instruments. Likewise for the comparison of the relative intensities (see section 6.1), this is done for 340, 440 and 500 nm (870 nm is excluded).

7.1 Data Preparation

Mandatory for a good alignment is the initial alignment phase when an instrument is set up at a new location. This alignment phase is characterized by a dense population of sun search routines, which are used to build up a database of leveling angles as mentioned above. This alignment phase took place at the beginning of the ICC (warm up phase), highlighted in gray in Figure 1.

A typical intensity variation for changing viewing elevation angles ($VEA = 90^\circ - VZA$) is given as red line in Figure 13 (here normalized at its maximum). The signal first descends slowly while pointing closer to the horizon (speaking from high to low VEA), with a sharp drop close to the horizon and is finally leveling out for radiation reflected from the ground. To get the transition point from sky to ground, RelInts at the selected nominal wavelengths [averaged around $\pm 1(2)$ nm for 1s (2s) spectrometers] for each VEA are derived using central differences. The normalized derivative to this curve is illustrated as light green line in Figure 13. The final HorEA (intercept of the gray vertical line in the figures with the x-axis) is estimated from the peak of a Gaussian fit into the normalized derivative (shown as green curve). This procedure is performed for all Pandoras at all selected wavelengths.

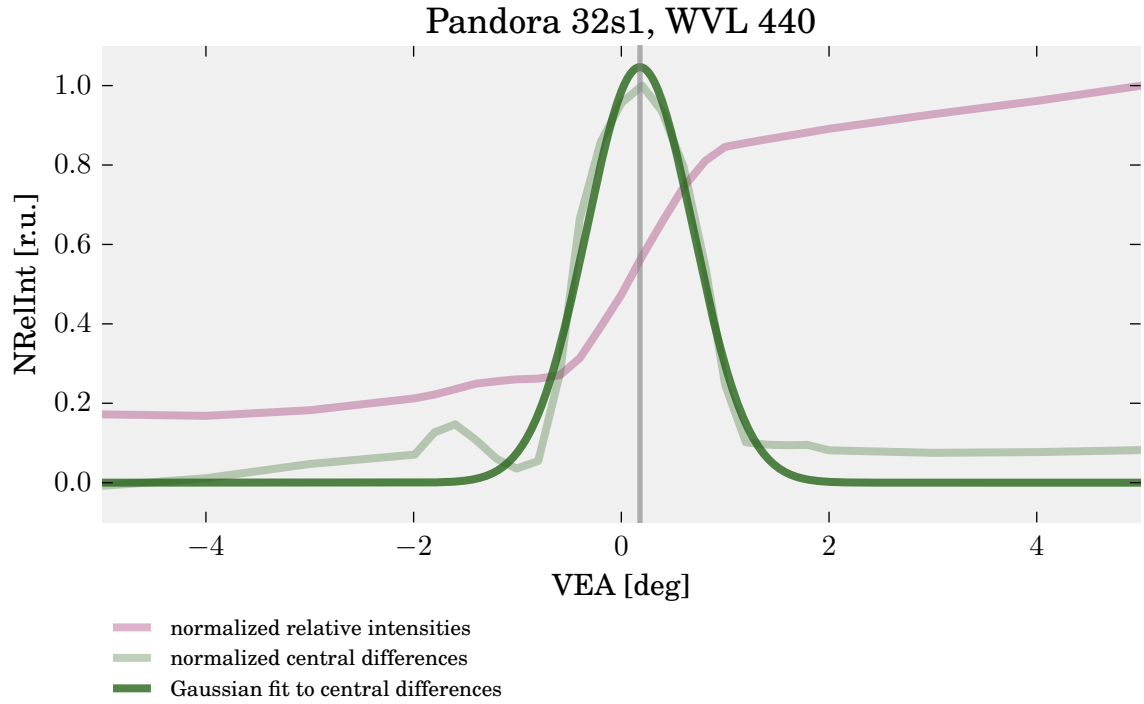


Figure 13: Retrieval of the elevation angle of the horizon (HorEA) based on EH routines. The red curve gives the (normalized) descending signal when pointing from 5 to -5° VEA. The normalized central differences from the signal curve is illustrated as light green curve, and a Gaussian fit in this curve as green line. The intercept of the gray vertical line with the x-axis gives the actual HorEA.

Data Filtering

For this comparison we want to include only events with comparable atmospheric conditions and where the sky is clearly distinguishable from the ground (note, dilution is always given due to vegetation). E.g. clouds at the horizon can be both enhance or mitigate radiance compared to clear skies and can further “displace” the apparent zenith position of the actual horizon. To circumvent this problems we include only EH routines where the absolute difference of the relative intensity i at VEA 5° to the mean value of all scans I is below 50 % of the standard deviation of all scans σ_I . That is

$$|i_5 - \bar{I}_5| < 0.5 \cdot \sigma_{I_5}. \quad (1)$$

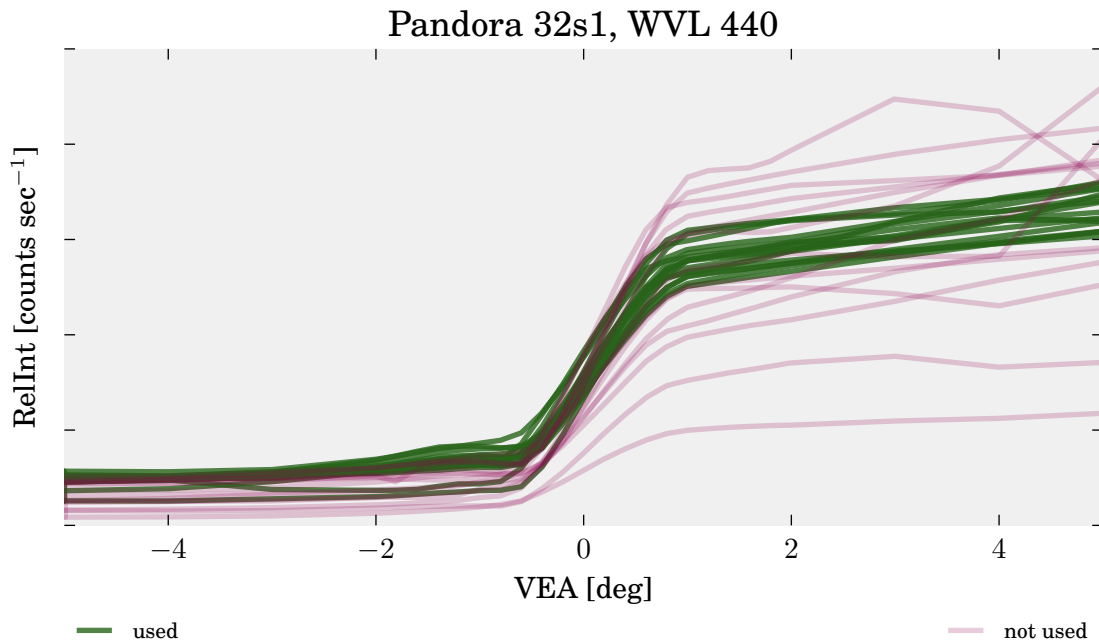


Figure 14: RelInts from all EH routines at 440 nm collected by Pandora 32s1. The VEAs within routine EH descend from 5 to -5 degrees. Only data exhibiting a comparable pattern are included in the comparison. By this we want to avoid cases, where the actual HorEA is smeared out by atmospheric conditions. Curves accepted by the selection criteria (1) are shown in green, the rejected curves in red.

Once the dataset is filtered, the pointing quality for each day (one EH routine per day has been measured) is analyzed individually. Since we are only interested in the agreement between the Pandoras rather than knowing the true HorEA, the values are corrected by the mean over all Pandoras on that day. The final measure for the pointing quality is the deviation from this mean $\text{HorEA}_{\text{Pan}} - \overline{\text{HorEA}}$.

7.2 Intercomparison Results

The instrument pointing comparison is summarized in Figure 15. Box-whisker plots gather $\text{HorEA}_{\text{Pan}} - \overline{\text{HorEA}}$ for all days, depicting the Pandoras in the columns and the nominal wavelengths 340, 440 and 500 nm in the rows. The whisker span the 10 to 90 interpercentile range, the boxes the 25 to 75 interpercentile range and the median is given as black bar within the boxes.

Nearly all Pandoras clearly agree within 0.10° for the 10 to 90 interpercentile range, only Pandora 118s1 and 128s2 agree within 0.15° . This holds true for all nominal wavelengths considered. We want to point out that the possibility to install the instrument at the ICC site (on top of a container, shared with other groups) is by far not as stable as it is usually given for a Pandonia site.

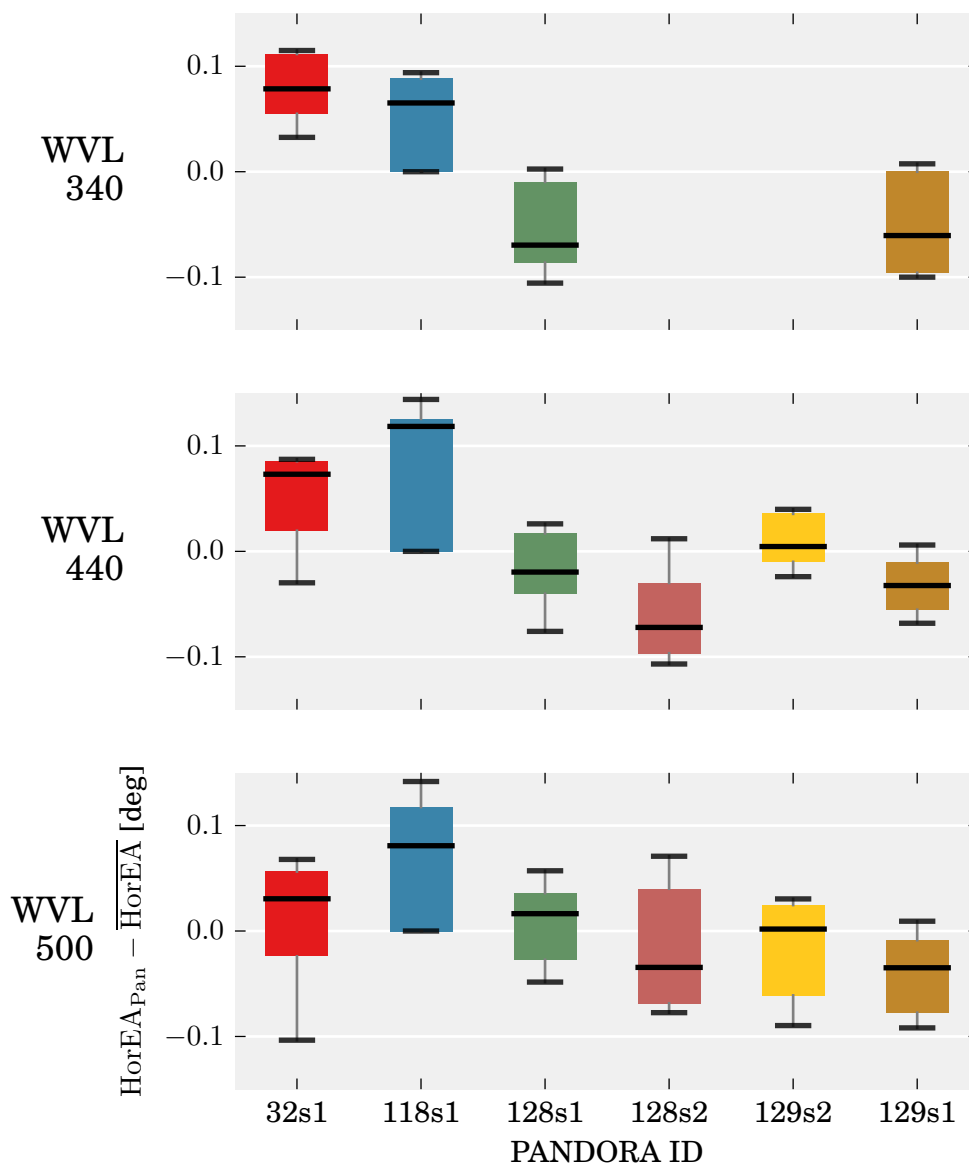


Figure 15: Instrument pointing comparison at nominal wavelengths 340 (top panel), 440 (middle panel) and 500 nm (bottom panel). Shown are the deviations of HorEA to the mean HorEA over all Pandoras for every day, condensed in a box-whisker representation. The whiskers give the 10 to 90 interpercentile range, the boxes the 25 to 75 interpercentile range. The Median is given as black bar within the boxes.

A Additional figures

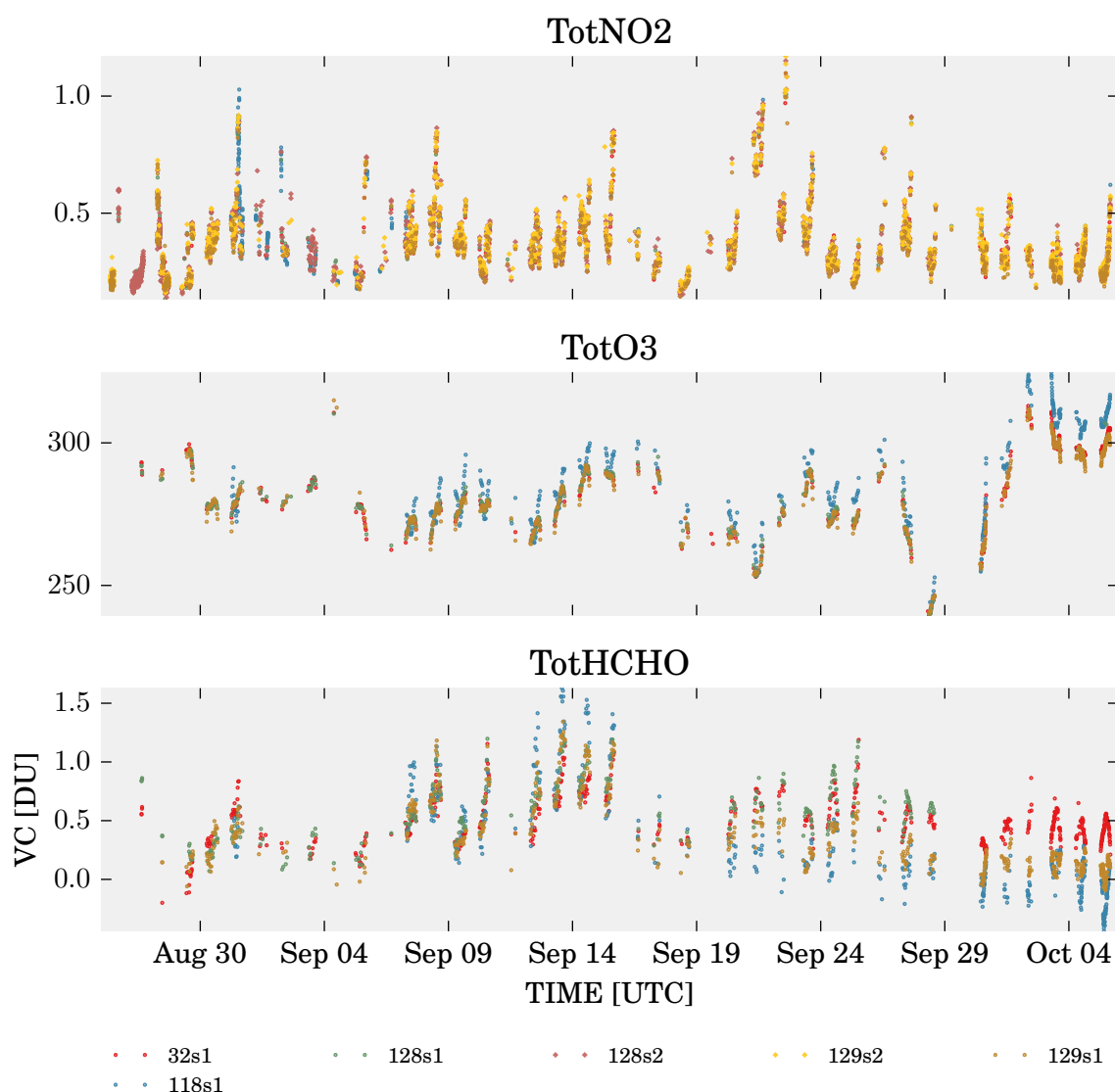
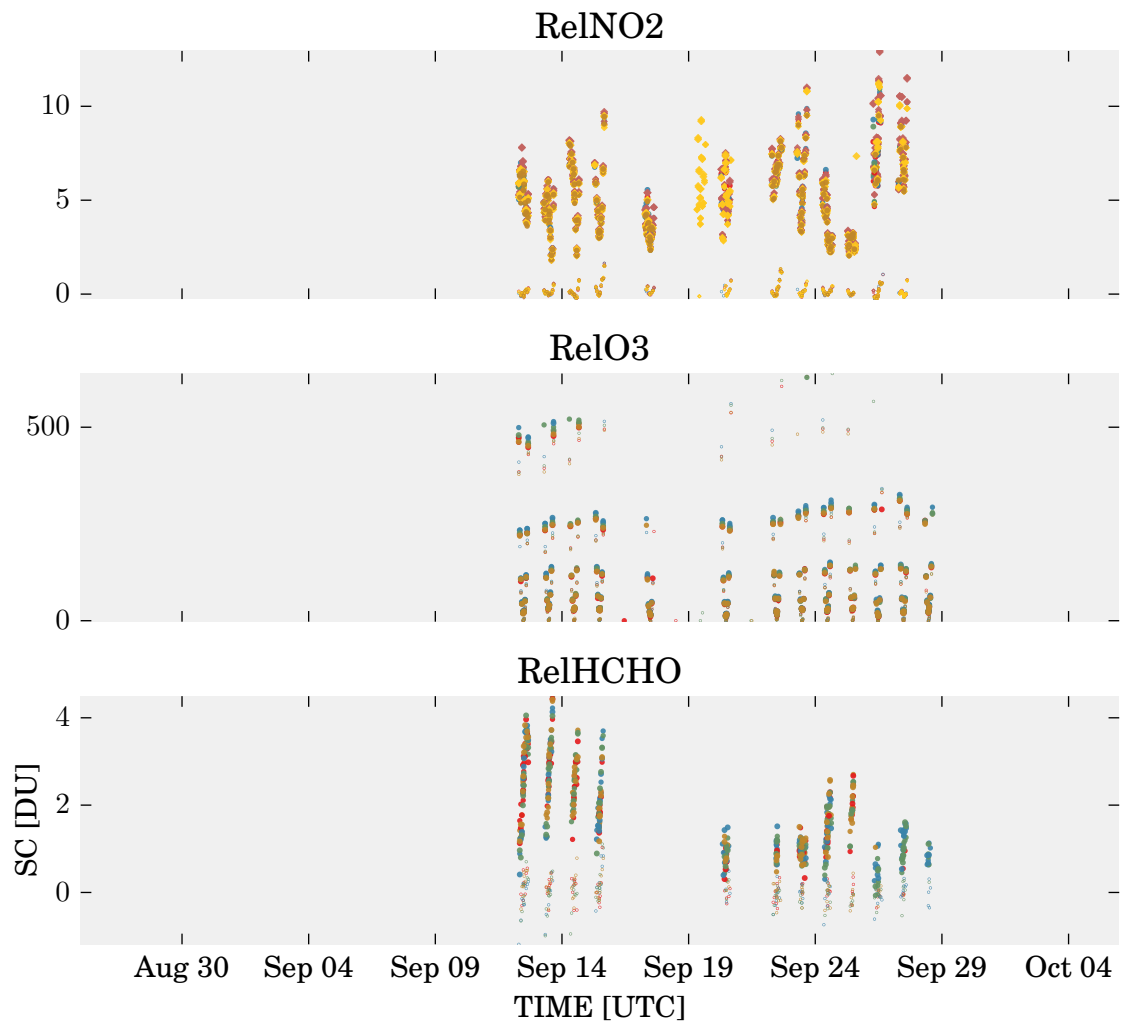


Figure 16: Full time series during the ICC for direct sun TotNO₂ (top panel), TotO₃ (middle panel) and TotHCHO (bottom panel) for all Pandora instruments. Datasets are filtered as listed in Table 7.



• 32s1, VZA0	• 129s2, VZA0	• 128s1, VZA88	• 32s1, VZA89	• 128s2, VZA89
• 118s1, VZA0	• 129s1, VZA0	• 128s2, VZA88	• 118s1, VZA89	• 129s2, VZA89
• 128s1, VZA0	• 32s1, VZA88	• 129s2, VZA88	• 128s1, VZA89	• 129s1, VZA89
• 128s2, VZA0	• 118s1, VZA88	• 129s1, VZA88		

Figure 17: Full time series for scattered sun RelNO2 (top panel), RelO3 (middle panel) and RelHCHO (bottom panel) for all Pandora instruments and VZAs. Datasets are filtered as listed in Table 9.

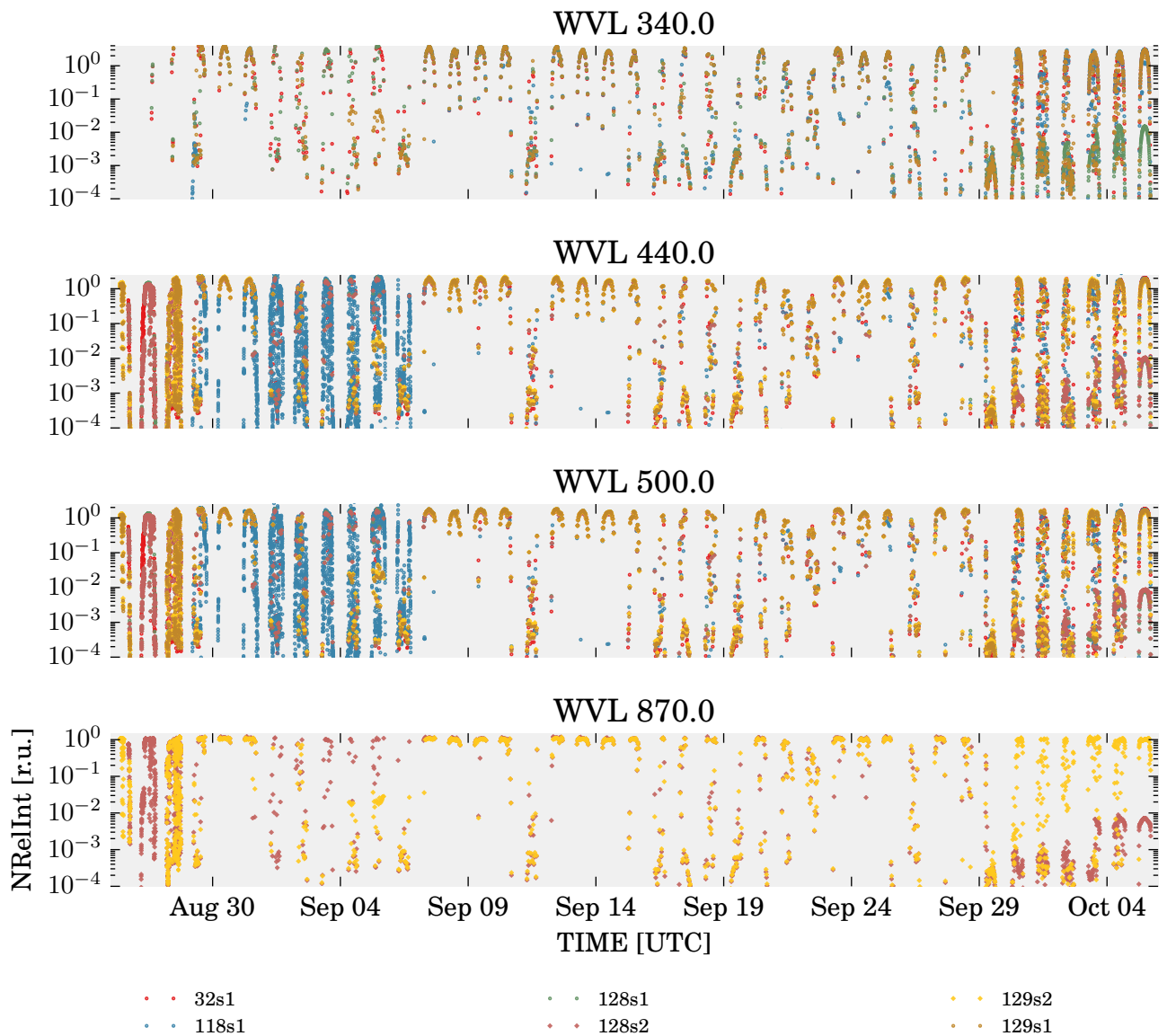


Figure 18: Full time series during the ICC for direct sun normalized relative intensities NRelInt for nominal wavelengths 340 (top panel), 440 (second panel), 500 (third panel) and 870 nm (bottom panel).

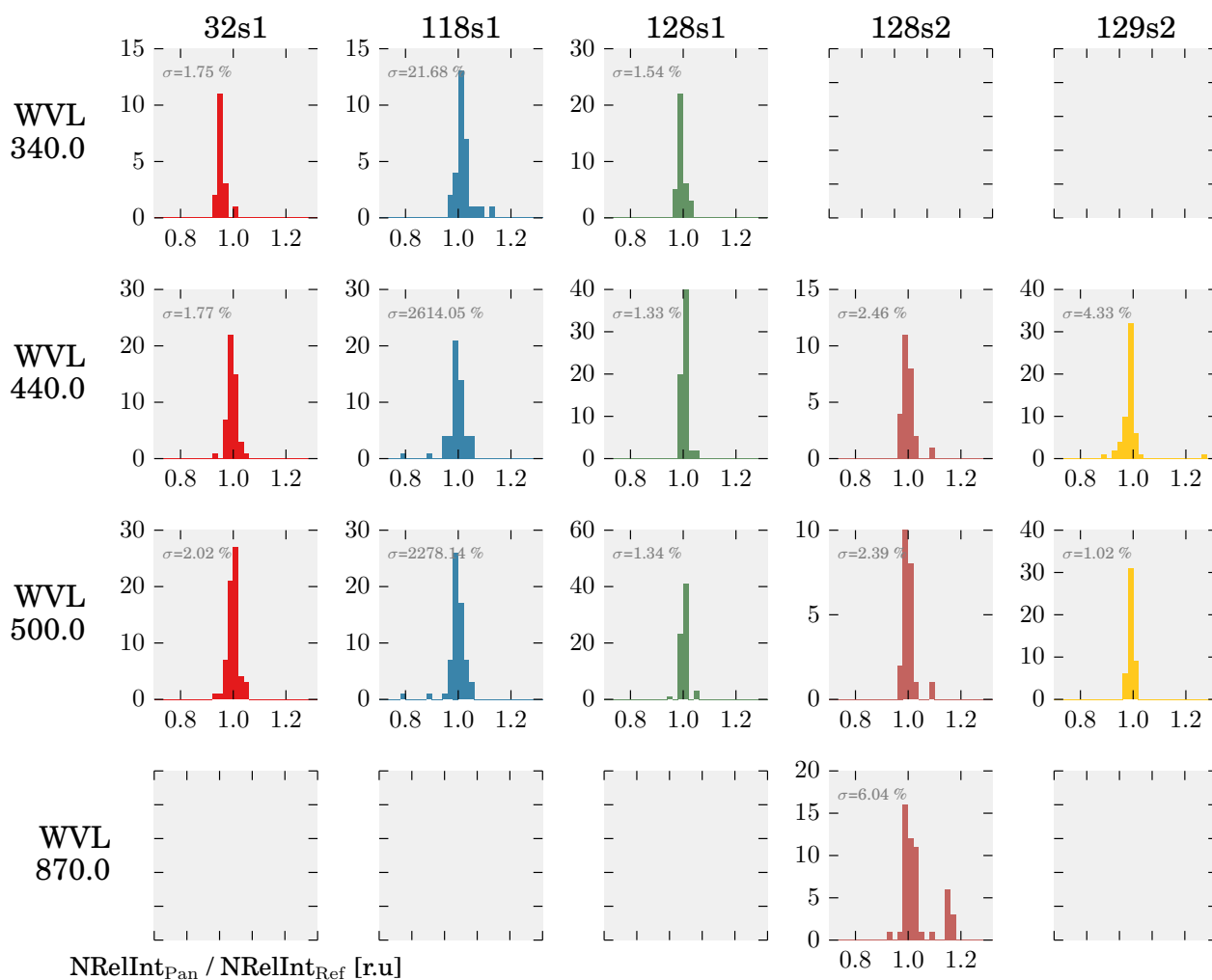


Figure 19: Histogram plots for the ratio $\text{NRelInt}_{\text{Pan}} / \text{NRelInt}_{\text{Ref}}$ for nominal wavelengths 340 (top panel), 440 (second panel), 500 (third panel) with Pandora 129s1 as reference and 870 nm (bottom panel) with Pandora 129s2 as reference. The data series is restricted to the evaluation period from August 29th to September 29th (that is excluding the warm up phase and the last week of the ICC). In addition all measurements using a ND filter are excluded for the S2 spectrometers. The standard deviation σ_{RelInt} is given as text in each subplot.