LuftBlick Report 2023008

Evolution of QA/QC Strategies

Technical Note on WP5 of FRM4AQ-2

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Prepared by

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1 Document Change Record

Issue	Date	Section	Observations
1	31 May 2023	All	First version
2	30 Nov 2023	4.4 5.2	Moved AMF-dependency minimization from development to applied into new Sec.4.4 Added data quality markers
3	30 May 2024	2, 5.2, 6	Added Appendix section describing data quality markers
4	30 Nov 2024	6.1	Added Markers 6.1.6 - 6.1.8
5	31 May 2025	6.1	Added Markers 6.1.9 - 6.1.11

1.1 Acronyms and Abbreviations

AMF	Air mass factor
BSS	Blick Software Suite
DQ	Data quality
FRM	Fiducial reference measurements
FRM4AQ	Fiducial reference measurements for air quality
NO_2	Nitrogen dioxide

PGN	Pandonia Global Network
QA	Quality assurance
QC	Quality control
QF	Quality flagging
QI	Quality indicator
QIT	Quality indicator threshold
QO	Quality operator
QP	Quality pilar
SO_2	Sulfur dioxide
$TotNO_2$	Total column amount nitrogen dioxide
$TropNO_2$	Tropospheric column amount nitrogen dioxide
vc	Total column amount
WP	Work package
wrms	Weighted root mean squared error based on measured uncertainty

2 Summary

The current QAQC strategies are built on the three quality pillars established during the previous FRM4AQ project. New strategies under development aim to enhance the detection and categorization of data quality issues, thereby reducing the time required for quality control and assurance. This improvement will be facilitated by creating a database of known data quality markers.

3 Introduction

3.1 General

This report is deliverable D6 of the ESA project FRM4AQ-2 as part of WP 5. It describes the evolution of quality assurance (QA) and quality control (QC) procedures applied on PGN related data products. The concept of this document aims to first introduce new QAQC strategies in the development Section (Section 5). After rigorous and successful testing, strategies in development can move into the applied Section (Section 4) in a later version. Changes and highlights will be summarized in Section 2.

3.2 Fiducial Reference Measurements

High quality reference measurements are crucial for satellite validation to provide independent ground-based observations, in order to characterize on-orbit characteristics:

“The suite of independent ground measurements that provide the maximum Return On Investment (ROI) for a satellite mission by delivering, to users, the required confidence in data products, in the form of independent validation results and satellite measurement uncertainty estimation, over the entire end-to-end duration of a satellite mission.” (Sentinel-3 validation team S3VT)

Consequently, so-called fiducial reference measurements (or FRMs), should fulfill the following concepts (Sentinel-3 validation team S3VT):

- FRM have documented SI traceability (eg. via round-robin characterisation and regular (pre-and post deployment) calibration of instruments) using metrology standards.
- FRM are independent from the satellite geophysical retrieval process.
- An uncertainty budget for all FRM instruments and derived measurements is available and maintained.

- FRM protocols, procedures and community-wide management practices (measurement, processing, archive, documents etc.) are defined, published openly and adhered to by FRM instrument deployments.
- FRM are accessible to other researchers allowing independent verification of processing systems.

Hereby, the uncertainty reporting plays an important role in validation concepts, which has been evolved for Pandora data products (Kreher et. al). A detailed description of different uncertainty sources that contribute to the reported total uncertainty of PGN data products, can be found in the BSS (BSS manual, Chapter 6, Data Uncertainty).

3.3 Quality pillars

The PGN QA/QC concept is based on three quality pillars (QP) to assess the data quality of each retrieval product (TN on Data Quality Flagging Generic Procedure Evolution, Chapter 3)

QP1 Each individual measurement of a data product,e.g. direct sun total NO_2, has its own classification into high / medium / low data quality, based on threshold exceedance of various quality indicators.

QP2 A time series of one retrieval product is used to determine instrumental changes in the field. A typical example is the evolution of the direct sun NO_2 wrms over time to detect sudden changes that are not related to atmospheric conditions.

QP3 This pillar is similar to QP2 to detect instrumental changes. Herein, time series of the same data product (e.g. total column amount NO_2 together with NO_2 wrms) or different data products (e.g. total column SO_2 amount together with O_3 temperature) are used to identify instrumental changes.

4 Strategies Applied

4.1 Data Quality Levels and Flagging

The processor of the Blick Software Suite (BSS) produces several processing levels from raw measurements (L0) to final level data:

- L0 to L1: Correction for instrumental characteristics which leads to corrected signals.
- L1 to L2Fit: Spectral fitting which leads to slant column amounts.
- L2Fit to L2: Conversion from slant columns to vertical columns, tropospheric amounts, surface concentrations, or profiles.

A detailed description can be found in the BSS manual. For each of those processing levels, different quality indicators (QI) exist. E.g., the L1 processor can derive a so-called atmospheric variability, which defines the variability of the atmosphere over the measurement duration. In particular, this quantity is achieved by making the ratio between the instrumental uncertainty, which is characterized by laboratory measurements, and the measured uncertainty, which is the standard deviation over the measurement duration. Expressed in percentage, this QI can serve as a decision basis to use only the best possible data.

Generally, each QI is defined by a certain-value range, which typically covers distinguishable regions for measurements that can be used with high or low confidence. Therefore, thresholds for quality indicators (QIT) are determined to separate low and high quality data, with an intermediate medium quality regime. An objective approach to determine such thresholds has been developed as part of the FRM4AQ-1[1] project, which is described in a technical note (TN on Data Quality Flagging Generic Procedure Evolution, Chapter 4.1.2). All QIs are listed in the BSS manual.

[1] Fiducial Reference Measurements for Air Quality [Contract and Statement of Work], ESA Contract No. 4000125841/18/I-NS, 2018.

Consequently, whenever a QI exceeds its QIT, it changes the data quality (DQ) from high (10) to medium (11), or from medium to low quality (12). Either only one, or even multiple QI's can be the trigger for individual measurements to be in one of those three DQ categories.

This also means that based on several QI, together with the objectively defined QIT, each retrieval product gets its own quality flag and DQ category automatically as part of the processor, which can be used easily for users. However, per definition, the first digit of the data quality number defines the quality assurance (QA) status, which defines a separate layer to provide confidence in the retrieval products (see Section 4.2 Quality assurance).

4.2 Quality Assurance

The quality assurance (QA) is currently a manual process done by the quality operator (QO). The QOs screen time series of data and QIs, dedicated aggregates and correlates this with metadata (like observations reported by local instrument operators). QA describes an additional layer of confidence that can be provided for a data product, which is added on top of the already existing DQ. For users, this is reported in the L2 data product as a change of the data quality from not-assured (two digits given, first digit = 1) to assured status (only one digit of 0/1/2)

- 10 to 0 (high quality)
- 11 to 1 (medium quality)
- 12 to 2 (low quality)

Furthermore, it might be possible that measurements are falsely labeled as high quality, since no QI is able to detect a specific or unknown issue (e.g., a bad instrument alignment for parts of the day, spider in the instruments telescope collimator, unknown spectral features,...). For these rare situations, it is possible to do a manual quality flagging (QF). This flagging changes the DQ, affecting again the first digit which becomes a 2:

- 10 to 20 (high quality)
- 11 to 21 (medium quality)
- 12 to 22 (low quality)

4.3 Quality Control

The quality control of data products is a routine task to observe the data quality in time. In the context of the PGN, this task is done by a QO. The goal of the QO. is to identify if an instrument needs human or remote intervention (e.g., if the instrument alignment pointing is lost), or if an instrument loses its calibration is not valid anymore. Both scenarios are impacting the data quality and can be detected by automated tools. Such tools and views have already been established in the FRM4AQ-1 project (TN on Data Quality Flagging Generic Procedure Evolution), which cover:

- Statistical break-point analysis for time series on aggregated data,
- Typical value range determination for QI,
- Warning system to highlight (potentially) critical datasets

The purpose of the applied tools is to minimize the time for an Q.O. to identify instrumental issues affecting the data quality. New tools and views which are implemented and developed as part of FRM4AQ-2 will be presented in the following sections

4.4 Tools and Views

4.4.1 Uncertainty-Based Out-of-Calibration Detection

For well calibrated data products, the diurnal variation of this product should not have any AMF dependency. It is possible, however, that due to certain environmental conditions U-shape or inverse-U shape patterns can be observed, but it is expected not to be systematic for many consecutive days. If such a systematic daily course exists, this would be the indication of a wrong calibration factor. In particular for (moderately) linear absorbers such as NO_2, HCHO, and SO_2, the following concept can serve as a detection if new field calibrations are required.

The idea of this strategy is to find the relative slant column amount that yields a minimum AMF-dependency of the total column amount (*Tot*). To realize that, the linear expression (Eq.1) is minimized. Herein, the absolute value of $\boldsymbol{\beta}_1$ should be minimized, which is achieved by optimizing the slant column amount (SC_{opt}) as defined in Eq.2:

Eq.1 $\quad \text{Tot} = \boldsymbol{\beta}_0 + \boldsymbol{\beta}_1 * \text{AMF}$

Eq.2 $\quad \text{Tot}_{\text{optimized}} = \text{Tot}_{\text{original}} + \text{SC}_{\text{opt}} / \text{AMF}$

An example of a sudden change in the daily course is illustrated for Pandora 209s1 at Izana (Figure Optimized NO_2 Column). Due to the remote location, a background stratospheric linear increase of the total column NO_2 is expected over the day (top graphic). If a slant column bias of +2.5e-5 mol/m^2 is assumed to happen on April 15th, the daily course of the original time series would change as in the bottom graphic.

Even on the first example day, the procedure would suggest a slightly larger SC_{opt} than for the original data. However, the optimized value is still within the reported uncertainty. In contrast, after April 15th, the optimized time series is showing the expected linear increase, and is clearly visible outside the reported 2-sigma uncertainty of the original time series.

With the proposed SC_{opt} used, the daily course is again showing the expected stratospheric linear increase for NO_2.

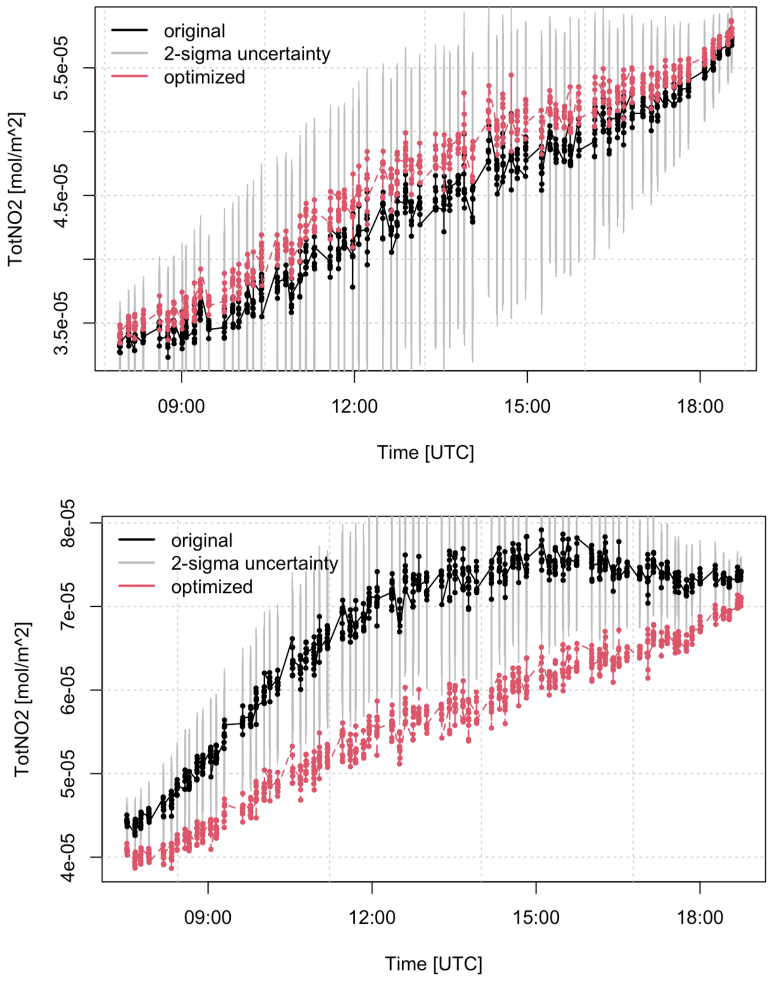


Figure Optimized NO_2 Column: Total column NO_2 amount on two different days for Izana, as expected (top) and with a positive slant column error (bottom).

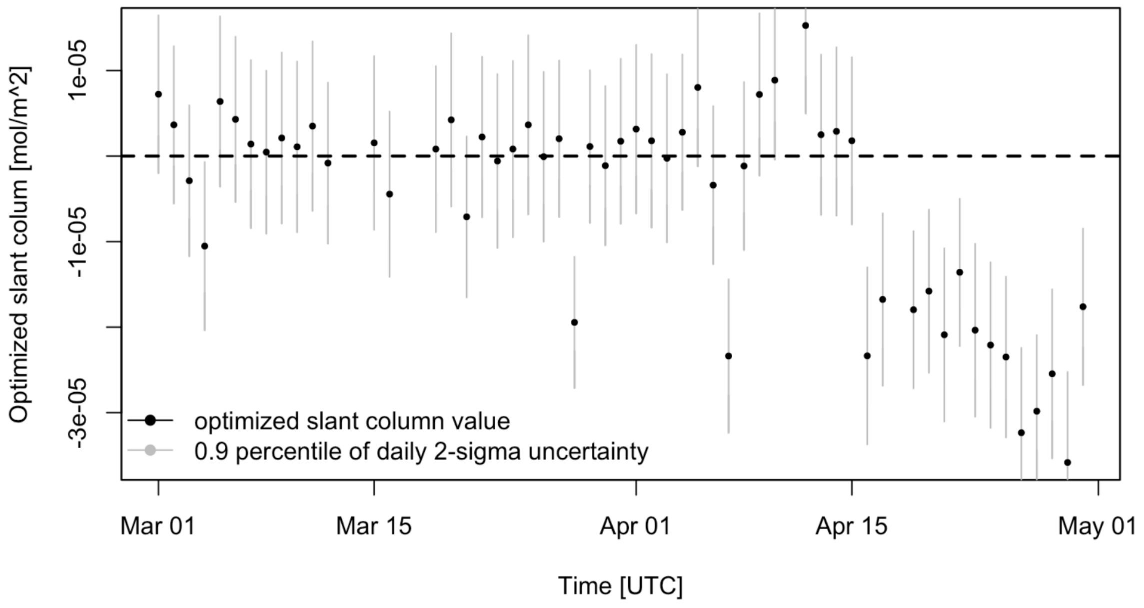


Figure Optimized slant column amount

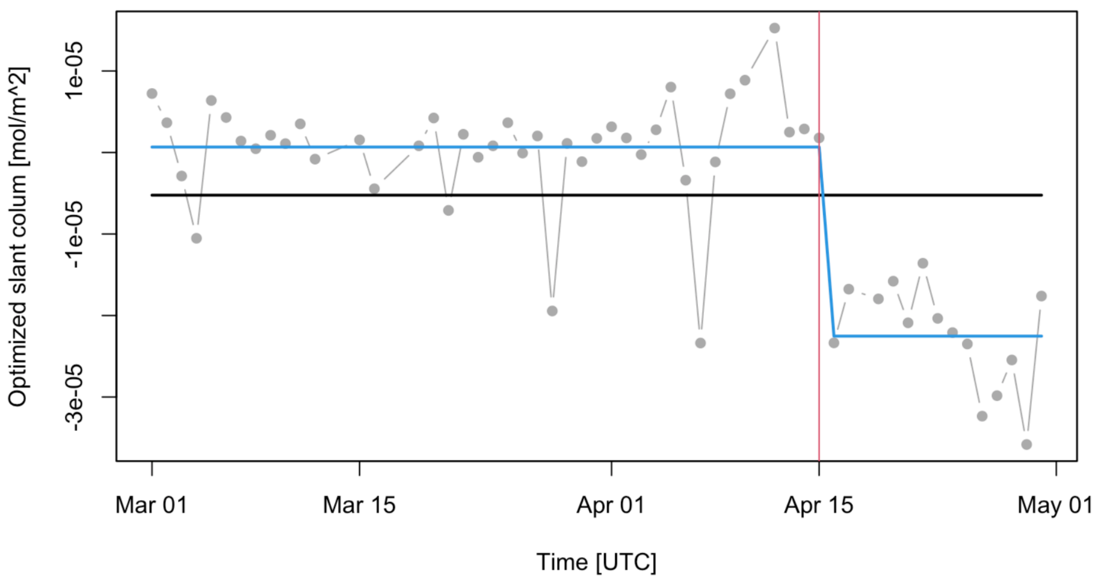


Figure Breakpoint analysis of optimized slant column amount: Black line illustrates a constant fit, the red line the introduced split, and the blue curve the two new constant fits.

The Figure Optimized slant column amount presents the obtained SC_{opt} for the time period from March 1st to May 1st 2023. The values are jumping around zero well within the reported 2-sigma uncertainty, which changes its pattern on April 15th. Furthermore, the date of such a sudden change can be detected with the break point analysis (TN on Data Quality Flagging Generic Procedure Evolution), as illustrated in Figure Breakpoint analysis of optimized slant column amount.

5 Strategies in Development

5.1 Residual Correlation-Based Flagging

The implemented quality flagging criteria used by the BSS are already well-evolved to put a label on each retrieval product. However, unknown sources impacting the DQ, present an exceptional group of issues that have to be considered. An issue which affects the retrieval output, and the DQ is falsely labeled as high quality, must be avoided.

A good proxy to assess the data quality is given by the wrms. It is a measure of how good the model agrees with the measurements. The wrms is expected to be as good as possible at the time of the selected reference, and in particular at small solar zenith angles. Consequently, when the solar zenith angle increases, the wrms is expected to increase as well due to effects not properly accounted for in the model. Therefore, the ideal wrms illustrate an U-shape (top graphic in Figure wrms cases) over the day.

If the wrms does not behave as expected, and changes over the day or season cannot be associated with changes in atmospheric conditions, instrumental features might be considered.

Such unusual behavior are exemplarily shown in Figure wrms cases, middle and bottom graphic. Both, the wiggly (oscillating) and flipped (inverse U) daily course of the wrms indicate a potential problem. However, it does not necessarily mean that it also affects the final retrieval output (e.g. total column NO_2). Therefore, it would be needed to correlate if such unexpected patterns are also propagated into the final data product.

A simple wrms threshold as used in QP1 is not feasible, as the overall baseline wrms can change over the season. Moreover, a fixed threshold is even more difficult to be defined for the flipped wrms. Therefore, it will be tested how to detect such cases already along the spectral fitting process, and correlate changes in the spectral residuals with potential changes in the final data product.

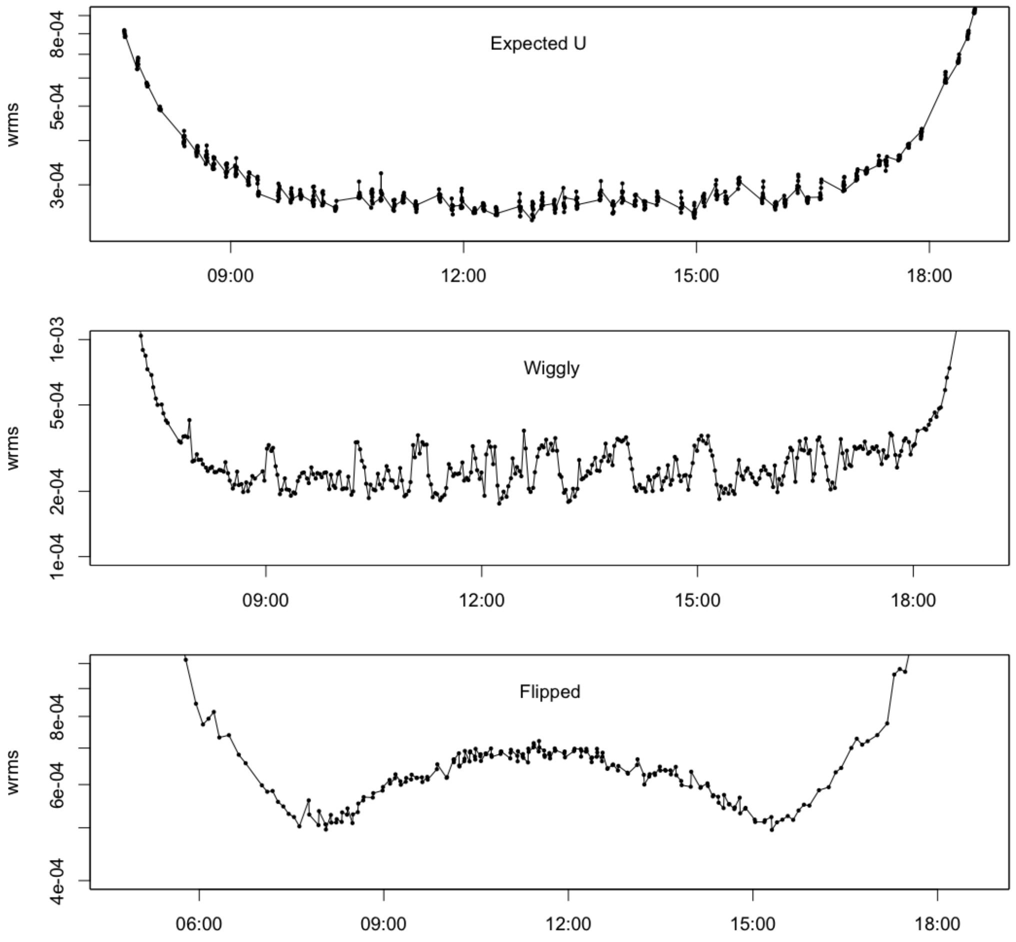


Figure wrms cases: daily timeseries of ideal U-shape (top), wiggly wrms (middle), and flipped (bottom).

5.2 Data Quality Marker

Data quality issues can have different origins which affect a PGN data product, which can be difficult to identify. The QI's used for single retrievals as part of QP1 provide already a very good first guess flagging, based on thresholds for each QI. However, these thresholds are PGN-generic and might not be instrument-specific and, therefore, not properly flagging affected periods. In exceptional cases, it is possible that none of the QI's from QP1 is capturing a quality issue. Nevertheless, most of the QI's have an expected characteristic and daily course. Together with other data products and their QI's, timeseries analysis, and derived quality parameters, it is possible to identify quality issues, by matching the observations with the expectation.

As an example, *losing the sun-alignment ('A')* for direct sun measurements shows up differently in the L2 data, compared to a *loose fiber on the spectrometer site ('B')*. While 'A' is seen in a sudden drop of the mean counts in the fitting window, 'B' is changing the illumination angle into the spectrometer and can show up in slit function related parameters, such as wavelength shift or resolution changes. But both examples would reveal enhanced wrms values in the spectral fitting. Examining the evolution of the wrms solely, is therefore not conclusive to understand the underlying problem, wherefore QP2 and QP3 are becoming even more important in this context.

This knowledge and pattern recognition allows us to label a period that has a dedicated problem, which we call a marker. The linkage between unusual behaving QI's and a marker is crucial to recognize an issue. But most importantly, the further linkage of a marker to a needed action, has to be defined, in order to solve an issue as fast as possible. While example 'A' requires the action of a new alignment, 'B' requires the fixation of the fiber on the spectrometer side. Both cases need some remote or local interaction with the instrument to collect proper L0 data again. Additionally, it is suggested to flag such problematic periods if needed as part of the quality assurance.

The concept of *affected quality indicator -> marker -> action* is therefore scalable in different ways:

- New QI's can be introduced to fine-tune a marker-definition which helps to separate markers:
  - QI from different official data products or quality products,
  - from derived QI, such as the difference of $TotNO_2$-$TropNO_2$,
  - from different processing levels: L2 ,L2Fit, L1, L0,
  - from calibration analysis output, such as magnitude of filter sensitivities.
- Multiple layers of needed actions can be introduced for different purposes:
  - Hardware interaction: e.g., cleaning entrance window, fiber alignment, fiber fixation,
  - remote access: e.g., re-alignment,
  - QA: QF of falsely labeled high quality data,
  - calibration analysis: e.g., change reference day, repeat wavelength calibration.

By feeding a database with this concept, one obtains a so-called marker network, as illustrated in the data quality marker network, where markers (blue) are linked via common quality indicators (red). Ultimately, each marker is perfectly specified by unique QI's, and having its own action(s) needed (green). Until this stage is reached, it is possible to derive a probability of observing a certain marker, conditional on the affected quality indicators.

Each marker description follows a standardized format to ensure clarity and consistency. The structure includes the following sections:

1. Description: A brief overview of the marker, describing the specific issue or anomaly.
2. Characteristics: Detailed observations and patterns associated with the marker, including how the issue affects quality indicators.
3. Potential Problem: A list of potential sources or causes of the problem.

4. Affected Quality Indicators: Specific quality indicators that are impacted by the issue. Hereby, the notation follows the idea of a unique identifier for blickP related output:
   - processing level (e.g. L2 -> rcode)
   - data product (e.g. HCHO from direct sun -> fus5)
   - processor version (e.g. p1-8)
   - output column (e.g. vertical column HCHO -> vc_HCHO)
5. Needed action category: Recommended actions to address the problem, categorized into the following groups:
   - HI (Hardware Interaction): Actions involving physical interaction with the instrument, such as checking fiber connections.
   - RC (Remote Check): Actions that can be performed remotely by network operators to verify and resolve issues.
   - QF (Quality Flagging): Steps to flag and document data quality issues for further analysis, which is defined by quality flags 20,21,22
   - CA (Calibration Analysis): Procedures required for calibration and ensuring the accuracy of the instrument's measurements.

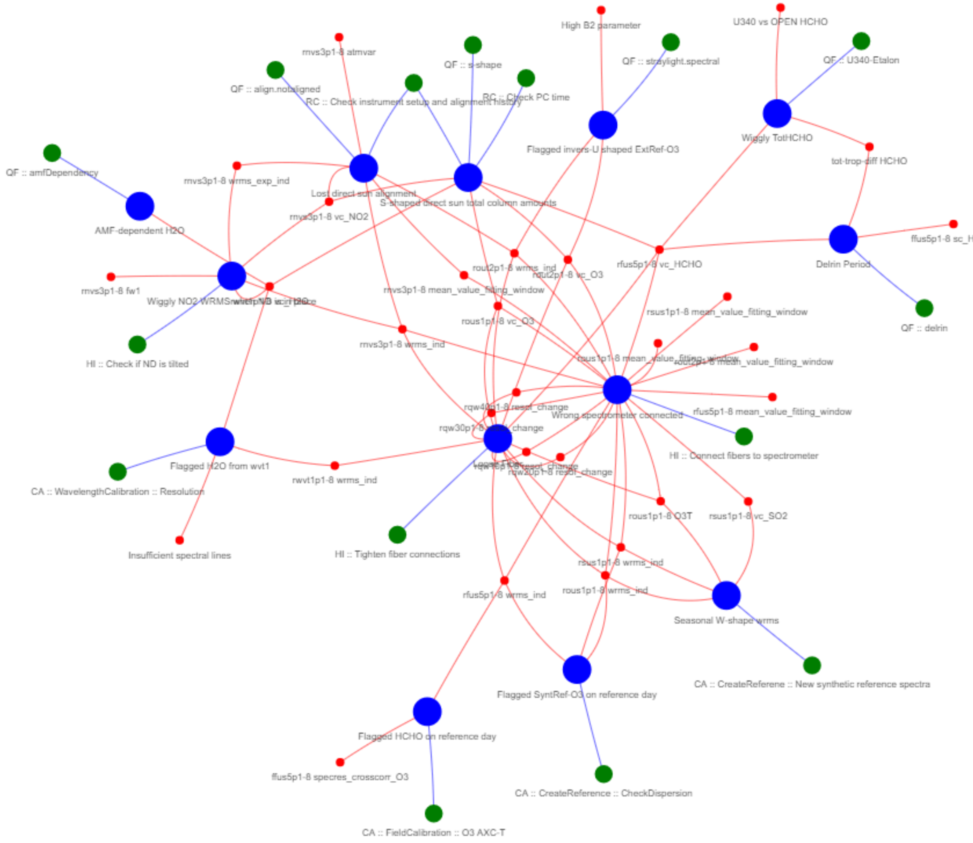


Figure Data quality marker network: quality indicators (red), markers (blue), actions (green)

This structured approach helps in systematically identifying, understanding, and resolving data quality issues. Already identified and documented markers are listed in Appendix 6.1 Data Quality Markers.

As illustrated in the data quality marker network, severe issues such as a loose fiber, are visible in many QI's, and therefore difficult to be separated from others. However, the probability of having such a marker is small if only 1 out of 10 specified QI's is affected. Another marker, which is perfectly specified by this single QI, is therefore the most likely source to describe why the data behave as they do.

This categorization and probability-based ranking serves as a decision-tree to support the calibration team, quality assurance / quality control team, in their routine business.

6 Appendix

6.1 Data Quality Markers

6.1.1 S-Shaped Direct Sun Total Column Amounts

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
Apparent S-shape in direct sun column amounts showing extraordinary unrealistic values that can range, e.g., 100-800 DU O_3 in a single day. It starts either unrealistically low or high and has an S or mirror-S shape.	• Observation: The most reasonable explanation is a wrong SZA/AMF calculation due to an incorrect PC time used, which is saved in the L0 file. Although the instrument can align with the sun using a proper alignment file, the SZA calculation is based on the date and time of the year. Therefore, using the wrong time causes the vertical columns to be wrongly calculated, although the slant columns are correct. • Impact: There might be cases (e.g., P25s1 HoustonTX) where this marker is also associated with a bad alignment, visible in the mean counts inside the fitting window.	• Wrong PC time used.	• rout2p1-8 vc_O3 • rous1p1-8 vc_O3 • rfus5p1-8 vc_HCHO • rnvs3p1-8 vc_NO2 • rwvt1p1-8 vc_H2O	• Quality Flag: QF :: s-shape • Remote Check: RC :: Check instrument setup and alignment history • Remote Check: RC :: Check PC time

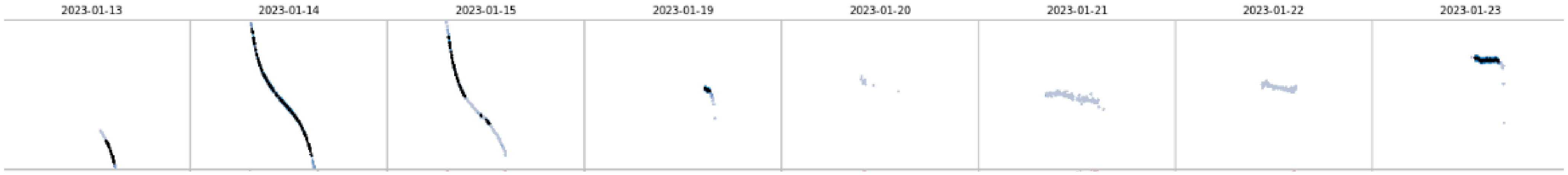


Figure S-shape in direct sun total column amount O_3

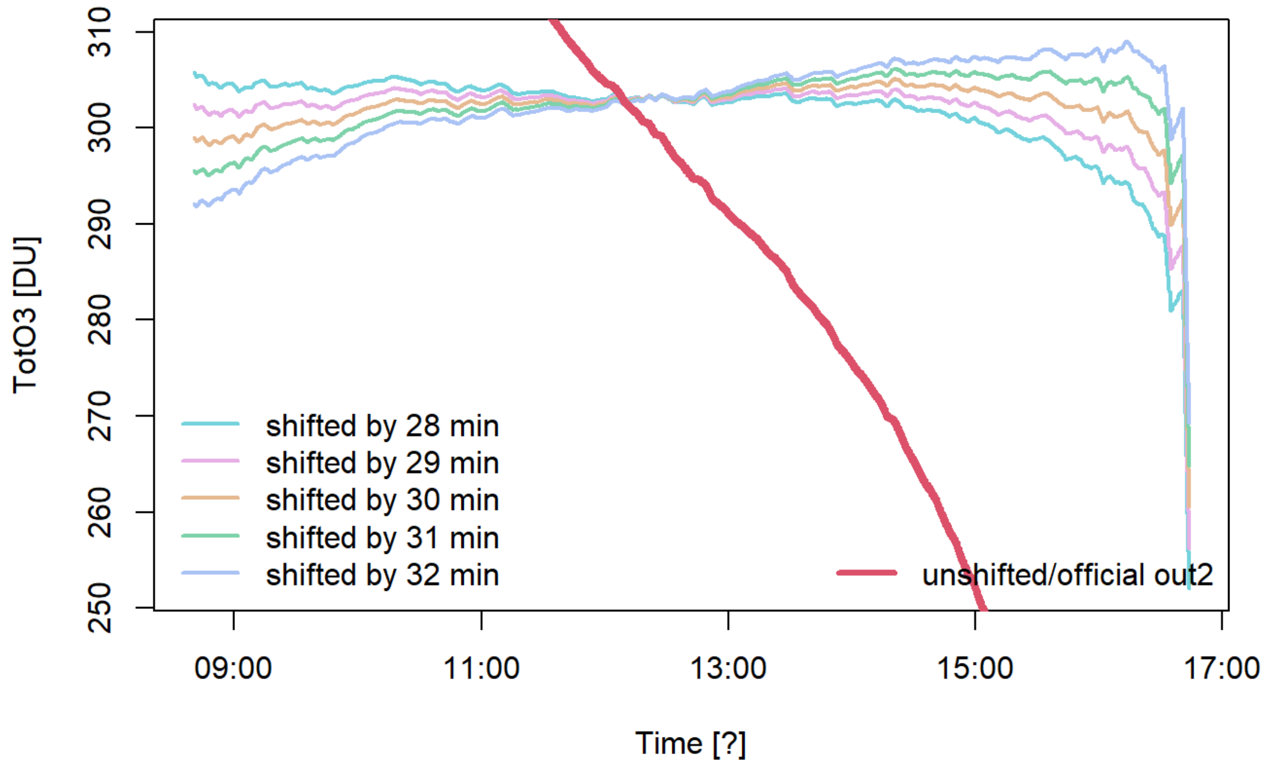


Figure S-shaped O_3 time-shifted

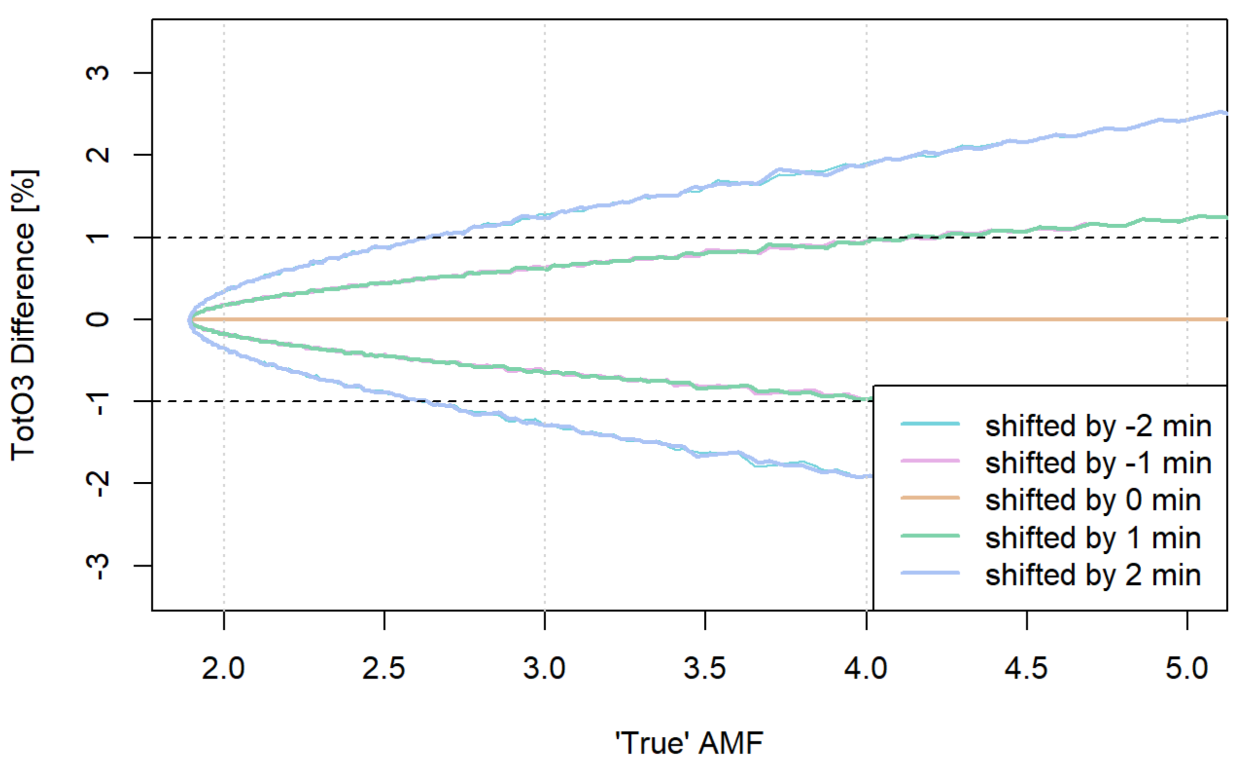
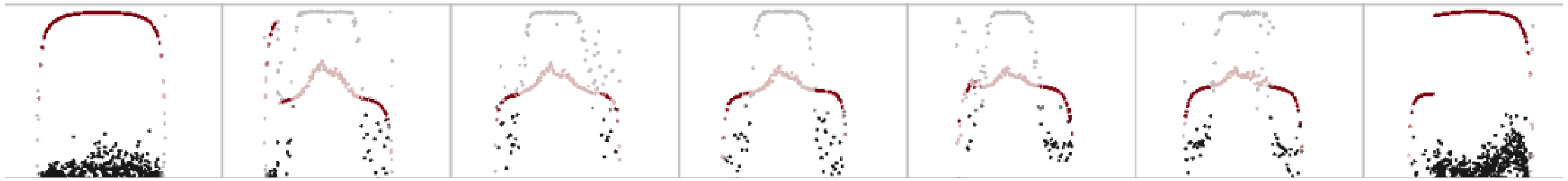


Figure Relative O_3 difference as a function of AMF

6.1.2 Lost Direct Sun Alignment

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
This marker indicates a loss of alignment during direct sun measurements.	• Observation: A noticeable sudden drop in counts within the mean counts of the fitting window. This affects multiple Quality Indicators (QIs), with the primary QI being the "mean counts inside the fitting window." • Pattern: Typically, this QI shows an upper envelope of the counts with a daily maximum around noon. By comparing this daily baseline to previous or subsequent days and analyzing the typical daily shape, structural changes become apparent. • Impact on QI: Other QIs are also impacted, and quality flags may be raised if certain quality limits are exceeded.	• The tripod is hit, causing the alignment history to be incorrect. • The alignment history is lost or deleted. • The tracker is stuck in a certain position due to incorrect cable layout, preventing movement. • The tracker motor (FLIR tracker) loses steps.	• rout2p1-8 wrms_ind • rnvs3p1-8 vc_NO2 • rnvs3p1-8 wrms_ind • rnvs3p1-8 wrms_exp_ind • rnvs3p1-8 atmvar • rnvs3p1-8 mean_value_fitting_window	• Quality Flag: QF :: align.notaligned • Remote Check: RC :: Check instrument setup and alignment history



6.1.3 Figure Lost alignment period showing mean counts inside fitting window (red) and atmospheric variability (black)

6.1.3 HCHO Outgassing of Delrin Components

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
HCHO outgassing from Delrin components affects direct sun HCHO retrieval (rfus5p1-8).	• Observation: Direct sun total column HCHO amounts show a pronounced daily cycle, particularly in summer when head sensor temperatures are high. This temperature increase causes internal HCHO release from Delrin components. • Pattern: The outgassing is visible as a linear increase in the slant column throughout the day. Additionally, there is a pronounced disagreement with the sky data product, which is not systematically biased and varies significantly from day to day. • Impact: The Delrin issue was identified in spring 2019. By summer 2019, SciGlob conducted initial tests with new filter wheels. From autumn 2019 onward, either new units were built with Nylon, or existing instruments were upgraded.	• Delrin filter wheels.	• rfus5p1-8 vc_HCHO • rfus5p1-8 sc_HCHO • tot-trop-diff HCHO	• Quality Flagging: QF :: delrin

6.1.4 Wrong Spectrometer Connected

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
This marker indicates that the wrong spectrometer is connected, leading to various issues with data quality. This marker is only relevant for Pandora 2S systems.	• Observation: A range of anomalies in data quality indicators due to the incorrect spectrometer being connected. This includes significant deviations in various parameters, since the measured optical setup is not equal as characterized in the laboratory. • Pattern: The quality indicators display unusual patterns, such as incorrect values and inconsistencies that suggest misconfiguration. This can range from enhanced spectral fitting residuals, unrealistic daily shapes and total columns amounts, AMF-dependencies for daily courses. • Impact on QI: Multiple quality indicators are affected and exceed quality limits, showing discrepancies that can be traced back to the wrong spectrometer connection. In particular slit function related parameters as the retrieved resolution change, and in-proper filterwheel transmission.	• Fiber connected to the wrong optical path	• rout2p1-8 vc_O3 • rout2p1-8 wrms_ind • rout2p1-8 mean_value_fitting_window • rous1p1-8 vc_O3 • rous1p1-8 wrms_ind • rous1p1-8 mean_value_fitting_window • rous1p1-8 O3T • rsus1p1-8 vc_SO2 • rsus1p1-8 wrms_ind • rsus1p1-8 mean_value_fitting_window • rfus5p1-8 vc_HCHO • rfus5p1-8 wrms_ind • rfus5p1-8 mean_value_fitting_window • rnvs3p1-8 wrms_ind • rnvs3p1-8 mean_value_fitting_window • rqw10p1-8 resol_change • rqw20p1-8 resol_change • rqw30p1-8 resol_change • rqw40p1-8 resol_change	• Hardware Interaction: HI :: Connect fibers to spectrometer

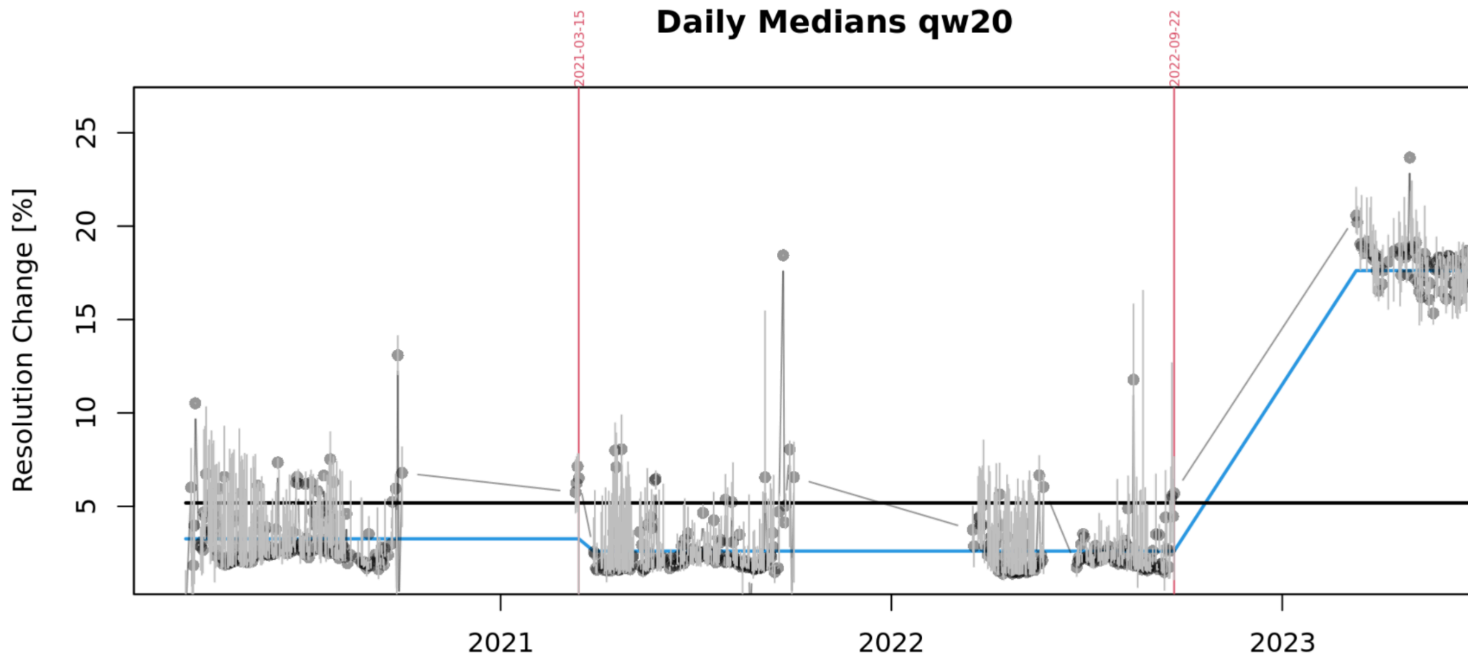


Figure Retrieved resolution change for wrong spectrometer connected

6.1.5 W-shape wrms on Reference Day

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
This marker describes the incorrect usage of a too high dispersion polynomial (npol=31 or 35) during the calibration analysis, mostly affecting UV retrievals (ous1, sus1) using the synthetic reference, resulting in most data being flagged out on the reference day.	• Observation: The flagging is primarily due to the wrms exceeding quality limits and /or showing flipped wrms . Case studies (e.g., P211 Agam) show that UV products like SO2 and O3 exhibit an enhanced W-shape of the wrms, as described in Figure wrms cases. It is also possible to observe a W-shape in the HCHO, but it is less affected since the fitting window is not at the lower end of the dispersion polynomial. • Pattern: The problem arises during the CreateReference action CheckDispersion when merging U340+DIFF and OPEN. The transition zone is "overfitted" due to the high polynomial, causing boundary effects impacting UV retrievals down to 305nm (O3 and SO2). Retrievals using the literature reference are not affected since it simply maps pixels to wavelengths, but the synthetic reference becomes incorrect.	• Dispersion polynomial set too high.	• rous1p1-8 wrms_ind • rous1p1-8 O3T • rsus1p1-8 vc_SO2 • rsus1p1-8 wrms_ind	• Calibration Analysis: CA :: CreateReference :: New synthetic reference spectra

6.1.6 AMF-dependent TotO3 from Literature Reference

Description	**Characteristics**	**Potential Problem**	**Affected Quality Indicators**	**Needed Action Category**
Pronounced inverse-U shape for the out2p1-8 vertical column amount.	A strong inverse-U shape, which typically goes in-line with an enhanced wrms well above the quality thresholds, so that no high quality data are given. If the calibration analysis also reveals a high B2 parameter at 325nm, the issue is related to spectral straylight, which is not corrected in p1-8. Therefore, explicit flagging is applied here. The pattern can also be obtained by in-field slit function changes, which does not therefore match the one characterized one anymore.	• uncorrected straylight in the calibration analysis • strong resolution changes	• rout2p1-8 vc_O3 • rout2p1-8 wrms_ind • B2@325nm	• Quality Flag: QF :: spectral.straylight

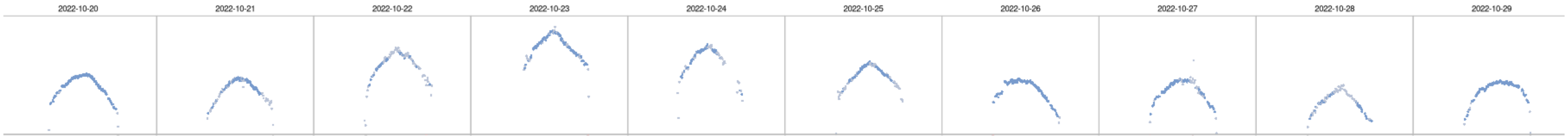


Figure Spectral straylight impact on total O3 column retrieved from literature reference: daily course of total column amounts for P209s1 Izana.

6.1.7 AMF-dependent TotH2O from Literature Reference

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
Repetitive amf-dependent total H2O daily course (rwvt1p1-8) not visible in sky data (rnvh3p1-8).	The ExtRef totH2O product (rwvt1p1-8) shows an amf-dependent daily course , repeating for many consecutive days or generally for the entire timeseries. In addition, this is typically not seen by the sky data product.	• In-proper sensitivity/ absolute calibration not captured by low order smoothing polynomial • In-proper resolution characterization at 500nm which is inside the fitting window of rwvt1p1-8 • strong resolution changes in the field • straylight	• rwvt1p1-8 vc_H2O • rwvt1p1-8 wrms • A2@500nm	• Quality Flag: QF :: amfDependency • Calibration Analysis: CA :: WavelengthCalibration :: Resolution

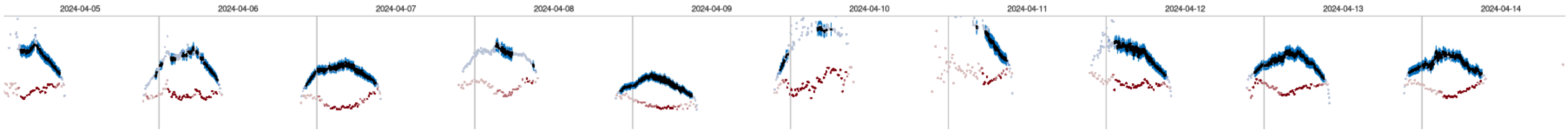


Figure AMF-dependent TotH2O columns for Incheon-ESC: high quality TotH2O (black dots), total uncertainty (blue bars), TropH2O (reddish dots).

6.1.8 Flagged TotHCHO on Reference Day

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
This marker describes a wrong O3 temperature obtained in the calibration with AXC-T. HCHO of fus5 is flagged (entirely) on the reference day.	HCHO wrms (rfus5p1-8) is not showing the expected U-shape wrms expected to go down to 1-2e-4 on the reference day. Instead it is either U-shaped exceeding the quality limits. Or there might be cases, which show a W-shape wrms. Looking into the spectral residuals, the reason for the high wrms is found in the O3 residuals, which are related to a wrong O3 temperature coming out from the O3 AXC-T calibration. The HCHO fitting window uses a climatological temperature in the retrieval. If this climatology is strongly different to the O3 temperature on the reference day, these residuals might show up.	• Wrong O3 temperature from the AXC-T • Uncorrected spectral straylight impacting the AXC-T	• rfus5p1-8 wrms_ind • ffus5p1-8 specres_crosscorr_O3	• Calibration Analysis: CA :: FieldCal :: AXC-T

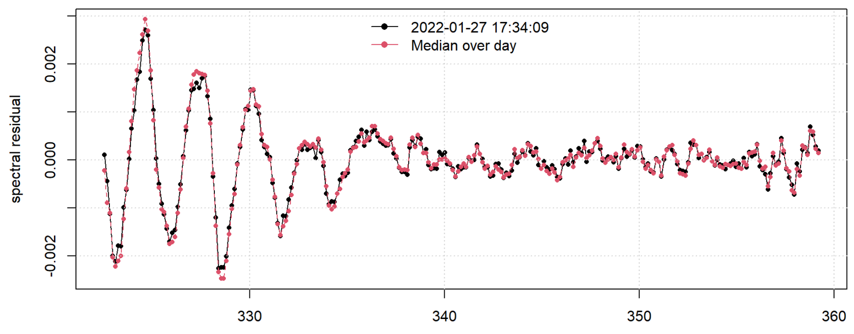


Figure Spectral O3 signal in rfus5p1-8 on reference day

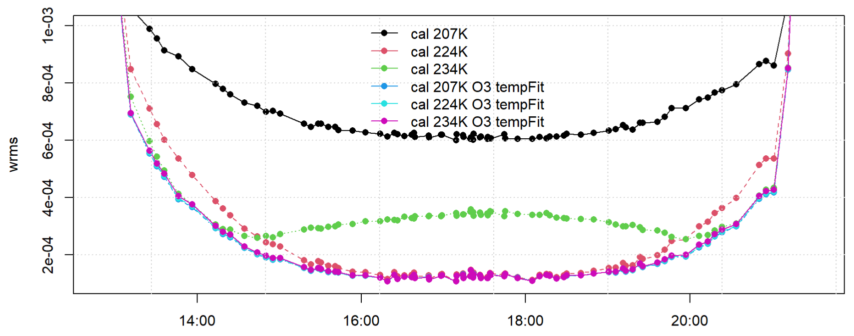


Figure rfus5p1-8 wrms pattern for different O3T reference temperatures

6.1.9 Condensation inside spectrometer

Description	Characteristics	Potential Problem	Affected Quality Indicators	Needed Action Category
This marker describes a critical situation when the spectrometer has water deposits on the optical elements.	H_2O Condensation in the spectrometer describes a severe impact on all retrievals due to deposit on the optical elements of the spectrometer. Typically, such a problem is visible in all data products and all quality indicators which show a drifting change over time. In particular, a strong resolution change in the quality window retrievals (qw) can be observed, as illustrated in Figure Condensation in the spectrometer.	• Instrument running at wrong temperature so that condensation can occur (e.g. too cold in very warm and humid environments) • Instrument exposed to strong varying daily conditions, either outdoor or indoor without air conditioning	• rnvs3p1-8 wrms_ind • rqw10p1-8 resol_change • rqw20p1-8 resol_change • rqw30p1-8 resol_change • rqw40p1-8 resol_change • rout2p1-8 wrms_ind • rout2p1-8 vc_O3 • rfus5p1-8 vc_HCHO • rfus5p1-8 wrms_ind • rwvt1p1-8 wrms_ind • rsus1p1-8 wrms_ind • rous1p1-8 wrms_ind • rous1p1-8 vc_O3 • rous1p1-8 O3T	• Hardware interaction: HI :: Sent back to manufacturer • Quality Flag: QF :: condensation

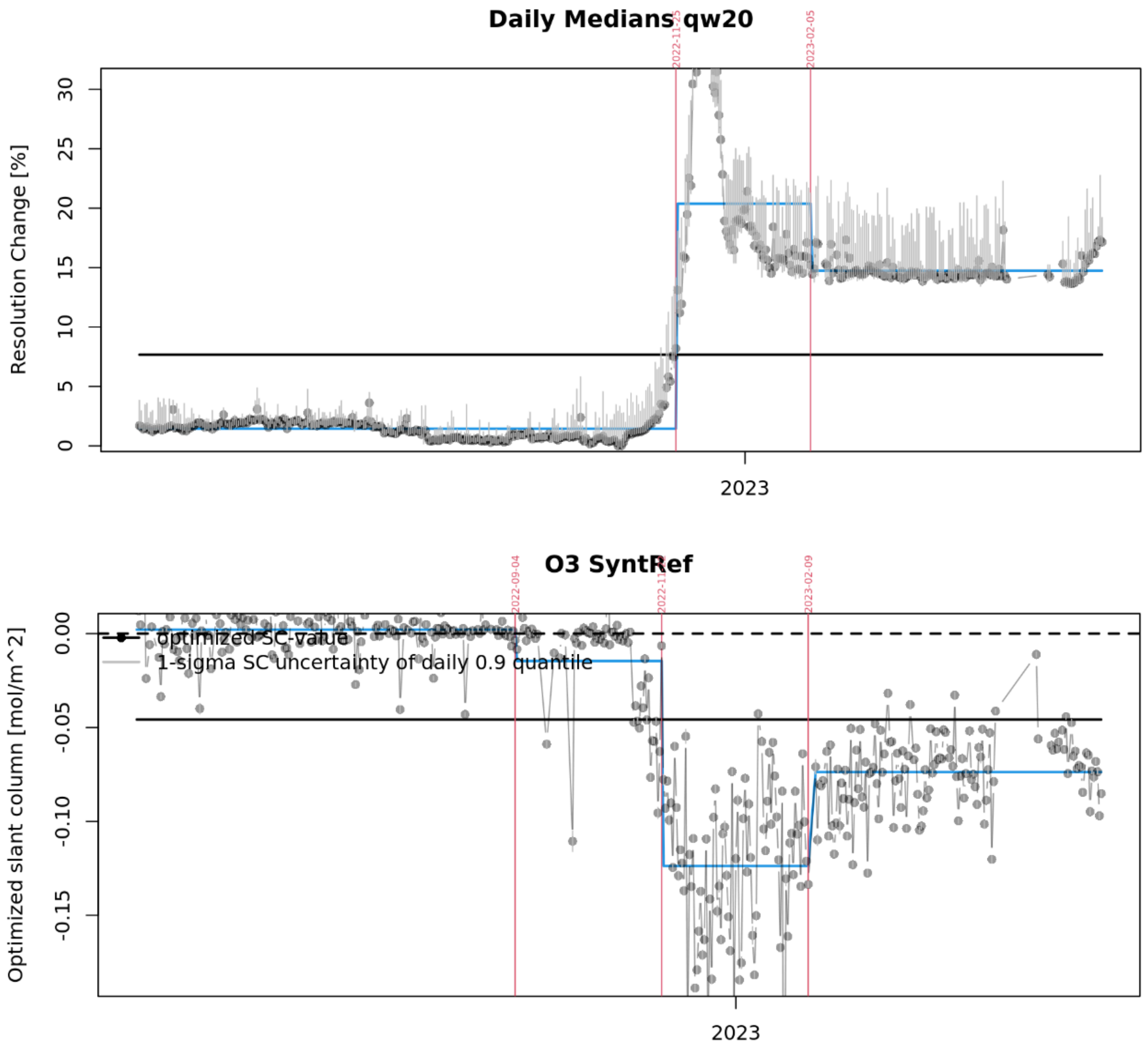


Figure Condensation in the spectrometer: P198s1 Kobe resolution change (top) between 350-420nm, and observed air mass factor dependency for direct sun total column O_3, expressed as the optimized slant column amount

6.1.10 Loose Fiber

Description	Characteristics	Potential Problem	• Affected Quality Indicators	Needed Action Category
This marker describes the situation of a loose fiber on the spectrometer side.	Loose fibers are affecting almost all data products and all quality indicators in a similar way as a wrongly connected fiber or condensation in the spectrometer, and represent a critical issue which needs to be solved immediately. In contrast to condensation, a loose fiber is typically visible in sudden jumps of a timeseries, most dominant in the resolution change of the quality windows, well above 10%. If properly connected, an immediate change back to an expected resolution change close to 0 can be observed. Typically all wrms quality thresholds are exceeded and jump back to lower values once the fiber is in its expected position, as marked by the lab personal.	• Fiber not properly tightened on the spectrometer side	• rnvs3p1-8 wrms_ind • rqw10p1-8 resol_change • rqw20p1-8 resol_change • rqw30p1-8 resol_change • rqw40p1-8 resol_change • rout2p1-8 wrms_ind • rout2p1-8 vc_O3 • rfus5p1-8 vc_HCHO • rfus5p1-8 wrms_ind • rwvt1p1-8 wrms_ind • rsus1p1-8 wrms_ind • rous1p1-8 wrms_ind • rous1p1-8 vc_O3 • rous1p1-8 O3T	• Hardware interaction: HI :: Tighten fiber connections • Quality Flag: QF :: loose_fiber

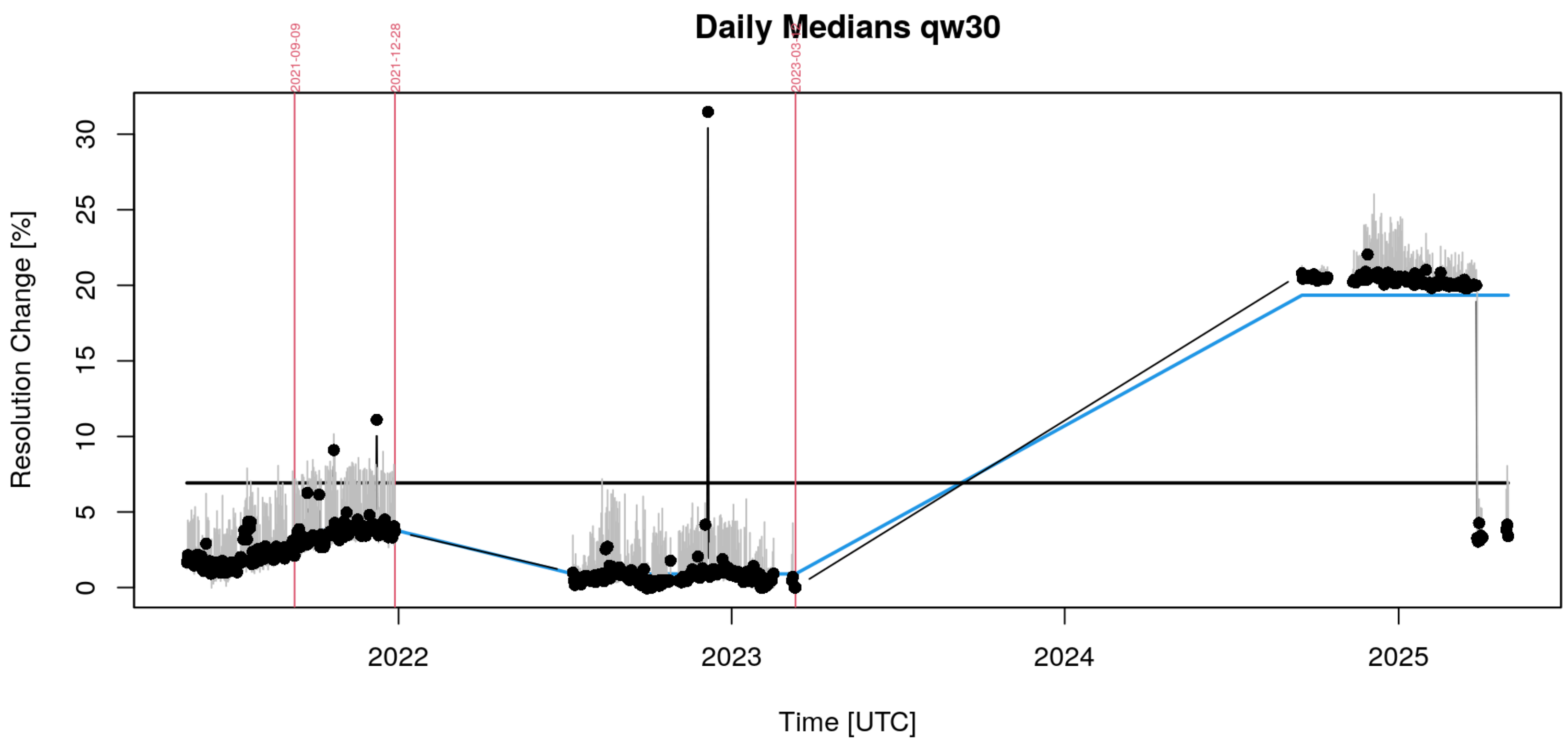


Figure Loose fiber: P40s1 WallopsIslandVA

6.1.11 Spectral Lamp Feature Lab MUI

Description	**Characteristics**	**Potential Problem**	**Affected Quality Indicators**	**Needed Action Category**
This marker describes a situation where a spectral feature in the L0Lab data occurs either in the L3 or in the L7 routine when a FEL-O lamp was used for Lab measurement.	If a lab measurement has been taken with a FEL-O lamp at the MUI lab in Innsbruck, a small bump or irregularity in the count rate (CCR) appears between pixels 880 and 920 in the L3 routine or, if the lamp has also been used in L7, between 393nm and 397nm. This is caused by the lamp itself, which has Aluminium emission lines. and has to be treated differently depending on whether it occurs in L3 or L7 analysis. Therefore, two action categories are defined to deal with the feature. If the spectral feature occurs in the L3 routine: Follow the feature as closely as possible. If a different lamp has been used in L7, it shouldn't be visible there anymore. You can look up which lamp was used	FEL-O Lamp of MUI Lab in Innsbruck having Al emission lines	• AnalyzeBright spectral feature for Innsbruck LabL0 • SensitivityCalibration spectral feature for Innsbruck LabL0	Calibration Analysis: CA :: AnalyzeBright :: PRNU :: Follow feature CA :: SensitvityCalibration :: Cut feature

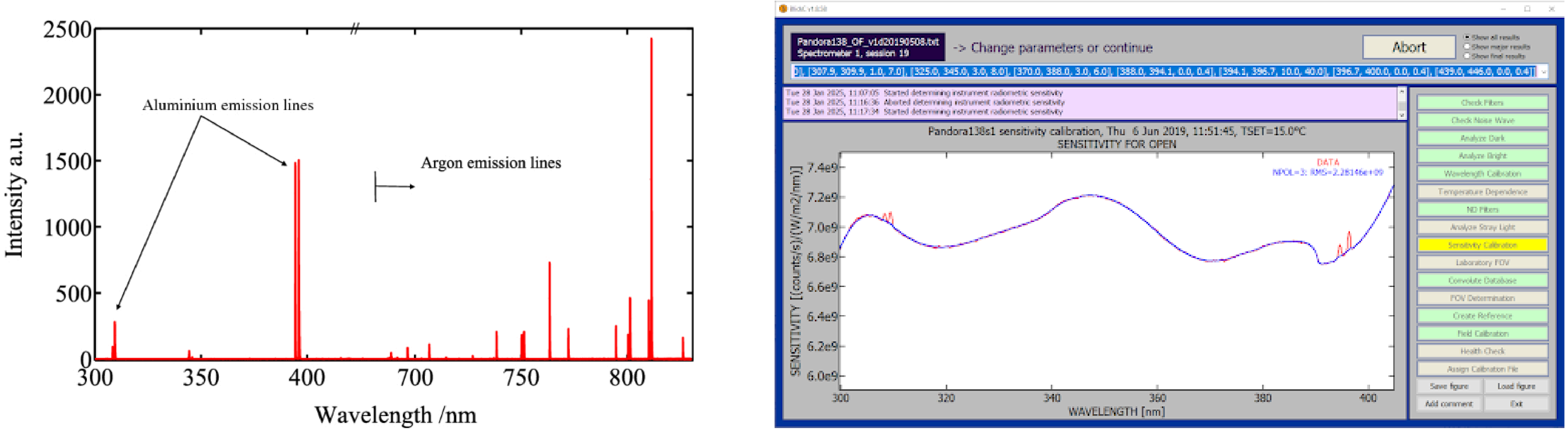


Figure Aluminium emission lines (left) observed during calibration analysis for P138s1