Product Quality README file for SCIAMACHY Level 1b version 8.0X dataset

Field	*Content*
Document Title	Product Quality Readme file: SCIAMACHY Level 1b version 8.0X dataset
Reference	ENVI-GSOP-EOGD-QD-16-0140, issue 1.0, 31/03/2016
Abstract	This document describes the major fields of improvement in the SCIAMACHY Level 1 baseline version 8.0X compared to previous version 7.0X, and details the Level 1b data set version 8.0X resulting from the full mission reprocessing campaign completed in 2016.
Applicability	This README file applies to the latest SCIAMACHY Level 1b consolidated products (SCI_NL__1P) generated with ESA processor baseline versions 8.01 and 8.02. The data set covers ENVISAT orbits from 02 August 2002 (orbit 2204) to 08 April 2012 (orbit 52867), and presents an upgraded processing stage flag "Y" (replacing the previous set of products with flag "W").
Reference Documents	[RD1] Input / Output Format (IODD): ENVISAT-1 SCIAMACHY Level 0 to 1b Processing, ENV-TN-DLR-SCIA-0005, issue 8, 2014. [RD2] Algorithm Description (ATBD): ENVISAT-1 SCIAMACHY L0-1c Processor Algorithm Theoretical Baseline Document for processor version 8, ENV-ATB-DLR-SCIA-0041, Issue 6, 2014. [RD3] ENVISAT-1 Product Specification: PO-RS-MDA-GS-2009, Volume 15, Issue 3M, 2016. [RD4] ENVISAT-1 Product Specification: PO-RS-MDA-GS-2009, Volume 05, issue 3E. [RD5] SCIAMACHY Command Line Tool Software User's Manual (SUM), ENV-SUM-DLR-SCIA-0071, issue 3C, 2015. Documents can be downloaded here.
Filled by	SPPA Engineer
Change log	The table below records history and status of the Product Quality Readme file.

Issue	Date	Change
1.0	31/03/2016	First release for new dataset version 8.0X

Content

Level 1 processor versions 8

The implementation of processor version 8 was completed after the end of the operational phase of the ENVISAT mission (April 8th 2012) and was used in the first post-operational data reprocessing campaign by ESA.

Within this document, the version of a processor baseline is often indicated with generic version number N.0X, pointing to the set of processors developed starting from baseline N.00 as natural evolution of the planned implementation, with possible baseline integrations fixing bugs and inconsistencies until a new major update with baseline version number N+1 is reached. For the current Level 1b baseline, version 8.0X indicates processor versions 8.00, 8.01, and 8.02.

The following algorithm changes have been implemented in the Level 1b version 8.01 processing baseline, compared to version 7.0X (see also ***Table 1***):

- As ENVISAT entered its post-operational phase (F), ESA reviewed the processor development strategy, removing the industrial implementation of the processor into the so-called Instrument Processor Facility (IPF). The instrument prototype processor (IPP) developed by DLR was thus chosen to become the "operational processor".
- The stray light matrix approach is extended to channels 3-8 leading to an improved stray light correction.
- The memory effect correction (MEC) for limb data is improved, correcting the estimate for the signal of the reset readout at new tangent heights. This is especially significant for measurements above 40 km tangent height.
- The scaling factor used for the non-linearity correction (NLC) for co-added data is corrected. In the previous version the NLC was wrongly calculated, when PMD signals were affected by high noise.
- The hot pixel correction for limb dark measurements is completely revised leading to more reliable results.
- The polarisation correction for occultation is switched off, since no reliable calibration data exist for this case, and since no significant amount of polarisation is expected in this mode.
- The states used for the dark calculation can now be selected in the configuration file. This is important for channel 8. Now only dark states with pixel exposure times between 0.125 and 1 second are used.
- The radiometric calibration uses a new approach: a physical model of the scanner unit including contamination layers (the scan mirror

model).

- The radiometric key data and the polarisation key data are updated from on-ground calibration data and adapted for the scan mirror model.
- The degradation is calculated using the scan mirror model that provides a scan angle dependent degradation correction. The degradation is now corrected in the Level 1 processing via m-factor application as part of the radiometric calibration.
- The mean PMD values contained in the product are now degradation corrected.

Item	Improvement	Affected channel
Stray Light	Matrix Approach extended	3-8
MEC	Correction improved for Limb data	1-5
Hot Pixel Detection	Improved Limb darks	All
Dark calculation	Dark states used are configurable	8
Key data update	New, consistent calculation	All
Radiometric calibration	Scan mirror model implemented	All
Degradation correction	Scan mirror model leads to scan angle dependent correction	All
Mean PMD values	Values are corrected for degradation	All PMDs

Table 1: Improvements for SCIAMACHY IPP version 8.01

A fix for processing baseline version 8.01 became necessary after it was discovered that corrupted or incomplete states within Level 0 products were transferred into Level 1b data. A new version of the SCIAMACHY Level 1 processor (IPP v8.02) was developed by DLR-IMF applying minor algorithms changes, and revising consistency checks on measurement states. IPP v8.02 drops corrupted states out of the resulting Level 1b products with behaviour similar to the version 7.04 processing.

Data Reprocessing

Data reprocessing is fundamental to improve the quality of existing data sets, and to generate coherent long-term series of geophysical parameters to be used for atmospheric applications, such as climate studies and trend analysis.

The SCIAMACHY consolidated Level 1b version 8.0X dataset is the result of the latest full-mission reprocessing campaign, completed in 2016. The new dataset represents the first complete reprocessing after the conclusion of the in-flight phase of the ENVISAT mission; it brings significant improvements to the quality of the Level 1b products with a new approach to compensate degradation. Figure 1 summarizes the history of the SCIAMACHY reprocessing campaigns, and positions the present 4th reprocessing campaign within the data processing evolution for the entire mission lifetime. Processing was performed using for the first time DLR Instrument

Prototype Processor: IPP versions 8.01 and 8.02. The reprocessed dataset covers the whole operational mission lifetime period, from the 2nd of August 2002 up to the 8th of April 2012. Users of SCIAMACHY Level 1b products are strongly recommended to migrate to the new reprocessed v8.0X dataset.

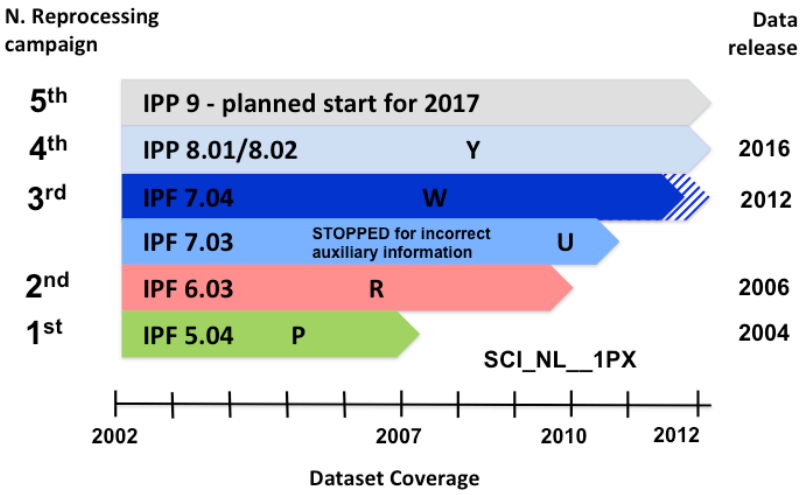

Figure 1 - History and details of the SCIAMACHY Level 1b reprocessing campaigns. The diagram reports for each reprocessing campaign the software version, the processing stage flag, the coverage, and the year of data release (on right side).

In general data reprocessing is performed as a single bulk processing for data over an entire mission, but, for its complexity, reprocessing is often accomplished in stages with post-processing activities (deltas) on limited subsets of data, integrating or correcting previous processing steps. This is the case of the SCIAMACHY version 8.0X dataset completed in three processing stages.

The initial reprocessing was accomplished at D-PAC for the full mission with baseline version 8.01. For the not negligible number of processing failures it was found that some Level 0 products require more than the 8 GB of RAM available at D-PAC; processing of specific orbits was thus successfully repeated in the development environment (DLR-IMF) on a 32 GB machine. In September 2015, a major issue was discovered in the SCIAMACHY Level 1b version 8.01 reprocessed data set. A significant number of Level 0 products containing incomplete states due to downlink or ground-station problems, resulted not compatible with the Level 1 version 8.01 processing generating incorrect Level 1b data. A new baseline was thus developed by DLR (IPP version 8. 02) introducing suitable patches to

- include state ID 67 measurements before July 20th 2003 having integration times incompatible with previous version 8 processing;
- fix states with missing scanner readouts (i.e. last geolocation missing);
- exclude truncated or perforated states;
- exclude measurements with a wrong combination of state ID and measurement category.

8288 SCIAMACHY Level 1b v8.01 products were identified as incorrect and required a corrective Level 0-1b delta reprocessing. As for the version 8.01 processing, data were generated both in the D-PAC (SCI_NL__1PYDPA*) and DLR-IMF (SCI_NL__1PYIMF*) environment due to different RAM requirements.

The new SCIAMACHY Level 1b dataset is the combination of products generated with baseline versions 8.01 and 8.02, and satisfying quality standards. ***Table 2*** reports the number of Level 1b products available for every year of the mission. In total 47715 products have been generated, with a total data volume of about 18 TB. An overview of the completeness of the SCIAMACHY consolidated Level 1b data set version 8.0X is provided here.

YEAR	L1b generated
2002	1789
2003	4689
2004	4972
2005	5042
2006	4773
2007	4966
2008	5120
2009	4987
2010	4966
2011	5052
2012	1359
	47715

Table 2: Number of SCIAMACHY Level 1b products (v8.01/8.02) obtained from the 4th reprocessing campaign.

The final dataset presents filenames characterizing the different processing stages of the reprocessing campaign, with different combinations of processing stage counter and processing centers.

SCI_NL__1PY**DPA**YYYYMMDD_HHMMSS_000000000000_00000_00000_**0000**.N1
SCI_NL__1PY**IMF**YYYYMMDD_HHMMSS_000000000000_00000_00000_**0001**.N1
SCI_NL__1PY**DPA**YYYYMMDD_HHMMSS_000000000000_00000_00000_**0002**.N1
SCI_NL__1PY**IMF**YYYYMMDD_HHMMSS_000000000000_00000_00000_**0002**.N1

Value 0000 identifies the first set of data generated at D-PAC with IPP 8.01, value 0001 identifies the corrective processing in the DLR-IMF 32GB environment with baseline 8.01, value 0002 distinguishes the processing with baseline version 8.02 both at D-PAC and DLR-IMF. ***Table 3*** presents the distribution of the Level 1b v8.0X products with respect to processing phase and processing center. Only one product per orbit is available in the Level 1b dataset.

center stage	DPA	IMF		IPP version
0000	39311	-	39311	8.01
0001	-	42	42	
0002	8281	81	8362	8.02
	47592	**123**	**47715**	

Table 3: Distribution of product types within the Level 1b v8.0X dataset.

Access to SCIAMACHY products can be provided to existing ESA Proposals and/or Registrations by contacting EO Helpdesk, or through a new user Registration on the ESA EOPI Portal.

The required storage space for the entire Level 1b version 8.0X dataset is 18 TB (uncompressed).

Processor Verification

The SCIAMACHY Quality Working Group and expert teams have verified the entire Level 1b dataset in order to ensure correct processing and content. Quality checks on the new Level 1b version 8.0X products revealed minor inconsistencies (listed in Section Known Processing Issues) that were not justifying baseline changes.

As part of the verification process required by ESA to assess the improvements obtained with the new processing baselines, a subset of orbits along the entire mission was selected in order to create a Diagnostic Data Set (DDS). These orbits (~5000) were processed up-to Level 2 products and were provided for inspection to the validation teams. Before commencing the Level 2 reprocessing of the full-mission, the DDS products were processed to Level 2 to permit QWG and validation teams to judge the quality of the finished products (evaluating the impact of Level 1 algorithm changes on the Level 2 products) and to verify the overall new SCIAMACHY processing chain: IPP 8.0X + SGP 6.0X. Validation reports were provided for the validation activities within the Multi-TASTE phase F project:

D. Hubert et al., Multi-TASTE Phase F Report “Delta-validation of SCIAMACHY SGP upgrade from V5.02 to V6.00”, TN-BIRA-IASB-MultiTASTE-Phase-F-VR1 issue 1, August 2015.

D. Hubert et al., "Multi-TASTE Phase F Final Report / October 2013 - December 2015", TN-BIRA-IASB-MultiTASTE-Phase-F-FR issue 2 revision A, 1 February 2016.

Both documents are available at
https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/cal/val/validation-activities/

Calibration options

Spectral Stray Light

The spectral stray light (channels 2-8) was initially described by means of focused ghosts and a uniform stray light component per channel. Fit residuals for ozone retrieval in channel 2 pointed towards residual stray light effects, clearest in the deep absorption lines and channel overlap region. As of version 8.0X, the spectral stray light for channels 2-8 is described as the sum of ghosts and non-uniform stray light in the form of a matrix.

Memory Effect

The memory effect correction (MEC) is an additive correction, which is applicable to data from channel 1 to 5, only. Physically, the actual readout of a detector pixel depends on its previous readout (memory). The amount of "memory" depends on the filling (i.e. the observed scene intensity). Due to an improved parameterization, former uncertainties for high dynamic range ground scenes could be removed. It is now accurate to ± 5 binary units [BU]. However, three situations remain, for which the memory effect can only be estimated:

- Memory effect of first readout in a state.
- Memory effect for the first limb readout at a new tangent height. The calculation for this case was corrected in version 8.0X and largely improved.
- Memory effect for co-added data.

In these conditions the correction is principally less accurate, because it depends on the previous readout, which is unknown in these cases; an associated error cannot be specified.

Non Linearity Effect

This effect, which is a pure infrared detector effect and which therefore only affects channels 6 to 8, was improved for co-added data: in the previous processor version, noise in the PMD data used to derive the correction for co-added data could lead to wrong correction value. This was corrected by discarding noisy PMD data before the calculation of the correction. Being an additive correction, it is very sensible to further Level 2 processing steps, which it helps to largely improve.

Dynamic Bad & Dead Pixel Mask

Due to the manufacturing of the IR detectors, individual pixels in the detector do not response or show an abnormal behavior (e.g. high noise or random change of the dark signal). During on-ground calibration, tests were made to identify those pixels. The result was put into a mask (DBPM) that shows for all pixels if they are usable (value 0) or if they are not (value 1).

After launch it was discovered that the IR detectors (especially channels 6+ to 8) were degrading with time, i.e. the number of abnormal pixels increased. The reason was most likely fast protons hitting the detector, when ENVISAT passed through the South Atlantic Anomaly (SAA) region. In the processor a dynamic bad pixel mask is included to account for the additional degradation. Note that the mask is still regarded as experimental and the retrieved products should be carefully inspected. Future versions of the processor will contain an improved mask.

Dark Signal Correction

For channels 1 to 5, no problems are known with the provided dark signal correction (note, however, the spatial stray light mentioned below under Known Instrument Features). The behavior of IR channels 6 to 8 on the other hand is much more complex. In difference to the visible channels, the integration time dependent part of the dark signal has a strong thermal background component, which, in addition, is modified with the ice layer, known as contamination. In order to assure best possible dark signal correction for this part of the spectrum, the dark states used for the determination of the dark signal can now be selected in the processor. This leads to an improved dark correction for channel 8.

Etalon Correction

The etalon is an interference pattern, introduced by the protective coating of channel 1 to 5 RETICON detectors, seen as “periodic” bumps in the uncorrected signal. Usually, these features are very stable, but may change after

- unintended interruptions/transitions to standby;
- planned interruptions like decontamination.

In the time between such an event and the next recalibration (a dedicated measurement is required, which usually is performed only once per week), the provided information will be wrong (i.e. it will lead to unintended spectral features in the calibrated radiance). The correction of changes in the etalon is now included in the degradation correction done with the m-factors. Therefore, the etalon correction should be no longer used, although it is still available for backward compatibility.

Spectral Calibration

Spectral calibration is the process to associate a wavelength to an individual detector pixel. It is achieved by looking to sources (special calibration lamp, sun) with known spectrum/spectral lines.

The spectral calibration quality is generally very good, except of channel 7 and 8 as well as for the channel overlap regions, where it is less good, due to systematic problems (e.g. insufficient number of calibration lines). An orbital dependency can be neglected. However, calibration quality might be affected by transient problems (see etalon).

Polarisation

Polarisation calibration is mandatory in case absolute calibrated radiance is required. In order to compensate for the polarisation sensitivity of the instrument, which has a different throughput for parallel and perpendicular polarized light, the atmospheric polarisation needs to be determined and compensated by sensitivity parameters, which were derived during on-ground calibration. The latter are also called polarisation key-data.

The quality of the polarisation therefore depends on both, the absolute values of the retrieved atmospheric degree of polarisation but also the correctness of instrument polarisation key-data. It also depends on further data treatment, whether the polarization correction improves the retrieval or not. Some recommendations:

- In case of full retrieval methods it is mandatory to apply polarisation.

- In case of monitoring data, polarisation calibration cannot be applied.
- In case of occultation data it is not recommended to apply polarisation, because the key-data do not properly consider the small aperture, which is used during the measurements. Therefore, a correction is no longer calculated in this case.
- Due to the approach, spectral features in the instrument polarization key-data can never be excluded to appear in the corrected signal. They might disturb DOAS type retrievals.

The polarisation correction degrades somewhat with time due to degradation in the PMD signals. This effect is now corrected using the scan mirror model. At the same time the polarization key data have been updated.

Radiance, Irradiance and Reflectance

Fully calibrated radiance of the observed ground scene is only one aspect of radiometric calibration. The quality of solar irradiance is also of great importance.

Revision and re-computation of involved calibration key-data widely removed the known offsets of SCIAMACHY solar irradiance. The agreement between reference spectra (Kuruzc, 2010) and SCIAMACHY is now in the order of 5% or better.

Due to the proven consistency between radiance and irradiance calibration parameters, the reflectance (sometimes also referred to as sun normalized radiance) too should benefit.

For the moment, the errors in SCIAMACHY reflectance (absolute) can be estimated as in the table below:

Channel	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**8**
	3%	4%	3%	2%	6%	4%	3%	3%

These numbers are based on comparison with DAK model, GOME, AATSR and MERIS data (ACVE-III). For channels 7 and 8 they are based on lunar observations in comparison with channels 2 to 6. However, a statistical verification of this aspect is still outstanding and might improve the figures.

Also, it is important to mention that even though there might still be uncertainties on the absolute value of the reflectance, these generally do not disturb DOAS type retrievals, which are insensitive to broadband offsets in the reflectance.

Degradation correction

The instrument degradation is corrected using a scan mirror model that models two contamination layers on the scanner surface(s). It uses in-flight data to determine the thickness of the layers and their change over time. From this parameter the degradation for each wavelength and scan angle is calculated. This correction is now applied in the Level 0-1b processing step and corrects the polarization sensitivity and the radiometric sensitivity stated in the product. Thus if the user applies the polarization correction or the radiometric correction, the degradation will be automatically corrected. The fully calibrated solar reference spectrum (identifier D0) in the product is also corrected for degradation. For a proper calculation of the reflectance, one must use this solar reference spectrum (D0) for radiometrically corrected Earth data and the not radiometrically corrected sun mean references (E0 or A0) for Earth measurements that were not radiometrically corrected.
Note that because the degradation correction is already contained in the Level 1b

product, the user must not use the m-factor corrections provided with the SciaL1c tool for Level 1b version 8.0X products (the option is still available for backwards compatibility when using Level 1b products version 7.04).

On-Ground Calibration Data (Key-Data)

The on-ground calibration of the instrument is represented in the so-called key data of the instrument. They are ultimately used to correct for polarization sensitivity of the instrument and to obtain absolutely calibrated spectra. Since processor version 8.01, an update to the stray light correction in channels 3 to 8 is available, which will benefit the radiometric calibration of these channels, in particular in the deep absorption lines. The radiometric and polarization key data were updated using on-ground calibration data.

Solar Reference Spectra

Handling of solar reference spectra has been adapted to special needs of trace gas retrievals. Following recommendations from verification scientists, solar spectra, obtained from both, ESM and ASM calibration measurements are provided in a calibrated and un-calibrated way (see table below). Spectra are distinguished by identifiers (i.e. first field in the solar reference global annotation data set record).

Globally, it is recommended to use a "not radiometrically calibrated" ASM diffuser spectrum (A0) for DOAS-type applications. This diffuser results in reduced spectral features, which is beneficial to DOAS type retrievals. This does of course not mean that different spectra from the list below couldn't be taken. However, all retrieval methods requiring absolute calibrated radiance and irradiance shall use the calibrated ESM diffuser spectrum (D0).

ID	Content	Remark
D0	ESM diffuser, calibrated, ND filter in	Absolutely calibrated spectrum.
D1	ESM diffuser, calibrated, ND filter out	Absolutely calibrated spectrum. However, it is only updated once per month.
D2	ASM diffuser, calibrated	This spectrum is pseudo calibrated i.e. the ESM diffuser BRDF is applied to the ASM diffuser measurement.
E0	ESM diffuser, un-calibrated, ND filter in	Radiometric calibration not applied. Corresponds to D0.
E1	ESM diffuser, un-calibrated, ND filter out	Radiometric calibration not applied. Corresponds to D1.
A0	ASM diffuser, un-calibrated	Radiometric calibration not applied. Corresponds to D2.
A1	ASM diffuser, un-calibrated	Additive offsets removed, as a function of wavelength; spectrum of 09.04.2003. This spectrum was provided already in the past and will remain in the product.
N1	Placeholder – not used	
N2	Placeholder – not used	
N3	Placeholder – not used	
N4	Placeholder – not used	
N5	Placeholder – not used	

Known Instrument Features

This section reports a list of known instrument features for version 8.0X products, which might get in conflict with intended data usage.

- Spectral feature around 480 nm caused by a change of a channel separating dichroic filter.
- Mid-scale spectral feature around 350 nm (channel 2), probably caused by non-uniformity of detector pixels. Size of the feature depending on the intensity distribution of ground scene.
- Light leak hampering all retrievals in channel 7.
- Varying throughput due to ice in channels 6, 7 and 8, partly compensated by m-factors.
- Spatial stray light resulting from scattering off the scan- and/or telescope-mirrors affects limb dark measurements around sunrise. Also other very high contrast scenes may be affected, like high bright clouds below the limb field of view. The spatial stray light extends to a few degrees and is wavelength and angle dependent.
- During time intervals where ENVISAT was working in Yaw Steering Mode (YSM) only a degraded pointing performance was achieved especially for limb and occultation data.
- Limb-Mesosphere states (ID 55) are treated as regular limb states in the calibration approach which is not optimised for that height region. It is recommended not to apply polarisation correction to these states.

Impact of ENVISAT Orbit Change

The following applies to limb tangent heights retrieved since orbit 45262 (27 October 2010). To account for the reduced orbit altitude after the ENVISAT orbit manoeuvre end of October 2010, ESM settings in the Basic Scan Profile table reflecting a fixed line-of-sight altitude had to be adjusted. This occurred with the upload of the new final flight configuration on 27 October 2010. A detailed description of the modifications is given in the Operations Change Request no. 48 (OCR_048). Note that the number of vertical steps was reduced by one, from 31 to 30. Verification of the modified configuration revealed that the tangent heights derived with the CFIs when viewing in limb type geometry did not fully comply with the specified values.

State (ID)	Nominal Orbit	
	Start	Stop
	Tangent height (km)	
limb (28-37,40,41)	-6.3	264
limb_mesosphere (27)	153.5	n.a.
mesosphere_thermosphere (55)	153.3	370
State (ID)	**Mission Extension Orbit**	
	Start	**Stop**
	Tangent Height (km)	
limb (28-37,40,41)	-6.2	270
limb_mesosphere (27)	158.2	n.a.

mesosphere_thermosphere (55)	158	350

Table 4: Executed tangent heights in several limb-type states for nominal and mission extension orbit. Note that "start" refers to the first altitude from where the line-of-sight immediately moves to the first measurement altitude, i.e. horizontal scan, by one vertical step of about 3 km. The column labelled "stop" indicates the altitude where the final dark current pointing occurs.

Between orbits 45262 and 45864 (07 December 2010) the states from ***Table 4*** were executed with Basic Scan Profile settings yielding to the listed start/stop altitudes. For the limb states 28-37 and 40/41 this is equivalent to a final horizontal scan at about 90 km.

State (ID)	Mission Extension Orbit	
	Start	Stop
	Executed (km)	
limb (28-37, 40, 41)	-2.7	263
limb_mesosphere (27)	152.3	n.a.
mesosphere_thermosphere (55)	152.3	370*

Table 5: Executed tangent heights in several limb-type states for the mission extension orbit with the new Basic Scan Profile table ESM settings as tested on 7 December 2010 and permanently uploaded in orbit 46340 (* this is an orbital mean value since the corresponding elevation angle is not Earth model corrected).

Between orbits 45865 and 45868 on 07 December 2010 four test orbits with slightly modified Basic Scan Profile ESM parameters were scheduled. Only the stop altitude for state 55 could not be tested because mesosphere/thermosphere states were not planned for that day. The achieved altitudes are those listed in **Table 5** and are considered acceptable.

Between orbits 45869 and 46339 (10 January 2011) the Basic Scan Profile settings as uploaded in orbit 45262 were operational again yielding the tangent heights from ***Table 4***. From orbit 46340 (11 January 2011) on the Basic Scan Profile parameters tested on 07 December 2010 were permanently uploaded generating a new final flight configuration with retrieved tangent heights as listed in **Table 5**.

Transient data quality degradation events

Decontamination intervals

During decontamination periods SCIAMACHY detectors were heated in order to remove contaminants. For the following time intervals SCIAMACHY was in decontamination mode (from start to stop of warm-up phase):

Orbit start/stop		Date start/stop		
2124	2175	27/07/2002	31/07/2002	
3746	3752	17/11/2002	18/11/2002	
4204	4428	19/12/2002	04/01/2003	
5718	5736	04/04/2003	05/04/2003	
6384	6420	21/05/2003	23/05/2003	

7574	7789	12/08/2003	27/08/2003	interleaved with transfer to HTR/RF
9407	9644	18/12/2003	03/01/2004	interleaved with transfer to HTR/RF
12031	12174	18/06/2004	28/06/2004	
14675	14860	20/12/2004	02/01/2005	
35574	35783	19/12/2008	03/01/2009	

Additional information can be found on the SOST web site (topic: Data Quality History): http://atmos.caf.dlr.de/projects/scops/

Any data products generated during these intervals are not to be used.

After decontamination has ended a cool down phase starts. Starting in 2003, the cool down phases are as follow (note: the first cool down period in 2003 was spoiled by an instrument anomaly):

Orbit start/stop		Date start/stop	
5736	5766	05/04/2003	07/04/2003
6420	6449	23/05/2003	25/05/2003
7789	7827	27/08/2003	29/08/2003
9644	9673	03/01/2004	05/01/2004
12174	12208	28/06/2004	30/06/2004
14860	14912	02/01/2005	05/01/2005
35783	35848	03/01/2009	07/01/2009

During these periods detector temperatures are not stable and data quality might be reduced.

Instrument Anomalies

After instrument switch-offs, detector temperatures needed some time to stabilise again. During these periods, the measurements of especially the IR detectors may be degraded. For a list of affected periods see SOST under “Data Quality History”.

Pointing Anomalies

During the following periods ENVISAT was operated in Yaw Steering Mode (instead of Stellar Yaw Steering Mode) which reduced the pointing accuracy:

Orbit start/stop		Date start/stop		
9280	9328	09-DEC-2003 10:00:00	12-DEC-2003 17:48:32	attitude tests

12070	12087	21-JUN-2004 07:56:33	22-JUN-2004 11:50:18	reduced pointing performance
45261	45353	27-OCT-2010 01:43:53	02-NOV-2010 10:25:00	orbit change

Other periods of potentially reduced pointing performance during e.g. orbit control manoeuvres are listed on SOST under "Data Quality History".

Known Processing Issues

This section reports the problems identified during verification of the SCIAMACHY consolidated Level 1b data generated with processing baseline 8.0X. The lists of products affected are available here.

Unprocessed Level 1 products

The number of unprocessed Level 1 products in data set version 8.0X is higher respect to the past reprocessing campaign (555 missing products in v8.0X dataset, evenly spread over the years). The new processor has revealed to be more sensitive to corrupted input Level 0 measurements (wrong sync word, corrupted ISP, downlink damages, incorrect reconsolidation, etc.). In these cases, the Level 1b files often inherited such problems with IPF v7.04, while IPP v8.0X processing does not produce a corresponding output Level 1b product. Processing failures are also a consequence of the IDL –> C++ porting occurred with the development of baseline version 8.0X, which applies a different filtering of corrupted/incorrect states. The capability to jump over the unprocessable part of the Level 0 files will be added in the next baseline.

MPH product error flag

In the new Level 1b version 8.0X dataset, MPH field PRODUCT_ERR reports value 1 according to ESA specifications. This flag has a different implementation respect to the version 7.04 products, and it does not indicate the level of confidence in the product, e.g. reporting errors occurred in the processing, but it declares the provision of additional information within the file (details in RD4).

The MPH PRODUCT_ERR field indicates if the presence of errors is tracked within the Level 1b product itself.

PRODUCT_ERR=0 means that information on errors is not provided.

PRODUCT_ERR=1 indicates that details on error condition are provided in SPH or SUMMARY ADS.

No filtering based on this flag has to be applied.

Incomplete states

Baseline v8.02 filters incomplete For some orbits filtering was not optimal, and some version 8.0X products still present incomplete states, with measurements duration shorter than expected. This issue affects all types of measurements: nadir, limb, occultation and monitoring states. Incomplete states are not discarded during processing and transferred to Level 1b files generating products with reduced data content. In these products, nadir states could have few ground-pixels missing, while

for occultation measurements first or last measurements of the state could be missing. A small subset of limb states results truncated with final planned dark measurement missing in the MDS. Limb dark states are not used operationally for leakage-correction so no impact on higher level processing is expected. Users of dark current calibrations from limb dark states are recommended to verify that the last available measurement in the limb state is indeed a dark measurement with tangent height reaching 150 km.

Incomplete states can be identified inspecting geolocation, comparing the actual number of geolocations ('num_rep_geo' from states GADS) to the expected number of geolocations, calculated from the state duration and the shortest integration time. A list of orbits with truncated limb states is reported as Annex. About 20% of the corrupted limb states are mesospheric states (cat 26/27), which are not used in the operational processing.

Different SPH start/stop latitude/longitude

For SPH start and stop latitude/longitude fields a different implementation has been introduced with processor versions 8.0X. Latitude and longitude for the sub-satellite track are now used, while version 7.04 adopted coordinates of the tangent ground point of the first measurement for the state of interest. The new implementation is more reliable and representative of the orbit coordinates. It is also in line with the requirements for SPH fields indicated in Product Specification Volume 15.

Missing usage of Restituted Attitude files (AUX_FRA_AX)

ENVISAT attitude file provides pitch, roll, and yaw of the satellite, and is required in the processing to accurately define the geo-location of the measurements. SCIAMACHY Level 1b products for 08 April 2012 (seven products on the last day of SCIAMACHY operations, orbits from 52861 to 52867) have been generated without ENVISAT Restituted Attitude auxiliary file as the last in-flight AUX_FRA_AX file generated does not supply suitable coverage for that day. When the AUX_FRA_AX information is missing, SCIAMACHY Level 1b products use attitude previsions and present a reduced quality in the pointing.

Anomalous data format

The ESA verification process comprises a screening to guarantee readability for every Level 1b data generated. For this task, the Common Data Access toolbox (CODA) is used verifying the data format. Level 1b products for days between 24 and 31 December 2002 resulted not fully compliant in the data format. These products did not pass the standard format check as SPH dataset descriptor for bad and dead pixel mask results written twice, with additional 280 bytes to the total file size. The CODA check inspection fails due to this size discrepancy. The structure of the binary part of the product is not compromised and higher level processing (Level 1b->2) results feasible.

In order to use CODA with the SCIAMACHY version 8.0X Level 1b dataset, the latest CODA definition file ENVISAT_SCIAMACHY-20140916.codadef specifying the new format has to be used.

Usage of Reference AUX file

The Level 1b version 8.0X baseline extracts calibration information of specific in-flight parameters from a calibration database. For some orbits along the mission, proper entries in the database do not exist (e.g. calibration measurements not yet performed, generation of calibration data failed after decontamination phases). In these cases, calibrations are extracted from begin-of-life reference auxiliary data files (ADFs). In particular, the processing of the first days of the mission for quasi-nominal in-flight conditions (i.e. August 2002) makes use of default values for the calibration parameters. In case very old ADFs are used with respect to measurement time, slightly reduced quality is expected. For the next reprocessing, the database search algorithm will be revised implementing a nearest neighbor selection of calibration records.

- Eleven consolidated Level 1b products for 02 August 2002 (orbits 2204-2215) were generated with PPG/ETALON information extracted from the reference auxiliary files as the corresponding calibration database entries start only for 2002-08-02 at 21:05.
- The A0 SMR spectrum enclosed into the Level 1b products is maintained constant over the period August-December 2002 as the first A0 diffuser SMR measurement occurred on 15 December 2002 at 14:11:57 (search for nearest neighbour database, forward selection allowed).
- Along the entire mission, 1400 Level 1b consolidated products were generated without updated in-flight average dead and bad pixel mask (DBPM) as measurements in the previous days were too sparse. DBPM calculation in fact uses individual masks for the last seven days (around 100 orbits) to calculate a smoothed average mask. For these orbits, DBPM from a reference auxiliary file was used. Products affected are indicated in the table below.

Mission interval	
Start	**Stop**
2291 (08-AUG-2002)	**3069 (01-OCT-2002)**
4267 (24-DEC-2002)	**4379 (31-DEC-2002)**
4380 (01-JAN-2003)	**4461 (06-JAN-2003)**
7672 (19-AUG-2003)	**7809 (28-AUG-2003)**
9528 (26-DEC-2003)	**9603 (31-DEC-2003)**
9604 (01-JAN-2004)	**9655 (04-JAN-2004)**
12123 (24-JUN-2004)	**12184 (29-JUN-2004)**
14773 (27-DEC-2004)	**14841 (31-DEC-2004)**
14842 (01-JAN-2005)	**14873 (03-JAN-2005)**
35672 (26-DEC-2008)	**35756 (31-DEC-2008)**
35757 (01-JAN-2009)	**35811 (04-JAN-2009)**

Sub-optimal selection of A0 SMR spectrum

For eight Level 1b consolidated products (year 2002) the selection and transfer of the A0 sun mean reference spectrum from the calibration database into Global Annotation Data Sets (GADS) enclosed into the Level 1b products result not optimal. In case more than one database entry exists for one day; the nearest neighbours search results not fully deterministic and the selection of the calibration parameter deviates from expectation. Orbits affected are from 2398 to 2401, and from 3272 to 3275. The impact on data quality is limited as A0 entries from contiguous days exist, and the calibration values derived are similar to the ones expected.

D0 SMR spectra inconsistency

For some orbits, the reference solar spectra (D0 SMR) enclosed into Level 1b v8.0X products present the Bad and Dead Pixel Mask (BDPM) applied. D0 spectra are usually not bad-pixel-corrected in the calibration database and should actually not be modified during the Level 0-1b processing. Nevertheless, whenever a SLS measurement (measurement category 10) is found in a Level 0 product, the D0 SMR spectrum is used to calculate new spectral coefficients; the solar spectrum results bad-pixel-corrected and transcribed into Level 1 GADS. This issue will be fixed in the next IPP version. Level 2 products are not impacted as bad-pixels are corrected for all Level 2 calculations.

Negative orbit-phases

Within the data set, the following products were found affected by negative orbit-phase values (within STATES GADS):

SCI_NL__1PYDPA20030219_061513_000045962014_00020_05084_0002.N1
SCI_NL__1PYDPA20050111_120950_000045132033_00410_14993_0002.N1
SCI_NL__1PYDPA20061223_112341_000045392054_00066_25170_0002.N1
SCI_NL__1PYDPA20070423_144106_000046022057_00297_26904_0002.N1
SCI_NL__1PYDPA20071211_131047_000045112064_00110_30224_0002.N1
SCI_NL__1PYDPA20091119_100827_000043682084_00237_40371_0000.N1

For these products, the iterative calculation of the orbit-phase via ESA CFI routines failed, returning an error and negative values. The orbit-phase is used for the determination of orbit-dependent part of leakage signal and for the orbit-phase dependent spectral calibration. In the case of negative values, orbit-phase zero is used.

Product format and tools

The SCIAMACHY Level 1b products generated with IPP v8.0X have an updated format. Owing to this, the BEAT, VISAN and CODA software have been updated in order to read the new products, allowing fields' extraction and data handling. Latest BEAT version 6.9.1, VISAN version 3.11.0 and CODA version 2.15.1 are aligned to the new specifications.

SciaL1c

SCIAMACHY Level 1b products are not fully calibrated Level 0 channel information in combination with calculated calibration data. The SCIAMACHY Calibration and Extraction Tool SciaL1c allows users to select specific calibration steps they like to apply to Level 1b data, obtaining fully or partially calibrated spectra within Level 1c

	products. Calibration can be combined with several filters to allow an extraction of special scenes or sub-set of measurement data, for example Nadir observations only. Current version (3.2) is designed to process Level 1b 8.0X products but backward compatibility to other product versions is provided. The SciaL1c tool incorporates new features adjusted to the SGP version 6.01 Level 1b-2 processing needs. In particular, it applies a new hot pixel mask detection algorithm and was adjusted reflecting the modified calibration scheme: degradation and etalon correction is now performed in the Level 0-1 processing step via m-factors (previously during Level 1-2 processing). Details of the changes can be found in the Software Release Note. SciaL1c 3.2 is available for the following platforms: • Linux on x86 • Linux on amd64 • Windows Executable files as well as complete documentation can be found here.
Acronyms	ADF Auxiliary Data File ASM Azimuth Scan Mechanism ATBD Algorithm Theoretical Baseline Document BEAT Basic ENVISAT Atmospheric Toolbox CFI Customer Furnished Items CODA Common Data Access Toolbox CTI Configuration Table Interface DDS Diagnostic Sata Set DBPM Dead and Bad Pixel Mask DORIS Doppler Orbitography and Radiopositioning Integrated by Satellite DLR-IMF Deutsches Zentrum für Luft- und Raumfahrt (German Aerospace Centre) D-PAC German PAC ENVISAT Environmental Satellite ESA European Space Agency ESM Elevation Scan Mechanism GADS Global Annotation Data Set IDEAS Instrument Data quality Evaluation and Analysis Service IODD Input / Output Data Definition IPF Instrument Processor Facility IPP Instrument Prototype Processor ISP Instrument Source Packet L0 Level 0 L1b Level 1b L2 Level 2 MDS Measurements Data Set MEC Memory Effect Correction MPH Main Product Header NDF Neutral Density Filter NLC Non-linear correction PMD Polarization Measurement Device QWG Quality Working Group SAA South Atlantic Anomaly SCIAMACHY Scanning Imaging Absorption Spectrometer for Atmospheric Chartography

	SGP SCIAMACHY Ground Processor SMR Sun Mean Reference SOST SCIAMACHY Operations Support Team SPH Specific Product Header SPPA Sensor Performance, Products and Algorithm SYSM Stellar Yaw Steering Mode YSM Yaw Steering Mode
WWW References	Additional information on the SCIAMACHY instrument, its data processing, anomalies, products' quality, calibration activities and validation campaigns can be found on-line. **Instrument operations** The list of events affecting the SCIAMACHY mission can be found on: SOST web-page at http://atmos.caf.dlr.de/projects/scops/ ESA SPPA portal at https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/mission-highlights **Processors documentation** https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/products-and-algorithms/products-information **Consolidated data sets** https://earth.esa.int/web/sppa/mission-performance/esa-missions/envisat/sciamachy/quality-control-reports/products-availability **Tools** The Basic ENVISAT Atmospheric Toolbox (BEAT) can be downloaded at: http://www.stcorp.nl/beat/ The new version of the SCIAMACHY Calibration and Extraction Tool SciaL1c, compatible with the Level 1b version 8 products, can be downloaded at https://earth.esa.int/web/guest/software-tools/content/-/article/scial1c-command-line-tool-4073
Inputs	SCIAMACHY Quality Working Group, SCIAMACHY Validation team, IDEAS+ (Instrument Data quality Evaluation and Analysis Service) team
Approver	Angelika Dehn (Angelika.Dehn@esa.int)
Annex	Products affected by truncated limb states within version 8.0X dataset (106 orbits). SCI_NL__1PYDPA20020806_022619_000057272008_00204_02262_0002.N1

	SCI_NL__1PYDPA20020822_035853_000060922008_00434_02492_0002.N1 SCI_NL__1PYDPA20020822_035853_000060922008_00434_02492_0002.N1 SCI_NL__1PYDPA20020913_072956_000059552009_00250_02809_0002.N1 SCI_NL__1PYDPA20030312_081145_000060492014_00322_05386_0002.N1 SCI_NL__1PYDPA20030403_114240_000059752015_00138_05703_0002.N1 SCI_NL__1PYDPA20030410_230621_000059992015_00245_05810_0002.N1 SCI_NL__1PYDPA20030413_080625_000060432015_00279_05844_0002.N1 SCI_NL__1PYDPA20030417_074049_000059992015_00336_05901_0002.N1 SCI_NL__1PYDPA20030511_233648_000057682016_00188_06254_0002.N1 SCI_NL__1PYDPA20030613_093311_000057582017_00151_06718_0002.N1 SCI_NL__1PYDPA20030624_120817_000057302017_00310_06877_0002.N1 SCI_NL__1PYDPA20030701_000400_000057652017_00403_06970_0002.N1 SCI_NL__1PYDPA20030808_064835_000060842018_00450_07518_0002.N1 SCI_NL__1PYDPA20040328_080617_000060482025_00279_10854_0002.N1 SCI_NL__1PYDPA20040418_020423_000060332026_00075_11151_0002.N1 SCI_NL__1PYDPA20040606_012813_000057302027_00275_11852_0002.N1 SCI_NL__1PYDPA20040630_103651_000057062028_00123_12201_0002.N1 SCI_NL__1PYDPA20040822_074615_000060342029_00379_12958_0002.N1 SCI_NL__1PYDPA20040825_111301_000060642029_00424_13003_0002.N1 SCI_NL__1PYDPA20041028_142303_000060202031_00340_13921_0002.N1 SCI_NL__1PYDPA20041112_181256_000060642032_00056_14138_0002.N1 SCI_NL__1PYDPA20041113_210237_000060772032_00072_14154_0002.N1 SCI_NL__1PYDPA20041210_133123_000060432032_00454_14536_0002.N1 SCI_NL__1PYDPA20050124_063413_000060292034_00092_15176_0002.N1 SCI_NL__1PYDPA20050129_021551_000060242034_00161_15245_0002.N1 SCI_NL__1PYDPA20050129_021551_000060242034_00161_15245_0002.N1 SCI_NL__1PYDPA20050129_021551_000060242034_00161_15245_0002.N1 SCI_NL__1PYDPA20050129_021551_000060242034_00161_15245_0002.N1 SCI_NL__1PYDPA20050129_021551_000060242034_00161_15245_0002.N1 SCI_NL__1PYDPA20050129_021551_000060242034_00161_15245_0002.N1 SCI_NL__1PYDPA20050129_021551_000060242034_00161_15245_0002.N1 SCI_NL__1PYDPA20050131_193850_000060392034_00200_15284_0002.N1 SCI_NL__1PYDPA20050131_193850_000060392034_00200_15284_0002.N1 SCI_NL__1PYDPA20050131_193850_000060392034_00200_15284_0002.N1 SCI_NL__1PYDPA20050131_193850_000060392034_00200_15284_0002.N1 SCI_NL__1PYDPA20050201_031855_000025762034_00204_15288_0002.N1 SCI_NL__1PYDPA20050201_031855_000025762034_00204_15288_0002.N1 SCI_NL__1PYDPA20050201_031855_000025762034_00204_15288_0002.N1 SCI_NL__1PYDPA20050516_094046_000057372037_00194_16781_0002.N1 SCI_NL__1PYDPA20050610_131510_000057742038_00053_17141_0002.N1 SCI_NL__1PYDPA20050615_035436_000034442038_00119_17207_0002.N1 SCI_NL__1PYDPA20050619_032840_000057772038_00176_17264_0002.N1 SCI_NL__1PYDPA20050712_130930_000057902039_00010_17599_0002.N1 SCI_NL__1PYDPA20050816_112445_000060202040_00009_18099_0002.N1 SCI_NL__1PYDPA20050909_084924_000060302040_00351_18441_0002.N1 SCI_NL__1PYDPA20050915_204508_000060322040_00444_18534_0002.N1 SCI_NL__1PYDPA20051116_181640_000060012042_00328_19420_0002.N1 SCI_NL__1PYDPA20060106_030713_000060312044_00047_20141_0002.N1 SCI_NL__1PYDPA20060118_051103_000060212044_00220_20314_0002.N1 SCI_NL__1PYDPA20060126_023849_000060402044_00333_20427_0002.N1 SCI_NL__1PYDPA20060223_043928_000060302045_00234_20829_0002.N1 SCI_NL__1PYDPA20060413_090128_000060002046_00437_21533_0002.N1 SCI_NL__1PYDPA20060710_075856_000057892049_00193_22792_0002.N1 SCI_NL__1PYDPA20060714_055236_000057922049_00249_22848_0002.N1 SCI_NL__1PYDPA20060721_035209_000057532049_00348_22947_0002.N1 SCI_NL__1PYDPA20060822_034222_000060012050_00305_23405_0002.N1 SCI_NL__1PYDPA20060929_070858_000060322051_00350_23951_0002.N1

	SCI_NL__1PYDPA20070404_041021_000060342057_00019_26626_0002.N1 SCI_NL__1PYDPA20070417_122506_000060442057_00210_26817_0002.N1 SCI_NL__1PYDPA20070421_115900_000060632057_00267_26874_0002.N1 SCI_NL__1PYDPA20070515_124529_000060762058_00110_27218_0002.N1 SCI_NL__1PYDPA20070523_024905_000025102058_00218_27326_0002.N1 SCI_NL__1PYDPA20070626_040552_000057802059_00205_27814_0002.N1 SCI_NL__1PYDPA20070801_101239_000060372060_00223_28333_0002.N1 SCI_NL__1PYDPA20070818_061717_000060202060_00464_28574_0002.N1 SCI_NL__1PYDPA20070901_071817_000060012061_00164_28775_0002.N1 SCI_NL__1PYDPA20070920_021853_000060322061_00433_29044_0002.N1 SCI_NL__1PYDPA20071211_192739_000060432064_00114_30228_0002.N1 SCI_NL__1PYDPA20071227_041911_000060312064_00334_30448_0002.N1 SCI_NL__1PYDPA20080104_032724_000060312064_00448_30562_0002.N1 SCI_NL__1PYDPA20080116_020958_000060432065_00118_30733_0002.N1 SCI_NL__1PYDPA20080308_081813_000059872066_00365_31481_0002.N1 SCI_NL__1PYDPA20080414_021237_000060632067_00390_32007_0002.N1 SCI_NL__1PYDPA20080521_075645_000057342068_00422_32540_0002.N1 SCI_NL__1PYDPA20080622_024810_000057782069_00376_32995_0002.N1 SCI_NL__1PYDPA20080628_094204_000057812069_00466_33085_0002.N1 SCI_NL__1PYDPA20080719_084214_000057962070_00265_33385_0002.N1 SCI_NL__1PYDPA20080727_042943_000057592070_00377_33497_0002.N1 SCI_NL__1PYDPA20080812_074325_000060342071_00107_33728_0002.N1 SCI_NL__1PYDPA20080917_234416_000008082072_00130_34252_0002.N1 SCI_NL__1PYDPA20081008_043110_000059882072_00420_34542_0002.N1 SCI_NL__1PYDPA20081027_043315_000060442073_00191_34814_0002.N1 SCI_NL__1PYDPA20081119_022937_000060402074_00018_35142_0002.N1 SCI_NL__1PYDPA20081119_055049_000060402074_00020_35144_0002.N1 SCI_NL__1PYDPA20081206_184140_000060212074_00271_35395_0002.N1 SCI_NL__1PYDPA20090216_105601_000060432076_00295_36421_0002.N1 SCI_NL__1PYDPA20090310_024141_000060312077_00104_36731_0002.N1 SCI_NL__1PYDPA20090319_094128_000060312077_00237_36864_0002.N1 SCI_NL__1PYDPA20090320_090943_000060312077_00251_36878_0002.N1 SCI_NL__1PYDPA20090512_144537_000060272079_00011_37640_0002.N1 SCI_NL__1PYDPA20090605_103408_000057752079_00352_37981_0002.N1 SCI_NL__1PYDPA20090627_122300_000057812080_00167_38297_0002.N1 SCI_NL__1PYDPA20090825_144602_000060202082_00011_39143_0002.N1 SCI_NL__1PYDPA20090918_084931_000060322082_00351_39483_0002.N1 SCI_NL__1PYDPA20091005_013228_000060322083_00089_39722_0002.N1 SCI_NL__1PYDPA20091016_022659_000060282083_00247_39880_0002.N1 SCI_NL__1PYDPA20091029_021828_000060202083_00433_40066_0002.N1 SCI_NL__1PYDPA20100125_043312_000060292086_00191_41327_0002.N1 SCI_NL__1PYDPA20100130_033552_000060392086_00262_41398_0002.N1 SCI_NL__1PYDPA20100306_083833_000059982087_00265_41902_0002.N1 SCI_NL__1PYDPA20100403_121853_000060342088_00167_42305_0002.N1 SCI_NL__1PYDPA20100514_104941_000060712089_00252_42891_0002.N1 SCI_NL__1PYDPA20100528_065300_000057762089_00450_43089_0002.N1 SCI_NL__1PYDPA20100601_080733_000057752090_00007_43147_0002.N1 SCI_NL__1PYDPA20110726_161007_000047653105_00026_49178_0002.N1