

ESO Phase 3 Data Release Description

Data Collection	ESPRESSO
Data Provider	ESO, Science Data Quality Group
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Abstract

This is the release of reduced spectra from the high-resolution echelle spectrograph ESPRESSO¹. The instrument is located at the Coudé focus of the VLT and can be used for observations with any of the UTs or with the incoherently combined beams from all four UTs. The spectrograph offers a wavelength range from 380 to 788 nm. The spectral resolution depends on the instrument mode. The median resolving power is 140000 in HR mode, 190000 in UHR, and 70000 in MR. The HR and UHR modes use the light from one of the UTs whereas the MR mode is used together with all four UTs. The spectrograph is fed with two fibres. One fibre (fibre A) is placed on the object. The second fibre (fibre B) can be used to either measure the sky background or to simultaneously collect light from a reference calibration source. A Fabry-Pérot (FP) cavity is the operationally used simultaneous reference which allows to measure the instrumental drift between the night-time observation and the daytime wavelength calibration.

This release is an open stream release. It is complete from start of operations on 2nd September 2018 until present. Data content is not fixed but grows with time as new data are being acquired and processed (with a delay of up to a few weeks).

Data have been reduced using the ESPRESSO pipeline version 2.2.1 or higher. It includes extraction of the spectrum, flat fielding, wavelength calibration, and flux calibration. Sky subtraction is only performed if fibre B is placed on sky. If the science target is not a QSO then an automated cross correlation with a stellar reference mask is executed in order to calculate the radial velocity (RV) of the observed object. Please note that systematic shifts of the RV values can occur between different versions of the pipeline. It is highly recommended to use only products from the same pipeline version for RV studies.

Data acquired from March 2025 onwards have been corrected for telluric absorption by water vapour. The pipeline version for these is 3.3.8 or later.

The ESPRESSO pipeline extracts a spectrum from a single exposure. If several exposures on the same target are executed within the same observing template then an additional reduction step is performed for this release. The extracted and flux-calibrated spectra of the single exposures are combined into a co-added spectrum with increased signal-to-noise ratio. The combined spectrum becomes the primary product; the single spectra are made available as associated files. For the co-adding step, the ESOTK pipeline is used (version 0.8.4 or higher).

¹ <https://archive.eso.org/docurl?ESPRESSO>

Release Content

The ESPRESSO release is a stream release. The content of the release grows with time as new data are being acquired and processed. The data are tagged "ESPRESSO" in the ESO archive user interface². The release contains data from all instrument modes and set-ups. First data have been published in April 2021.

Data Selection

Data selection is based on the following rules:

- instrument = ESPRESSO
- category (DPR.CATG) = SCIENCE
- observing technique (FITS key DPR.TECH) = ECHELLE
- type (DPR.TYPE) = OBJECT,SKY or OBJECT,FP.

Processing of the ESPRESSO science data has a success rate of nearly 100%, only very few input raw files are rejected. No selection is made on the basis of the observing mode (visitor or service). Data with 'test programme IDs' starting with '60' or '060' are not processed.

Settings. Data from all instrumental modes (HR, UHR, and MR) and with all detector binning values are processed.

Data sets and input files. Processing of ESPRESSO science data is based on single exposures: every science exposure is pipeline-processed and results in an extracted, flux-calibrated spectrum. Often, a science observation consists of a single exposure. However also regularly, several exposures on the same object are executed within the same template. In such a case, an additional processing step is executed after the reduction of the single exposures. All spectra resulting from the same observing template as defined by the same TPL.START keyword are co-added into a combined spectrum. This step is performed independently of the original intent of the observation, i.e. whether the intention was to add the exposures in order to get a higher signal-to-noise ratio or to study a time series. In any case, all individual single-exposure spectra are available in addition to the combined spectrum as associated files. Observations from different OB (Observing Block) executions on the same target are not combined.

² https://archive.eso.org/wdb/wdb/adp/phase3_spectral/form
https://archive.eso.org/scienceportal/home?data_collection=ESPRESSO

Release Notes

Pipeline Description

A detailed description of the ESPRESSO pipeline can be found in the pipeline user manual which is available from the ESO pipeline web pages³. The initially released data set was processed with version 2.2.1 of the pipeline. The actual version used for processing can be found in the header of any product in the keyword “PROCSOFT”.

Combination of spectra from single exposures is done with the `esotk_spectrum1d_combine` recipe. A detailed description is available from the ESO pipeline web pages⁴. The initially released data were processed using version 0.8.4 of the ESOTK pipeline.

Data Reduction and Calibration

Reduction steps. Data reduction includes bias subtraction, flat fielding, correction for the Echelle blaze function, wavelength calibration, extraction of the spectrum, merging of Echelle orders, and flux calibration. Since pipeline version 3.3.0, also a correction for telluric absorption is performed. This applies to data acquired from March 2025 onwards.

Wavelength calibrations. Wavelength calibration is achieved in two steps. The Fabry-Pérot (FP) light source provides a high number of evenly distributed lines for an accurate relative wavelength calibration. The absolute wavelengths are determined by an exposure with a Thorium-Argon (Th-Ar) hollow-cathode lamp. ESPRESSO is also equipped with a laser frequency comb (LFC) which can be used alternatively to the Th-Ar lamp. Because the LFC was only partially available since start of operations and since its stability is not yet fully characterised, only Th-Ar exposures are taken for the wavelength calibration in this release.

Wavelengths in the “WAVE” column of the output products are expressed in vacuum.

Barycentric correction. The wavelengths in the science spectrum are correct to the barycentre of the solar system.

Correction for instrumental drift. The ESPRESSO spectrograph is fed with two fibres simultaneously. Fibre A is placed on the scientific object. Fibre B can be used to record the FP source during the science exposure. For these observations, the instrumental drift between the science observation and the daytime wavelength calibration is calculated and corrected in the wavelength solution.

Sky subtraction. Alternatively to simultaneously measuring the FP with fibre B, this fibre can be used to measure the sky background which is then subtracted within data reduction. The relative efficiency between fibres A and B is determined via daylight sky flats and corrected at the sky subtraction step. The sky cannot be subtracted if fibre B is on the FP.

Contamination induced by the FP. When fibre B is used to measure the FP light, the strong FP lines can produce contamination on the detector at the position of fibre A. This effect is measured with dedicated calibration frames and is corrected.

Cleaning of cosmic ray hits. Cosmic ray hits are cleaned from the spectra using kappa-sigma clipping.

Spectrum extraction. The spectra are extracted using the optimal extraction algorithm using cross-dispersion order profiles that are obtained from the spectral flat fields.

Flux calibration. Extracted spectra are always flux calibrated by the pipeline. According to the ESPRESSO calibration plan, spectroscopic flux standards are observed with each telescope every few weeks. Exact measurements of the actual atmospheric conditions in a specific night are, there-

³ Under the ESPRESSO pages available at <https://www.eso.org/sci/software/pipelines/>

⁴ Under the ESOTK pages available at <https://www.eso.org/sci/software/pipelines/>

fore, not available. For this release, sets of standard stars have been identified that are representative for a given time period. All science observations from such a period have then been calibrated with the same set. The telescopes of the science and the standard star observations are matched.

Telluric correction. Telluric lines are corrected since pipeline version 3.3.0. The correction includes only water vapour absorption.

Radial velocity calculation. The espresso science recipe computes the cross-correlation function (CCF) of the extracted spectrum in wavelength-order space with respect to a binary template of a given spectral type. The radial velocity (RV) is then obtained from a Gaussian fit to the CCF. Template masks for F-, G-, K-, and M-type stars are available within the pipeline. The results are written into the “HIERARCH ESO QC CCF *” header keywords of the output products; the measured RV value can be found in “HIERARCH ESO QC CCF RV”, the corresponding error in “HIERARCH ESO QC CCF RV ERROR”, and the used mask in “HIERARCH ESO QC CCF MASK”. If the spectra have been corrected for telluric absorption then the values of the CCF keywords correspond to the corrected spectrum.

Combination of spectra. For the combination of spectra, the generic recipe `esotk_spectrumld_combine` is used. All input spectra are normalised to the flux level of the first input spectrum. For the combination, kappa-sigma clipping is used with $\kappa = 10$. Note: combined spectra do not contain the header keywords from the radial velocity calculation. Please refer to the individual spectra which are available as ancillary products.

Calibrations used for data reduction. Table 1 lists the required calibration types that are needed for the reduction of science data. Please see the pipeline user manual for further details.

Table 1. ESPRESSO calibrations

Type	Purpose
Bias	Measures the residual, fixed pattern of the detector bias. (The bias level is measured in the overscan regions of the detector.)
Dark	Hot pixel map.
Detector (LED) flat fields	Bad pixel map.
Order definition flat	Defines the position of the orders on the detector.
(Spectroscopic) flat field	Echelle blaze function per order.
Wavelength calibration (FP and Th-Ar)	Wavelength solution. Calibrations with (fibre A, fibre B) = (FP, FP), (Th-Ar, FP), and (FP, Th-Ar) are used for this release..
Contamination	Measures the contamination from the FP source on fibre B.
Sky flat fields	Give the relative efficiency of fibre B with respect to fibre A. Only used in science reduction if fibre B is on sky.
Standard stars	Absolute flux calibration.

All calibrations used in this release have been processed with pipeline version 2.2.1 or higher. Calibration and science data for ESPRESSO are always processed with compatible pipeline versions.

Products

The primary ESPRESSO science data product is a 1D spectrum with merged Echelle orders. The file has one table extension. It is the result of either a single exposure or a combination (“stacking”) of spectra resulting from individual exposures. The table columns contain the extracted flux, the wavelength, the error of the flux, and some additional quantities.

There are several additional files which are associated to the primary product:

- 1) an extracted spectrum of fibre B (sky spectrum or FP);
- 2) the cross-correlation function from the calculation of the radial velocity, not produced if target is a QSO;

- 3) the drift matrix between the science exposure and the wavelength calibration, only in case fibre B is on FP;
- 4) a tar file with additional pipeline products that are needed to run the DAS⁵ (data analysis) pipeline of ESPRESSO, it includes the Echelle blaze function and files with extracted spectra for each Echelle order (as 2D images in wavelength-order space);
- 5) a PNG plot file that visualizes the primary product and provides quality control (QC) information;
- 6) all extracted spectra from the individual exposures if the primary product is a co-added spectrum; then also the files under items 1 to 3 are provided for each exposure.

The primary products contain some header keywords with information related to the OB and the QC process. They are listed in Table 2.

Table 2. FITS keywords added to the primary product

Parameter	Values	Meaning
<i>OB-related information:</i>		
VM_SM	SM or VM	Data taken in Service Mode or Visitor Mode; VM data are less constrained in terms of OB properties; they have no user constraints defined and therefore no OB grades.
OB_GRADE	A/B/C/D; X	Immediate grade given by night astronomer, considering ambient conditions checked against user constraints (VM data are formally graded X meaning 'unknown').
OB_COMM<n>	Free text	Any optional comments added by the night astronomer, together with the approximate UT hh:mm (truncated after 200 characters).
<i>QC-related information:</i>		
QC_COMM<n>	Free text	Comments about quality issues

Data Quality

Master calibrations. All used master calibrations have been quality-reviewed and certified at the time of acquisition.

Review and certification of science products. ESPRESSO spectra are reviewed and certified by a process that involves both automatic scoring and random human-supervised certification. The automatic quality-control system scores

- the fulfilment of the calibration plan with respect to the wavelength calibration;
- the saturation of (parts of) the observation;
- and the quality of the combination process in case of co-added spectra.

The measured values are compared to reference values and scored. A non-zero score flags a potential issue. Any non-zero score is reviewed. Upon review, comments can be entered. They are intended to be informative, but they don't claim completeness. The comments are propagated to the product headers (in the keywords QC_COMM<n>).

Preview plots. For each science target, a preview plot is available as quick look. It is delivered as ancillary file together with the main product. An example for a single spectrum is shown in Figure 1 and an example for a combined spectrum in Figure 2.

The plot for a single spectrum shows as top panel the full extracted spectrum (in blue) and a re-binned version (in orange) of the same spectrum. The positions of prominent spectral features (H α , H β , H γ , H δ , H ϵ , and Na D) are marked with dashed lines. Directly below, the spectrum of the signal-to-noise ratio (SNR) and the quality spectrum are plotted. Values of greater than 0 for the latter indicate an issue with the extracted spectrum which could, for example, be due to saturation in the input. The three plots at the bottom show details of the spectrum for three spectral windows.

⁵ See ESPRESSO-DAS pages available at <https://www.eso.org/sci/software/pipelines/>

The plot for a combined spectrum has one more panel. It shows the two input spectra with the lowest and highest average flux together with the co-added spectrum. This panel allows to infer how much the flux of the input spectra varied during the observation sequence.

At the bottom of each plot, a set of QC parameters applicable to the product are printed:

- the total exposure time of the observation, from header keyword “TEXPTIME”;
- the number of exposures on the target (keyword “NCOMBINE”) and, for combined spectra only, the square root of this number;
- the average SNR of the spectrum;
- the average wavelength binning;
- the seeing during the observation (keyword “HIERARCH ESO TEL<N> IA FWHM”);
- the number of saturated pixels in the (first) input frame;
- the time difference between science and the wavelength calibration (delta time wave A);
- and the RV results from the cross-correlation (keywords “HIERARCH ESO QC CCF RV”, “HIERARCH ESO QC CCF RV ERROR”, and “HIERARCH ESO QC CCF MASK”).

For a combined product, the following parameters are added:

- the average contribution of the input spectra to the co-added spectrum; this number should be close to the number of combined exposures;
- the SNR of the co-added (stacked) spectrum;
- the average SNR of all input spectra;
- and the improvement of the SNR in the co-added spectrum, i.e. $\text{SNR}_{\text{coadd}} / \text{SNR}_{\text{single}}$; this number should be close to the square root of the number of combined exposures.

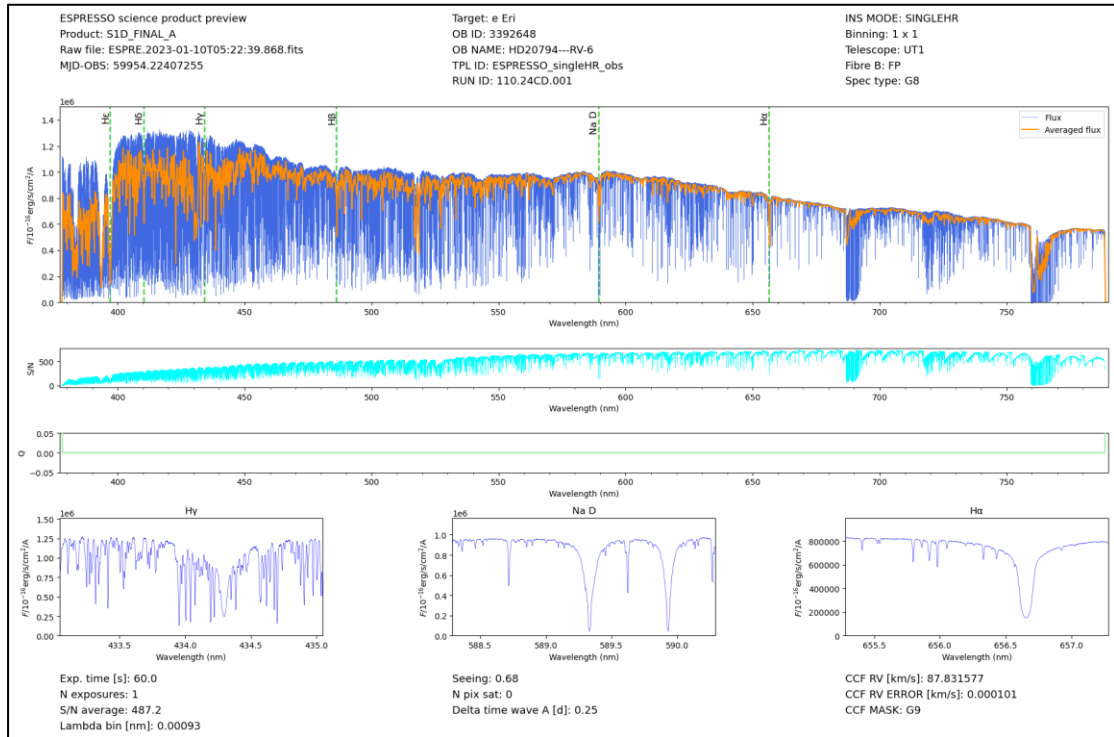


Figure 1. Preview plot associated to a single-exposure spectrum. See text for explanation

Co-added spectra. Multi exposures on the same target are combined if they have been measured within the same template, i.e., if the files have the same TLP.START header key value. Combination is executed independently from the original science goal of the observation. For studying temporal variations, the products from the individual exposures are provided as ancillary files.

RV values for co-added spectra. The RV value that is shown in the QC plots for co-added spectra is only indicative and cannot be used for RV studies. The user is referred instead to the products from the individual exposures which are available as ancillary products.

Data Format

File Types

The data set for each observation consists of one primary product file, several ancillary FITS files, a tar archive, and one preview plot. The number of ancillary files depends on the source for fibre B (FP or sky), whether or not cross correlation was performed, and whether the primary product comes from a single exposure or is a co-added spectrum. Table 3 and Table 4 give an overview of the provided files.

Table 3. Primary and ancillary products for spectra from a single exposure

Type	Product category HIERARCH ESO PRO CATG and PRODCATG	Num- ber	Primary or an- cillary?	Description
fits	S1D_FINAL_A SCIENCE.SPECTRUM	1	Primary	Flux-calibrated spec- trum of the target (fi- bre A)
fits	S1D_FINAL_B ANCILLARY.SPECTRUM	1	Ancillary	Extracted spectrum of fibre B
fits	CCF_A ANCILLARY.CCF	0..1	Ancillary	Cross-correlation func- tion, without telluric correction; not pro- duced for QSOs
fits	CCF_TELL_CORR_A ANCILLARY.CCF	0..1	Ancillary	Cross-correlation func- tion, with telluric cor- rection; not produced for QSOs
fits	DRIFT_MATRIX_B ANCILLARY.DRIFT	0..1	Ancillary	Drift between science exposure and wave- length-calibration, only in case fibre B is on FP
tar		1	Ancillary	Tar archive with addi- tional fits files
png		1	Ancillary	Preview plot

Table 4. Primary and ancillary products for co-added spectra

Type	Product category HIERARCH ESO PRO CATG and PRODCATG	Num- ber	Primary or ancillary?	Description
fits	S1D_STACK_A SCIENCE.SPECTRUM (for data earlier than March 2025)	1	Primary	Flux-calibrated, co- added spectrum of the target (fibre A)
fits	ESOTK_SPECTRUM_IDP_FOR- MAT SCIENCE.SPECTRUM	1	Primary	Flux-calibrated, co- added spectrum of the target (fibre A)

fits	S1D_FINAL_A ANCILLARY.SPECTRUM	1..N	Ancillary	Flux-calibrated spectra for each of the N exposures
fits	S1D_FINAL_B ANCILLARY.SPECTRUM	1..N	Ancillary	Extracted spectra of fibre B
fits	CCF_A ANCILLARY.CCF	0..N	Ancillary	Cross-correlation function, without telluric correction; not produced for QSOs
fits	CCF_TELL_CORR_A ANCILLARY.CCF	0..N	Ancillary	Cross-correlation function, with telluric correction; not produced for QSOs
fits	DRIFT_MATRIX_B ANCILLARY.DRIFT	0..N	Ancillary	Drift between science exposure and wavelength-calibration, only in case fibre B is on FP
tar		1	Ancillary	Tar archive with additional fits files
png		1	Ancillary	Preview plot

The tar archive⁷ that is delivered as an ancillary file contains pipeline products which are needed by the ESPRESSO DAS recipes. The content of the tar file is listed in Table 5.

Table 5. Content of the tar archive

Type	Product category HIERARCH ESO PRO CATG	Number	Description
fits	S2D_A	1..N	Extracted spectra for each order, not flux-calibrated, divided by blaze function
fits	S2D_BLAZE_A	1..N	Extracted spectra for each order, not flux-calibrated, not divided by blaze function
fits	S2D_SKYSUB_A	0..N	Extracted spectra for each order, sky-subtracted, not flux-calibrated, divided by blaze function; only if fibre B is on sky
fits	BLAZE_A	1	Blaze function

The ORIGFILE product name for observation from March 2025 onwards follow a naming convention which is

ESPRESSO_<PRO CATG>_<DATE-OBS>.fits

Using the header keywords `HIERARCH ESO PRO CATG` and `DATE-OBS`. The value of `DATE-OBS` can deviate by a millisecond from the time stamp given in the `PROV1` header keyword.

The ORIGFILE product names for observations before March 2025 follow a naming convention which is

ES_<TYPE>_<OBS_ID>_<DP_ID>_<RES>_<BINX>x<BINY>_<TEL>.fits

See Table 6 for details. An example ORIGFILE name would be

⁷ When extracting the tar archive on the command line of Linux machines, it is advised to use a command like

```
tar -xvf ./ES_SFLX_2147913_2018-11-09T07:18:46.594_UHR_1x1_U3.fits
```

in order to avoid confusion due to the presence of colons in the file name.

ES_SFLX_2147913_2018-11-09T07:18:46.594_UHR_1x1_U3.fits

for a single-exposure spectrum from OB 2147913, observation started at 07:18:46.594 (UT) on 9 November 2018. The ultra-high resolution (UHR) mode was used with a detector binning of 1x1. The telescope for the observation was UT3. The archive user may wish to read the ORIGFILE header key and to rename the archive-delivered fits files accordingly.

In addition to the fits products, also the preview plots are delivered as ancillary files. They come in the PNG image format. Data from March 2025 onwards follow a naming convention which is

ESPRESSO_<PRO CATG>_<DATE-OBS>.png

Earlier data follow the naming conventions

r.ESPRESSO.<DP_ID>_<NNNN>.png

for single-exposure spectra and

r.ESPRESSO.<DP_ID>_com_<NNNN>.png

for co-added spectra, <DP_ID> is the time stamp of the (first) exposure and <NNNN> is a running number with leading zeros (e.g. '0000', '0001', ...).

Table 6. ORIGFILE naming convention for observations before March 2025

Component	Description
ES	ESPRESSO product
<TYPE>	Product type. See Table 3, Table 4, and Table 5
<OBS_ID>	OB ID of the observation (header key <code>HIERARCH ESO OBS ID</code>)
<DP_ID>	Time stamp in UT of the first exposure of the stack in the format <YEAR>-<MONTH>-<DAY>T<HOUR>:<MINUTE>:<SECOND>.<MILLISECOND>
<RES>	Spectral resolution: either HR, UHR, or MR
<BINX>	Detector binning in x (cross-dispersion) direction: 1, 2, 4, or 8
<BINY>	Detector binning in y (dispersion) direction: 1, 2, or 4
<TEL>	Telescope: U1, U2, U3, or U4 for HR and UHR; U1234 ⁸ if all for four UTs are used for MR

File structure and size

The primary ESPRESSO product is a FITS file with one table extension. The table columns for single-exposure spectra and co-added spectra are given in Table 7 and Table 8, respectively. File sizes of the primary products are between 8 and 53 MB.

Table 7. Table columns of single-exposure spectra

Column	Unit	Description
WAVE	Å	Wavelength (in vacuum)
FLUX	erg/cm ² /s/Å	Extracted flux; sky-subtracted if fibre B is on sky, otherwise not sky-subtracted; <i>corrected for telluric absorption (for pipeline versions 3.3.6 or later)</i>
ERR	erg/cm ² /s/Å	Error of flux
QUAL	None	Quality. Values above 0 may indicate issues with data, e.g. saturation
SNR	None	Signal-to-noise ratio of extracted spectrum
WAVE_AIR	Å	Wavelength (in air)

⁸ There are few cases where not all four telescopes were available. Then, a value like “U234” can be found.

FLUX_EL	Counts	Extracted electrons per wavelength bin, not sky-subtracted; telluric correction not applied
ERR_EL	Counts	Corresponding error
QUAL_EL	None	Corresponding quality
FLUX_CAL	erg/cm ² /s/Å	Extracted flux, not sky-subtracted; telluric correction not applied
ERR_CAL	erg/cm ² /s/Å	Corresponding error
QUAL_CAL	None	Corresponding quality
FLUX_CAL_SKYSUB	erg/cm ² /s/Å	Extracted flux, sky-subtracted; only present if fibre B is on sky; telluric correction not applied
ERR_CAL_SKYSUB	erg/cm ² /s/Å	Corresponding error
QUAL_CAL_SKYSUB	None	Corresponding quality
FLUX_EL_SKYSUB	Counts	Extracted electrons per wavelength bin, sky-subtracted; only present if fibre B is on sky; telluric correction not applied
ERR_EL_SKYSUB	Counts	Corresponding error
QUAL_EL_SKYSUB	None	Corresponding quality
FLUX_TELL_EL	Counts	Extracted electrons per wavelength bin, not sky-subtracted; telluric correction applied
ERR_TELL_EL	Counts	Corresponding error
QUAL_TELL_EL	None	Corresponding quality
FLUX_TELL_CAL	erg/cm ² /s/Å	Extracted flux, not sky-subtracted; telluric correction applied
ERR_TELL_CAL	erg/cm ² /s/Å	Corresponding error
QUAL_TELL_CAL	None	Corresponding quality
FLUX_TELL_CAL_SKYSUB	erg/cm ² /s/Å	Extracted flux, sky-subtracted; only present if fibre B is on sky; telluric correction applied
ERR_TELL_CAL_SKYSUB	erg/cm ² /s/Å	Corresponding error
QUAL_TELL_CAL_SKYSUB	None	Corresponding quality
FLUX_TELL_EL_SKYSUB	Counts	Extracted electrons per wavelength bin, sky-subtracted; only present if fibre B is on sky; telluric correction applied
ERR_TELL_EL_SKYSUB	Counts	Corresponding error
QUAL_TELL_EL_SKYSUB	None	Corresponding quality

Table 8. Table columns of co-added spectra

Column	Unit	Description
WAVE	Å	Wavelength (in vacuum)
FLUX	erg/cm ² /s/Å	Co-added flux; sky-subtracted if fibre B is on sky, otherwise not sky-subtracted; corrected for telluric absorption (for pipeline versions 3.3.8 or later)
ERR	erg/cm ² /s/Å	Error of flux
SNR	None	Signal-to-noise ratio of extracted spectrum
QUAL	None	Quality. Values above 0 may indicate issues with data, e.g. saturation
CONTRIB	None	Number of contributing input spectra

Acknowledgement Text

All users are kindly reminded to notify Mrs. Grothkopf (esodata at eso.org) upon acceptance or publication of a paper based on ESO data, including bibliographic references (title, authors, journal, volume, year, and page numbers) and the program ID(s) of the data used in the paper.

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Based on data obtained from the ESO Science Archive Facility with DOI(s) :
<https://doi.eso.org/10.18727/archive/21>.