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Copernicus Climate Change Service

# Product User Guide and Specification (PUGS) – ANNEX C for product CH4_GOS_SRPR (v2.3.9, 2009-2019)

## C3S_312b_Lot2_DLR – Atmosphere

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# History of modifications

| Version | Date | Description of modification | Chapters / Sections |
|---|---|---|---|
| 1.3 | 20-October-2017 | New document for data set CDR1 (2009-2016) | All |
| 2.0 | 4-October-2018 | Update for CDR2 (2009-2017) | All |
| 3.0 | 12-August-2019 | Update for CDR3 (2009-2018) | All |
| 3.1 | 03-November-2019 | Update after review by Assimila: Some typos corrected and references added. | All |
| 4.0 | 18-August-2020 | Update for CDR4 (2009-2019) | All |

# Related documents

| Reference ID | Document |
|---|---|
| D1 | Main PUGS:<br><br>Buchwitz, M., et al., Product User Guide and Specification (PUGS) – Main document for Greenhouse Gas (GHG: CO2 & CH4) data set CDR 4 (2003-2019), project C3S_312b_Lot2_DLR – Atmosphere, 4.0, 2020.<br><br>*(this document is an ANNEX to the Main PUGS)* |
| D2 | **TRD GAD GHG, 2020:** Buchwitz, M., Aben, I., Armante, R., Boesch, H., Crevoisier, C., Hasekamp, O. P., Wu, L.., Reuter, M., Schneising-Weigel, O., Target Requirement and Gap Analysis Document, Copernicus Climate Change Service (C3S) project on satellite-derived Essential Climate Variable (ECV) Greenhouse Gases ($CO_2$ and $CH_4$) data products (project C3S_312b_Lot2), Version 2.11, 9-April-2020, pp. 80, 2020. |
| D3 | Related ATBD:<br><br>Wu, L., et al.: Algorithm Theoretical Basis Document (ATBD) – ANNEX C for product CH4_GOS_SRPR (v2.3.9, 2009-2019), C3S project C3S_312b_Lot2_DLR, v4.0, 2020. |

# Acronyms

| Acronym | Definition |
|---|---|
| ATBD | Algorithm Theoretical Basis Document |
| CAR | Climate Assessment Report |
| C3S | Copernicus Climate Change Service |
| CCI | Climate Change Initiative |
| CDR | Climate Data Record |
| CDS | (Copernicus) Climate Data Store |
| CRG | Climate Research Group |
| D/B | Data base |
| EC | European Commission |
| ECMWF | European Centre for Medium Range Weather Forecasting |
| ECV | Essential Climate Variable |
| EO | Earth Observation |
| ESA | European Space Agency |
| EU | European Union |
| EUMETSAT | European Organisation for the Exploitation of Meteorological Satellites |
| FP | Full Physics retrieval method |
| FTIR | Fourier Transform InfraRed |
| FTS | Fourier Transform Spectrometer |
| GCOS | Global Climate Observing System |
| GEOSS | Global Earth Observation System of Systems |
| GHG | GreenHouse Gas |
| GOSAT | Greenhouse Gases Observing Satellite |
| IPCC | International Panel in Climate Change |
| IUP | Institute of Environmental Physics (IUP) of the University of Bremen, Germany |
| JAXA | Japan Aerospace Exploration Agency |
| KIT | Karlsruhe Institute of Technology |
| L1 | Level 1 |
| L2 | Level 2 |
| L3 | Level 3 |
| L4 | Level 4 |
| LMD | Laboratoire de Météorologie Dynamique |
| MACC | Monitoring Atmospheric Composition and Climate, EU GMES project |
| NA | Not applicable |
| NetCDF | Network Common Data Format |
| NIES | National Institute for Environmental Studies |
| NIR | Near Infra Red |

| | |
|---|---|
| NOAA | National Oceanic and Atmospheric Administration |
| Obs4MIPs | Observations for Climate Model Intercomparisons |
| ppb | Parts per billion |
| ppm | Parts per million |
| PR | (light path) PRoxy retrieval method |
| PVIR | Product Validation and Intercomparison Report |
| QA | Quality Assurance |
| QC | Quality Control |
| REQ | Requirement |
| RMS | Root-Mean-Square |
| RTM | Radiative transfer model |
| SNR | Signal-to-Noise Ratio |
| SRON | SRON Netherlands Institute for Space Research |
| SWIR | Short Wave Infra Red |
| SZA | Solar Zenith Angle |
| TANSO | Thermal And Near infrared Sensor for carbon Observation |
| TANSO-FTS | Fourier Transform Spectrometer on GOSAT |
| TBC | To be confirmed |
| TBD | To be defined / to be determined |
| TCCON | Total Carbon Column Observing Network |
| TIR | Thermal Infra Red |
| TR | Target Requirements |
| TRD | Target Requirements Document |
| URD | User Requirements Document |
| WMO | World Meteorological Organization |
| Y2Y | Year-to-year (bias variability) |

# General definitions

Table 1 lists some general definitions relevant for this document.

Table 1: General definitions.

| Item | Definition |
|---|---|
| $XCO_2$ | Column-averaged dry-air mixing ratios (mole fractions) of $CO_2$ |
| $XCH_4$ | Column-averaged dry-air mixing ratios (mole fractions) of $CH_4$ |
| L1 | Level 1 satellite data product: geolocated radiance (spectra) |
| L2 | Level 2 satellite-derived data product: Here: $CO_2$ and $CH_4$ information for each ground-pixel |
| L3 | Level 3 satellite-derived data product: Here: Gridded $CO_2$ and $CH_4$ information, e.g., 5 deg times 5 deg, monthly |
| L4 | Level 4 satellite-derived data product: Here: Surface fluxes (emission and/or uptake) of $CO_2$ and $CH_4$ |

## Scope of document

This document is a Product User Guide and Specification (PUGS) for the Copernicus Climate Change Service (C3S, https://climate.copernicus.eu/) greenhouse gas (GHG) component as covered by project C3S_312b_Lot2.

Within this project satellite-derived atmospheric carbon dioxide ($CO_2$) and methane ($CH_4$) Essential Climate Variable (ECV) data products have been generated and delivered to ECMWF for inclusion into the Copernicus Climate Data Store (CDS) from which users can access these data products and the corresponding documentation.

The GHG satellite-derived data products are:

- Column-averaged dry-air mixing ratios (mole fractions) of $CO_2$ and $CH_4$, denoted $XCO_2$ (in parts per million, ppm) and $XCH_4$ (in parts per billion, ppb), respectively.
- Mid/upper tropospheric mixing ratios of $CO_2$ (in ppm) and $CH_4$ (in ppb).

This document describes the C3S product CH4_GOS_SRPR.

This product is the $XCH_4$ Level 2 product as retrieved from GOSAT using algorithms developed at SRON, The Netherlands.

## Executive summary

This document is the Product User Guide (PUG), which is a deliverable of the C3S project. This document describes the RemoteC $XCH_4$ PROXY data product (CH4_GOS_SRPR) so that it will be clear for the user how to use the product. The description includes quality flags and metadata, data format, product grid, known limitations, bias correction, and the product (column) averaging kernels and a description how to use them.

# 1. Product description

The Japanese Greenhouse gases Observing SATellite (GOSAT) was launched on 23rd January 2009 (*Yokota et al., 2009)* by JAXA, the Japanese Space Agency. GOSAT provides the first dedicated global measurements of total column $CO_2$ and $CH_4$ from its SWIR bands, *Yoshida et al., 2010*. It is equipped with two instruments, the Thermal And Near Infrared Sensor for carbon Observations - Fourier Transform Spectrometer (TANSO-FTS) as well as a dedicated Cloud and Aerosol Imager (TANSO-CAI).

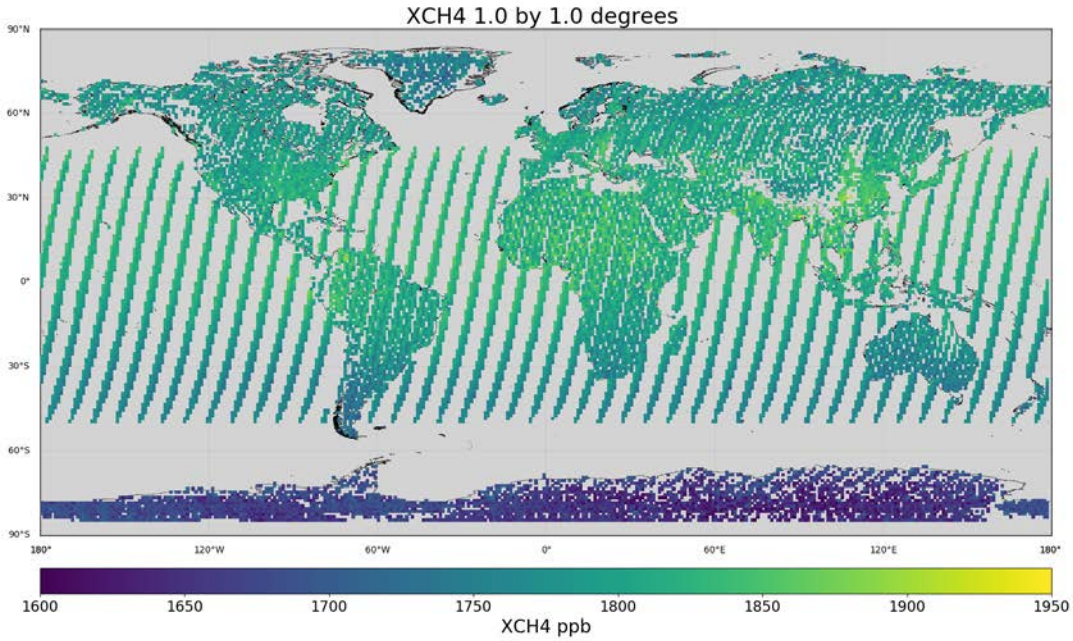
The TANSO-FTS instrument has four spectral bands with a high spectral resolution 0.3 $cm^{-1}$, three of which operate in the SWIR at around 0.76, 1.6 and 2.0 µm providing sensitivity to the near-surface absorbers with the fourth channel operating in the thermal infrared between 5.5 and 14.3 µm providing mid-tropospheric sensitivity.

The measurement strategy of TANSO-FTS is optimized for the characterization of continental-scale sources and sinks. TANSO-FTS utilizes a pointing mirror to perform off-nadir measurements at the same location on each 3-day repeat cycle. The pointing mirror allows TANSO-FTS to observe up to ±35° across track and ±20° along-track. These measurements nominally consist of 3 across track points spaced ~100km apart (although measurements are possible with 1, 3, 5, 7 or 9 across track points) with a ground footprint diameter of approximately 10.5 km and a 4 second exposure duration. Whilst the majority of data is limited to measurements over land where the surface reflectance is high, TANSO-FTS also observes in sunglint mode over the ocean within ±20° of the sub-solar latitude.

The CH4_GOS_SRPR product is retrieved from GOSAT TANSO-FTS NIR and SWIR spectra using the RemoTeC algorithm that has been jointly developed at SRON and KIT. The algorithm retrieves simultaneously $XCH_4$ and $XCO_2$. For the retrieval, we analyze four spectral regions: the 0.77 µm oxygen band, two CO2 bands at 1.61 and 2.06 µm, as well as a CH4 band at 1.64 µm. Within the retrieval procedure the sub-columns of $CO_2$ and $CH_4$ in different altitude layers are being retrieved. To obtain the column averaged dry air mixing ratios XCO2 and XCH4 the sub-columns are summed up to get the total column which is divided by the dry-air columns obtained from ECMWF model data in combination with a surface elevation data base. As the PROXY retrievals perform a non-scattering retrieval, the retrieved XCH4 column cannot be used directly, as effects of aerosol scattering modify the light path. To correct for this, in the PROXY approach, the retrieved XCH4 column is divided by the retrieved XCO2 column at the 1.61 µm band and then multiplied by a XCO2 total column obtained from LMD flask-based inversions. As the LMD flask inversions were not yet available at the time of delivery of this product, we extrapolated the 2015 model XCO2 values by 3 ppm (the growth rate in 2016). The retrieved XCH4 has been extensively validated with ground based TCCON measurements. To further improve accuracy a bias correction has been developed based on TCCON comparisons. We use the GGG2014 release of the TCCON data (**Wunch et al. 2015)**.

More details on the technical aspects of the retrievals can be found in the ATBD Annex-C (*D3*).

Figure 1: Global $XCH_4$ for the 2009-2019 period for the CH4_GOS_SRPR product on a 1 by 1 degree resolution.



# 2. Target requirements

Table 1: Target requirements for $XCH_4$.

| Random and systematic error requirements for $XCH_4$ | | | | | |
|---|---|---|---|---|---|
| **Parameter** | **Req. type** | **Random error** ("Precision") | | **Systematic error** | **Stability** |
| | | Single obs. | $1000^2$ km$^2$ monthly | | |
| $XCH_4$ | G | < 9 ppb | < 3 ppb | < 1 ppb (absolute) | < 1 ppb/year (absolute) |
| | B | < 17 ppb | < 5 ppb | < 5 ppb (relative §)) | < 2 ppb/year (relative §)) |
| | T | < 34 ppb | < 11 ppb | < 10 ppb (relative #)) | < 3 ppb/year (relative #)) |

Table 1 shows the target requirements for $XCH_4$ (Threshold, Breakthrough and Goal) as derived in the Target Requirements Document (TRD) (*D2*).

# 3. Data usage information

## 3.1 Product Content and Format

The RemoteC XCH4 data product is stored per day in a single NetCDF file. Retrieval results are provided for the individual GOSAT spatial footprints, i.e. no averaging has been applied. The product file contains the key products, i.e. the retrieved column averaged dry air mixing ratio XCH4 with and without bias correction. Information relevant for the use of the data is included in the data file, like the vertical layering and averaging kernels. Also, the parameters that are retrieved simultaneously with XCH4 are included (e.g. surface albedo), as well as retrieval diagnostics like retrieval errors, quality of the fit.

Table 2: Common variables for the CH4_GOS_SRPR product

| Name | Type | Dim. | Units | Description |
|---|---|---|---|---|
| | | | | |
| solar_zenith_angle | float | n | degrees | Angle between line of sight to the sun and local vertical |
| sensor_zenith_angle | float | n | degrees | Angle between the line of sight to the sensor and the local vertical |
| time | float | n | seconds | Seconds since 1970-01-01 00:00:00 |
| longitude | float | n | degrees_east | Center longitude |
| latitude | float | n | degrees_north | Center latitude |
| pressure_levels | float | n, 5 | hPa | Pressure levels |
| pressure_weight | float | n, 4 | | Layer dependent weights needed to apply the averaging kernels |
| xch4 | float | n | 1e-9 | Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb |
| xch4_uncertainty | float | n | 1e-9 | 1-sigma uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane |
| xch4_averaging_kernel | float | n, 4 | | Normalized column averaging kernel |
| ch4_profile_apriori | float | n, 4 | 1e-9 | A priori dry-air mole fraction profile of atmospheric methane |
| xch4_quality_flag | int | n | | Quality flag for XCH4 retrieval, 0 = good, 1 = bad |

Table 3: Product specific (additional) variables for the CH4_GOS_SRPR product

| Name | Type | Dim. | Units | Description |
|---|---|---|---|---|
| | | | | |
| flag_landtype | int | n | | 0 = land, 1 = ocean |
| flag_sunglint | int | n | | 0 = no sunglint, 1 = sunglint |
| gain | char | n | | gain setting of sensor, H = gain H, M = gain M |
| exposure_id | int | n | | Exposure identification number of the sounding |
| l1b_name | char | n, 44 | | Name of the Level 1B file of the sounding |
| signal_to_noise_window | float | n, 4, 2 | | Signal to noise ratio per retrieval window and for both polarization directions |
| dry_airmass_layer | float | n, 4 | m-2 | Dry airmass per layer |
| altitude | float | n | m | Vertical altitude above the surface |
| air_temperature | float | n, 5 | K | The bulk temperature of the air at each level |
| surface_altitude_stdv | float | n | m | Standard deviation of the surface elevation within the sounding |
| x_wind | float | n, 5 | m s-1 | Eastward wind velocity |
| y_wind | float | n, 5 | m s-1 | Northward wind velocity |
| chi2 | float | n | | Chi-squared value of the sounding |
| optical_thickness_of_atmosphere_layer_due_to_ambient_aerosol | float | n, 4 | | Scattering optical thickness per retrieval window |
| raw_xch4_err | float | n | 1e-9 | 1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric methane |
| h2o_column_1593 | float | n | m-2 | Retrieved total water column at 1593 nm |
| h2o_column_1629 | float | n | m-2 | Retrieved total water column at 1629 nm |
| h2o_column_2042 | float | n | m-2 | Retrieved total water column at 2042 nm |
| surface_albedo_758 | float | n | | The retrieved albedo at 758 nm |
| surface_albedo_1593 | float | n | | The retrieved albedo at 1593 nm |
| surface_albedo_1629 | float | n | | The retrieved albedo at 1629 nm |
| surface_albedo_2042 | float | n | | The retrieved albedo at 2042 nm |
| intensity_offset_o2a | float | n | W cm-2 | The retrieved intensity offset in the O2A band |
| raw_xch4 | float | n | 1e-9 | Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before scattering correction |
| xch4_no_bias_correction | float | n | 1e-9 | Retrieved column dry-air mole fraction of atmospheric methane (XCH4) in ppb before bias correction |
| raw_xco2 | float | n | 1e-6 | Retrieved column dry-air mole fraction of atmospheric carbon dioxide (XCO2) in ppm before scattering correction |
| xco2_apriori | float | n | 1e-6 | A priori dry-air mole fraction of atmospheric carbon dioxide |
| co2_profile_apriori | float | n, 4 | 1e-6 | A priori dry-air mole fraction profile of atmospheric carbon dioxide |
| xco2_averaging_kernel | float | n, 4 | | Normalized column averaging kernel for carbon dioxide |
| raw_xco2_err | float | n | 1e-6 | 1-sigma statistical uncertainty of the retrieved column-average dry-air mole fraction of atmospheric carbon dioxide |

## 3.2 Quality Flags and Metadata

There is a quality flag "xch4_quality_flag" included in the data file. The quality flag can have 2 values:

- 0: retrievals for **H-gain**, **M-gain** or **sunglint** data, quality has been checked
- 1: data should not be used (e.g. bad fit to data, residual cloud contamination)

For a GOSAT ground pixel to be processed by the RemoTeC PROXY algorithm it has to fulfill the following criteria: GOSAT nominal quality flags should be good and the standard deviation of the elevation in the pixel should be less than 1000 meters (to filter out the most extreme terrain). After the retrieval the data that fulfill the following criteria are flagged as '0':

- Number of iteration steps in retrieval < 10.
- $\chi 2$ of fit < 7.
- SNR > 50.
- Standard deviation of surface elevation within GOSAT ground pixel should be < 150 m
- SZA < 75°.
- 0.98 < CO2 (1.6 micron) / CO2 (2.0 micron) < 1.15
- 0.88 < O2 (retrieved) / O2 (prior) < 1.035
- 0.9 < H2O (1.6 micron) / H2O (2.0 micron) < 1.5

## 3.3 Bias Correction

From comparison with TCCON it was found that the error in XCH4 correlates with the retrieved albedo $\alpha$ at 1.6 um in band 2. Based on this correlation the following bias correction has been developed for XCH4:

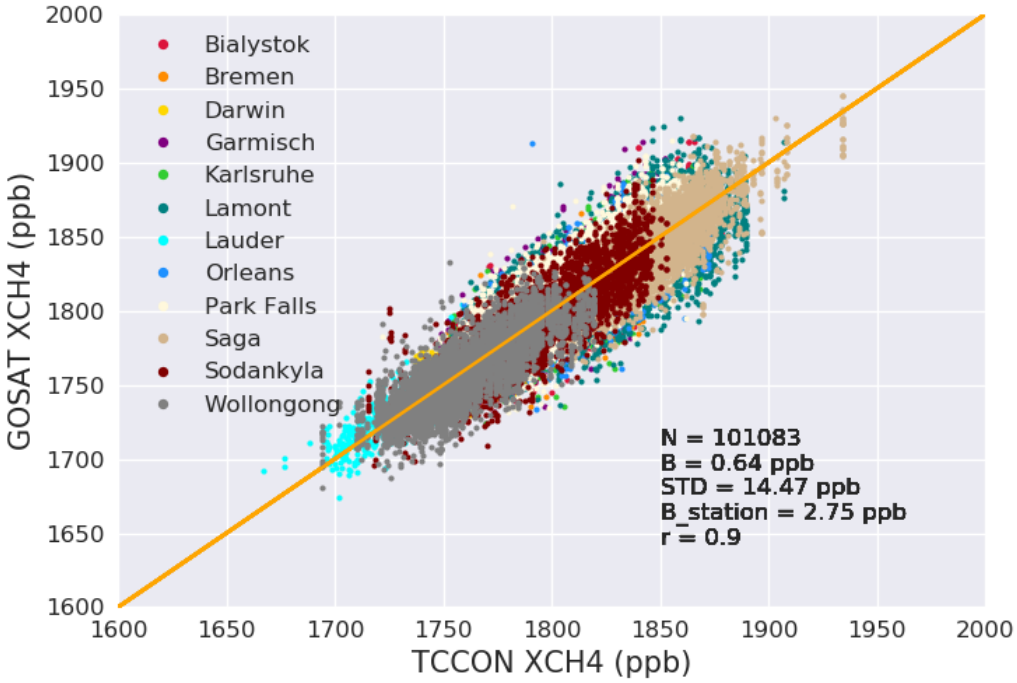
$$XCH4_{corr} = XCH4 * (a + b * \alpha)$$

with a = 0.9869 , b = 0.01788 for **H-gain** data and a=0.98446 , b = 0.01892 for **M-gain** data.
The bias correction parameters are obtained from fits to the GOSAT-TCCON differences. For **sunglint** observations we apply a global offset as a bias correction:

$$XCH4\_corr = XCH4 * a$$

With a = 0.992557.

Figure 2: Co-located GOSAT-TCCON XCH4 measurements for gain H measurements.



## 3.4 Recommended data usage

It is strongly recommended to only use the bias-corrected data in: "xch4" except if users explicitly correct for biases themselves (e.g. in an inverse modeling framework). Here, it should be noted that the bias correction has been developed independently for the different GOSAT-FTS instrument settings **(H-gain**, **M-gain**, **sunglint**).

**Also, use only data over land (land_type=0) except for sunglint cases**.

If the data are to be compared with other XCO2 and/or XCH4 data for which vertical profile information is available (e.g. inverse modeling, comparison to models, comparison to measured profiles), the column averaging kernels should be used. Here it should be noted that **the column averaging kernels are to be applied to layer sub-columns (m-2)** , as these are the quantities directly retrieved in the RemoTeC algorithm. For model comparisons the retrieved XCO2 should be compared to $[VCO2]'_{model}/[VAIR]_{model}$ where $[VAIR]_{model}$ is the total dry air column provided by the model and $[VCO2]'_{model}$ is the model total CO2 column after applying the column averaging kernel, viz.:

$$[VCO2]'_{model} = [VCO2]_{prior} + \mathbf{a}^T(\mathbf{x}_{model} - \mathbf{x}_{prior})$$

where $[VCO2]_{prior}$ is the prior CO2 total column used in the retrieval, $\mathbf{x}_{model}$ is the vertical CO2 profile from the model (as sub-columns) and $\mathbf{x}_{prior}$ is the prior vertical profile from the retrieval. For application of the column averaging kernel the model vertical profile should be re-calculated on the vertical grid of the retrieval (preferred) or the averaging kernel has to be interpolated to the vertical grid of the model.

## 3.4 Tools for Reading the Data

The data are stored in Netcdf format which can be read with standard tools in the common programming languages (IDL, Matlab, Python, Fortran90, C++, etc).

## 3.5 Known Limitations and Issues

- The data retrieved for the H-gain instrument settings are considered highest quality and are well validated. In the "raw" retrievals (i.e. before bias correction) there is a bias between **H-gain** and **sunglint** and **M-gain** retrievals, respectively. Although these biases have been corrected in the bias-corrected products, there may still be a small residual bias left, especially due to the limited number of validation sites for **sunglint** and **M-gain** retrievals.
- The 2nd half of December 2014 and the whole of January 2015 have no data due to the GOSAT satellite being in calibration mode after switching to the backup pointing system.

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