SOFTWARE

CHROMATEC ANALYTIC

BUILD 4.0

USER MANUAL

214.00045-51I

VERIFICATION AND QUALIFICATION

Revision 02.12.2025

Table of contents

1 Introduction 4
2 Checkout 5
2.1 Noise Calculation 5
2.2 GC checkout 6
2.3 MSD checkout 7
3 IQ/OQ/PQ qualification 9
3.1 Installation qualification (IQ) 9
3.2 Qualification of functioning (OQ) 10
3.3 Performance qualification (PQ) 11
3.4 Preparation to work 12
3.5 Tools and materials 12
3.6 Qualification protocol 13
3.6.1 Login with Internet access 13
3.6.2 Login without Internet access 13
3.6.3 Protocol editing. Basic sections 14
3.6.4 Special sections 19
3.6.5 Creating a protocol 20

1 INTRODUCTION

This manual is intended for service engineers working with chromatographs manufactured by JSC SDO "Chromatec". The manual describes the operations required for the verification and qualification of IQ/OQ/PQ equipment and software.

2 CHECKOUT

Metrological verification of chromatographs of the "Crystal" and "Chromatec-Crystal" series is carried out according to the instructions of the following documents:

- GOST 8.485-83 "Analytical gas laboratory chromatographs. Methods and means of verification".
- GOST 26703-93 "Analytical gas chromatographs. General technical requirements and test methods".
- RD 214.2.840.030-01D Chromatograph "Crystal 2000M". Verification procedure.
- RD 214.2.840.043-03D is a hardware and software complex for medical research based on the chromatograph "Chromatec-Crystal 5000". Verification procedure.
- RD 214.2.840.073D Chromatograph "Chromatec-Crystal 9000". Verification procedure.

Preparatory work must be carried out before the verification:

- external inspection: compliance with the completeness of the complex, serviceability of mechanisms and fasteners, clarity of marking;
- preparation of appropriate solutions (samples);
- checking the tightness of gas lines, from the carrier gas cylinder to the Pressure regulators and digital flow controllers, from pressure regulators and digital flow controllers to detectors, inlets and valves;
- checking the inlet, detector and column thermostats for heating from 300 to 400 °C and cooling;
- preparation of columns in accordance with the regulatory documentation for analysis (conditioning);
- conditioning of chromatograph filters and auxiliary devices (compressor, hydrogen generator, external filter unit).

For more information about the above actions, see the "Chromatograph Operating Manual", as well as the analysis manual (if there is such a manual for your analysis).

2.1 Noise Calculation

Noise calculation can be performed without performing the entire checkout calculation.

To calculate the noise, record the chromatogram of the blank analysis (without entering a sample). The recommended duration of the chromatogram is 30 minutes.

According to the **Verification Procedure**, the interval at which noise should be measured is 10 minutes.

In the chromatogram passport, specify its purpose – **baseline**.

{video analytic_noise_calculation}

2.2 GC checkout

- Create instrumental method and processing method.
- Get a chromatogram of the blank analysis and calculate noise level.
- Perform at least five tests of the calibration mixture.
- In the processing method, fill in the table of components and processing parameters.
- Go to the report settings, add the section "GC/HPLC checkout" and set its parameters:

{video analytic_checkout Checkout}

- Specify the type of chromatograph, enter its serial number and the numbers of all detected detectors.
- Select the detector version (not all detectors have it).
- Specify the name of the column. If the column is capillary, enable the corresponding option.
- Set the measurement conditions.
- Select the component for which the detection limit will be calculated.
- Select the components for which the Standard Solution will be calculated (if necessary).
- Select the type of detection limit calculation: **standard**, **volume%** or **HPLC** (calculation of detection limit for chromatograph "Chromatec-Crystal HPLC 2014").
- Specify split ration of the sample in the input port (set in instrumental method).
- Specify the extraction coefficient in accordance with the Verification procedure.
- Specify the concentration units.
- When checking TCD, set the flow rate of the carrier gas, temperature and ambient pressure.
- Adjust the noise evaluation parameters. It is recommended to set an auto-search interval of 10 minutes, taking into account the drift.
- Select the chromatogram from which the noise will be calculated. It should have the designation "Baseline".
- Save the method.
- After setting up the method, go back to the "Analytic", open open batch of chromatograms that will be used for verification.

 Create a report.

2.3 MSD checkout

- Create instrumental method and processing method.
- Get a chromatogram of the blank analysis and calculate noise level.
- Perform at least five analyses of a sample containing hexachlorobenzene.
- Go to the report settings, add the section "MS checkout".
- Save the method.
- Select the batch of recorded chromatograms.
- Go to the "MS: Signal/Noise" page.
- Specify the type of analysis.

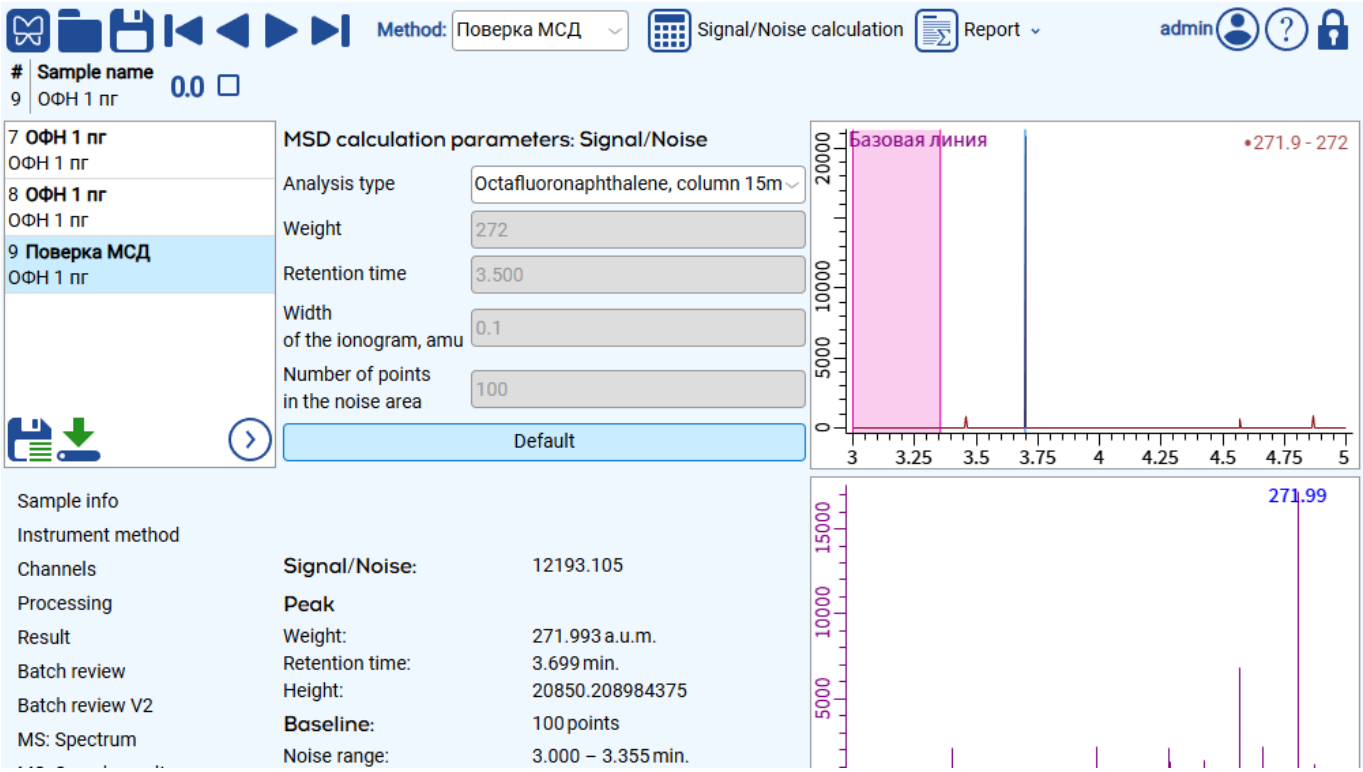


Fig. 2.1 – Signal/Noise calculation

Click "Signal/Noise Calculation".

For the correct calculation, it is necessary to set the column length and the test substance. The program has 6 preset values: for columns with a length of 15 m and 30 m, and test substances: octafluoroaphthalene, hexachlorobenzene and benzophenone.

After performing the calculation, create a report.

{video analytic_ms_checkout MS checkout, signal/noise}

The **Custom** analysis type allows you to enter an arbitrary mass and an approximate retention time for the peak, according to which the signal-to-noise ratio will be calculated.

Parameters for determining the signal-to-noise ratio:

Smoothing. Allows you to select the degree of smoothing of the chromatogram (there is no smoothing by default).

Number of points in noise area. Sets the width of the noise section, expressed in the number of scans (by default – 100 scans).

Width of the ionogram. The width of the mass range according to which the chromatogram will be formed, a.e.m.

A chromatogram with a mass range of a given width selected to determine the signal-to-noise ratio is displayed on the upper graph. The chromatogram is limited in time by the range around the desired peak: 1.5 minutes in both directions from the peak.

The calculated values are shown at the bottom of the window:

Peak. Peak parameters. They are determined by the chromatogram and do not depend on the calculation parameters.

Baseline. The value of the baseline, the boundaries and width of the noise section, the standard deviation from the baseline in the noise section are displayed.

3 IQ/OQ/PQ QUALIFICATION

The qualification of laboratory equipment and software guarantees their "validity", i.e. suitability for the implementation of user tasks.

IQ-OQ-PQ qualification procedure can be performed by service engineers authorized by JSC SDO Chromatec".

The run of the qualification program is possible only if you have a digital certificate of a service engineer.

JSC Chromatec products may contain upgraded parts in accordance with new developments or may be subjected to minor modifications not reflected in this document.

The general qualification plan and acceptance criteria for the chromatograph are listed below. The plan and eligibility criteria may differ for other qualification objects, in this case it is necessary to be guided directly by the qualification protocol.

3.1 Installation qualification (IQ)

Qualification of installation of equipment manufactured by JSC SDO Chromatec consists of the following stages:

1. Initial inspection of the device: checking the completeness of delivery, checking the absence of damage to the device.
2. Identification of the device. It is confirmed that the delivery of the device was carried out correctly, in accordance with the order specification.
3. Checking the installation of the device. The compliance of the device location conditions with the required ones is checked, the correct connection of gas lines, their tightness is checked. The correct connection of the cables and the dispenser is confirmed (if available).
4. Checking the initialization of the device. The device is being turned on and peripheral devices are being initialized.

3.2 Qualification of functioning (OQ)

When qualifying the operation, the operability of the software and the device is checked. The full list of tests and acceptance criteria of the results are given in the table below.

Test		**Acceptance criteria**
Checking the relevance of software versions and firmware		
Checking the compliance of the hash code of metrologically significant modules with the standard		Hash Code matching
Leakage test	Tightness of the pressure reducer at 0.4 MPa	Gas pressure change ≤ 0.05 MPa
	Tightness of electronic DFC	Gas consumption (without gas supply) ≤ 0.3 ml/min Gas consumption (on a regulator with a plug installed) = 0.3 ml/min
	Checking the tightness of the system with DFC at a flow rate of 30 ml/min	Gas flow (on a regulator with a plug installed) ≤ 0.8 ml/min
Checking the stability of maintaining the pressure of the carrier gas		Visual control of the absence of pulsations and pressure surges
Checking thermostats	Column oven	Temperature fluctuations ≤ ±0,03 °C
	Inlets	Temperature fluctuations ≤ ±0,2 °C
	Detectors	Temperature fluctuations ≤ ±0,1 °C
Checking the correctness of instrumental method transmission		Compliance of the set parameters with the fixed ones
Checking the work of the DFC	Compliance of the set flow rate with the actually measured	Gas flow difference < 0.3 ml/min (optional check)

3.3 Performance qualification (PQ)

At this stage, the metrological characteristics of the detectors are checked. The acceptance criteria are listed below.

Test	Parameters and configuration	Acceptance criteria
Detectors noise evaluation	FID	≤2×10^{-14} A
	ECD	≤1×10^{-12} A
	FPD	≤2×10^{-11} A
	TCD	≤1×10^{-7} V
	CCD	≤6×10^{-6} V
	PID	≤1×10^{-13} A
	NPD	≤2×10^{-13} A
	PDD	≤$1,2\times10^{-4}$ V
	HID	≤1.3×10^{-11} A
Baseline drift is determination	FID	≤4×10^{-13} A/h
	ECD	≤8×10^{-11} A/h
	FPD	≤4×10^{-10} A/h
	TCD	≤2×10^{-5} V/h
	CCD	≤$1,2\times10^{-4}$ V/h
	PID	≤2×10^{-11} A/h
	NPD	≤2×10^{-11} A/h
	PDD	≤$6\times10^{-}$ V/h
	HID	≤$1,3\times10^{-10}$ A/h
Detection limit determination	FID	≤2×10^{-12} g/s
	ECD	≤3×10^{-14} g/s
	FPD	≤2×10^{-13} gP/s ≤1×10^{-12} gS/s
	TCD	≤2×10^{-9} g/ml
	CCD	≤8×10^{-10} g/ml
	PID	≤$2,5\times10^{-13}$ g/s
	NPD	≤2×10^{-14} gP/s
	PDD	≤3×10^{-13} g/s
	HID	≤$4,5\times10^{-12}$ g/s
RSD,% determination	FID	≤2% (6% for capillary column)
	ECD	≤4%
	FPD	FPD-P ≤6%. FPD-S ≤10 %

Test	Parameters and configuration	Acceptance criteria
	TCD	≤2%
	CCD	≤2%
	PID	≤5%
	NPD	≤4%
	PDD	≤4%
	HID	≤2%

3.4 Preparation to work

To perform the equipment qualification procedure, make sure that all the required tools and accessories are available.

You will need stickers for qualification certificates. They are supplied when ordering the qualification procedure.

The list of necessary equipment is given in the qualification protocol itself and may be different for different qualification scenarios.

The scenario is determined by the choice of the qualification object (chromatograph, software, automatic dispenser, mass spectrometric detector).

Copies of certificates of used measuring equipment must be attached to the protocol.

3.5 Tools and materials

- Logbook:
  "Chromatec-Crystal 5000": 214.2.840.043ФО.
  "Chromatec-Crystal 9000": 214.2.840.073ФО.
- "Laboratory Gas Chromatographs" User manual 214.2.840.039(075)UM parts 1, 2 and Installation instruction.
- Performance verification procedure:
  Chromatec-Crystal 5000: 214.2.840.043-03D.
  Chromatec-Crystal 9000: 214.2.840.073D.
- Qualification stickers.
- Spare parts and accessories (spare parts) 214.4.060.245.
- Digital voltmeter.
- Thermometer.
- Remote temperature sensor
- Flow meter.
- Capillary column* BPX5 15 m × 0.25 mm × 0.25 microns or similar, with characteristics no worse than those proposed.
- Sample for testing**. The test samples are selected according to the verification procedure 214.2.840.043-02D and the configuration of the device.

* If there is regulatory documentation for the MVI according to GOST 8.563-96, the technical characteristics of the columns must comply with the requirements of the section on measuring instruments of the MVI.

** In the presence of regulatory documentation for MVI according to GOST 8.563-96, samples must comply with the requirements of the section on samples of MVI. The following measuring instruments are available: GSO 10956-2017 heptane in non, Electron capture detector test sample 18713-60040; Standard flame ionization detector GC, conventional hydrocarbons C14, C15 and C16, 0.033 wt.% in hexane, 18710-60170; NPD standard in isooctane, 18789-60060.

3.6 Qualification protocol

- In "Chromatec Navigator" go to the "Administration" page.


Click on the button "IQ/OQ/PQ Qualification Protocol".

3.6.1 Login with Internet access

- Enter your surname, name and number of the certificate.
- Click "OK". With a successful entrance, the "Qualification" page will open.

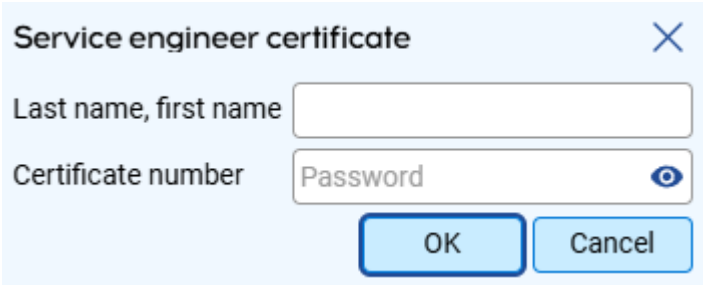


Fig 3.1 – Entering data of the service engineer (with Internet access)

3.6.2 Login without Internet access

- Enter your surname, name and number of the certificate.
- Scan the QR code with a smartphone.
- Follow the received link.
- In the browser on the smartphone, a site will open on the page of which the access code will be indicated.
- Enter this code in the request window.
- Click "OK". With a successful entrance, the "Qualification" page will open.

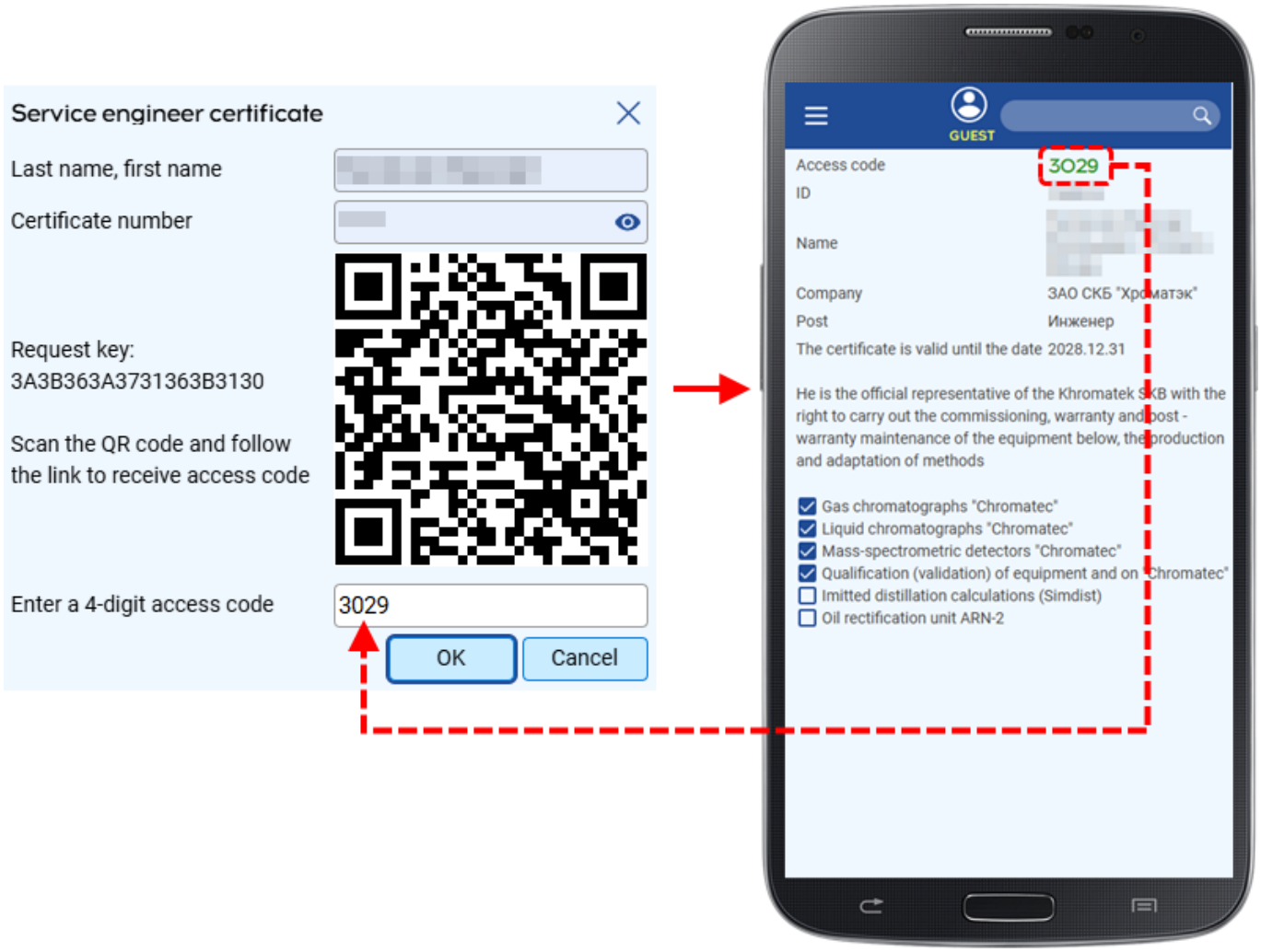


Fig 3.2 – Entering data of the service engineer (without Internet access)

3.6.3 Protocol editing. Basic sections

The "Qualification" page opens. On it, click the "Select Protocol" button. Select the protocol type.

- A dialogue for entering the protocol variables will appear on the screen. Set the variables.
- Click "OK".

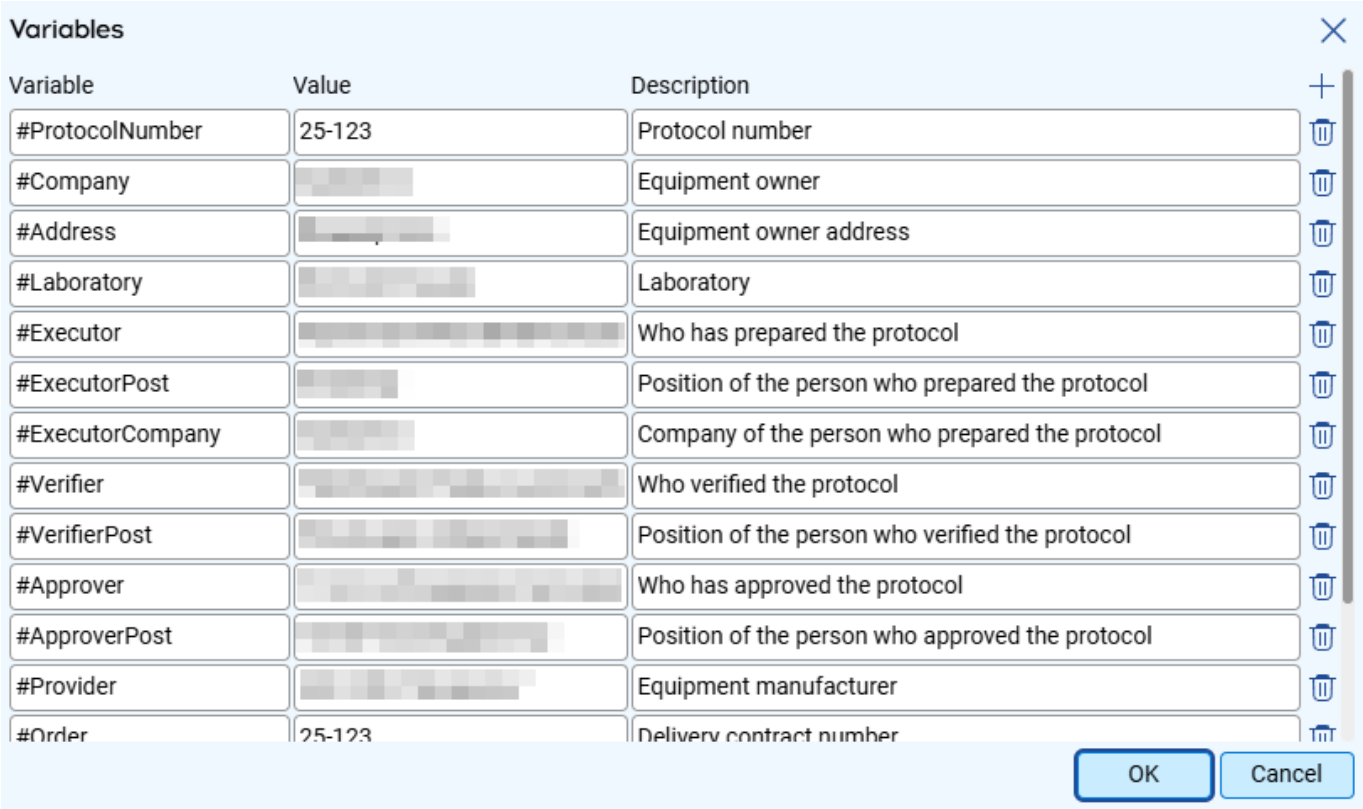


Figure 3.3 – Set variables

The protocol editor will open:

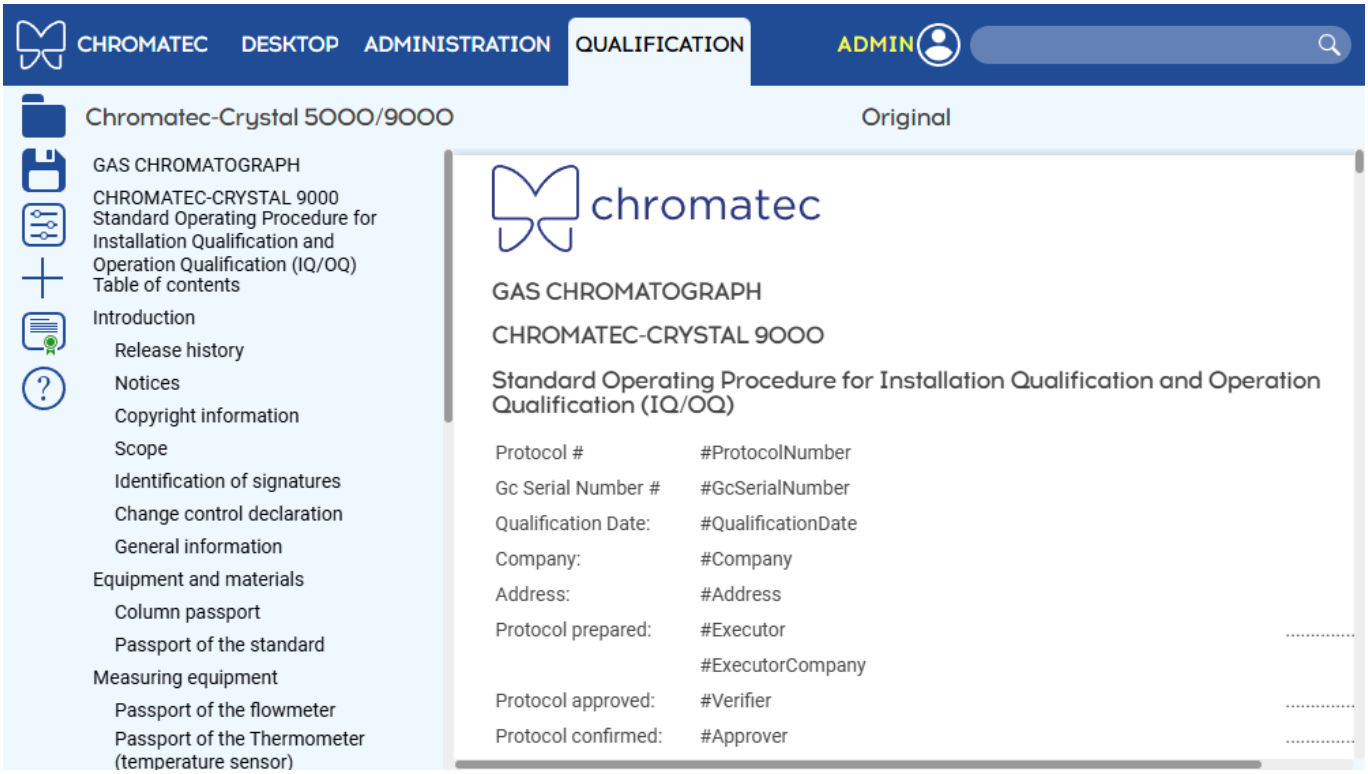


Fig 3.4 – Protocol editor

You can highlight each section of the protocol (paragraph, table, marked or numbered list, images entering in SVG, PNG, JPG formats and edit their content.

For each section, when isolating, a toolbar appears. For everyone, it contains the option "from the new page" and the section deletion button.

Some sections are forbidden to remove. For them, this button is blocked.

If we enable the option “from the new page”, then in the final protocol in PDF this section this section will be printed from the new page, and the icon will appear in the editor on the left .

To add the section, click on the "Add" button on the left side panel and select the type of section. The new section will be added after allocated. If there are no selected sections, then the new will be added to the end of the protocol.

Paragraphs and headlines

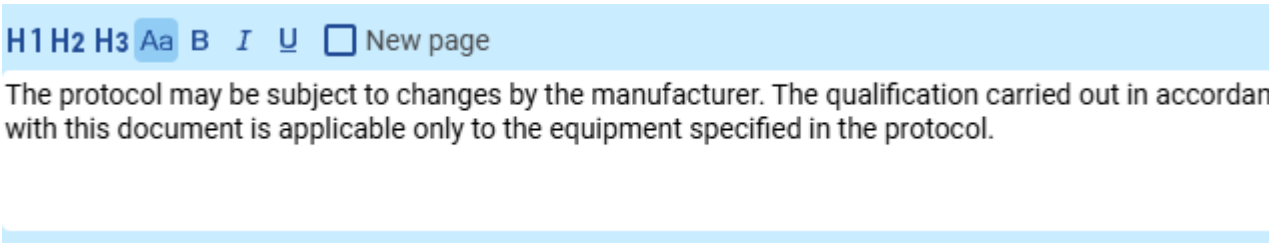


Fig 3.5 – Paragraph and headlines settings menu

For a simple text, you can change the type – paragraph, heading of the first, second or third level. The text allows the use of html tags:

-   – semi -fat.
-   – italics.
- <u></u> – emphasized.

Marked and numbered list

For lists, you can select the type, add or remove the element.

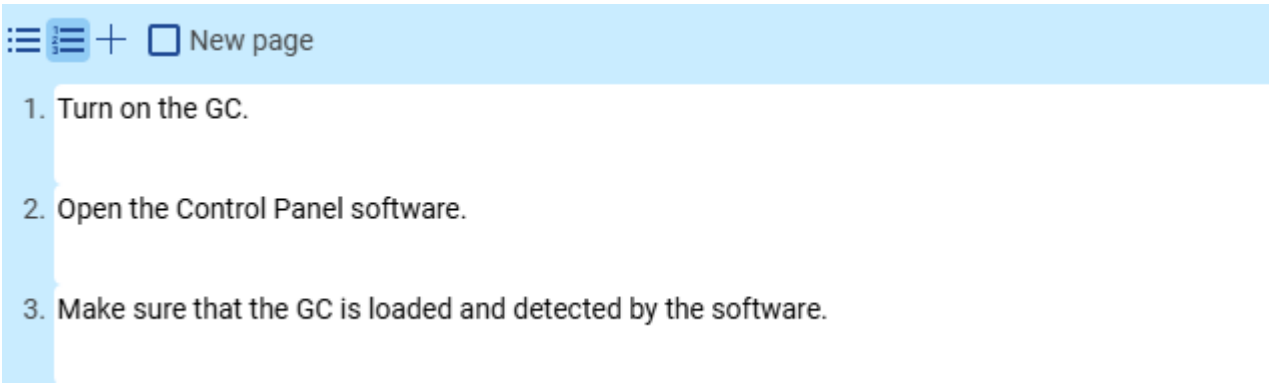


Fig 3.6 – Marked and numbered lists settings

Tables

For the table in the settings menu, you can specify whether it has a frame or not. You can display the panel of the column width settings.

The width of the column can be indicated clearly by setting the value in the pixels. You can set the value of auto – auto -haired, or indicate * – stretch the column to fill all the free space on the sheet.

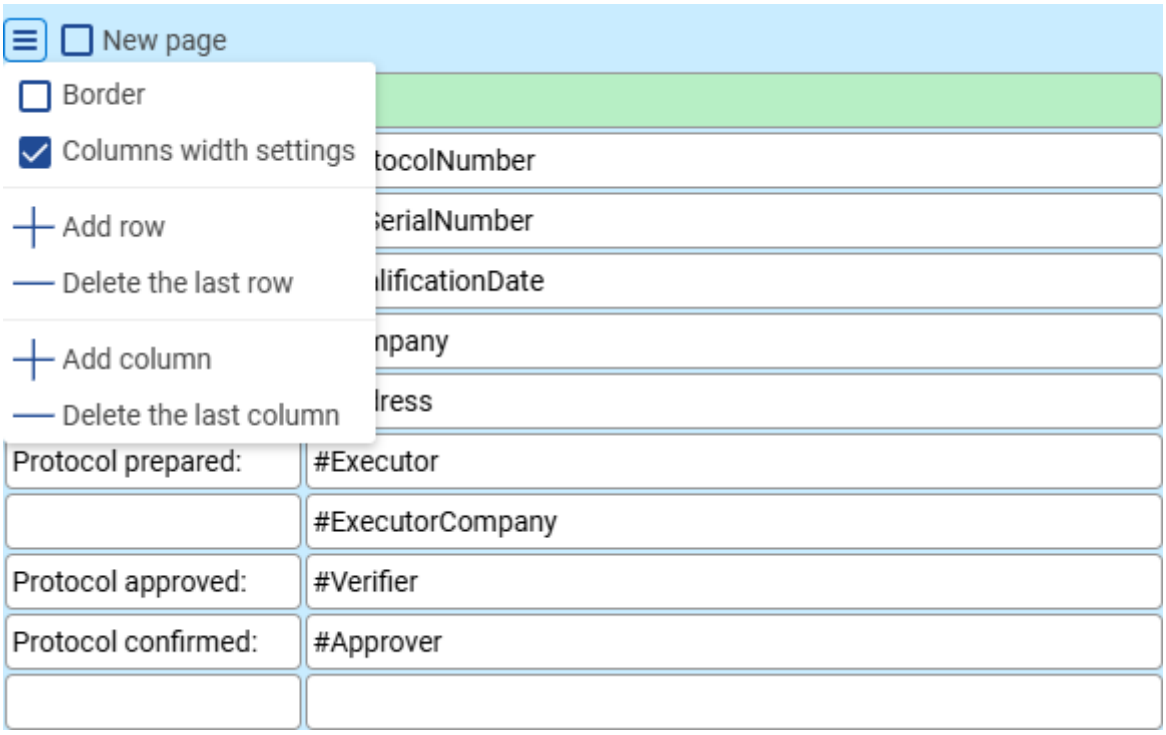


Fig 3.7 – Table settings menu

You can add and remove columns and lines.

Images in SVG format

SVG is a vector image format that provides high clarity during printing. In this format, you can save chromatograms and diagnostic charts to insert them into the protocol in the places where it is required.

To insert the image, press the corresponding button on the section toolbar and select the SVG file.

SVG image file is not selected

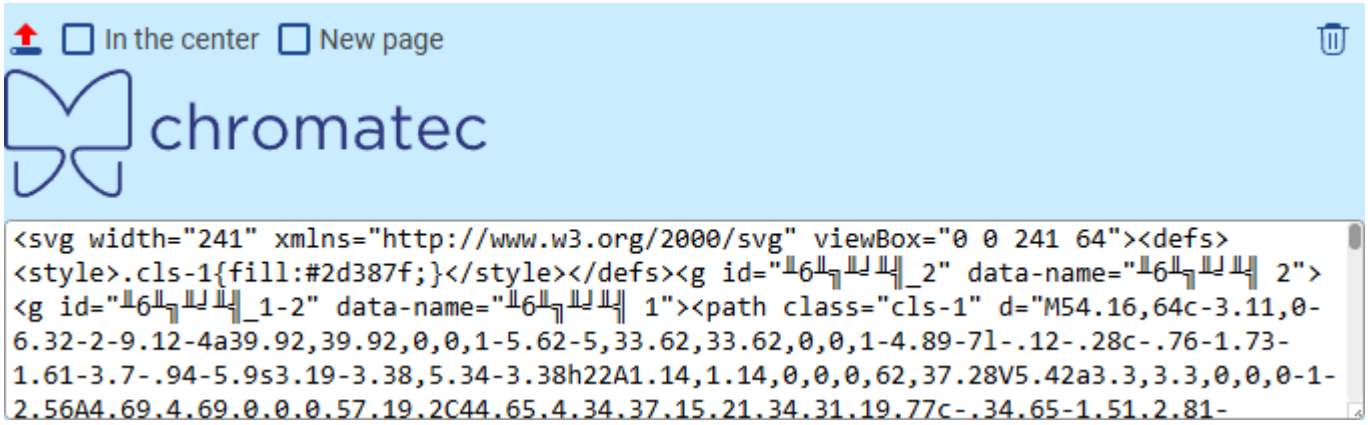


Fig 3.8 – SVG insert menu

Images in PNG and JPG format

You can insert images into the protocol - scans of documents, photos, etc.

To insert the image, press the corresponding button on the section toolbar and select the PNG or JPG file.

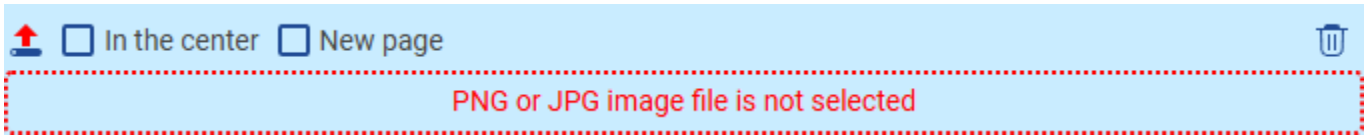


Fig 3.9 – PNG/JPG insert menu

3.6.4 Special sections

You can add special sections to the protocol:

- Reports in CSV, TXT, A4R formats (own format "Chromatec Analytic 4").
- Audit protocols.
- Table with information about the main software modules "Chromatec Analytic 4".
- A table with information about metrologically significant modules "Chromatec Analytic 4".

To add a special section, click on the "Add" button on the left side panel, select the "Special Section" item and then the type of section.

If there are already tables with information about the software modules of the " Chromatec Analytic 4" in the protocol, then they will not be in this menu.

Reports

- To insert a report (for example, verification) in the protocol, it must first be created in the CSV, TXT or A4R formats.
- Add the section.
- The block "The report is not added" will appear. Click on it.
- The program will redirect you to the report viewing page.
- Select an interesting report.
- Return to the qualification page by clicking on the corresponding button on the top panel of the navigator (figure below).



Fig 3.10 – The upper Navigator panel when choosing a report

Audit

To insert a fragment of the audit report into the protocol:

- Add the section.
- The block "A report on the audit is not added" will appear. Click on it.
- The program will redirect you to the audit page.
- Choose with the help of filters an interest fragment of the audit magazine.

Return to the qualification page by clicking on the corresponding button on the top panel of the Navigator (the figure above).

3.6.5 Creating a protocol

The qualification procedure may take a long time. Do not forget to save the entered data periodically.

After all the protocol parameters are configured and the necessary files are added, click on the "Create Protocol" button.

The protocol will be created in PDF format and opened on a separate browser tab.

Print it out and put the necessary signatures, attach a sticker.

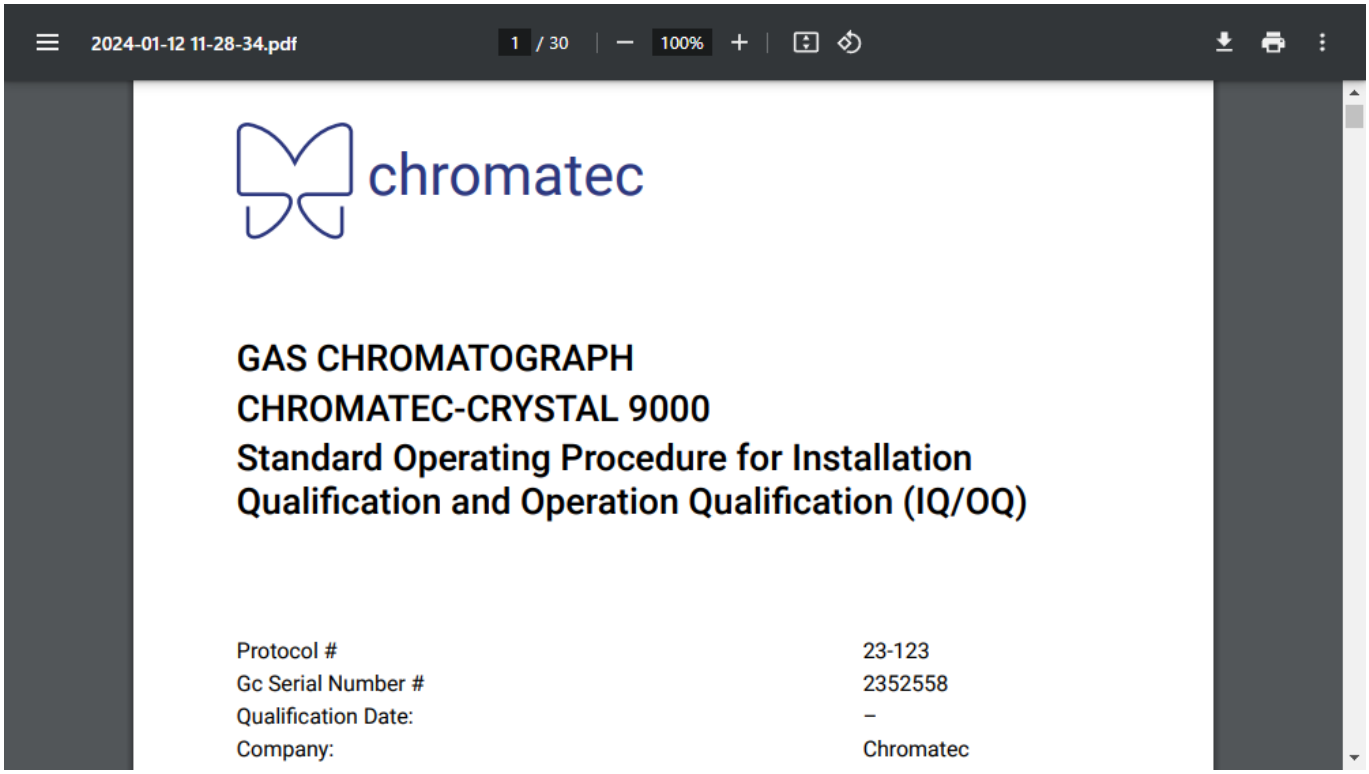


Fig 3.11 – Qualification protocol

The created qualification protocol is available in the Chromatec Navigator report repository

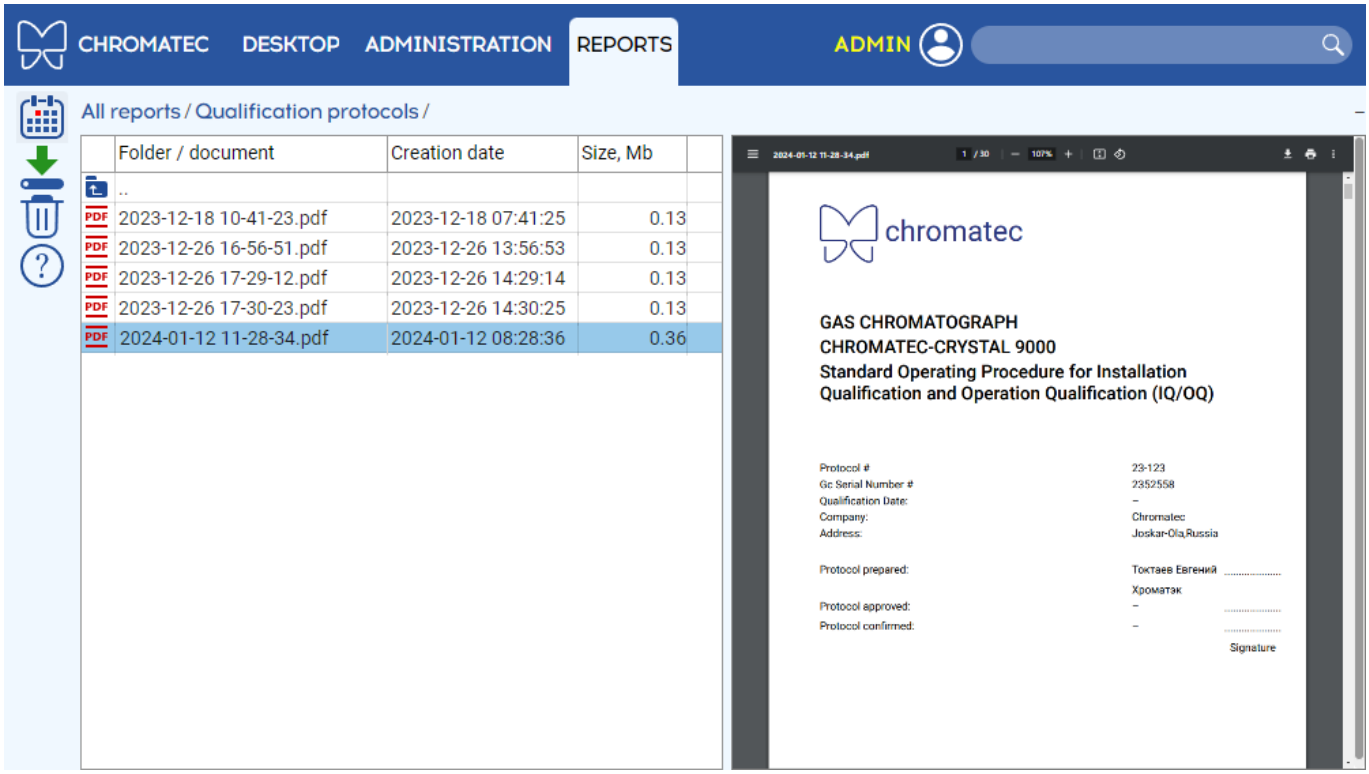


Fig 3.12 – Qualification protocol in the report repository