

SOFTWARE

CHROMATEC ANALYTIC

BUILD 4.0

USER MANUAL

214.00045-51I

PROCESSING OF CHROMATOGRAMS AND SPECTRUM

PROCESSING METHODS AND REPORTS

Revision 31.07.2026

Table of contents

1 General information 6
1.1 Project 6
1.1.1 Creating a project 6
1.1.2 Selection of chromatograms 7
1.1.3 Selection of methods 8
1.1.4 Import and export of chromatograms 9
1.1.5 Import of chromatograms from Analytics 3.x 10
1.1.6 Caching chromatograms 10
1.2 Processing Program Settings 12
1.2.1 General settings 12
1.2.2 Sample info settings 13
1.2.3 Infobar settings 14
1.2.4 Channel settings 15
1.2.5 Result table settings 15
1.2.6 MSD settings 16
1.2.7 Graph settings 19
2 Chromatogram 22
2.1 Working with graphs 22
2.1.1 Image quality 22
2.1.2 Axes tooltips 23
2.1.3 Chromatogram labels 24
2.1.4 Graphs scaling 24
2.1.5 Channels 25
2.1.6 Multichannel chromatogram 26
2.1.7 Shift 27
2.1.8 Manual peak adjustment 28
2.1.9 Switching views of the main window 28
2.1.10 Saving a graph as SVG 28
2.2 Instrument method 29
2.3 Sample info 30
3 Method 31
3.1 Method type 32
3.2 Calibration levels 33
3.3 Calibration control 34
3.4 Channels 37
3.5 Filtration 37

3.5.1 LOP-filter 38
3.5.2 Adaptive filter 38
3.5.3 Gauss filter 38
3.5.4 Median filter 39
3.5.5 Second order filter 39
3.5.6 Peak inversion 39
3.6 Components 39
3.6.1 Group 39
3.6.2 Rules for identifying components 40
3.6.3 Concentration 40
3.6.4 Internal standard 41
3.6.5 Function selection 41
3.6.6 Multirow changing 43
3.7 Processing plug-ins 43
3.7.1 Peak detection 44
3.7.2 Configuring quantitative analysis 49
3.7.3 Peak parameters 52
3.7.4 Group intervals 55
3.7.5 Gas sample volume 55
3.7.6 Air correction 56
3.8 Custom formulas 57
3.8.1 Examples of formulas 58
3.8.2 Mathematical functions in formulas 58
3.8.3 Debugging formulas 59
3.9 Report 61
3.9.1 Report Templates 61
3.9.2 Main settings 61
3.9.3 Header and signature 63
3.9.4 Sample info 63
3.9.5 Instrument method 64
3.9.6 Input data 64
3.9.7 Components 64
3.9.8 Calibration 67
3.9.9 Chromatograms 68
3.9.10 Audit trail 69
3.9.11 Auto report at the end of the analysis 69
3.10 Calculation 69
4 Analysis processing 71

4.1 Performing analyses 71
4.1.1 General analysis 71
4.1.2 Analysis with an internal standard 71
4.1.3 Identification 72
4.2 Process parameters 72
4.3 Batch review 73
4.3.1 Summary table of results 73
4.3.2 Results in the summary table 73
4.3.3 Chromatogram grid 74
4.3.4 Batch review V2 74
4.4 Batch processing 76
4.5 Qualitative mass spectrometric analysis 76
4.5.1 Working with spectrum 76
4.5.2 Performing a manual search 76
4.5.3 Performing an automatic search 77
4.6 Report 79
4.6.1 Report creation 79
4.6.2 Viewing saved reports 79
4.6.3 Reports comparision 80
4.6.4 Digital signature 81

1 GENERAL INFORMATION

The qualitative and quantitative composition of the sample according to chromatographic or mass spectrometric analysis is determined in "Chromatec Analytic" software.

Often it is required not only to determine the qualitative and quantitative composition of the sample but also to perform any additional operations with the obtained chromatographic or mass spectrometric data.

1.1 Project

In Chromatec Analytic 4, chromatograms are stored in a relational database called a "project". You can create an unlimited number of projects. It is recommended to create a own project for each analytical task.

1.1.1 Creating a project

A new project can be created at any time. It is usually created in the "Scheduler" at the stage of creating a sequence of analyses, but this can also be done in the "Analytic", in the dialog for selecting chromatograms and methods.

Projects can be displayed as a simple list or a tree structure. In the latter case, they can be grouped:

- by user IDs,
- by the name of the laboratories (set when creating projects),

In addition, the user can create a tree structure of projects at his discretion. The number of "tree branches" is unlimited.

By default, the user sees only those projects that he created himself, but can also display everything.

The video below shows how to create a project and configure the display of projects.

{video analytic_create_project Project, create project}

If you have many projects, you can quickly find the one you need using a filter. Click anywhere in the list of projects and start typing the name of the one you are interested in. Projects will be filtered by the entered text.


In the upper right corner of the chromatogram selection dialog, the service message server operation indicator is displayed.


This kind of indicator has at the time of connection to the message server.


This kind of indicator has if the connection to the message server failed.

1.1.2 Selection of chromatograms

After selecting a project, a selection of chromatograms is available to you.

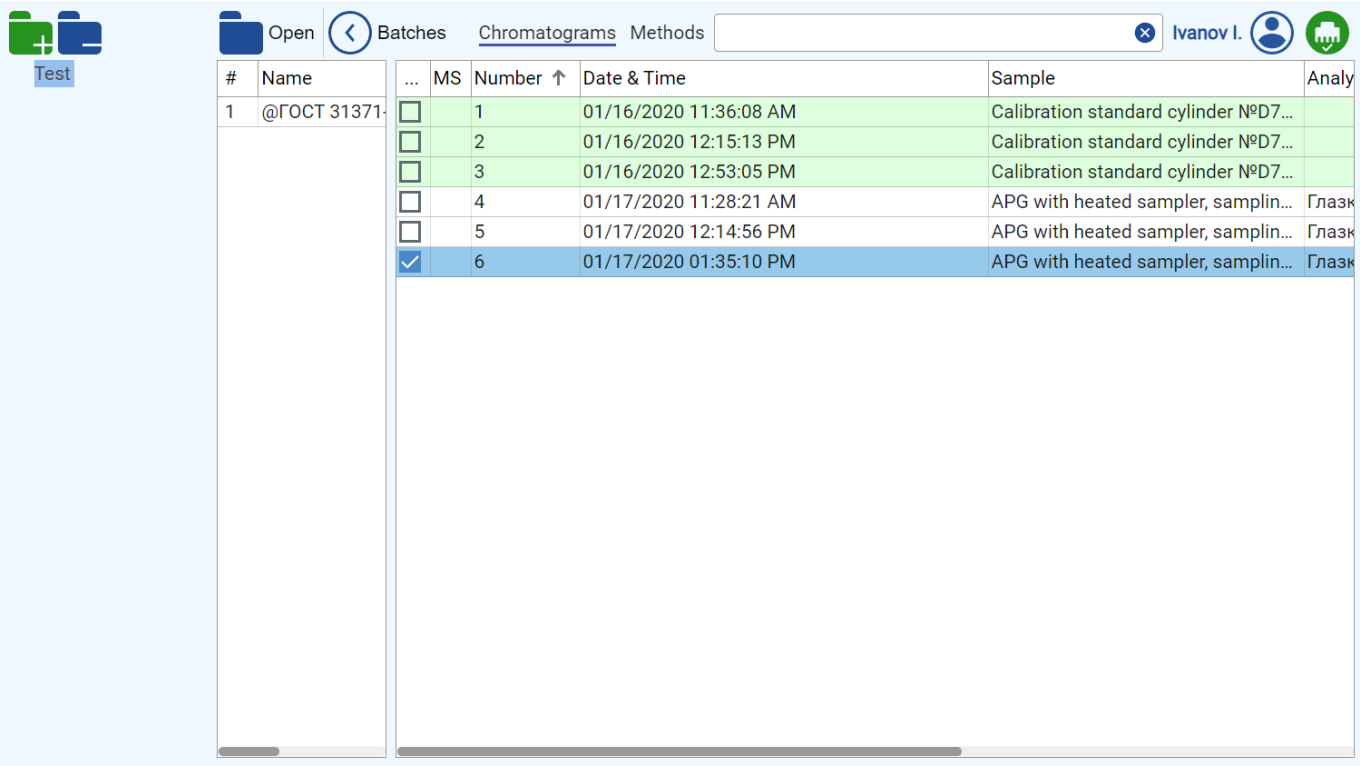


Fig 1.1 – Selection of chromatograms

In Chromatec Analytic, you can work with batches of chromatograms – open several at once for joint processing and construction of summary reports.

The batches are needed to quickly select the chromatograms of interest. For example, all chromatograms recorded during the execution of the sequence of analyses by the Scheduler (they receive a unique group number). You will only have to select a batches in the corresponding column.

You can create batches of any composition and use not only numbers as a name, but also any text designations that are convenient for you.

To form a new batch from the selected chromatograms, right-click in the table and select "Save as batch".

To open the selected chromatograms, click on the corresponding button above the tabs.

In the list of chromatograms, the analysis time can be displayed taking into account the clock belt.

	MS	Number	Date & Time UTC
☐	§	1	08.03.2023 15:27:34
☐	§	2	08.03.2023 15:27:34
☐	§	3	08.03.2023 16:14:19
☐	§	4	08.03.2023 17:01:21
☐	§	5	08.03.2023 17:48:01
☐	§	6	08.03.2023 18:34:47
☐	§	7	08.03.2023 19:21:57
☐	§	8	08.03.2023 20:07:43
☐	§	9	08.03.2023 20:53:27
☐	§	10	08.03.2023 21:39:18
☑	§	11	08.03.2023 22:25:10
☑	§	12	08.03.2023 23:12:28
☑	§	13	08.03.2023 23:59:13

	MS	Number	Date & Time UTC(+03:00)
☐	§	1	03/08/2023 06:27:34 PM
☐	§	2	03/08/2023 06:27:34 PM
☐	§	3	03/08/2023 07:14:19 PM
☐	§	4	03/08/2023 08:01:21 PM
☐	§	5	03/08/2023 08:48:01 PM
☐	§	6	03/08/2023 09:34:47 PM
☐	§	7	03/08/2023 10:21:57 PM
☐	§	8	03/08/2023 11:07:43 PM
☐	§	9	03/08/2023 11:53:27 PM
☐	§	10	03/09/2023 12:39:18 AM
☑	§	11	03/09/2023 01:25:10 AM
☑	§	12	03/09/2023 02:12:28 AM
☑	§	13	03/09/2023 02:59:13 AM

Fig 1.2 – Date and time of analysis taking into account the clock belt

1.1.3 Selection of methods

A list of processing methods is available on the "Methods" tab.

There are no instrumental methods in this list. In Chromatec Analytic 4, the processing method and the tool method are different entities.

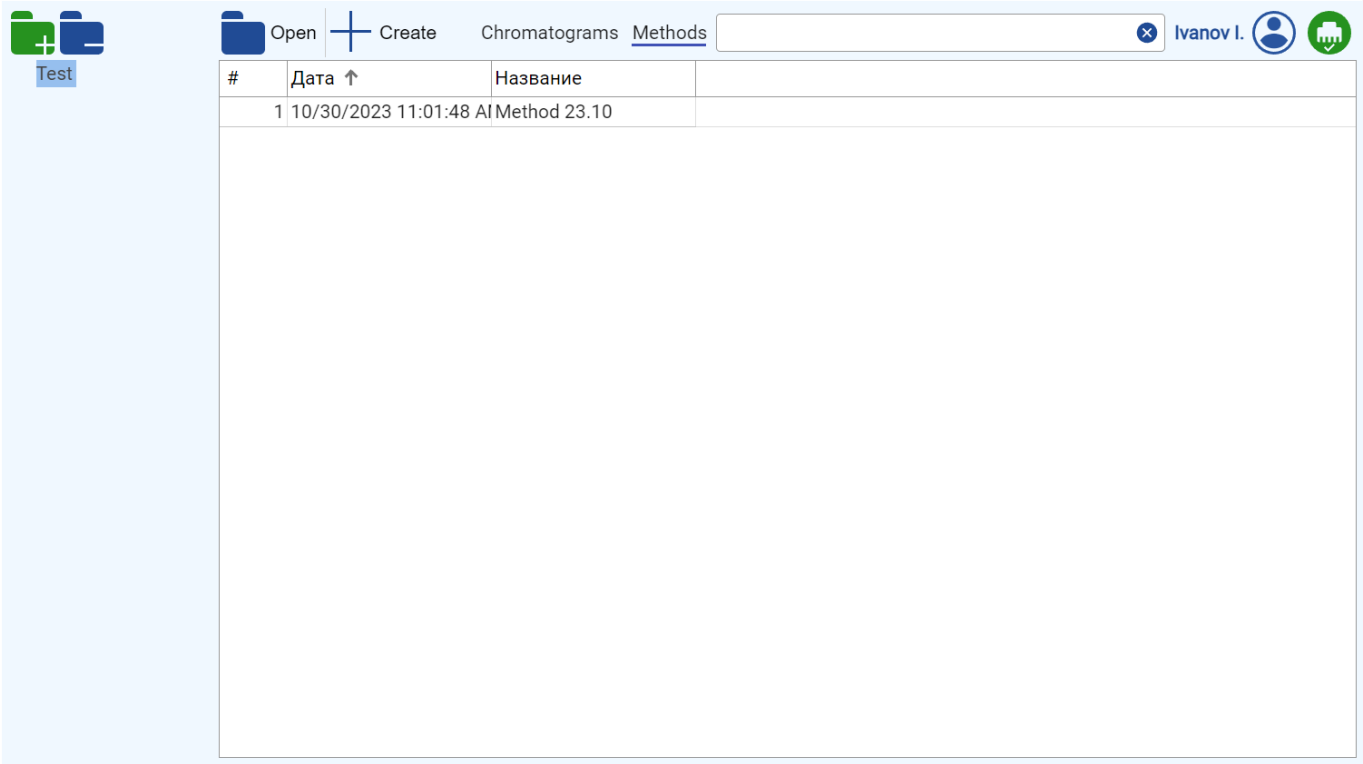


Fig 1.3 – Selection of methods

To edit the method, select it on this tab and click "Open". The method editor page opens.

1.1.4 Import and export of chromatograms

You can import chromatograms and methods obtained from third-party sources into the project, for example, by e-mail, or on computers outside your network.

Import and export commands are available in the right-click context menu.

The "Export " command allows you to upload the selected chromatograms to an archive that can be transferred to another computer or sent by e-mail.
At the same time, it is proposed to configure the binding of chromatograms and methods (figure below):

- "Add chromatogram methods" – this option will allow you to archive all the methods for the selected chromatograms. **It doesn't make sense to export chromatograms without methods!**
- "Add method chromatograms". If you are exporting a method, it is appropriate to add to the archive the chromatograms on which it was created.



Fig 1.4 – Creating an archive of chromatograms and methods

The "Export to the CDF" team allows you to convert the selected chromatograms into an open CDF format. Chromatograms in this format can be open in chromatographic for other manufacturers. When converting for each channel, a separate file will be created. All files received will be packed in the TAR archive.

The Import command allows you to download chromatograms and methods from files:

- TAR
- ZIP
- 7Z
- CDF

The video below shows the import/export process:

{video analytic_import_export_chromatogram Import, chromatogram import, export, chromatogram export}

If downloading chromatograms does not work on a Linux computer, the possible reason is the lack of access rights. This can happen if the tar archive is brought from another computer. In this case, you need to perform the following actions:

- Launch the terminal.
- Enter the **mc** command. The "Midnight Commander" program opens.
- In the "File" menu, select "Access Rights".
- Enable the options – "Read for others", "Write for others", "Run/search for others".

- Click "Install".

1.1.5 Import of chromatograms from Analytics 3.x

You can import chromatograms from Chromatec Analytic 3.1 software using a converter. This converter is available on a USB drive with the software installation package. It can also be downloaded from the official Chromatec website.

The converter only works on Windows! If you previously worked on a Windows computer, and now you have been given a Linux computer, perform the import in advance, before replacing the computer.

Chromatograms can be uploaded directly to the server (you need to create a project for this).

If the server is not available from the computer on which the chromatograms in the Analytic 3.x format are located, convert them to the tar archive. The resulting archive can be transferred on a USB drive to the computer from which Analytic 4.0 is available and imported into the project there.

Although Analyst 4 chromatograms contain the instrument method, when converting from Analyst 3 it will not be in the resulting chromatograms.

Tool method version 3 (*.mthx file) can be loaded to the chromatograph without conversion using the "Import" command in the "Control Panel".

1.1.6 Caching chromatograms

By default, chromatograms are cached to speed up loading. In normal operation, this process is invisible to the user, but if you are importing a large project, then when you first open it, the list of chromatograms can take a long time to build. But in the future, it will be much faster.

However, in the event of any emergency, you may not see any previously obtained chromatograms.

In this case, refresh the cache. To do this, right-click in the list of projects and select "Update cache" from the menu.

The use of the cache can be disabled in the program settings.

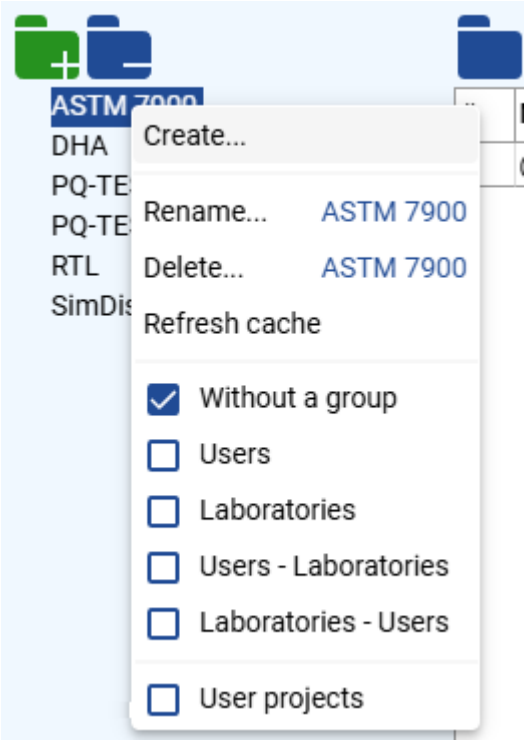


Fig 1.5 – Cache update

1.2 Processing Program Settings

1.2.1 General settings

- **Read only**. If set to "Yes", then no user actions with chromatograms will be saved. In normal operation, this option should not be enabled. It is needed for various debugging needs.
- **Automatically hide MS tabs**. If you set it to "No", then the tabs of the main window (on the left side panel) that are needed for working with MS data will always be shown. In normal mode, they are only displayed if the selected chromatogram contains MS data.
- **Maximum number of chromatograms**. A limit is set on the number of chromatograms in a batch. If you need more than 20, you can change this number.
- **Use chromatogram cache**. Enabling this option allows you to speed up the loading of the chromatogram list.
- **Reload page**. If the option is enabled (by default), then when navigating through chromatograms, the page is updated every 10 chromatogram loads. This prevents possible memory leaks.

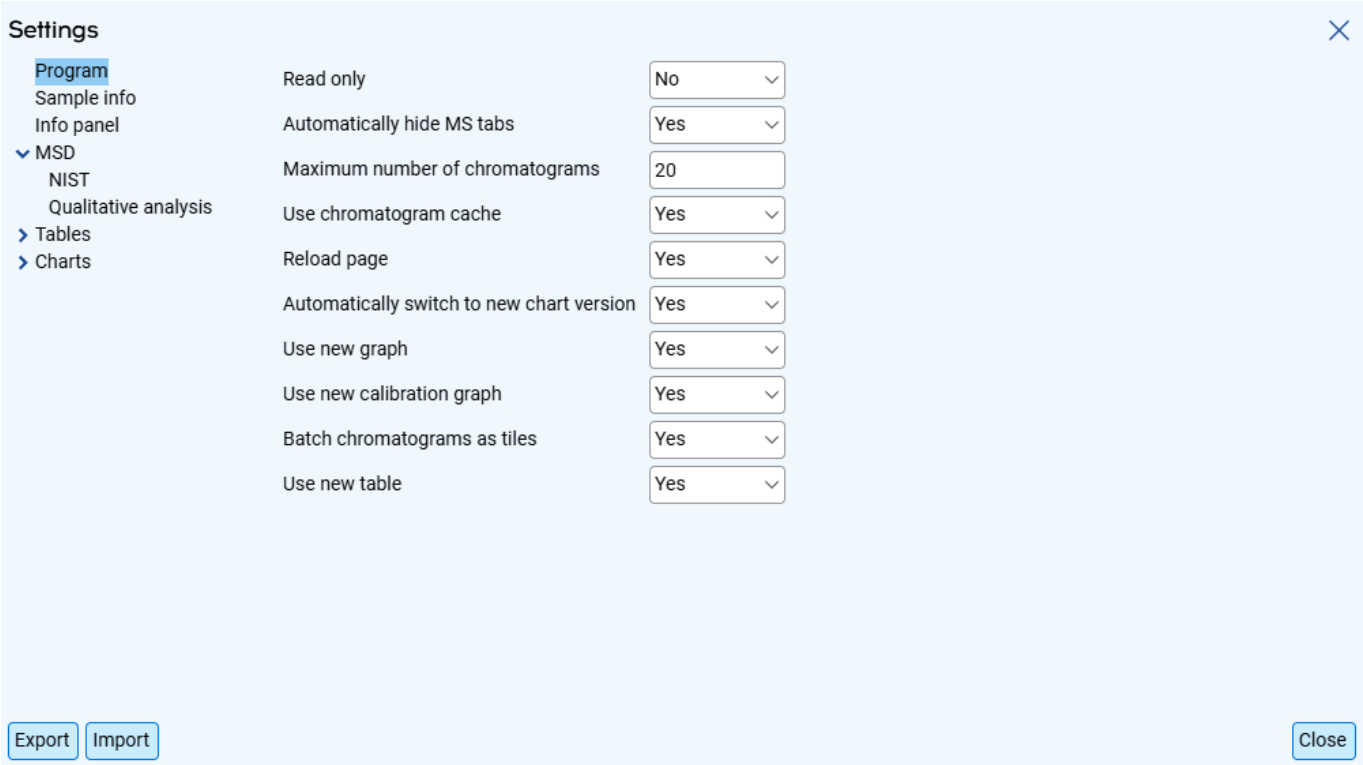


Fig 1.6 – General settings

- **Use new graph.** In the "Chromatec Analytic" build 2024.09.06, a new chromatogram graph has been introduced. You can return to the old one by selecting "No". The option is available temporarily.
- **Use new calibration graph.** The option is similar to the previous one.
- **Batch chromatograms as tiles.** The option allows you to present the batch of chromatograms not in the form of a table, but in the form of tiles (see the figure below). This can be handy if you have long sample names.

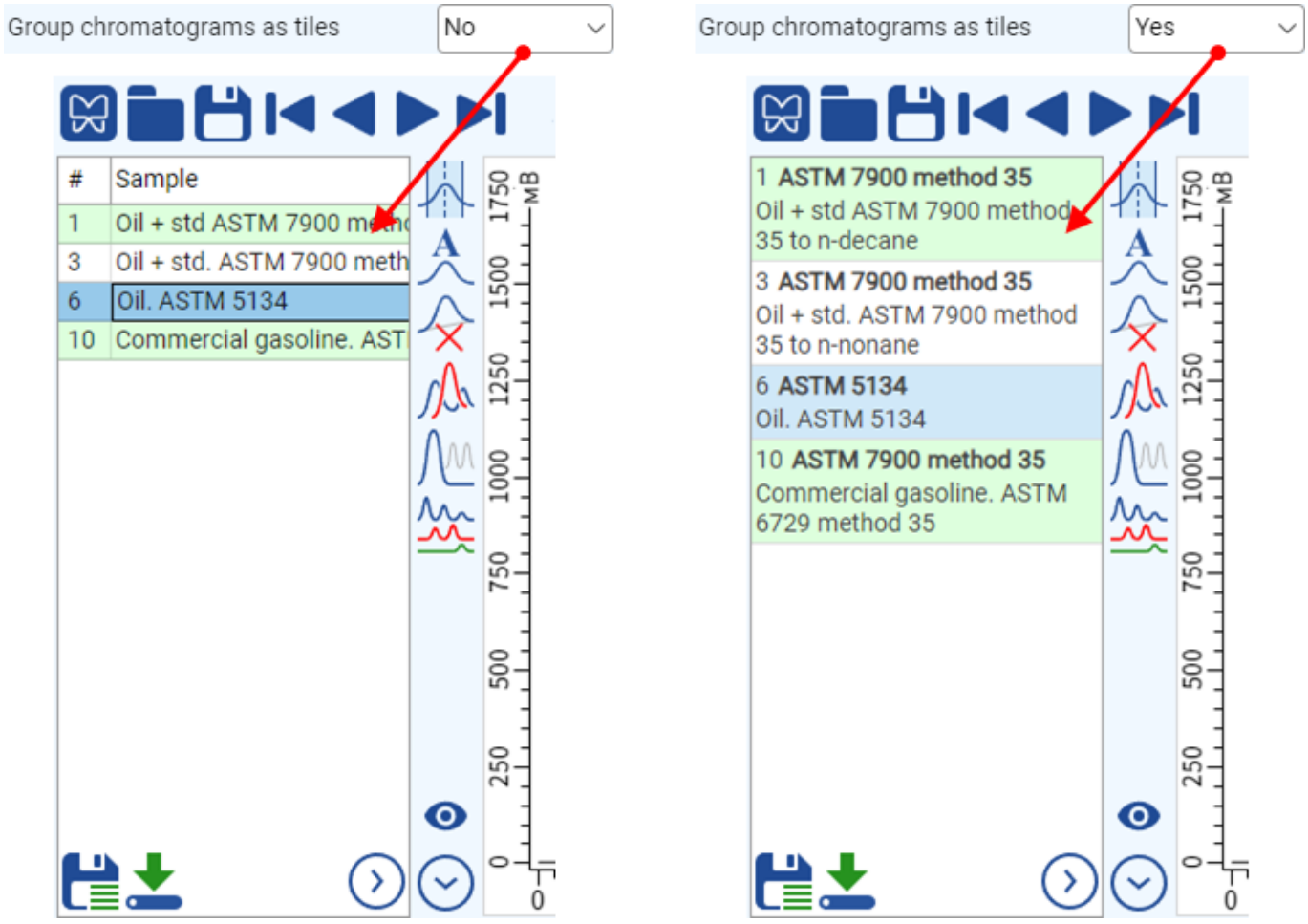


Fig 1.7 – Chromatograms of the batch in the form of a table or tiles depending on the setting

1.2.2 Sample info settings

In this section, you can enable/disable the display of chromatogram passport parameters.

The order of the parameters can be changed by moving them with the mouse.

You can add your own parameters to the sample info. To do this, click the appropriate button. Additional settings will appear:

Name of the parameter.

Visible. Enables/disables the display of the parameter in the chromatogram passport.

Order. You can specify a number, but it is more convenient to move the parameter in the list with the mouse.

Type of parameter:

- string,
- number,
- date and time,
- multiline text,
- Boolean value ("Yes", "No"),
- number with tolerance.

Key. The designation by which the parameter can be accessed in user formulas. Set the name of your parameter in English as the key, or simply write it down in Latin transliteration. Spaces are not allowed.

Default parameter **value**.

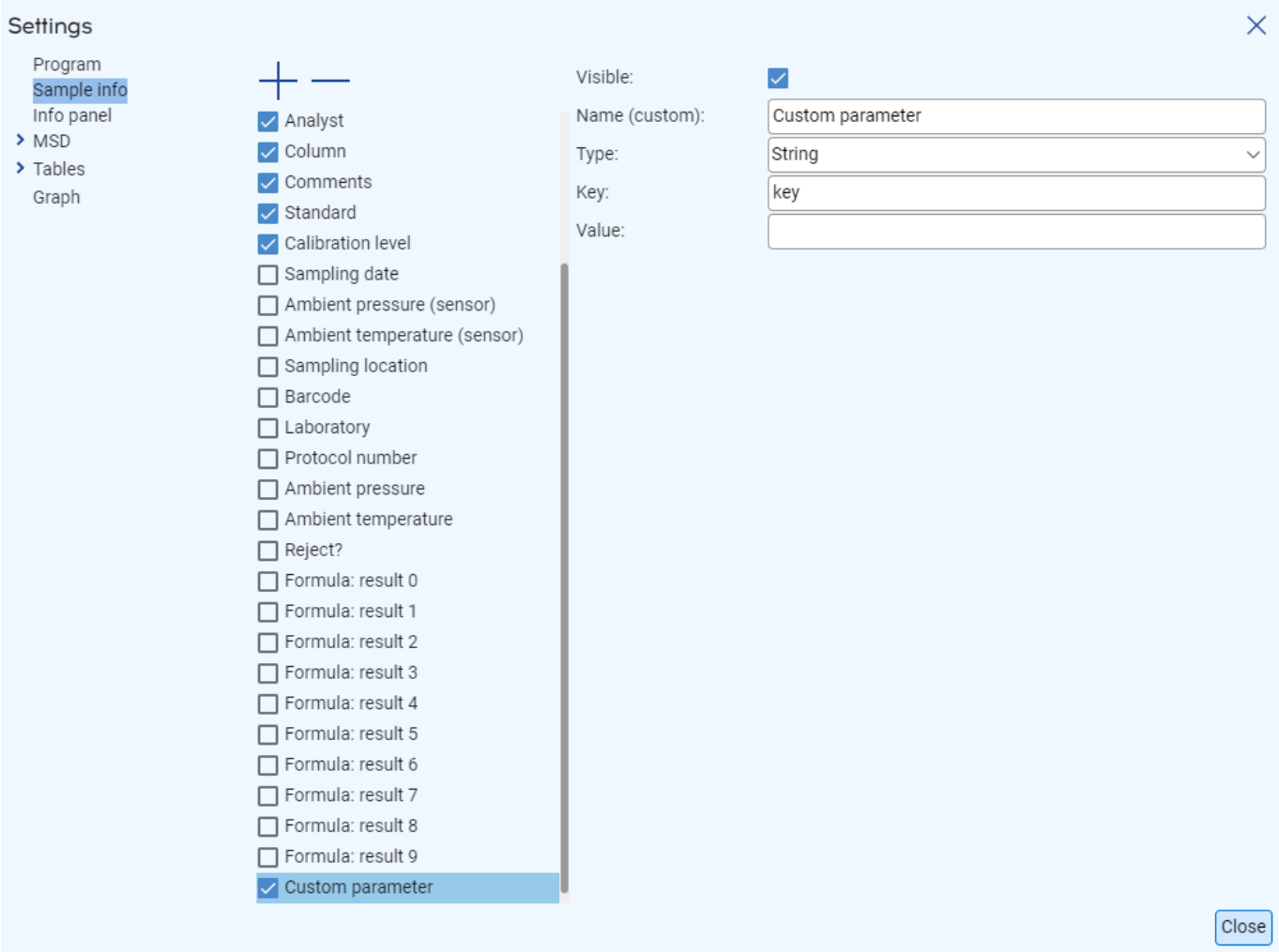


Fig 1.8 – Sample info settings

1.2.3 Infobar settings

In this section, you can set the display of sample info parameters on a special quick access information panel. It is located on the top toolbar.

The infobar is hidden by default. To show it to her, turn on the “Visible” option.

{video analytic_infobar Infobar}

1.2.4 Channel settings

In this section you can configure the channel table: visibility of columns, their order and the format of rounding numeric values.

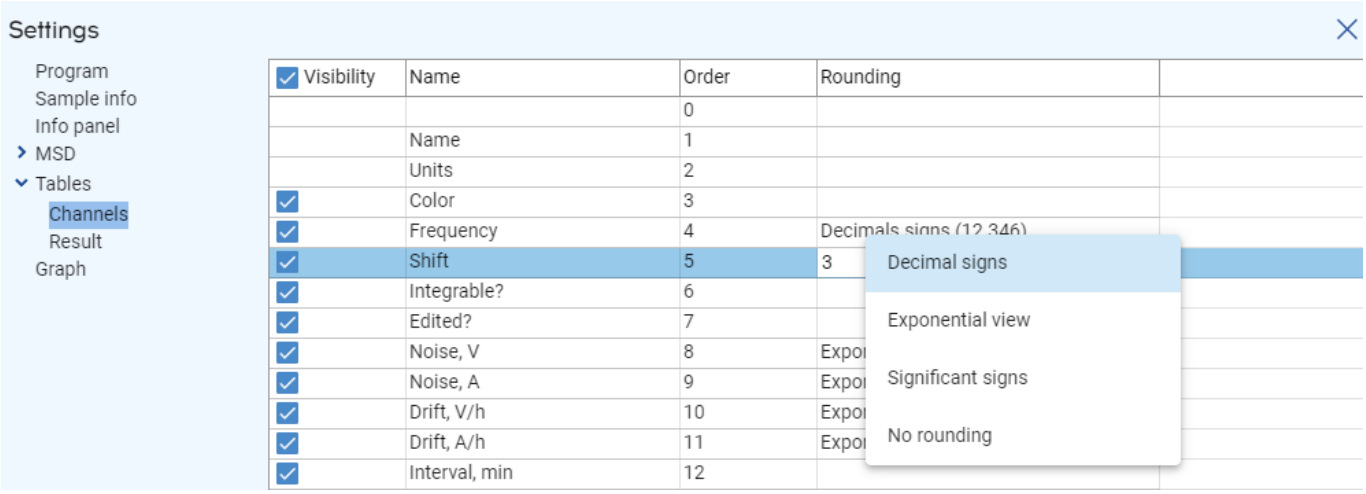


Fig 1.9 – Channel settings

1.2.5 Result table settings

In this section, you can configure the results table: the visibility of columns, their order and the format of rounding numeric values.

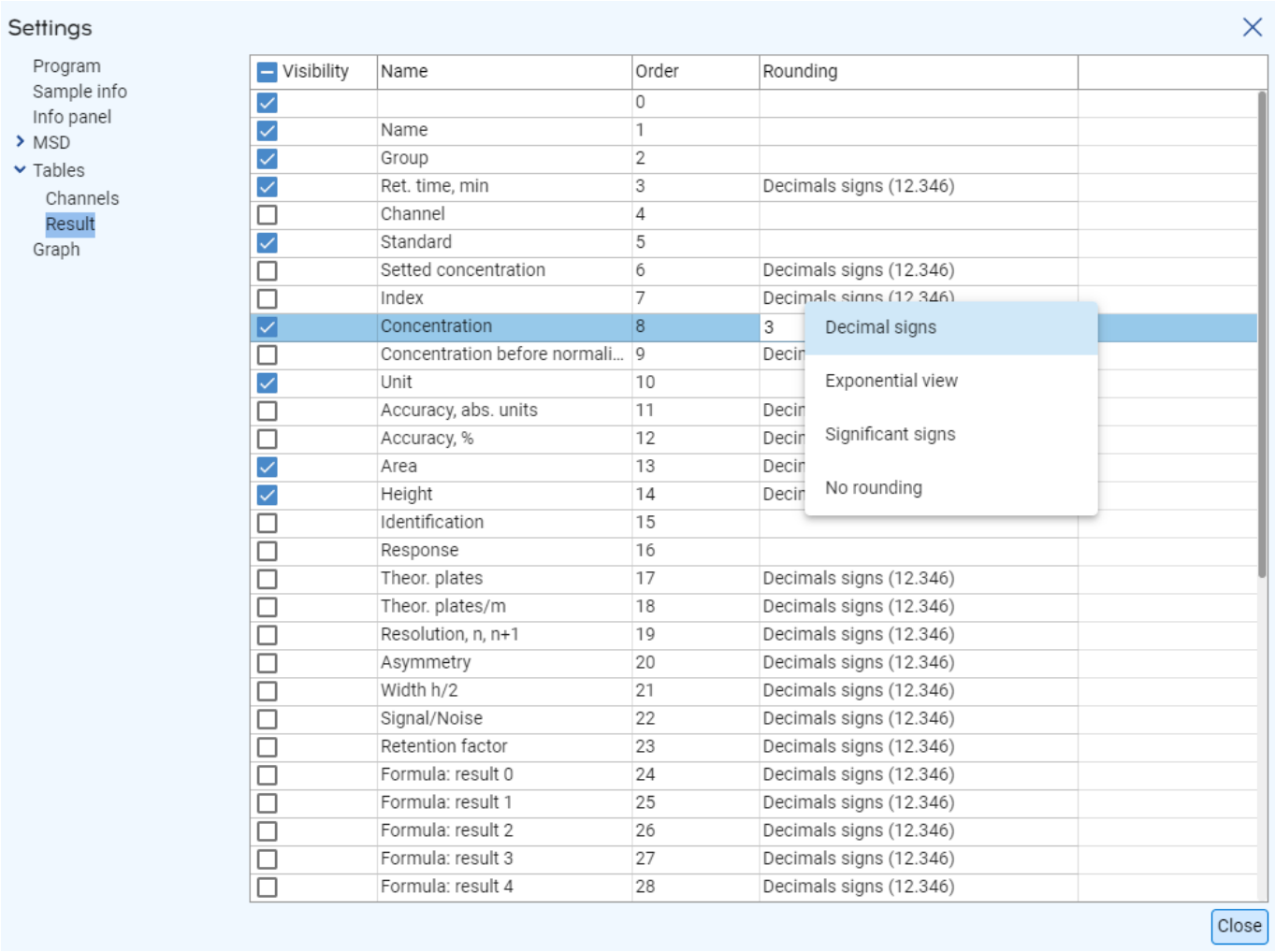


Fig 1.10 – Result Table Settings

1.2.6 MSD settings

NIST

A group of search settings for the NIST mass spectrum library.

To work with this library, it must be installed on each local computer where chromatograms are processed.

{video analytic_ms_setting_lib NIST}

The table shows the available spectrum libraries. To allow a library search, select it in the list.

Search type:

- **By correspondence.** This type of search is suitable for a spectrum for which it is known that there is a match in one or more libraries selected for the search.
- **Ordinary.** This type of search is set by default. Uses several (up to 4) pre-search criteria. Finds more candidates for subsequent search than "Fast"**.**
- **Fast.** Uses a single pre-search algorithm, in which an approximate comparison occurs.

- **Exclude rare compounds.** Reduces the probability of "rare" connections in the candidate list. A compound is considered "rare" if there are few references to other chemical libraries in which it is present in the information about it.
- **By similarity**. Use this type of search if you are sure that the spectrum has no matches in the libraries selected for search. The algorithm will search for library spectra similar to the presented spectrum.
- **Simple.** Uses 4 preliminary search criteria, but it is preferable for spectra obtained from molecules close in structure to the analyzed compound.
- **Combined.** Mixed search using the principles of simple search and neutral loss spectrum.
- **Neutral losses.** This type of search uses mass estimation. molecular ion. The search results will include compounds with similar neutral loss spectra (starting from the molecular ion mass).

Pre-search type:

- **By default.** The usual search.
- **Fast.** The search is similar to "Default", but the number of results is about 3 times less.
- **No.** The pre-search is disabled, so the main search takes longer. This can be useful if a preliminary "Default" search does not give good matches.
- **Molecular mass.** A detailed search is also applied immediately, but only compounds with the specified molecular weight are included in it.

A group of **Restrictions** parameters allows you to reduce the number of output matches (candidates).

Don't display matches with Match (R Match) less... Exclude from the list of candidates all connections for which the value of Match (or R Match) is less than the specified one.

Don't display matches with a probability less than... Exclude from the list of candidates all connections with a probability less than the specified one.

Maximum number of candidates. Limit the list of candidates to the first few with the highest probabilities.

If the libraries are not in the list, install the service to work with NIST.

Qualitative analysis

The mass interval. The program searches for peaks only on a chromatogram of a specified mass/mass range. Use this parameter if you are looking for a substance with a known mass of an ion.

Time interval. The program automatically searches for peaks in both chromatograms for the total ion current and all selected separate (individual) ions. If you are looking for a substance for which the masses of the characteristic ions are known, enter the required mass range of the individual ion.

The assignment of other parameters is similar to that described in section "Peak detection".

Spectrum improvement

The use of spectrum improvement significantly improves the quality of compounds identification by spectral libraries.

If the **Spectrum improvement** option is disabled, then the spectrum at the peak is taken as the peak spectrum. If this option is selected, the spectrum obtained using the spectrum refinement or background subtraction algorithms will correspond to the peak.

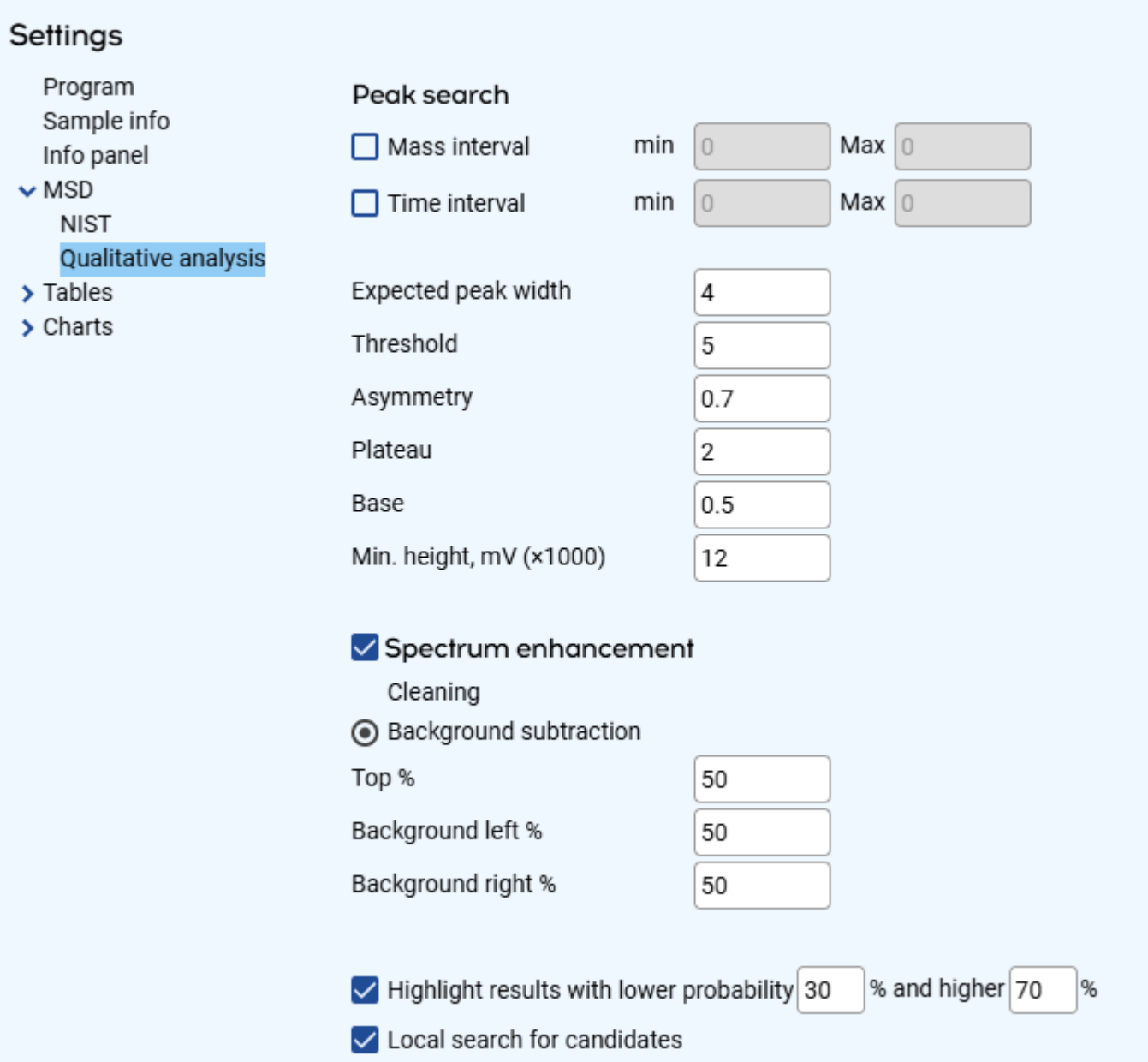


Figure 1.11 – Qualitative analysis settings

Refine. Chromatograms of all masses are analyzed for the presence of peaks. Only masses with chromatograms that have peaks with the same retention time are included in the resulting spectrum. This algorithm gives good results for high intensity peaks.

Background subtraction. Averaging the spectra of the peak points followed by subtracting the averaged spectrum of the background. This algorithm gives good results for both high and low intensity peaks.

Top. Specifies a segment of the peak (1 ... 100% of the peak width), which averaged points determine the spectrum of the substance.

Left background region. Specifies the segment to the left of the peak base (0 ... 200% of the peak width), which averaged points determine the spectrum of the substance. In order not to subtract the background on the left, set the value of this parameter to zero. The spectra of the background to the left and right of the peak are averaged and subtracted from the peak spectrum.

Right background region. Specifies the segment to the right of the peak base (0 ... 200% of the peak width), which averaged points determine spectrum of the substance. In order not to subtract the

background on the right, set the value of this parameter to zero. The spectra of the background to the left and right of the peak are averaged and subtracted from the peak spectrum.

1.2.7 Graph settings

A group of settings for displaying graphs of chromatograms, spectra, and calibrations.

Here you can set the thickness of the lines, radii of various reference points, indents, and rounding of the data displayed on the graphs.

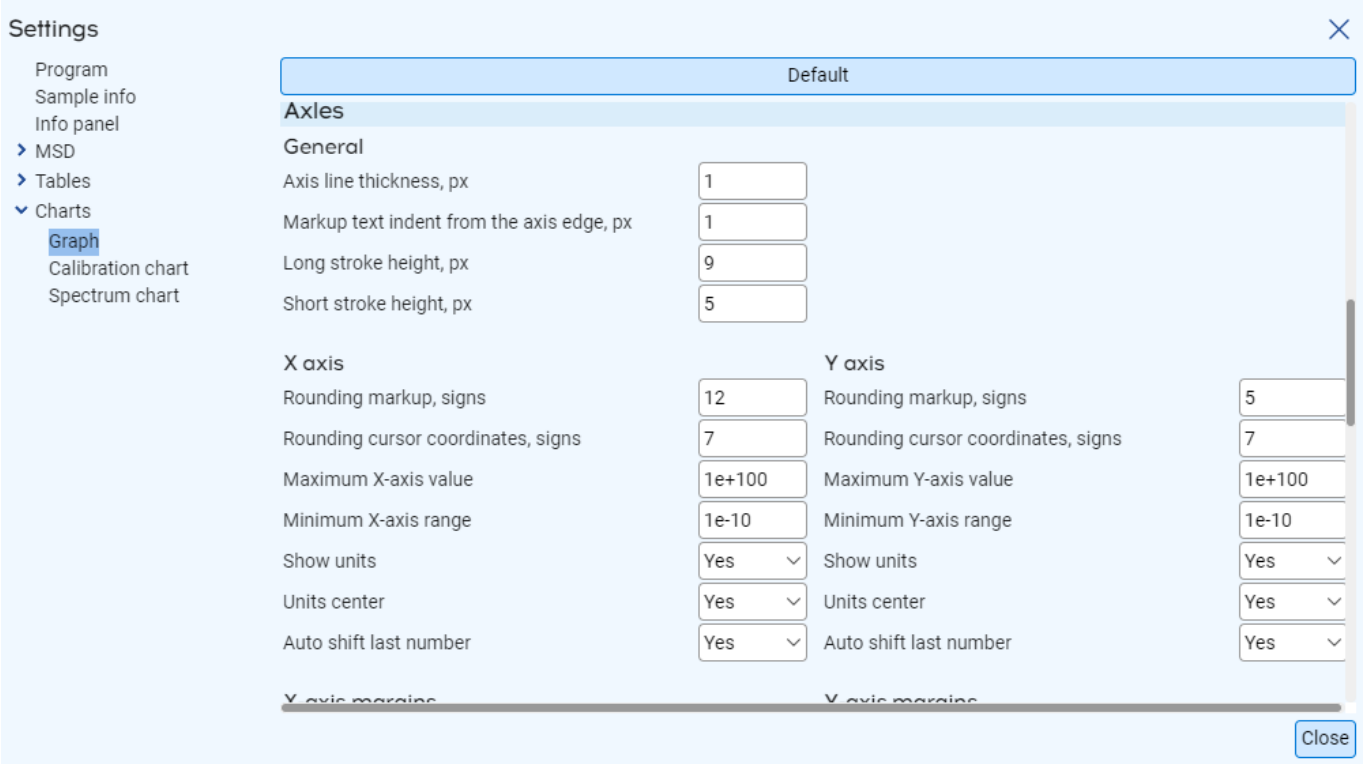


Fig 1.12 – Graph settings

We recommend using the default values. Descriptions of the purposes of all parameters are not given in the help; most of them are intuitive. The figures below explain the purpose of some specific parameters.

You can change the value of any parameter and evaluate how it will affect the display of the chromatogram, spectrum or calibration graph.

Using the "Default" button you can always restore the original values.

X-axis margins		Y-axis margins	
Top to graph area, px	5 (1)	Left to axis, px	25 (5)
Top to data (autoscale), px	10 (2)	Left to data (autoscale), px	30 (6)
Bottom to axis, px	26 (3)	Right to graphics area, px	5 (7)
Bottom to data (autoscale), px	30 (4)	Right to data (autoscale), px	10 (8)
Left from cursor position, px	2	Top from cursor position, px	2
Right from cursor position, px	2	Bottom from cursor position, px	2
Markup text margin, px	11	Markup text margin, px	9

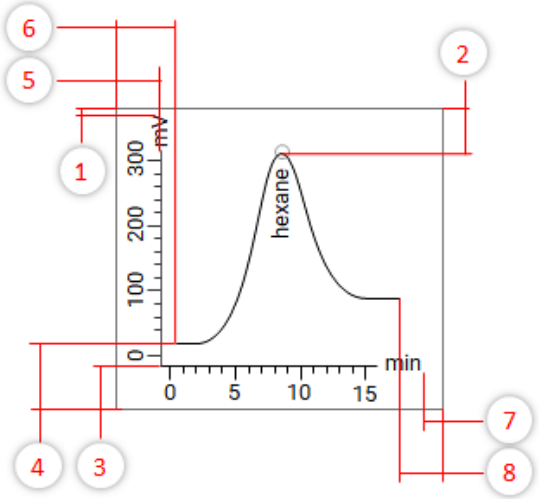


Fig 1.13 – Margins

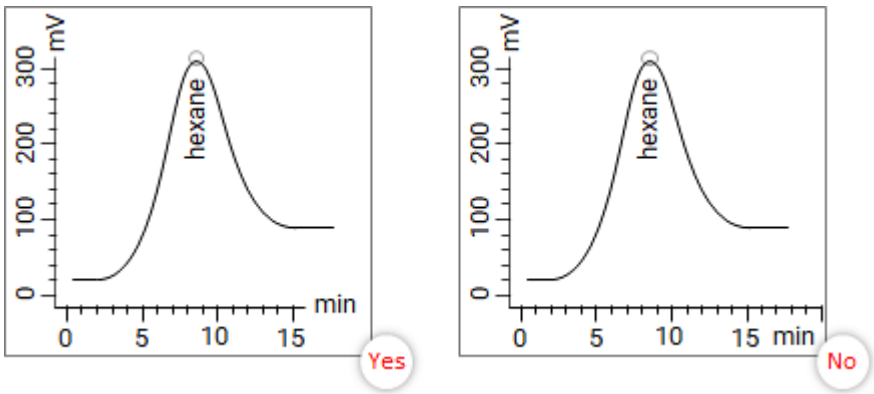


Fig 1.14 – Is units center by X-axis?

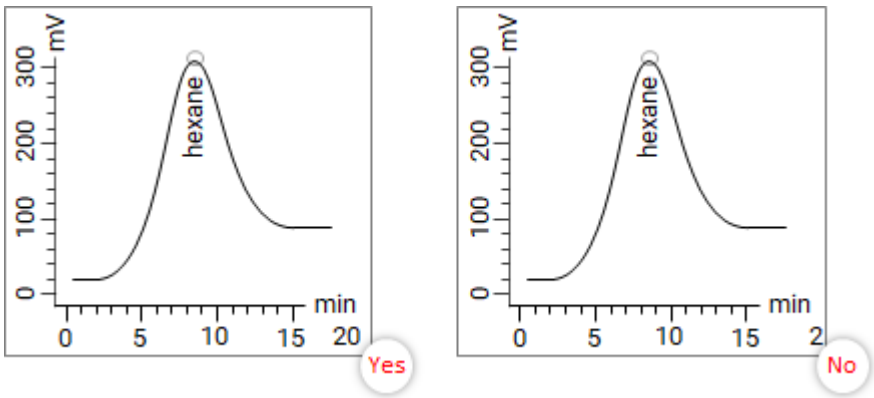


Fig 1.15 – Autoshift last number

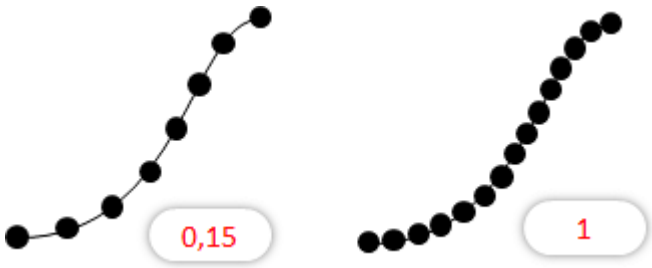


Fig 1.16 – Ratio of number of points to window width

The parameters of the calibration graph are basically similar to the parameters of the main one.

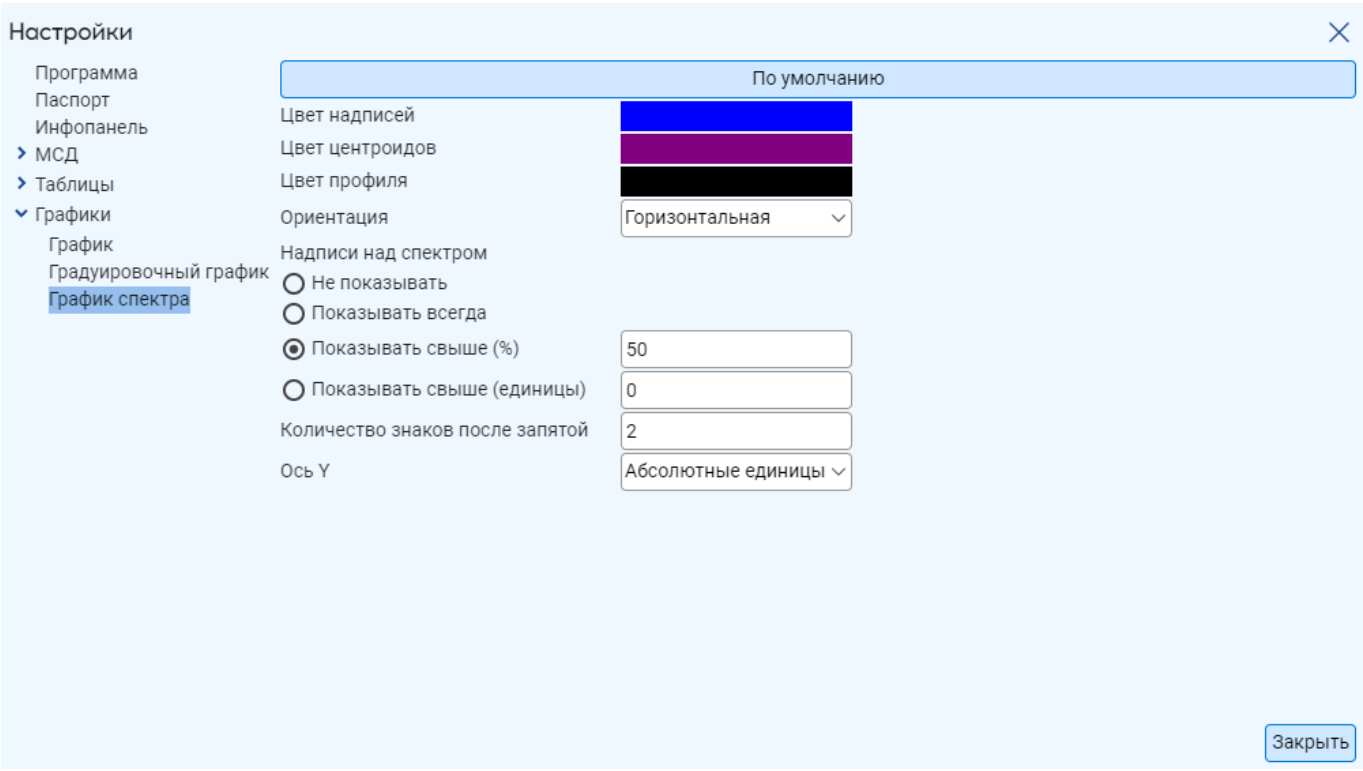


Fig 1.17 – Graph spectrum settings

2 CHROMATOGRAM

2.1 Working with graphs

2.1.1 Image quality

The chromatogram graph is displayed in reduced quality for faster performance, but you can increase it if you need to copy it to paste it into a document.

To do this, right–click on the graph and select "Enable high quality (rendering slower)" in the context menu. In the same place, you can switch back to low quality for faster drawing of the graph.

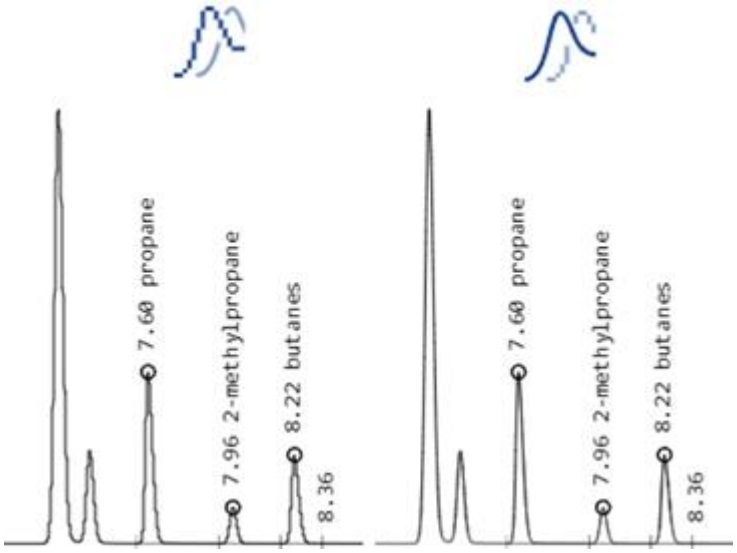


Fig 2.1 – Graph in reduced quality (left) and increased (right)

The graph is always displayed in high quality in the report.

The rendering speed is especially noticeable when scaling large chromatograms.

2.1.2 Axes tooltips

If you hover the cursor over the graph axis, three values will be displayed:

- The minimum value on the graph at the current scale for the selected axis.
- Range (the difference between the maximum and minimum value in the current scale).
- The maximum value on the graph at the current scale for the selected axis.

Hints are highlighted in green.

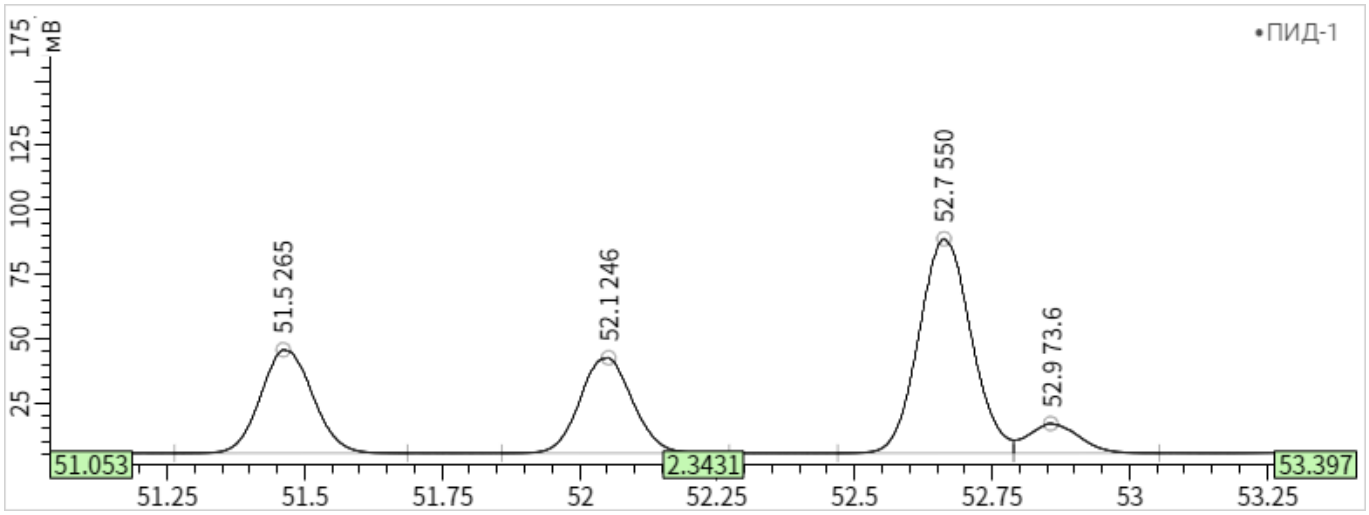


Fig 2.2 – Axis tooltips on hover

You can enable the display of cursor coordinates. To do this, click on the chart with the middle mouse button (wheel).

The cursor will take the form of a crosshair, and its current coordinates will be shown on the axes on a yellow background:

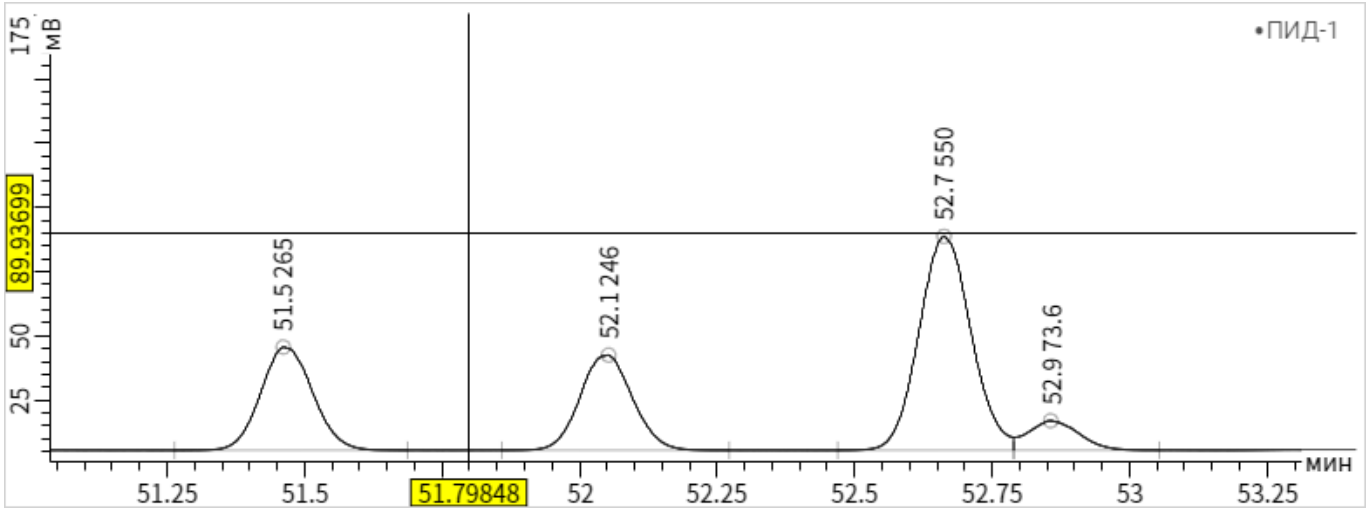


Fig 2.3 – Cursor coordinates

To exit the mode of displaying cursor coordinates, simply click anywhere on the chart with the left mouse button.

2.1.3 Chromatogram labels

To display the labels of interest above the peaks, click the corresponding button on the sidebar and select the necessary parameters in the menu that appears. Also, here you can set the orientation of the inscriptions– horizontal (by default) and vertical.

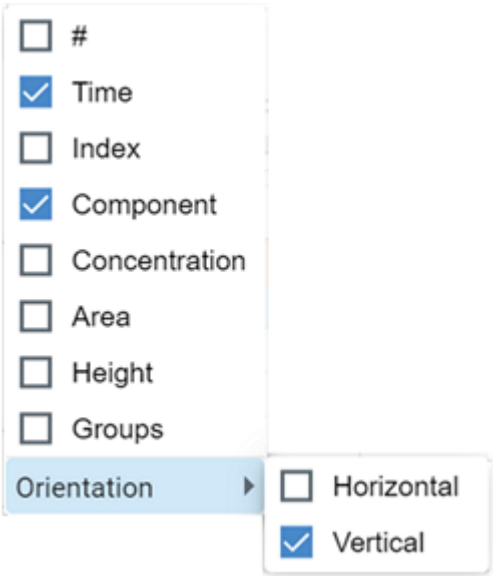


Fig 2.4 – Menu of inscriptions above the peaks

{video analytic_chromatogram_labels Labels on the chart, labels above the peaks, show hidden labels above the peaks }

Peak groups can be set using the Grouping Intervals process.

2.1.4 Graphs scaling

By default, the scale is automatically set in such a way that the entire graph is visible.

- In order to enlarge a certain part of the graph, click the left mouse button in one of the corners of the area of interest and, without releasing, move the mouse pointer to the opposite corner.
- After you release the mouse button, the selected area will increase to the size of the window.

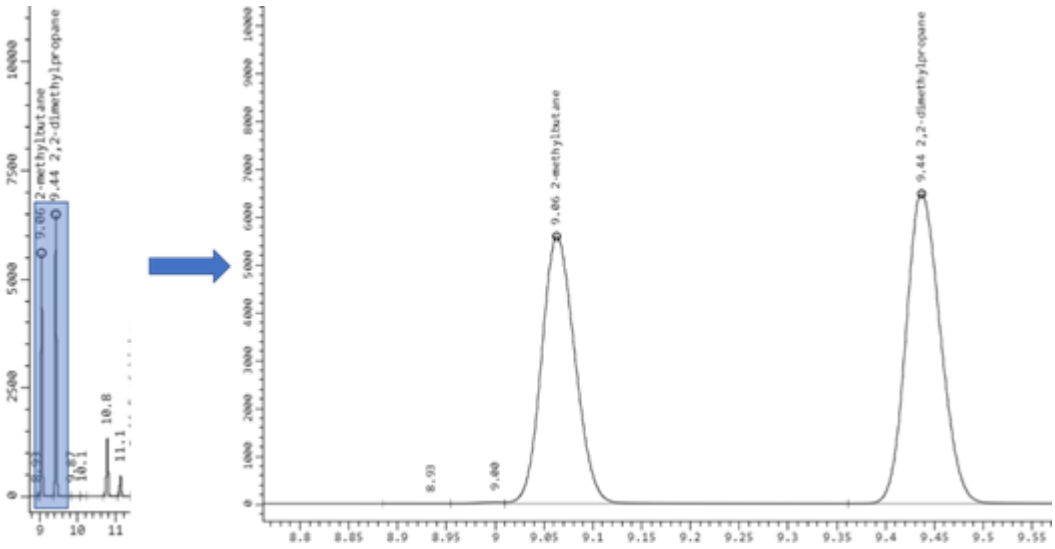


Fig 2.5 – Selection of the chromatogram area

In order to return to displaying the entire graph on the screen, double-click on it (the cursor should be outside the peak boundaries).

In an area where there is a lot of data (for example, in noise), it is difficult to perform a box selection, since the priority in this situation is to grab and move the channel with the mouse (the cursor looks like this:). To still highlight a section of the chromatogram with a frame, press and hold **SHIFT**.

If you double-click on the vertical axis, the portion of the chromatogram currently visible on the screen will be scaled vertically to the size of the window.

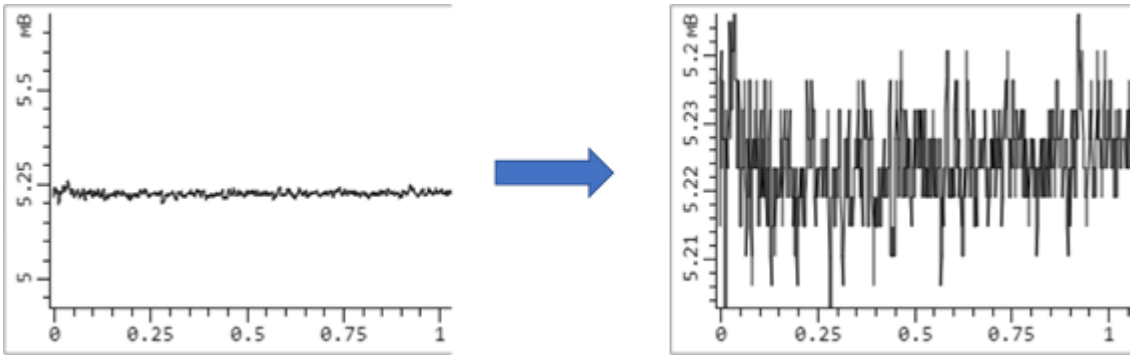


Fig 2.6 – Scaling the selected area vertically only

Scrolling the mouse wheel over one of the axes allows you to scale the graph only relative to this axis.

Scrolling the wheel above the graph scales it vertically.

{video analytic_chromatogram_zoom Zoom}

2.1.5 Channels

The Channels tab is available both in the method editor and in the Chromatec Analytic main window.

Here you can:

- Enable/disable channel display (including using the filter in the header of the corresponding column of the table).
- Choose channel color.
- Adjust the shift in minutes.
- Disable the Edited flag so that the program can perform an automatic peak search, which is blocked if at least one peak has been edited manually.

	Name	~shared~Chanr	Color	Frequency	Shift	Integrable?	Edited?
Detectors							
☑	FID-1	мВ		25.000	0.000	Yes	No
☑	TCD-1	мВ		25.000	0.000	Yes	No
☑	TCD-2	мВ		25.000	0.000	Yes	No
☑	TCD-3	мВ		25.000	0.000	Yes	No

Fig 2.7 – Channels

2.1.6 Multichannel chromatogram

In the case of a multichannel chromatogram, the channel graphs are arranged one above the other. In this case, one of the channels is drawn on top of the others and is active. Axis signatures refer only to the active channel, since in general the channel scales may not coincide and generally have different units of measurement.

You can move the channel up and, therefore, make it active by clicking on its chart or using the menu in the upper right corner of the chart.

On the side panel of the graph there are buttons for commands that perform the following actions:

 Show all channels at the active scale. 

 Switch the transparency of inactive channels. 

 Split channels vertically.

{video analytic_channels_selection Channels}

Additional channel controls are located on the "Channels" tab. Here the operator can:

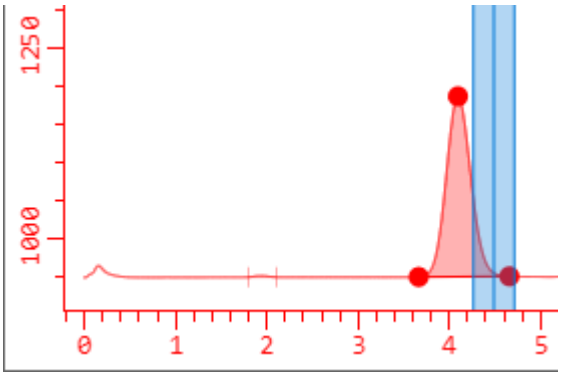
- Enable/disable channel display (including using the filter in the header of the corresponding column of the table).
- Choose channel color.
- Adjust the shift in minutes.
- Turn off the "Edited" flag so that the program can perform an automatic search for peaks.

The fact is that when performing manual peak marking adjustments, further peak search becomes impossible, because operator intervention in chromatogram processing has the highest priority. If you

need to cancel the manual adjustment of the markup, then you should set the "Edited" = "No" sign for the channel.

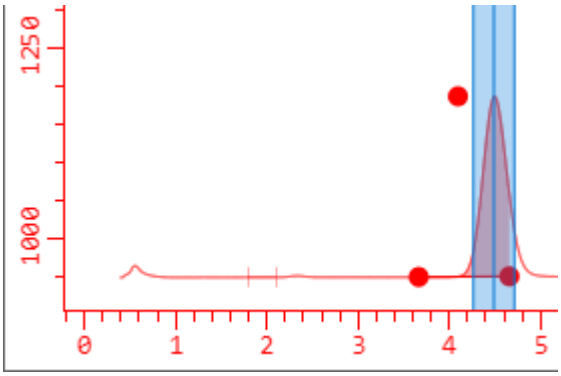
2.1.7 Shift

The **shift** parameter can be changed. This can be convenient for input errors if the operator hesitated when pressing the start button. Selection of shift helps avoid the need to adjust component retention times.

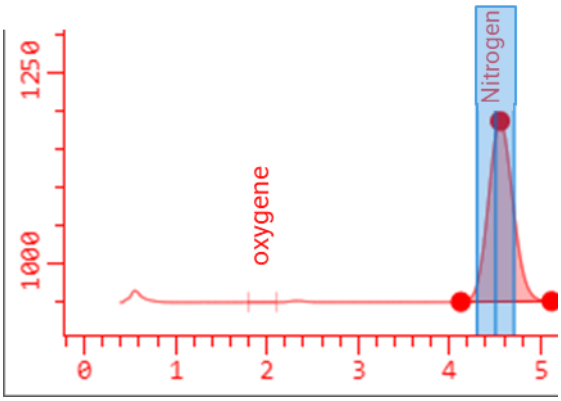


Example:
The method specifies the retention time of the nitrogen component – 4.5 min.
But the real retention time turned out to be 4.1 min.

But the real retention time turned out to be 4.1 min.



The operator set the value of the "shift" parameter to 4.5 min.



After performing the calculation, the peak was identified as "nitrogen", while the method remained unchanged.

It is advisable to use this procedure when the change in the retention time is random, for example, as a result of an operator error.

However, if the nature of the changes is systemic (column aging) – change the retention time in the method.

You can change the shift using the mouse. To do this, press (and hold) the **SHIFT** + **SPACE** keys and move the channel with the mouse in the desired direction.

You can shift one channel relative to another. For example, the autosampler AS-2M (3D) injects a sample into the Inlet-1, after which it injects a sample into the Inlet-2 in the same analysis. The chromatogram on channel 2 is shifted relative to channel 1 for the time during which the sampler took a sample after the

first injection (at this time, the delay set by the operator may enter). If a negative shift is specified for channel 2, the peaks can be combined in time with the peaks on channel 1.

2.1.8 Manual peak adjustment

It is not always possible to achieve automatic adjustment of chromatogram peaks with the help of the **Peak detection** operation setting. To eliminate this problem directly on the chromatogram graph, you can visually adjust the position of the specific points of the peak.

{video analytic_manual_peak_correction manual peak correction}

You can switch to peak adjustment mode by pressing **CTRL**.

If you are on the "MS: Spectrum" page, then moving the cursor with the left mouse button pressed and the **CTRL** key will highlight a section of the chromatogram with a marker, which is used for background subtraction when manually searching through MSD data.

2.1.9 Switching views of the main window



In the main window "Chromatec Analytic" you can switch the following types:

- **By default.** The classic view is a chromatogram graph on top, a table of results (or a table of channels, or a description of the instrument method) on the bottom.
- **Calibration of the component.** When this type is selected, a calibration graph of the selected component appears to the right of the chromatogram. The area and quantity of the selected component are displayed on it with a red label.
- **All components.** When this type is selected, the peak of each component is displayed in its own small window. This view allows you to quickly assess the correctness of the markup of all components.

{video analytic_view_switch Analytic view switch}

2.1.10 Saving a graph as SVG

If you need to insert a chromatogram into your specific report or presentation, you can save it in the SVG vector format, which is supported by popular office packages and provides high-quality images when resized in word processors.



Right-click on the chromatogram and select "Save graph as SVG" from the menu. You can also press the key combination SHIFT+CTRL+S. A dialog for setting image dimensions will appear. By default, they correspond to the current ones. If you wish, change them. Click OK to save the SVG file.

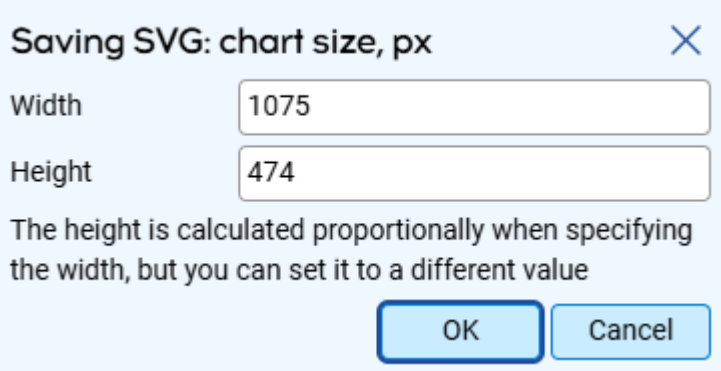


Fig 2.8 – Set image size when saving SVG

2.2 Instrument method

The "Instrument method" tab displays a description of the instrument parameters (GC/MS/Autosamplers) used to perform the analysis, as well as the chromatograph configuration.

This data is read-only, it cannot be edited.

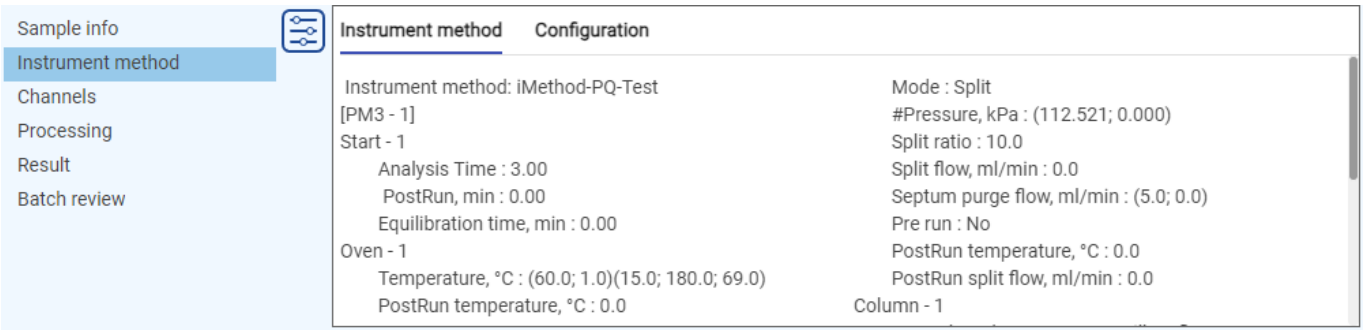


Fig 2.9 – Instrumental method

The instrument method is stored in the chromatogram not only as a text description, but also in a special format that allows it to be transferred to the instrument. To do this, you need to save it in the connection, and it will become available for selection in the corresponding Control Panel dialog.

To do this, open the main menu of "Chromatec Analytic" and select "Upload the method to the instrument". The dialog shown in the figure below will open. In this dialog, select the connection you are interested in and click OK.

The list displays only running connections available to this user.

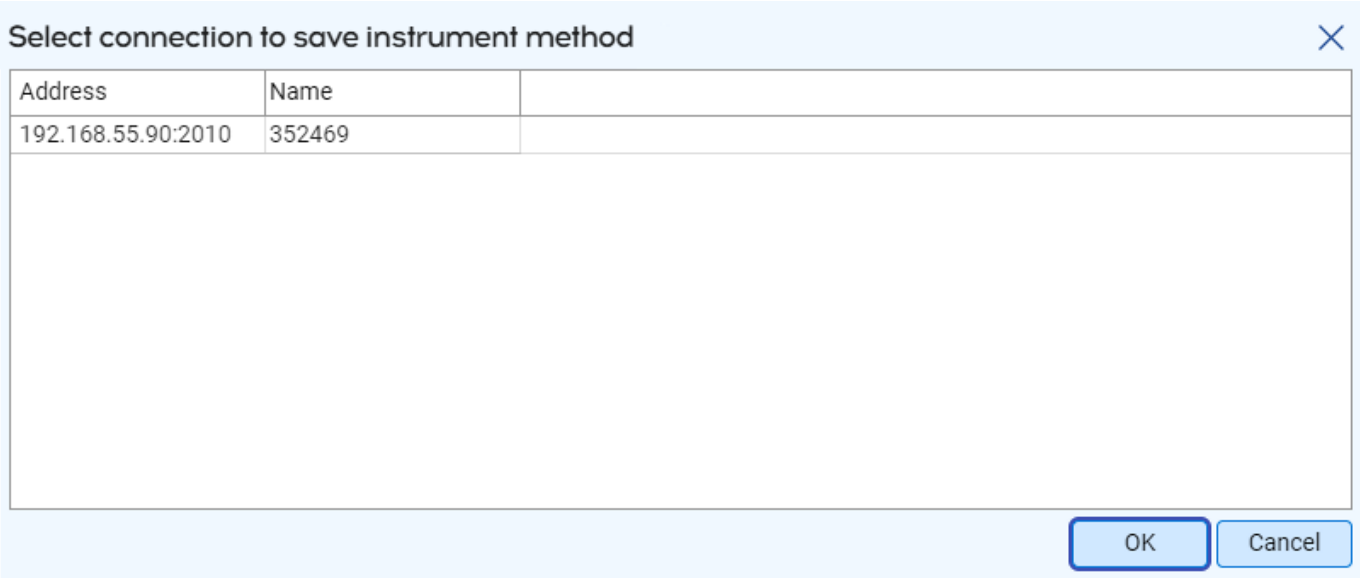


Fig 2.10 – Save the instrument method. Select connection

2.3 Sample info

Sample Info is filled in in the Scheduler when setting the sequence of analyses. When the chromatogram has already been recorded, you can change it in the "Analytic" by selecting the appropriate tab.

If the analyzed sample has internal standards and undetectable components, then their concentrations are also set in the passport. Well -known concentrations are also set here for assessing accuracy (absolute or relative deviation of the measured concentration from the known given).

{video analytic_sample_info_concentrations Internal standard concentration, undetectable component concentration, a given concentration, calculation of accuracy}

3 METHOD

The method should be created at the stage of setting up the sequence of analyses. However, you can create new methods and edit existing ones at any time.

To open the method editor from the processing program, click on the Method link next to the method selection drop-down list.



Fig 3.1 – The upper toolbar of the processing software

The method editor opens:

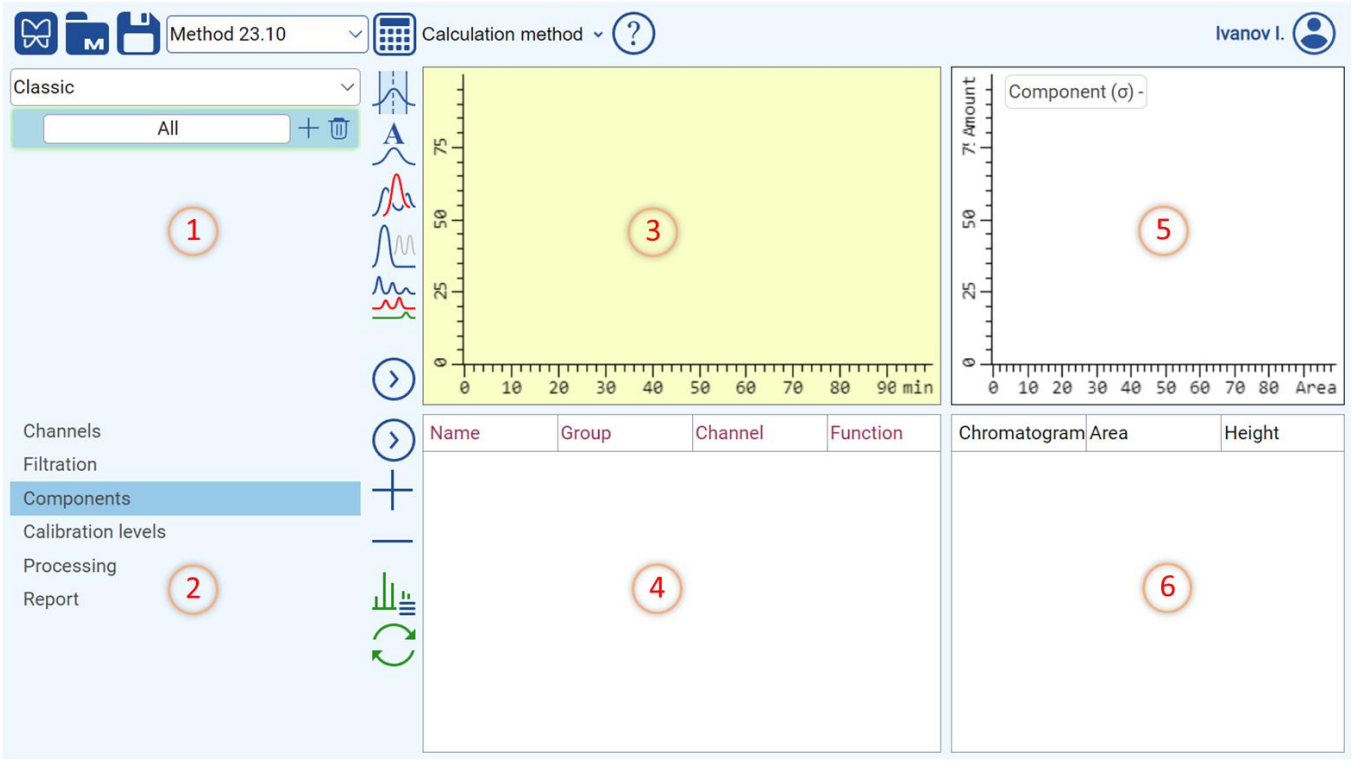


Fig 3.2 – The method editor

The method editor contains the following areas:

1. Panel of calibration levels.
2. Bookmarks bar. The contents of areas 4 and 6 depend on the selected bookmark.
3. The graph of the chromatogram corresponding to the one selected in panel 1.
4. The area depends on the selected bookmark. For the "Components" tab, a table of components of the selected calibration level is displayed here.
5. Calibration graph of the selected component.
6. Table of calibration points.

When choosing a method, the processing of an open chromatogram using this method will be performed immediately.

Algorithm for creating the method.

3.1 Method type

In "Chromatec Analytic 4" two types of method:

- Classic. Used for most tasks, selected by default.
- Channel generator. It is used when working with a single-quadrupole mass spectrometric detector.

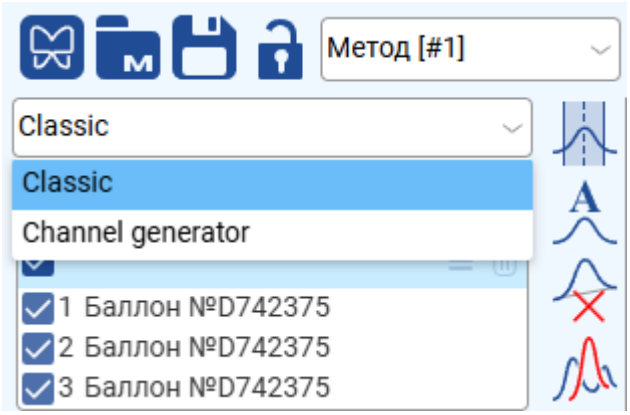


Figure 3.3 – Method type selection

When creating a method based on the search results (according to the mass spectrometric data with a single-quadrupole MSD), the “channel generator” is automatically turned on. The table of components (name, retention time, component mass, relative intensity) from the MS: Search Results will also be automatically filled out.

When choosing the type of "Channel generator" method, the following condition is checked – if the channel points with a constant frequency differs from real points by more than one second, then such a channel is considered poor and will not be created.

Also, a channel will not be built if "Window, %" in the "Components" table is too large in the component, i.e. If the window includes neighboring components where there was a scan of similar masses (nr, α-bhc and γ-bhc have similar spectra/masses), while the segments do not overlap in the instrumental method of MSD.

The algorithm of the method with a sign of the channel generator:

- At the time of time (holding the ± window, %) the program for building a channel on the main ion (first mass) is searching for mass M/Z 1.
- The main ion extracts from this segment.
- Next, checks the condition – is it possible to generate a channel with a constant frequency – after which the channel displays.

3.2 Calibration levels

On the left side of the method editor page there is a panel of calibration levels.

A calibration level is a group of points in a calibration graph that have the same concentration.

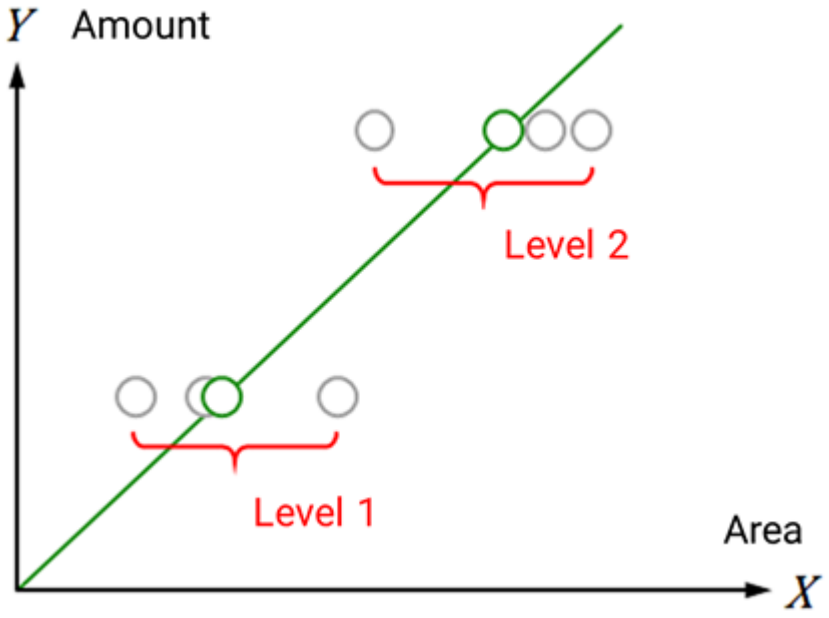


Fig 3.4 – Levels on the calibration graph

In Chromatec Analytic 4, the calibration level is a software structure that combines the components of a sample that have the same concentration set.

Each point entering the level corresponds to a specific chromatogram. In the context of calibration, the chromatogram and the calibration point will be considered synonymous.

There is always at least one calibration level, since components cannot be added without it.

When adding components to the table with the corresponding button, they are added to the selected calibration level. And if the level does not exist, then it is automatically created.

The calibration level will be created even if this method is created without calibration. For example, if it is a normalization method or one of the variants of the method with an internal standard. This is done for the uniformity of the method settings.

If you don't need to create multiple grading levels in your method, then you don't have to think about this entity. It will exist in the method, but your interaction with it will not be required.



A – all calibration levels are selected, B –"level 1 is selected", C – chromatogram #13 (calibration point) in "Level 1" is selected.

Fig 3.5 – Calibration Levels Panel

In order to add a new level, click the corresponding button in the top row of this panel (where it says "All").

To remove the entire level or one calibration chromatogram from the method, press the corresponding button. It is different for each level or chromatogram.

Here, by deleting the chromatogram, you simply exclude it from the method. It is not physically deleted. The same chromatogram can be included in different methods.

This button opens a menu with the following commands:

Add analysis. The command allows you to select a chromatogram to be included in the calibration.

Import from level. The command allows you to import calibration points to the current level from any other.

Update point data. The command allows you to recalculate the chromatograms corresponding to the calibration points.

{video method_calibration Method calubration}

3.3 Calibration control

- In the method editor, go to the "Components" tab".
- Select the component for which you want to show the calibration.

A calibration graph of the selected component will appear. On it, you can visually assess the dispersion of calibration points, as well as determine the value of the control parameter.

The following are used as control parameters:

- Relative standard deviation, RSD %.
- Coefficient of determination, R^2.
- Accuracy, %.

The accuracy is shown in the table below the graph.

RSD and R^2 are shown in the upper left corner of the graph.

Only one of the control values is displayed. To view everything and/or select something else to show, click on the control parameter and select the desired one in the menu that opens.

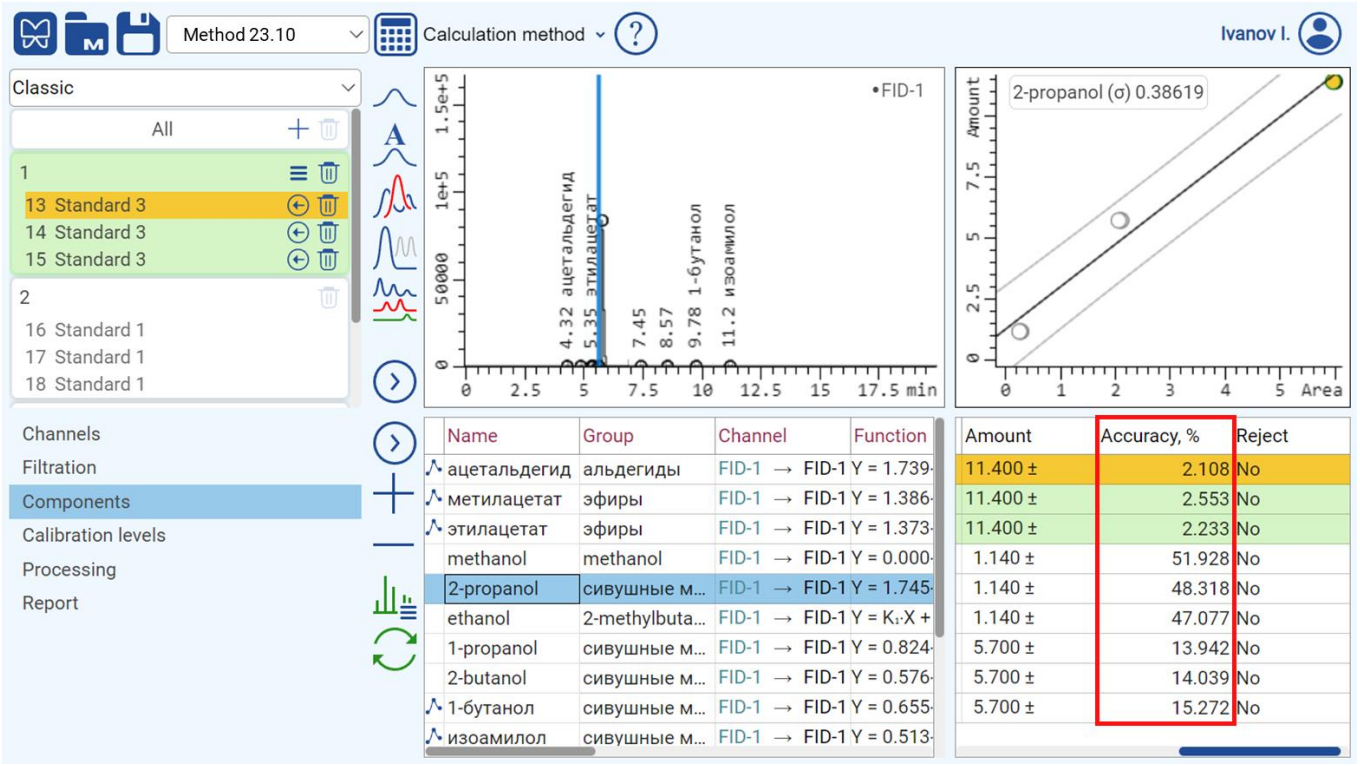


Fig 3.6 – Calibration control

When the mouse cursor is over the control parameters, a statistics window appears. You can secure it by pressing the "lock" button.

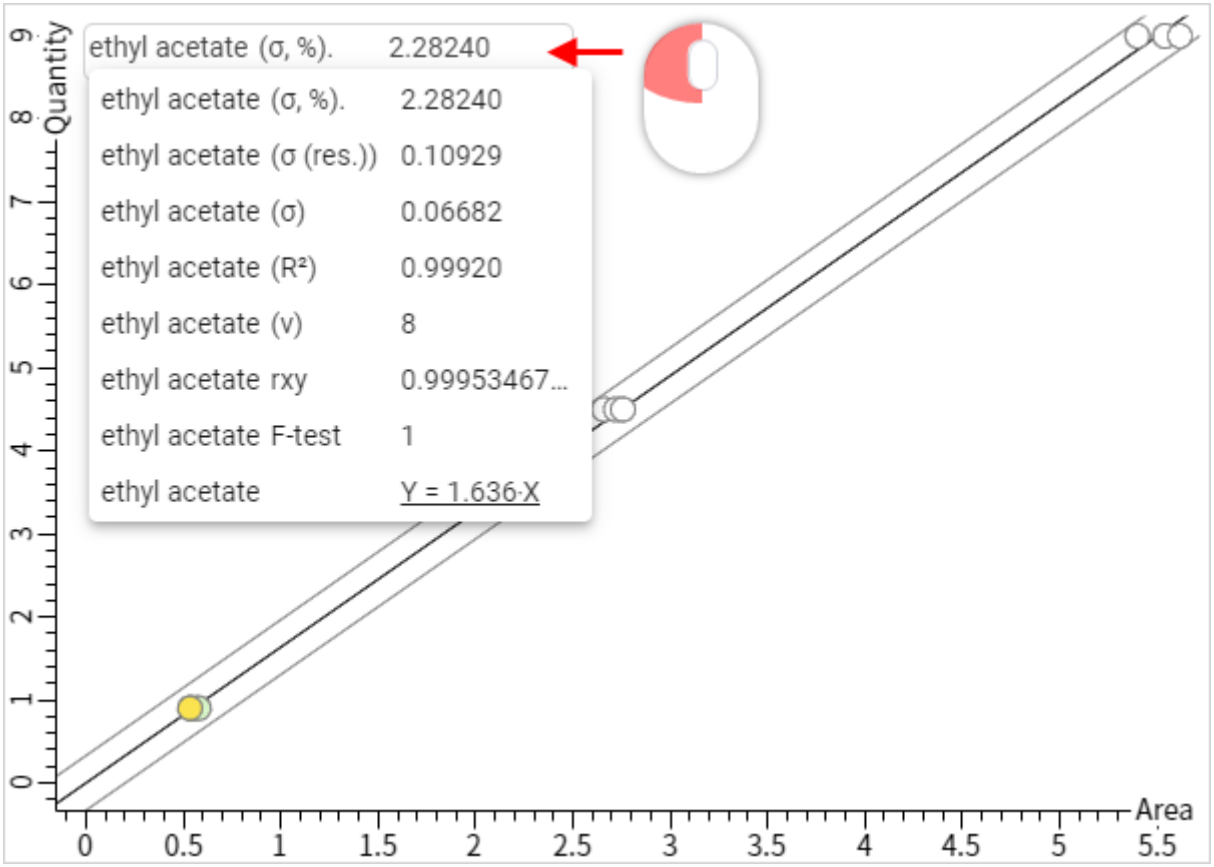


Fig 3.7 – Calibration control. Selecting a control parameter (left click on the control parameter)

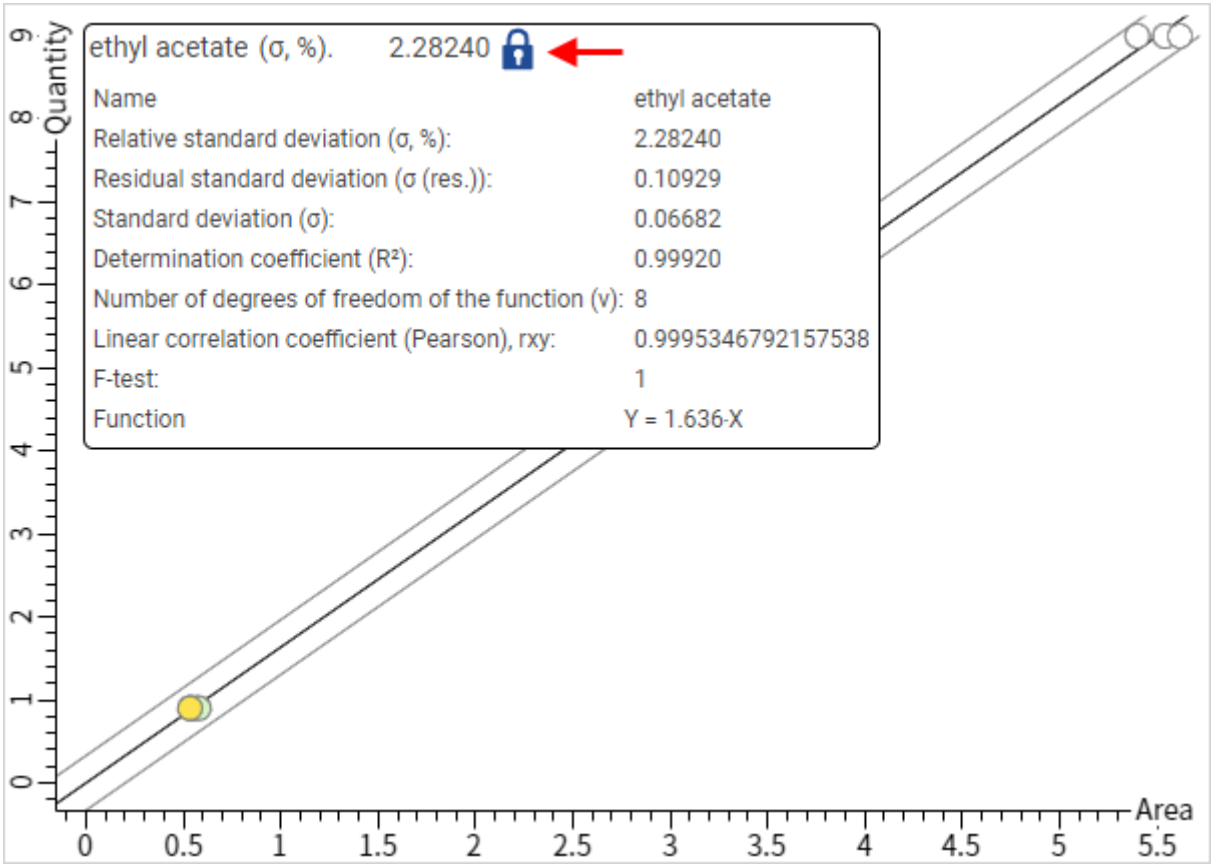


Fig 3.8 – Calibration control. Pin statistics

3.4 Channels

The Channels tab is available both in the method editor and in the Chromatec Analytic main window.

3.5 Filtration

There are a number of noise filtering methods that differ in the principle of operation. Most of them consist in performing certain transformations over a chromatogram point, and the result depends on the values of neighboring points. The number of adjacent points located to the right or left of the transformed point is called the half-width of the filtering window.

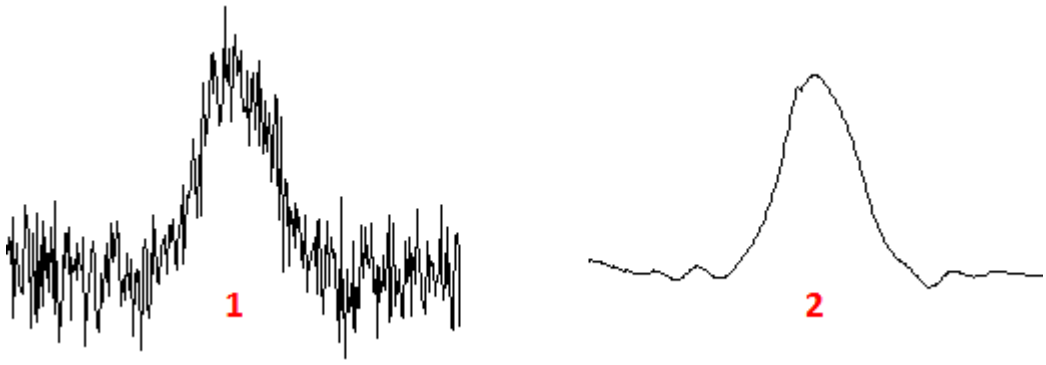


Fig 3.9 – Chromatogram 1) before filtration, 2) after filtration

Since any filtering distorts the shape of peaks, its use is justified only at high noise values. At the same time, it is recommended to start selecting the half-width of the filter window from one and gradually increase it until a satisfactory result is obtained.

When setting up the filtering operation, it is important to pay attention to the fact that, simultaneously with the suppression of zero-line noise, the areas (heights) of the peaks are not distorted. To estimate the response distortion, select the narrowest peak analyzed.

In "Chromatec Analytic 4" filters are used:

- LOP-filter (local-optimal polynomial filter).
- Adaptive filter.
- Gauss filter.
- Median filter.
- 2nd order filter.

In addition, the filters include the operational line correction:

- Peak inversion.
- Drift compensation.

{video method_filtration Filtration}

{embed filters 1020 562}

3.5.1 LOP-filter

The LOP-filter is based on the assessment of the error in the measurement of each point on the chromatogram. Due to the polynomial interpolation of the signal, noise is effectively suppressed. Unlike other methods, the filter takes into account the form of chromatographic peak and retains it unchanged.

Filter with constant dispersion well removes noise, which has constant value throughout the chromatogram. If the noise scope changes during the analysis, for example, when programming the column temperature, it is preferable to use filtration with variable dispersion. However, the effectiveness of noise removal in the variable dispersion method will be worse than with constant dispersion.

The window width is determined by the width of the chromatographic peak. With an increase in the width of the noise window, the chromatogram is more suppressed, however, with too high values, the distortion of chromatographic peaks begins.

The coefficient adjusts the assessment of noise dispersion, which affects the confidence interval and smoothing the base line.

Parameter	**Range**	**Default**	**Discretion**
Window width, points	1 – 1000	1	1
Coefficient	0 – 10	1.5	0.01

3.5.2 Adaptive filter

It does not distort the form of peaks, does not reduce their area.

Noise filtration is carried out by approximation of the source data near the smoothed sample of the third degree polynoma. The width of the approximation window changes from 5 to 40 counts, depending on the nature of the current section of the chromatogram.

It works faster than a LOP-filter, gives out a close result.

The disadvantage – on sharp front fronts of peaks, distortions can occur.

Filter without parameters.

3.5.3 Gauss filter

The average balanced value of all points inside the window with a weight distributed according to the Gauss function with the center in the middle of the window is calculated, the result is used as a new detector response. The peaks after smoothing become lower and wider, their area does not change.

The value of the half -chewing of the window during tuning should be selected minimal and gradually increase it to optimal.

Gaussov Filter, compared with the median, gives the best visual smoothing of peaks, but smells the noise of the basic line.

3.5.4 Median filter

The median filter effectively suppresses emissions on the chromatogram, while the hemisphere of the filter window should be less than the width of the largest emissions. The values of the points inside the filtering window are sorted in an increase in order and the point corresponding to the middle of the window is replaced by another value that falls into the center of the sorted array.

3.5.5 Second order filter

The filter serves to suppress high -frequency noise on the chromatogram. When using the filter, select the cut frequency as high as possible, because in this case, the distortion is minimal.

It is regularly used during the checkout procedure.

3.5.6 Peak inversion

{video method_peak_inversion Peak inversion, inversion}

3.6 Components

3.6.1 Group

You can set a group for each component. The group allows you to summarize the concentrations and areas of components in the report.

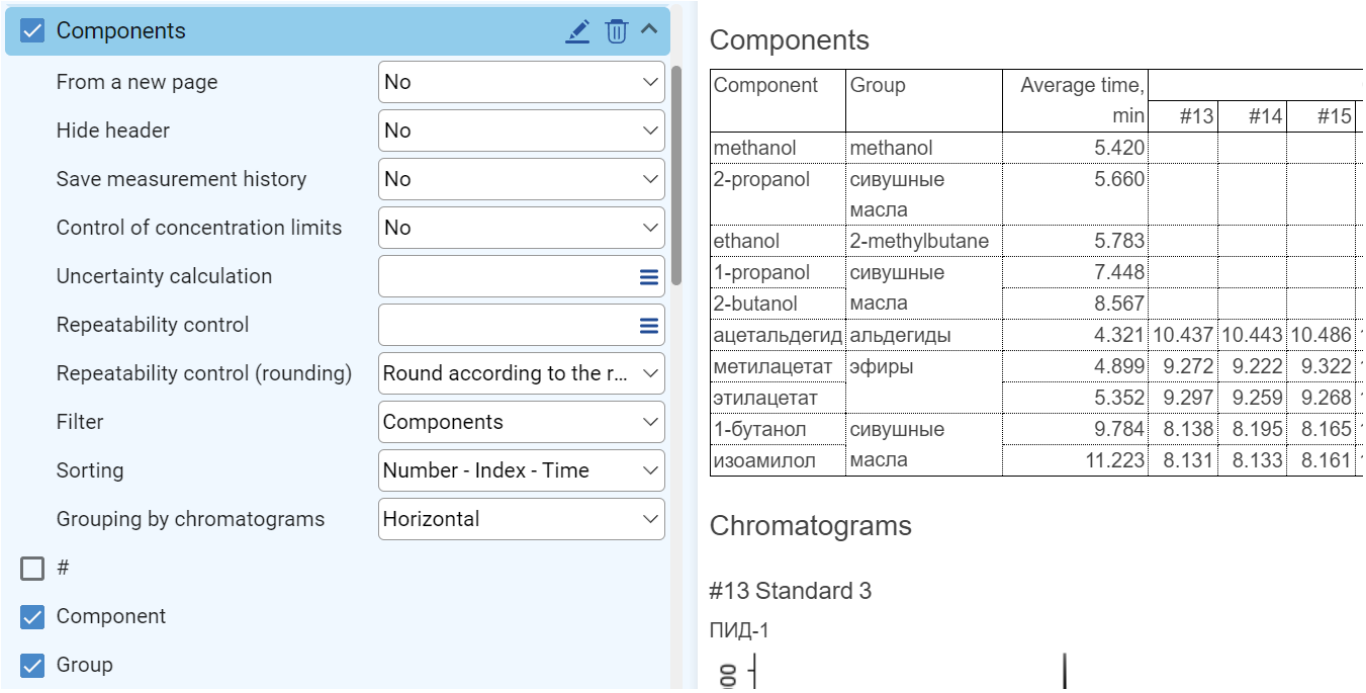


Fig 3.10 – Summing up areas by groups in the report

3.6.2 Rules for identifying components

The rules for identifying components are set in the "Identification" column. By default, it is hidden and you need to enable it before you start working.

{video method_table_show_hidden Show hiddencolumns, table settings}

According to the method of identification, the component can be:

- ordinary,
- reference,
- undetectable
- confirming.

By default, all components have the attribute – **ordinary**.

You can create a table of components in the method even before recording chromatograms. However, in this case, you do not know the exact retention times and with a high probability the peaks on them will not be identified. In addition, they may remain unidentified in case of any hardware problems or operator error.

However, you can always adjust the retention time of the component so that peak identification works – link the peak and the component.

{video method_peak_component_binding Binding peak to component}

An **undetectable component** is a component that is not eluted on the chromatogram of the analyzed sample, but is artificially taken into account in the quantitative calculation of chromatographic analysis. The retention time of non-detectable components is set to 0. They are added to the table in order to set the concentration value (it must be known in advance). It can participate in the general calculation.


Click the button on the sidebar to add a undetectable component.

- A new entry will appear in the table. Specify the name of the undetectable component.
- Set the time, it is 0.
- In the "Identification" column, specify the type – "Undetectable".
- The "confirming" attribute is used for identification on two channels.

3.6.3 Concentration

By default, the concentration set and measured is displayed together with the error (uncertainty).

If the uncertainty is not needed, it can be hidden.

{video method_table_concentration Concentration}

3.6.4 Internal standard

When using a quantitative calculation by the internal standard method, set for all components a link to the component, which is the standard. There may be several standards.

Set the name of the standard in the Standard Name column. At the standard itself, this cell should be empty! If there is no such column, it needs to be shown.

	Name	Function	Standard name
	A	Y = 0.032·X - ...	
	B	Y = 0.049·X - ...	A
	C	Y = 0.169·X - ...	A
	D	Y = 0.211·X - ...	A
	E	Y = K_1·X	A

Fig 3.11 – Set of the internal standard (here the standard is component A)

3.6.5 Function selection

To perform a quantitative calculation, each component must have a function specified. The type of function is determined by the features of the analysis methodology.

To select a function, open the list in the corresponding cell.

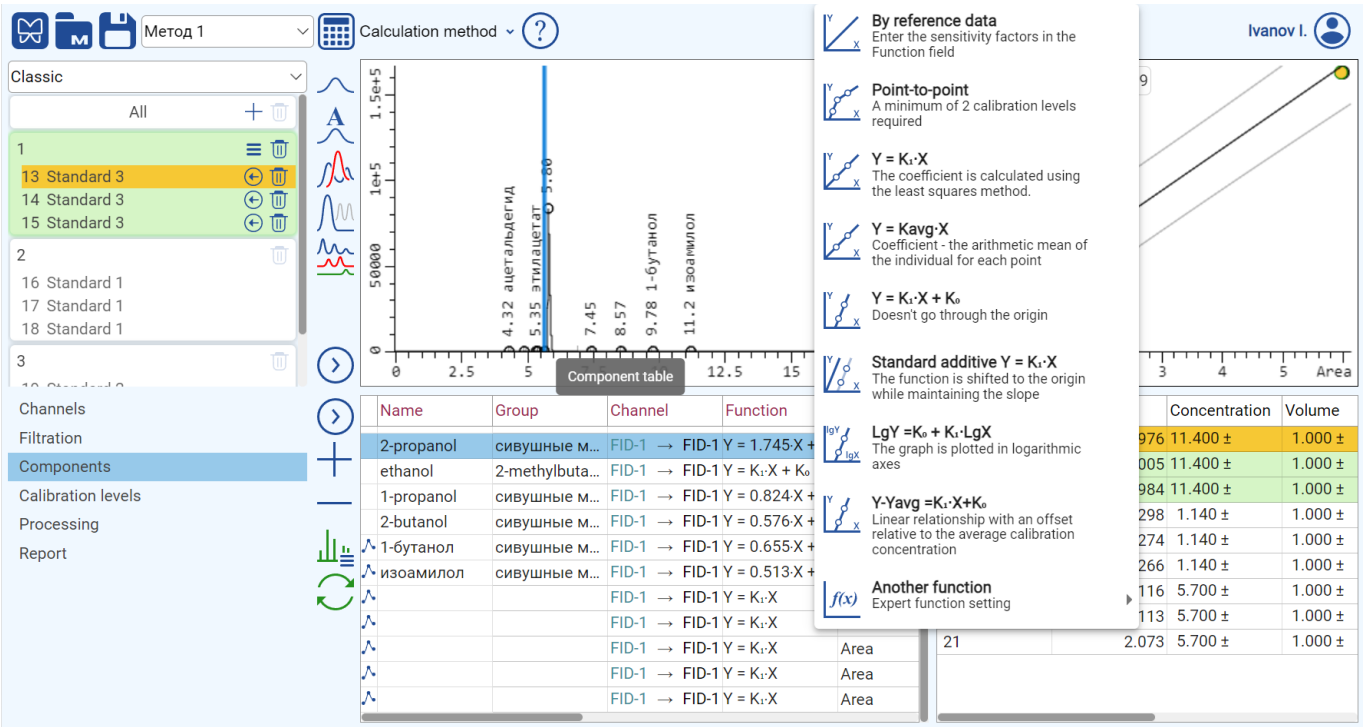


Fig 3.12 – Function selection

Table 3.1 – Calibration functions

Function	Description
By reference data	This function should be selected when the component is not calibrated, and the calibration factor is entered from the reference data provided in the methodology. It is used for analyzes by methods of internal normalization, external and internal standard.
Point-to-point	The function is used to plot a broken calibration curve for multipoint graduations. It is used when other functions do not provide the necessary calibration accuracy.
$Y = K_1 X$	Linear function. Used in most analyzes by default. The coefficient K1 is calculated by the method of least squares.
$Y = K_{1avg} X$	Linear function similar to the previous one. Differs in the way of K_1 calculation. Here it is defined as the arithmetic average of all coefficients individually calculated for each point.
$Y = K_1 X + K_0$	Linear function that does not pass through zero.
$LgY = K_1 LgX + K_0$	Logarithmic function. Used when working with an FPD-S detector (sulfur channel).
Standard additive	This function is used to account for the unknown content of the calibrated component in the solvent. It is used only for a linear relationship between the detector response and the amount of component in the sample. See the Calibration section for details.

If none of the functions in this list is suitable for this technique (for example, a quadratic function is required), select the Another function setting.

- If the component is not calibrated, select a function for it according to the reference data.
- Instead of "1" enter the values of the correction factors given in the methodology (relative sensitivity coefficients) in these cells.

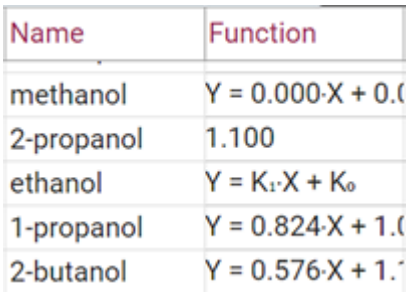


Fig 3.13 – Selecting a function by reference data

3.6.6 Multirow changing

When there are many components in the table and you need to fill in the same value for any parameter (for example, units of measurement or the value of a function), it is convenient to use a batch change of rows. To do this, call the corresponding function in the context menu of the table, which opens by right-clicking on the column.

{video analytic_table_settings Table settings}

3.7 Processing plug-ins

Chromatogram processing is the sequential execution of several processes. These processes are also called plugins. By default, there are two processes in the queue on the "Processing" tab:

- Peak detection.
- Quantitative calculation.

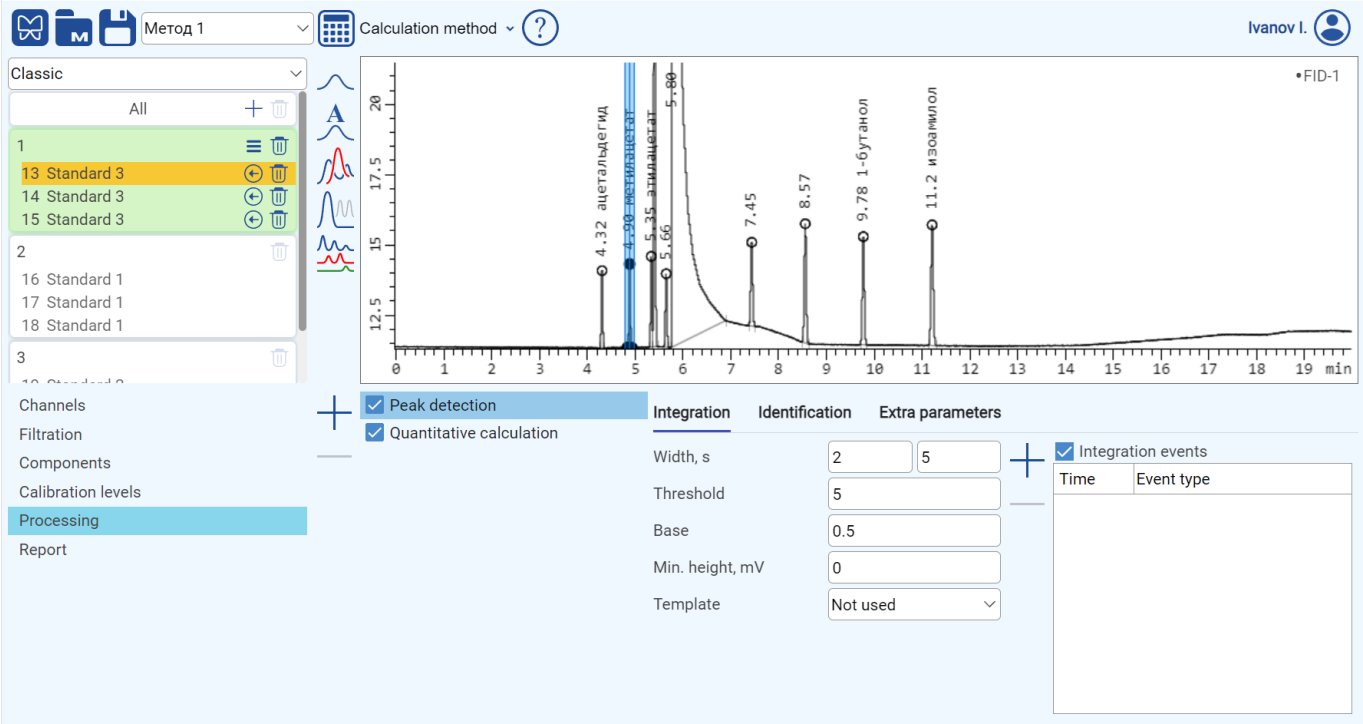


Fig 3.14 – Processing Parameter Settings

To perform various analytical tasks, you can add additional processes to the queue. To do this, click the corresponding button on the sidebar and select the desired calculation from the list.

3.7.1 Peak detection

Purpose of the **Peak detection** operation:

- Integration (marking of peaks on the chromatogram, calculation of their heights and areas).
- Identification (comparison of found peaks with expected components).

To configure the peak search, go to the **Processing** tab and select the **Peak detection** operation in the list. ".

Integration

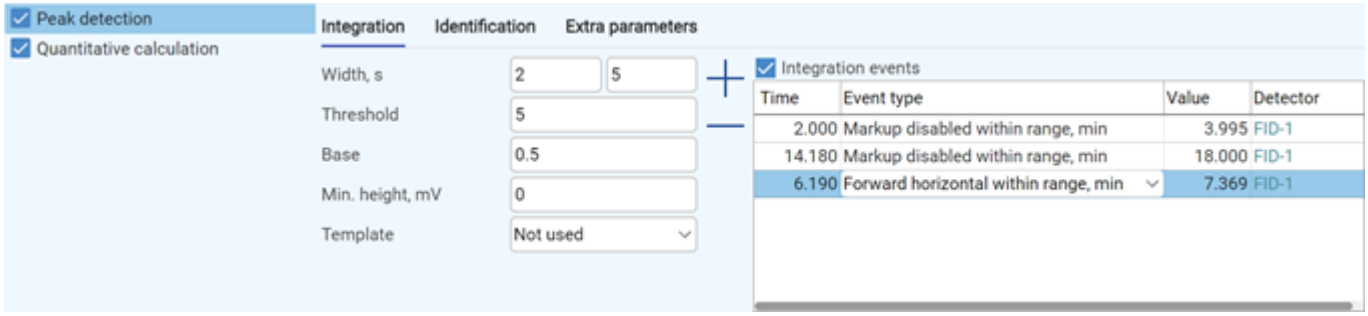


Fig 3.15 – Peaks detection parameters. Integration

In the ideal case, markup setting is reduced to four parameters:

Width – is a parameter determines how wide (in seconds) the peak of the chromatogram must be in order for the program to integrate it. If this parameter is small, wide peaks are perceived by the program as drift and are not marked. Since the peaks near the end of the chromatogram are broadened, the width of the peak at the beginning may not be sufficient to detect them, so two values are specified – the width at the beginning and at the end.

Threshold – is a criterion for detecting the onset of the peak. If the value of the derivative at each point of the chromatogram exceeds the level set by this parameter, it is considered that the peak began at that point.

Base – is a parameter describes what space should be between the two peaks, so that the program considers them to be separate. The parameter value is not specified in seconds, but in fractions of width. Thus, if the width in this area is 2 s, and the base is 0.4 of width, then this means that there must be an empty space between the peaks for at least one second in width, otherwise, they will be considered merged. The recommended value is 0.1.

Min height – The program can consider any noise of the zero line as a peak, which is inconvenient. It is recommended to set the minimum height of the peaks (in millivolts). Peaks below this threshold will not be marked on the chromatogram. This parameter requires adjustment for a specific chromatogram.

If you click on the **Width** parameter, the program selects the optimal peak width for this chromatogram. You need to click on the link several times until the digits stop changing..

Integration events

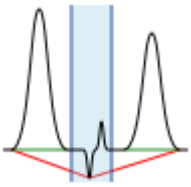
Sometimes the selection of integration parameters in order to achieve the correct marking of the peaks is not possible on the entire chromatogram, but only on some of its sections. In other cases, the

chromatogram may contain peaks that are not subjected to the calculation, and their markings may interfere with the visual perception of the chromatogram. **Integration events** can be used to fine tune the peak markings on the chromatogram.

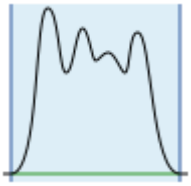
Integration events allow you to set the values of the parameters listed above even more subtly, thus, the operator can further influence the procedure of peaks detection on the chromatogram. The event can be set both for an individual detector and all detectors simultaneously.

When defining integration events, it is convenient to use a marker. It allows you to specify the time from which the event will be executed, as well as visually change its boundaries (for events running at a certain interval).

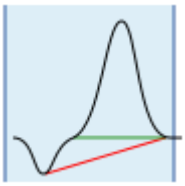
Application of integration events (red line – markup before applying the event, green line – mark up the result of applying the event, blue bar – marker position):



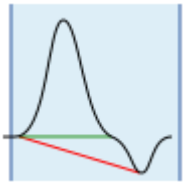
Markup disabled within range, min
This event is used more often than others. It helps to remove the markup in those places where the baseline is drawn incorrectly or the markup is simply redundant there. As the parameters of the event, the start and end time of the interval is set.



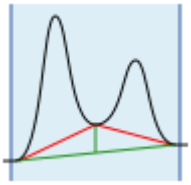
One peak within range, min
If you need to mark a group of peaks as one (for example, to calculate the total area of poorly separated isomers), you should use this event. As the parameters of the event, the start and end time of the interval is set.



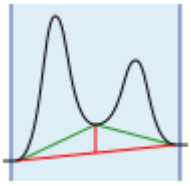
Backward horizontal within range, min
A horizontal line is drawn from the peak end to the intersection with the chromatogram or baseline. It is used when the peak goes right after the troughs (negative peak) and they are separated not so well it. As the parameters of the event, the start and end time of the interval is set. The initial peak must fall entirely within the event interval, otherwise, it will not be processed.



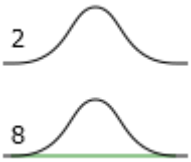
Forward horizontal within range, min
A horizontal line is drawn from the beginning of the peak to the intersection with the chromatogram or baseline. The start and end times of the interval are specified as event parameters. The initial peak must fall entirely within the event's action interval, otherwise the event will not be executed.



Merged peaks within range, min
All peaks at this interval will be marked as merged, i.e. with a vertical line between the points of their beginning and end. As the parameters of the event, the start and end time of the interval is set.

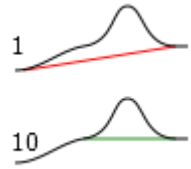


Valley to valley within range, min
All peaks, even physically merged, will be marked as separate. As the parameters of the event, the start and end time of the interval is set.



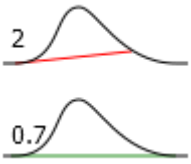
Width, s

Set the expected width of the peak in seconds. If the width is too small, the program may take the peak for the drift of the zero line. In this case, the markup will not be performed.



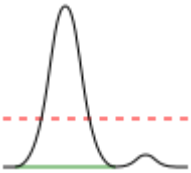
Threshold

The detection criterion of the peak onset. If the value of the derivative at each point of the chromatogram exceeds the level set by this parameter, it is considered that a peak began at that point.



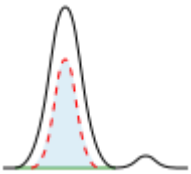
Asymmetry

The ratio of the threshold on the rear slope of the peak to the threshold on the front slope. The significance of the threshold for the rear slope of the peak may be set different from the threshold for the front slope. This parameter sets the ratio of these thresholds. If the specified parameter is 0.7 (recommended value), then this means that the threshold on the rear slope of the peak is 0.7 of the threshold on the front slope of the peak.



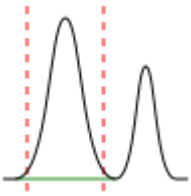
Min height, mV

The minimum allowable height of the detected peak. Peak suppression with a height less than the specified value. At the same time, the value of the parameter equal to 0 means that the suppression of the peaks is turned off.



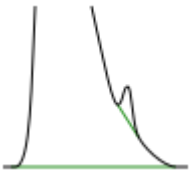
Min area, mV*s

The minimum allowable area of the detected peak. When detecting peaks, it is possible to suppress peaks which area is smaller than the specified one. At the same time, the value of the parameter equal to 0 means that the suppression of the peaks is turned off.



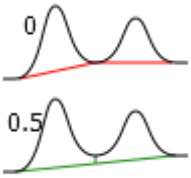
Min width, s

Peaks with width less than the specified value are not marked.



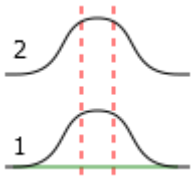
Peak-rider

The parameter used to identify the peak as a rider, separated from the main peak with tangential descent. The value of this parameter indicates how many times the second peak must be less than the first one to become a rider. If the value of the parameter is 0, the riders are not detected. The recommended value of this parameter is 0, but if there is still the need to detect riders, it is possible to set the parameter value in the range from 5 to 10.

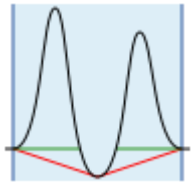


Base

The minimum width of the plateau on the descent peak, sufficient to complete the peak and identify the baseline. The unit of measurement is the current value of the "Width" parameter. The end of the peak is determined by the decrease of the derivative below the threshold and if the derivative value remains low during a period that exceeds the value of the Base parameter, then the peak is considered to have gone back to the baseline. Otherwise, merged peaks will be recorded. The recommended parameter value is 0.1, if the value is 0, all peaks will be marked as separate.



Plateau in percent of width
The maximum plateau width at the top of the peak. The unit of measurement is the current value of the "Width" parameter. Near the peak top, the derivative becomes lower than the threshold and may stay at this level during the time specified by the "Plato" parameter. If the corresponding period of time is longer, then this feature on the chromatogram is interpreted not as a peak, but as a rise of the baseline to a new level. The recommended value is 2.



Base through within range, min
For all peaks, a baseline is drawn at this interval. It crosses the chromatogram without rounding the "trough" if present. This event is used in conjunction with the "Merge Peaks on the interval" event. It is desirable that the intervals of both events coincide.

In case of the change in peak retention times, integration events may not be performed correctly. To ensure that event boundaries are shifted to the same intervals as the retention time shift, it is convenient to create reference peaks. The program will determine how the event boundaries should be shifted according to the position of the reference peak.

It is recommended to choose the reference peak from among those located near the end of the chromatogram..

Setting the reference peaks is described in the Component Identification Rules section.

To add a new event, click the button to the left of the integration event table.

- Click on the **Event Type** cell to open the list of available.
- Select the event.
- Use the mouse to adjust the limits of the interval when this event will be executed.

{video analytic_integration_events Integration events}

Identification

The purpose of identification is to establish the correspondence between the predetermined components and the detected peaks in the chromatogram.

In the **Peaks Detection** dialog, go to the **Identification** section.

Dialog settings are suitable for most tasks, there is no need to change most of them.

Holdup time is set when identifying components by retention indices. Holdup time is displayed in the "Control Panel" on the Diagnostics tab for the corresponding column.

If you are identifying components by retention indices and there are no peak points for any component (i.e. there is no component in the sample or component is not marked), turn on the **Use non-peak reference component** option.

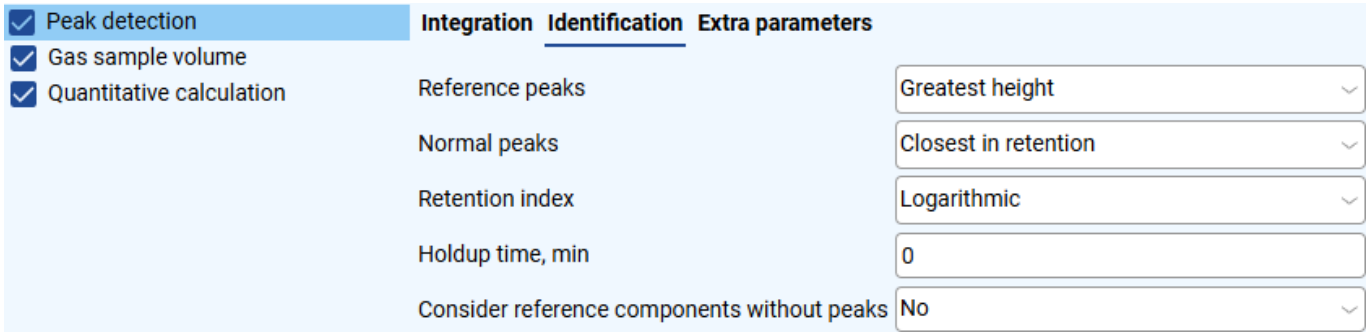


Fig 3.16 – Peak detection parameters. Identification

Peak detection extra settings

The **Extra parameters** tab contains the following detection settings:

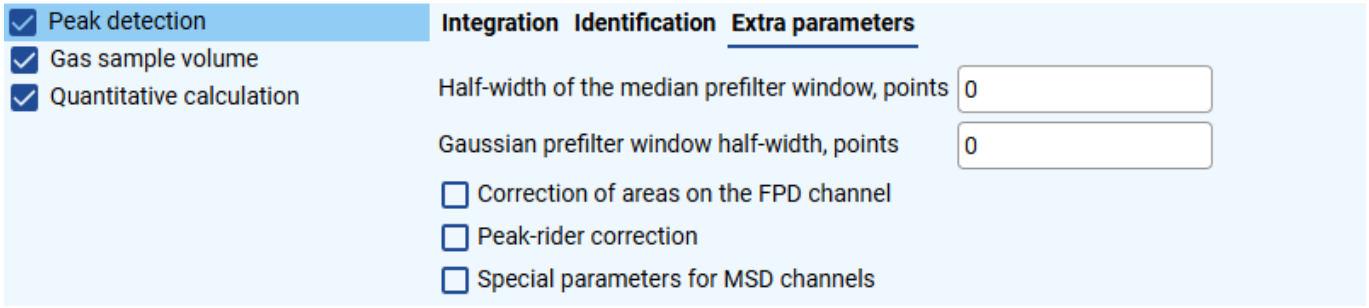
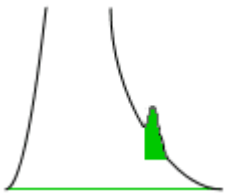


Fig 3.17 – Peak detection extra settings

Median and Gaussian prefilters allow you to pre-smooth the zero line for a more reliable determination of the start and end points of the peak in noise. Prefilters can be used individually or together. The recommended value of the half–width of the window is 2 points. If the value is set to 0, the corresponding prefilter is not used.

If the "Correction of areas on the FPD channel" option is enabled, the linearization of the FPD detector will be applied (when working with FPD, a linear function can be used for calibration).



Peak rider correction. Enabling this option allows to **calculate the area** of the riders, as shown in the figure below. At the same time, graphical markup of the peaks does not change.

3.7.2 Configuring quantitative analysis

The purpose of the operation is to calculate the concentrations of components and percentages.

Go to the **Processing** tab

Select the operation **Quantitative analysis** from the list.

Select calculation method:

- **External standard**. The calibration function is calculated for all components for which the concentration is known. For the other components, relative sensitivity factors are used and the standard is indicated.
- **Internal standard**. It can be applied with calibration or without it.
- **Internal standard with effective volume**. It is applied with calibration only.
- **Without calibration**. Used for percentage and internal normalization. Calibration functions are not calculated. Relative coefficients are set for all components. If they are unknown, then set to 1.

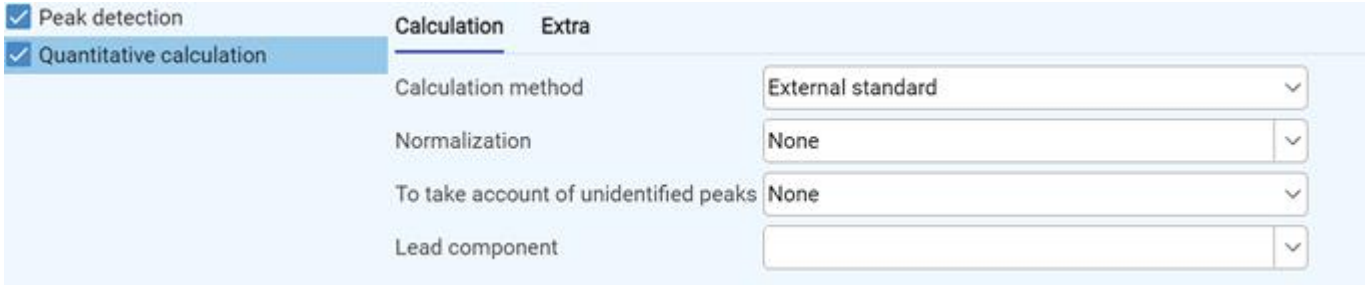


Fig 3.18 – Quantitative analysis parameters

Normalization of results

If you want to normalize the result after performing the calculation, specify the normalization option::

- None.
- 1.
- 100.

You can also set another normalization value.

Internal and percentage normalization in this dialog are configured in the same way. They differ by the presence of relative sensitivity coefficients in the **Function** field of the component table for the case of internal normalization. For percentage normalization, relative coefficients can be omitted.

For methods with calibration, normalization can be optionally enabled, for methods without calibration, it is always included.

If you perform percentage normalization and there are unidentified peaks on the chromatogram, in the **To take account of unidentified peaks** list, select the Area value.

When using sensitivity correction factors for **identified** peaks, consideration of unidentified should be used with caution. The result of such a calculation may be incorrect..

Calculation of the main substance concentration

Sometimes, as a result of the analysis, it is necessary to present the percentage composition of the sample, in which the concentrations of impurities are calculated, and the main component is calculated by the formula:

$$C_0 = 100\% - \sum (C_{avg})$$

In order for the program to perform such a calculation, specify the name of the component of interest in the **Lead component** field.

Extra calculations

The **Extra** tab contains rarely used quantitative calculation parameters.

If you perform parallel analyzes of an unknown sample, set the method for **calculating** the average concentration:

- **Arithmetic average** (the average concentration will be determined as the arithmetic average of the selected measurements).
- **Equally accurate** (can be used if the Sample Volume is strictly the same in all parallel analyzes).
- **Unequall accurate** (it is necessary to apply if the sample volume in parallel analyzes varies).

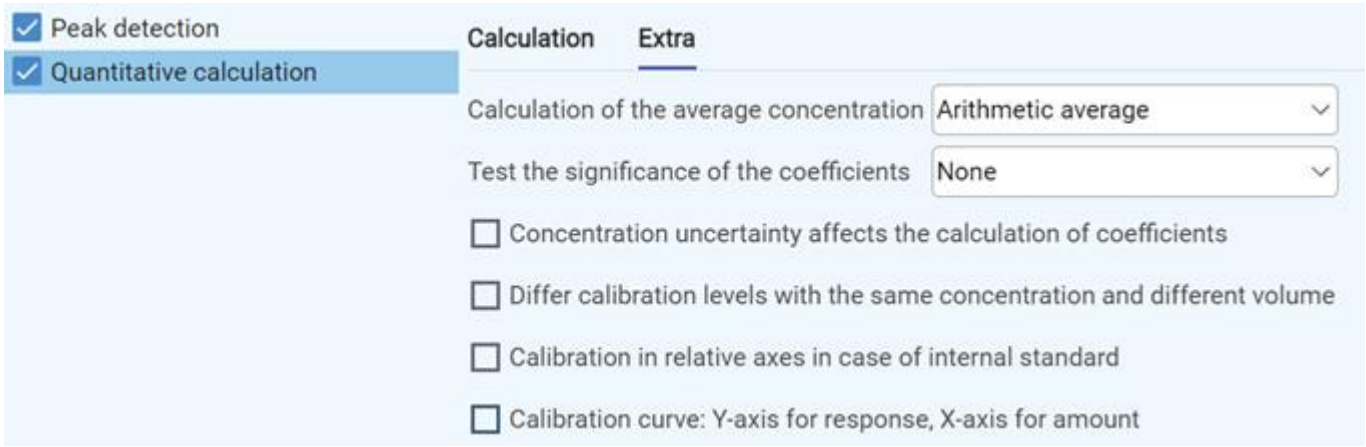


Fig 3.19 – Quantitative analysis parameters. Extra calculations

In order to make sure that the calibration function is selected correctly, select the method for **testing the significance of the coefficients**:

- None.
- All.
- Boundary.

If necessary, enable the option – **Concentration uncertainty affects the calculation of the coefficients**.

If the option **Calibration in relative axes in case of internal standard** is enabled, then the calibration function for all components except the standard takes the form:

$$Q' = F(S')$$

Where:

$$Q' = \frac{Qi}{Q\text{st}}$$

$$S' = \frac{Si}{S\text{st}}$$

Qi and Si – amount and response of the i-th component.

Qst и Sst – amount and response of the standard.

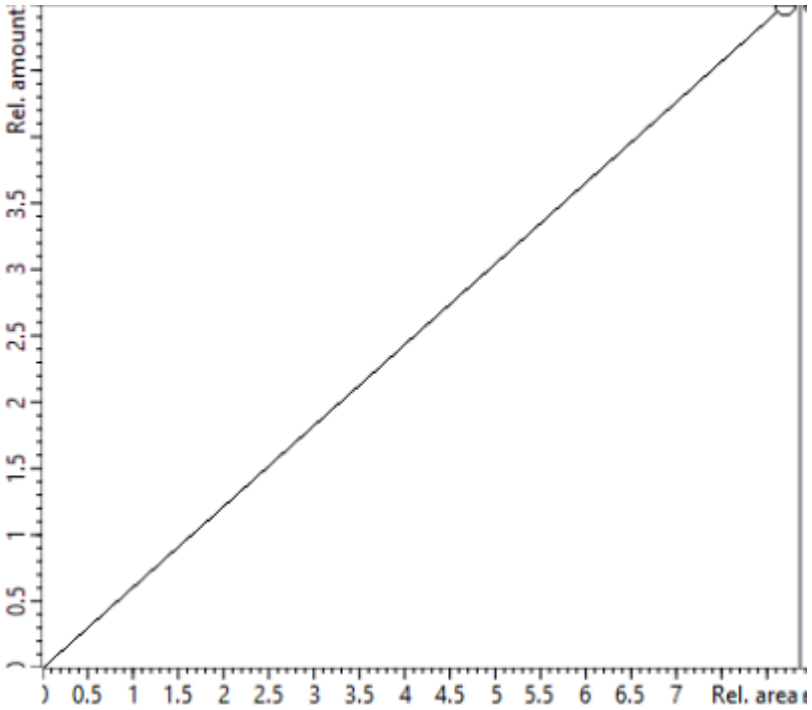


Fig 3.20 – Calibration in relative axes

The standard calibration remains in absolute axes.

This option can be used for both internal and external standards.

In the Chromatec Analytic software, the dependence of the quantity on the response is applied by default. This is done for ease of perception. The fact is that when conducting analyses, a known quantity that is convenient to consider as an argument of a function is precisely the response, the peak area. If you need to use a direct dependence of the response on the amount of substance, enable the option "**Calibration curve: Y axis for response, X axis for amount**".

If necessary, add additional calculations to the queue of processing operations.

After setting the parameters, perform the calculation.

{a=method_peak_parameters}

3.7.3 Peak parameters

Chromatec Analytic allows you to automatically calculate the following parameters of chromatographic peaks:

- Signal/Noise
- Width of peaks at half height
- Number of theoretical plates
- Peak resolution
- Peak asymmetry

To calculate them, add the operation "Peak Parameters" to the queue of processing operations.

The calculation result is displayed on the tab of the same name in the main window. To display the columns of peak parameters, you must first enable their visibility in the table settings.

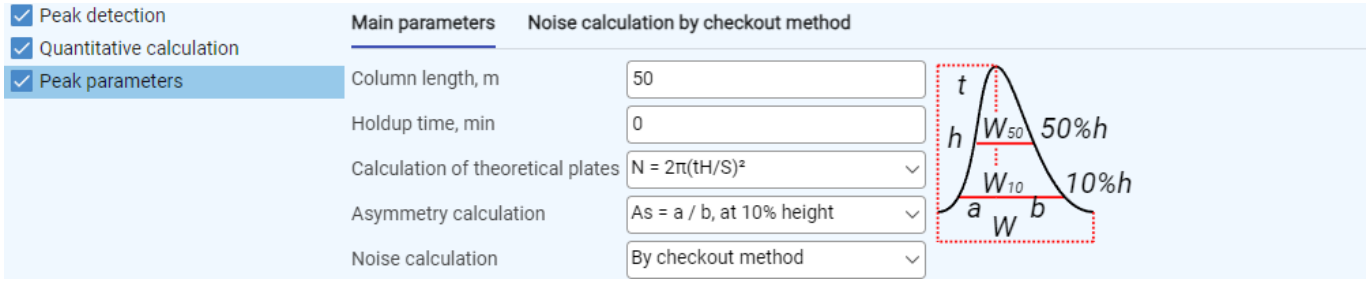


Fig 3.21 –Peak parameters

To calculate the number of theoretical plates, set the column length.

You can choose the following formulas for calculating plates:

$$N = 2\pi\left(\frac{t \times h}{S}\right)^2$$ The method of areas and heights

$$N = 5.54\left(\frac{t}{W_{0.5}}\right)^2$$ Width at half height method

$$N = 16\left(\frac{t}{W}\right)^2$$ Tangential method

$$N = 47.1\frac{\left(\frac{t}{W_{0.1}}\right)^2}{\frac{b_{0.1}}{a_{0.1}} + 1.25}$$ Exponentially modified Gaussian method

Where:

t – retention time, min.

h – height, mV.

S – area of the i-th peak, mV*s.

W – peak width at 13.4% height.

$W_{0.5}$ – peak width at half height, min.

$W_{0.1}$ – peak width at 10% height, min.

$a_{0.1}$ – the width of the left half of the peak is 10% of the height.

$b_{0.1}$ – the width of the right half of the peak is 10% of the height.

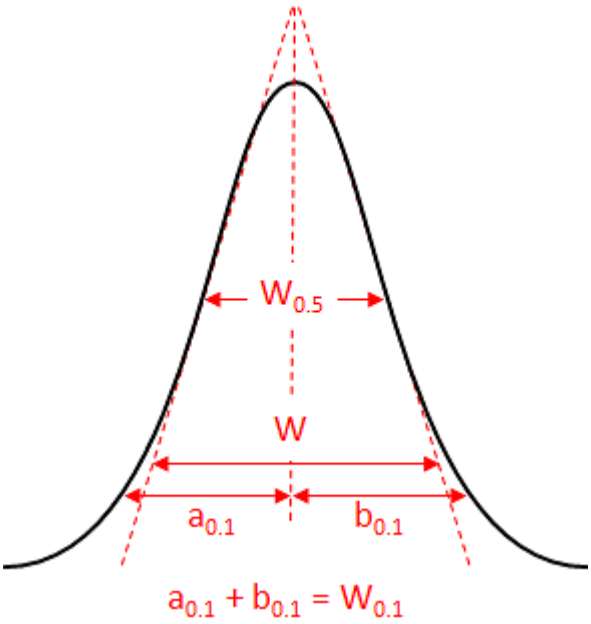


Fig 3.22 – Peak parameters

It is recommended to use the width method at half height, since this parameter can be calculated most accurately for the case of incompletely separated peaks.

The number of theoretical plates per meter of length is calculated by the formula:

$$N' = \frac{N}{L}$$

Where:

L – column length, m.

The resolution (degree of separation) of peaks is calculated by the formula:

$$R = \frac{2(t_2 - t_1)}{1.699(W_2 + W_1)}$$

Where:

t_1 and t_2 – retention times of the first and second peaks.

W_1 – width at half the height of the first peak.

W_2 – width at half the height of the second peak.

In the literature on chromatography , another calculation formula often appears:

$$R = \frac{2(t_2 - t_1)}{\lambda_2 + \lambda_1}$$

Where:

λ_1 and λ_2 – width at the base of the first and second peaks.

The resolution value is calculated for peaks **n** and **n+1**, where n is the ordinal number of the current peak.

The peak asymmetry can be calculated using one of the formulas to choose from:

- As = a/b, at 10% height
- As = (a + b) / 2A, at 5% height

To calculate the Signal to Noise ratio, a noise calculation is performed. Noise can be calculated in two ways:

- By checkout method.
- By amplitude over the interval.

If the “Noise calculation” parameter is set to "By checkout method", then the "Noise calculation by checkout method" tab appears. Go to it and specify the noise search interval. You can specify it explicitly or set it to autosearch.

To correctly calculate noise in amperes, as well as take into account drift, you should select the device model, verification method, detector type and its modification.

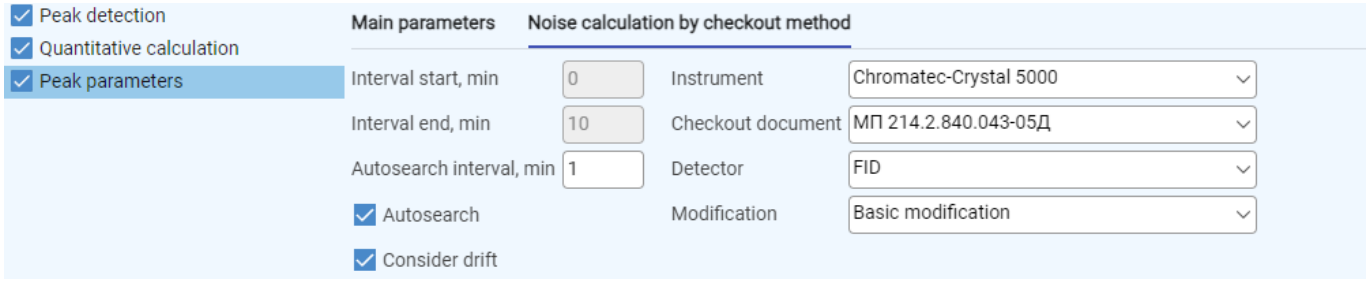


Fig 3.23 – Peak parameters. Calculation of the Signal/Noise ratio

If the "Noise calculation" parameter is set to "By amplitude on interval", set the interval.

3.7.4 Group intervals

The process is used to group peaks at specified retention time intervals, which allows summation of component concentrations within a group and convenient graphical representation of groups.

The process adds the areas of unidentified peaks in the interval to the area of the presenter. The original areas will be occupied. The identified peaks are ignored by the process.

- Add the process to the queue

Add a new group interval.

- Use the markers on the graph to adjust the boundaries of the interval.
- Set the group name for the peaks that fall within this interval. The group name will not change for peaks for which it is already set in the **Components table**.
- Specify the name of the lead component.

Perform the calculation.

You can enable color highlighting of groups.

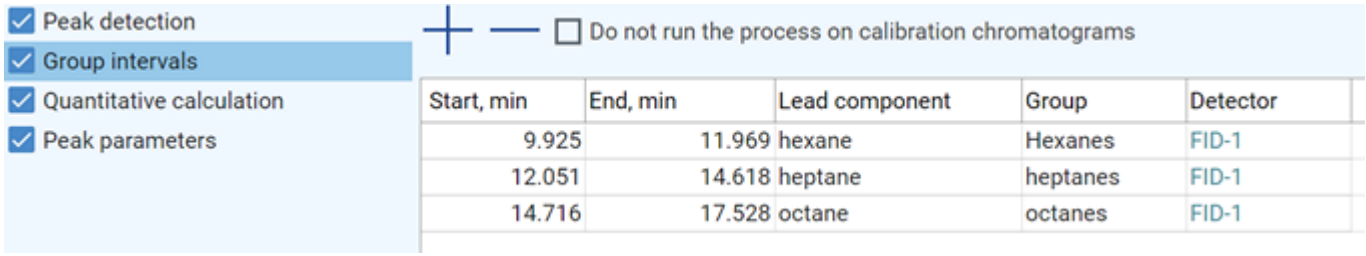


Fig 3.24 – Group intervals

3.7.5 Gas sample volume

The process is used to take into account the temperature and pressure of the gas sample when entering into the chromatograph.

- Add the process to the processing queue
- Set the **loop Volume, ml**.
- Set pressure and temperature under standard conditions, select units of measurement.
- If atmospheric pressure is maintained in the valve loop, enter its value or enable the option from the sensor (if it is installed in the chromatograph).
- If excessive pressure is maintained in the valve loop, set its value.
- Set the valve temperature.

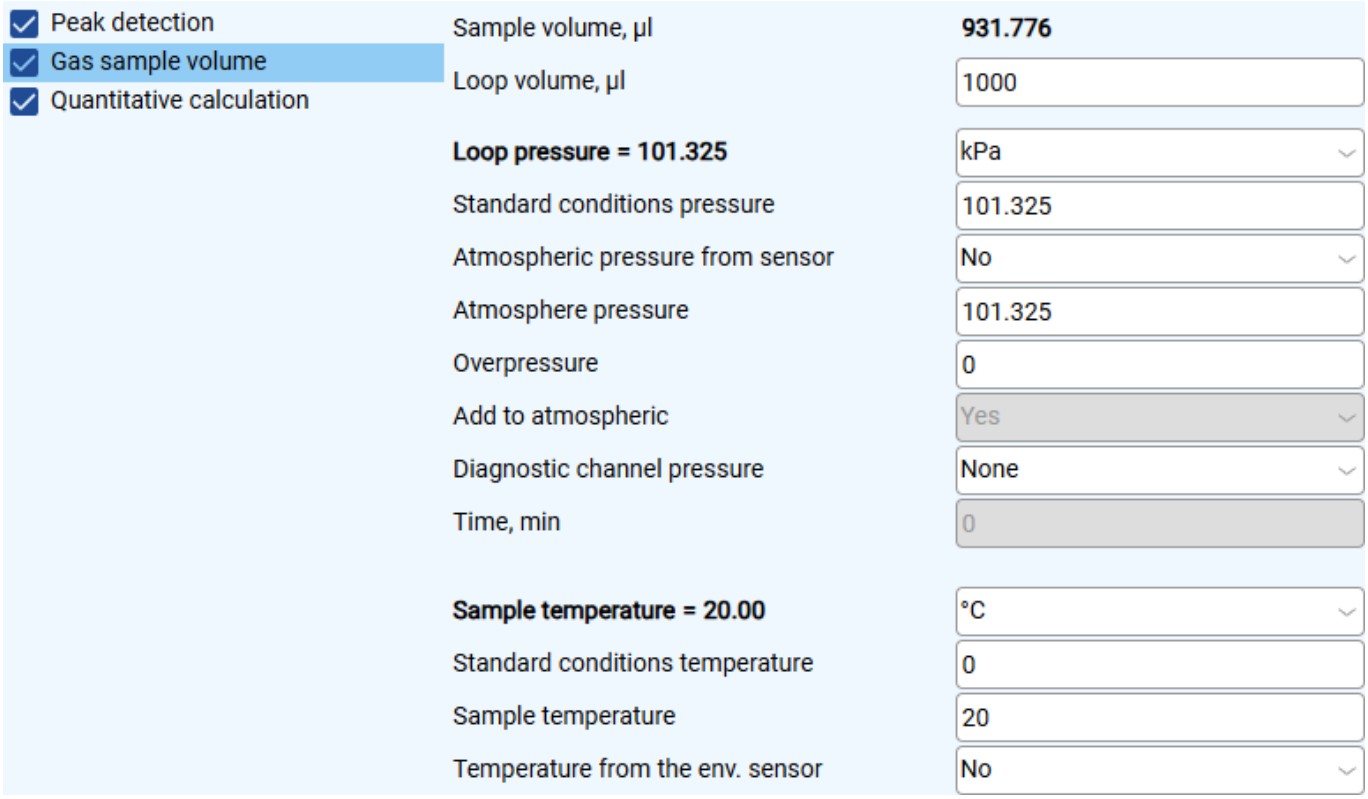


Fig 3.25 – Process settings "Gas sample volume"

3.7.6 Air correction

The process subtracts air from the sample using the formula:

$O_2^* = O_2 - O_2 = 0$

$N_2^* = N_2 - (A/B) \cdot O_2$

Where:

O_2, N_2 – oxygen and nitrogen, respectively, before correction,

O_2^*, N_2^* – oxygen and nitrogen, respectively, after correction,

A, B – coupling coefficient.

If the calculation results in a negative nitrogen value, no correction is made.

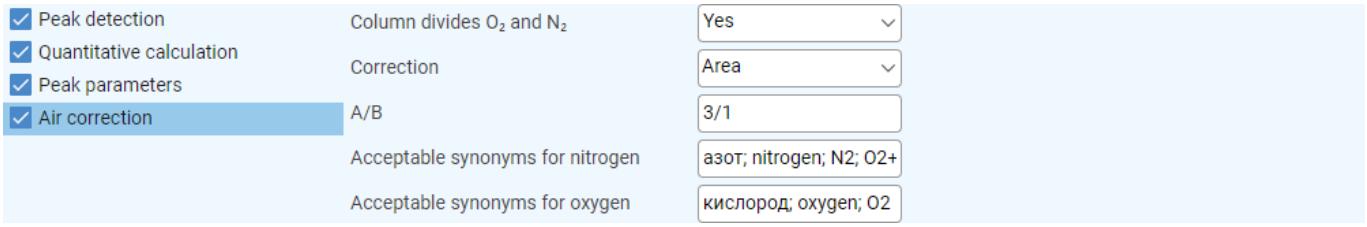


Fig 3.26 – Process settings "Air correction"

3.8 Custom formulas

Chromatec Analytic 4 allows you to create custom formulas.

In the formulas, you can:

- use any specified and calculated chromatogram data,
- enter additional parameters, for example, any constants from regulatory documents,
- use data filters, for example, to create a selection based on certain component names,
- use cycles, for example, to sum up areas or concentrations in preliminary calculations,
- use conditions for a number to get into the range,
- convert numbers to strings,
- debug formulas, i.e. get the values of variables at various stages of calculations,
- you can create 10 custom formulas and show their result in a report.
- In formulas, 10 additional user-defined numbers can be used to enter data that is not provided for in Chromatec Analytic 4.
- import and export formulas for insertion into other methods, sending by mail, etc.

Formulas in Chromatec Analytic 4 are configured using a graphical interface.

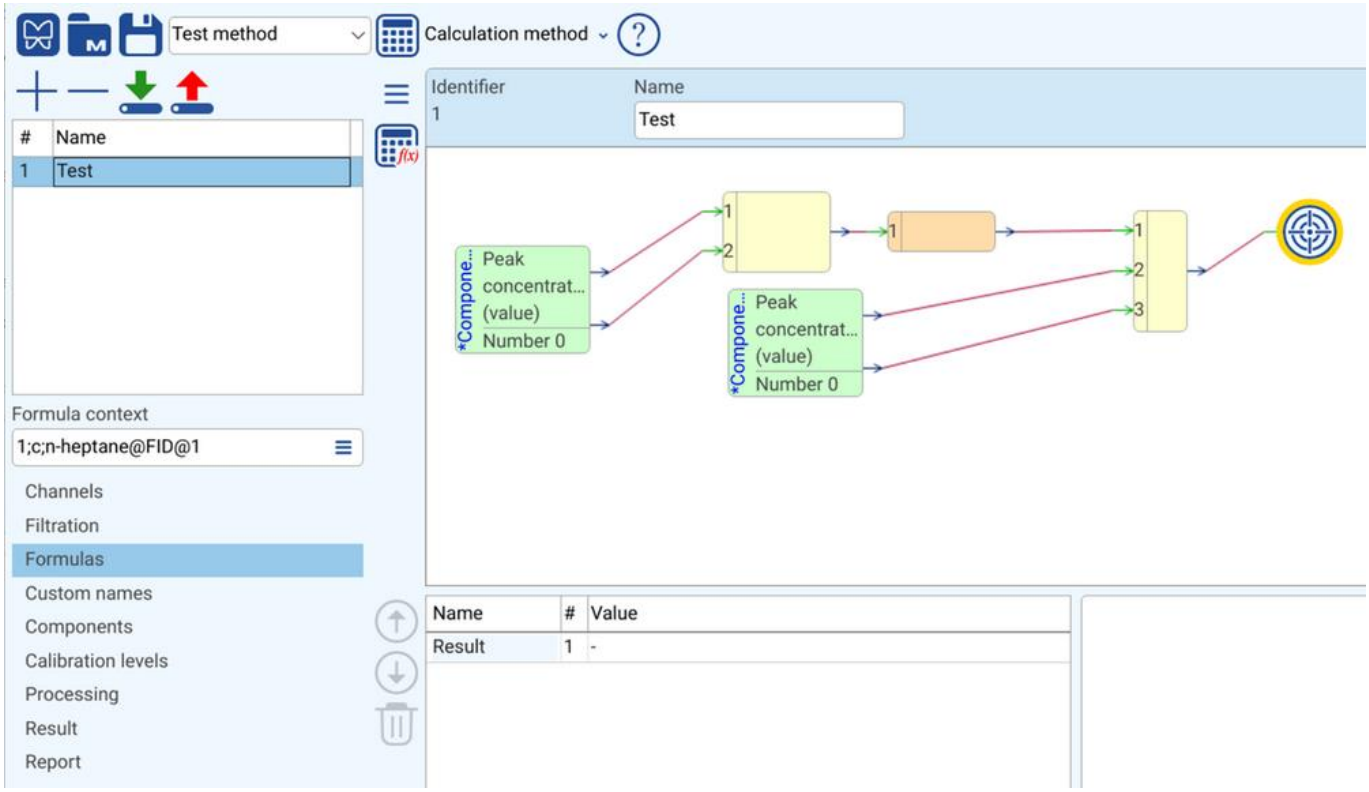


Fig 3.27 – User Formula Editor

3.8.1 Examples of formulas

Preparing input data, creating a formula:

{video method_formula1 Formulas}

Multiplication by a coefficient with normalization:

{video method_formula2 Multiplication by a coefficient with normalization }

Individual rounding:

{video method_formula3 Individual rounding }

Concentrations out of range:

{video method_formula4 Concentrations out of range }

3.8.2 Mathematical functions in formulas

You can use functions in formulas. In the table below, in1 is the first input of the formula, in2 is the second input of the formula

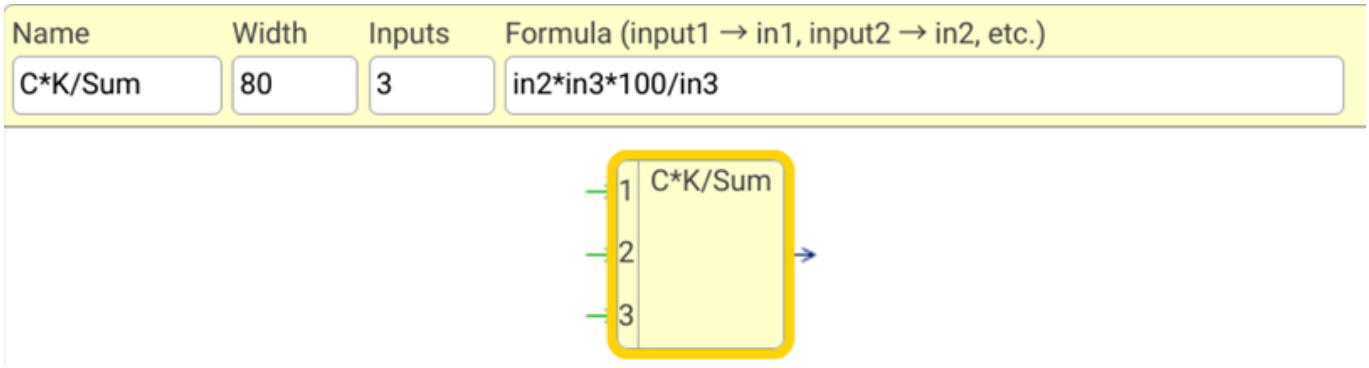


Fig 3.28 – Formula

You can specify a name for the formula and other auxiliary blocks. It is necessary only for the convenience of visualization. If there are many formulas, then you will see what each one does. You can enter any text in the title.

Function	**As set in the formula editor**
$in1^2$	in1*in1 or in1^2
$in1^{in2}$	in1^in2
$\sqrt{in1}$	in1^0.5

$\|in - in2\|$	abs(in1-in2)
$\ln in1$	ln(in1)
$\log in1$	log(in1)
$\sin in1$	sin(in1)
$\cos in1$	cos(in1)
$\mathrm{tg}\, in1$	tg(in1)
$\mathrm{ctg}\, in1$	ctg(in1)
Special functions:	
Find out the sign of a number	sign(in1) – returns -1 or 1
Rounding to a specified number of characters	round(in1;n) – here n is the number of characters
Rounding to a given number of significant digits	roundmean(in1;n) – here n is the number of digits

3.8.3 Debugging formulas

To debug a formula, it is convenient to put any component in the context so that you can immediately see how the calculations are going.

For this:

- Click on the "Formula Context" field.
- Select the chromatogram and the component from which the data will be taken for operational debugging.
- Click "Apply".

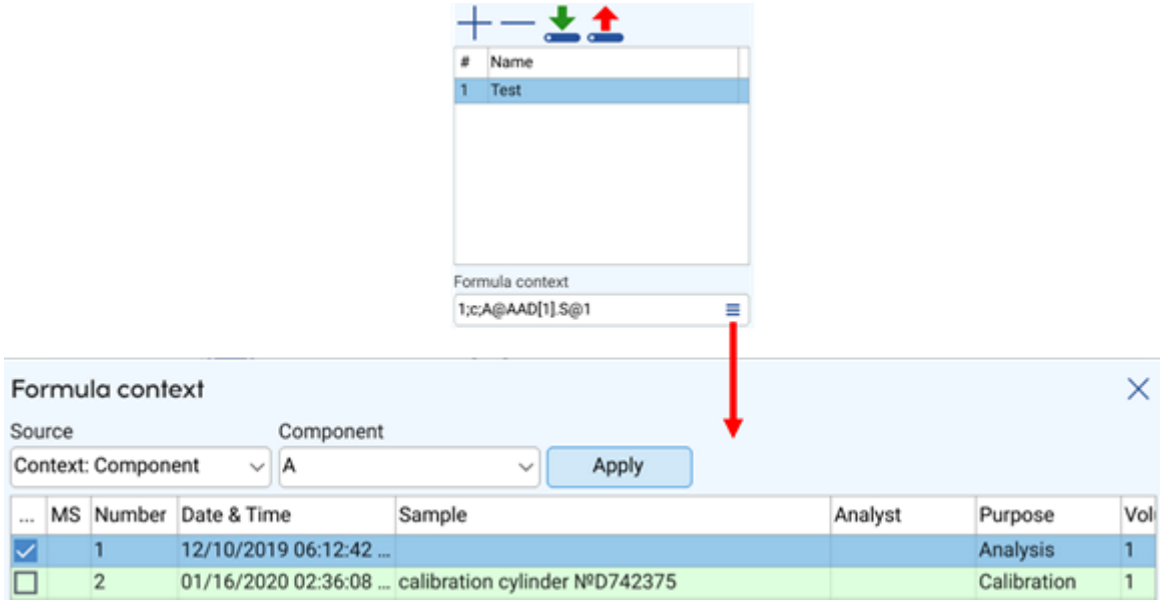


Fig 3.29 – Setting the context of the formula for debugging

To view the result of intermediate calculations for a block:

- Right-click on this block and select the menu item "Add output to view..."

Click on the calculation button using the formula.

- The result will be shown in the table under the formula editor (see the picture below).

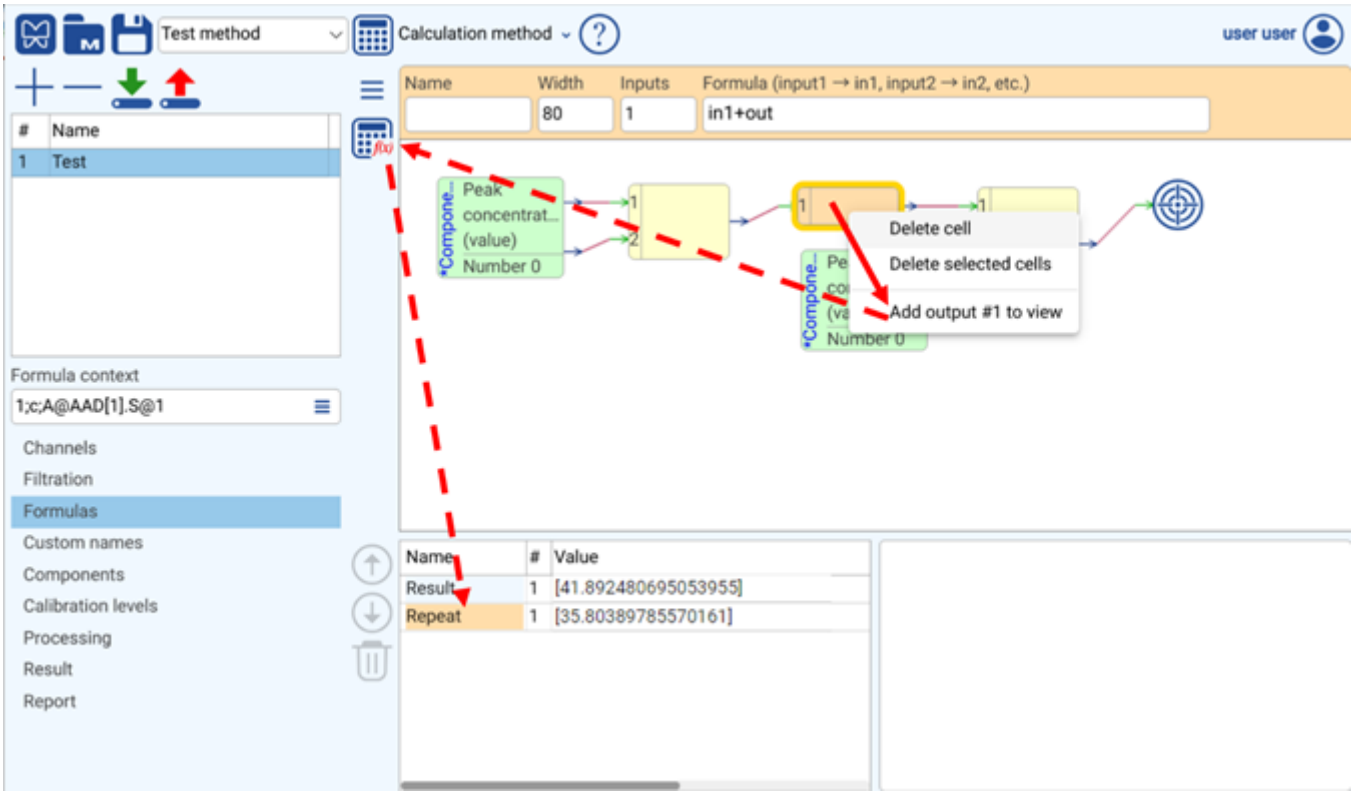


Fig 3.30 – Viewing the results of intermediate calculations

After setting up the user's formulas, you need to:

- Select the customized formulas on the Components page in the columns "Formula 0, Formula 1 ...". To do this, you need to enable the display of hidden columns.
- On the "Processing" tab, add the "Calculation of user formulas" process to the queue.

3.9 Report

To configure the report, go to the corresponding tab on the sidebar of the method.

In the right part of the window there is a preview of the future report. It is rebuilt when any parameter of the report is changed.

The preview is formed on the basis of chromatograms added to the method. During the analysis, the report will be based on the selected batch of chromatograms.

In the left part of the report settings dialog there is a list of sections with parameter settings.

Sections are collapsible blocks, inside which the parameters of the sections are located. You can change the order of sections by dragging them with the mouse. The same can be done for some parameters – those that are responsible for displaying columns in tables.

{video method_report_settings Report settings}

3.9.1 Report Templates

The report template in Chromatec Analytic 4 is a set of sections selected by the user. In most tasks, one template is enough, but the method can contain an unlimited number of them.

The video shows how to create and use templates using the example of setting up a checkout report.

{video analytic_checkout Checkout}

3.9.2 Main settings

Report formats. You can generate a report in several formats at the same time:

- PDF
- HTML
- CSV
- TXT
- XLSX
- JSON
- A4R. Service format. It preserves the intermediate report structure from which the formats in the list above are created.
- TEST. Service format. Used by developers to create test data.

Template XLSX. The option is available if XLSX is selected in the report format list. Clicking on the parameter row will open a dialog (see figure below). Here you can upload a *.xlsx file that will serve as a template. With the template, you can completely customize the look and feel of the report to your requirements.

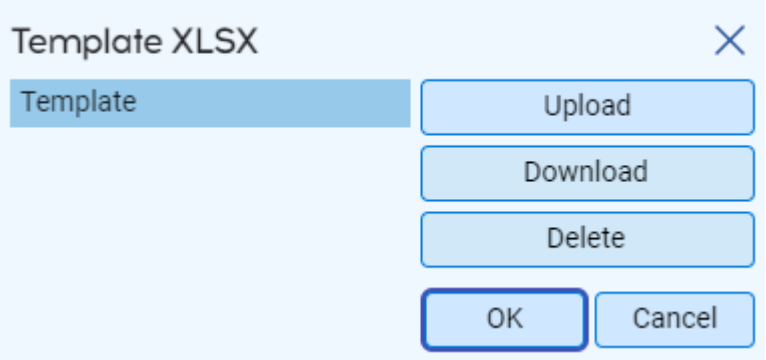


Fig 3.31 – XSLX template upload and selection

Base font size, pt. Set the font height in tables and text blocks. The font height of the headings is automatically set relative to the base.

Font family. You can choose the font:

- Sans Serif. Sans-serif font.
- Serif. Serif font.
- Monospace. Monospaced font.
- Chinese. Chinese font (for Chinese localization of the interface and report).

PDF: Page orientation. Portrait or landscape. PDF only.

PDF: Page margins, cm. Set the margins values in centimeters. PDF only.

PDF: Header left, Header right, Footer left. Only for PDF. You can set any permanent text in the headers and footers. The page numbering is displayed in the lower right footer.

If you want the header and footer to not appear on the first page, add 2+ at the beginning of the footer text

Show thousands separator. For large numbers, a space is added between the digits. For example: 123456789 → 123 456 789.

Group components for app. calcs. If this option is enabled, the components will be combined into the specified groups in special calculations.

Calculation of averages. Ignore null values. Enabling this option allows you to ignore zeros when calculating the arithmetic mean *in some calculations*.

Display null components in the report. Enabling this option allows you to display in the report components whose concentration is zero *for some calculations*.

Show time in UTC. If the date and time are displayed somewhere in the report, then after the main title there will be information about the time zone. The time in the report will be shown according to this setting. For example, if the value of the parameter = "No", then the report will include the message: "The time in the report is indicated in the UTC (+03:00)."

Measurement history (Trend). Enabling this option will allow you to save the results of some calculations for later viewing on a special chart – trend.

3.9.3 Header and signature

You can customize the title and signature of the report. Layout customization options:

- You can use HTML tags to implement complex layout.
- You can insert images.


The layout can be created in an XLSX file (using MS Excel or its equivalent) and imported.

{video method_report_header_layout Report header layout}

You can use variables:

- **#title**. Inserts the word "Report" into the layout.
- **#analyst**. Inserts the operator's last name into the layout.
- **#date**. Inserts the report creation date into the layout
- **#qrcode**. Inserts a QR code into the layout.
- **#qrfit**. Sets the size of the QR code.

To insert a QR code, add the text #qrcode=Some text in the desired place on the layout.

For example, the following code will create a link to the SKB Chromatek website:

#qrcode=https://chromatec.ru

This QR code only supports Latin script and numbers!

By default, the QR code will be placed in a square with a side of 100px. To change the size, write anywhere in the layout: #qrfit=Number. For example, #qrfit=150.

You can save the layout on your computer as a JSON file and load it from the saved file in the settings of another method.

3.9.4 Sample info

Specify whether to display this section from a new page.

If necessary, you can hide the section header.

By default, matching rows are grouped in the sample info data table. You can turn off grouping.

Mark the data of the chromatogram sample info to be shown in the report. For numeric values, adjust the rounding format.

3.9.5 Instrument method

This section is a description of the chromatograph instrumental method with which this analysis was obtained. The instrument method is taken from the first chromatogram in the selected group.

Specify whether to display this section from a new page.

If necessary, you can hide the section header.

3.9.6 Input data

When this section is included, a table of calculated concentrations of components, as well as their average values, will be added to the report.

You can enable the option to check the composition for homogenety. The composition is homogeneous if the same components are present on all selected chromatograms.

The section is most often used in conjunction with special calculations.

3.9.7 Components

This section displays a table of components in the report.

Calculation results and input data can be shown here (for example, a given time, function, multiplier).

Section Parameters:

Control of concentration limits. If the option is enabled, the result of the concentration calculation will be compared with the boundary values (minimum-maximum), which you can set in the table of components in the method. If the calculated value is outside the specified boundaries, then the report will display not it, but the result in the form of ">X.XXX" or "<X.XXX". In this case, the result is highlighted in red italics.

Filter. The option specifies which components to display in the report. By default, only identified peaks are displayed (i.e. peaks with a name).

Sorting. The option specifies how the components in the table will be sorted. By default, components are sorted first by ordinal number, then by retention index, then by retention time.

Grouping by chromatograms. Sets the style of the final table – vertical or horizontal display of data from multiple chromatograms:

Component	Average time, min	Concentration									Unit	Detector
		#13	#14	#15	#16	#17	#18	#19	#20	#21		
acetaldehyde	4.321	0.011	0.011	0.011	0.001	0.001	0.001	0.005	0.005	0.005	мг/дм3	ПИД-1
methylacetate	4.899	0.010	0.010	0.010	0.001	0.002	0.001	0.005	0.005	0.005	мг/дм3	ПИД-1
ethylacetate	5.352	0.010	0.010	0.010	0.001	0.001	0.002	0.005	0.005	0.005	мг/дм3	ПИД-1

Fig 3.32 – Horizontal grouping of results

Component	Average time, min	Concentration	Unit	Detector
acetaldehyde	4.321	0.011	мг/дм3	ПИД-1
		0.011	мг/дм3	ПИД-1
		0.011	мг/дм3	ПИД-1
		0.001	мг/дм3	ПИД-1
		0.001	мг/дм3	ПИД-1
		0.001	мг/дм3	ПИД-1
		0.005	мг/дм3	ПИД-1
		0.005	мг/дм3	ПИД-1
		0.005	мг/дм3	ПИД-1
methylacetate	4.899	0.010	мг/дм3	ПИД-1
		0.010	мг/дм3	ПИД-1
		0.010	мг/дм3	ПИД-1
		0.001	мг/дм3	ПИД-1
		0.002	мг/дм3	ПИД-1
		0.001	мг/дм3	ПИД-1
		0.005	мг/дм3	ПИД-1
		0.005	мг/дм3	ПИД-1
		0.005	мг/дм3	ПИД-1

Fig 3.33 – Vertical grouping of results

Next, a list of available parameters is displayed in the section. Check the boxes that you want to show in the report.

For some parameters, you can show totals (sum) and set the rounding format.

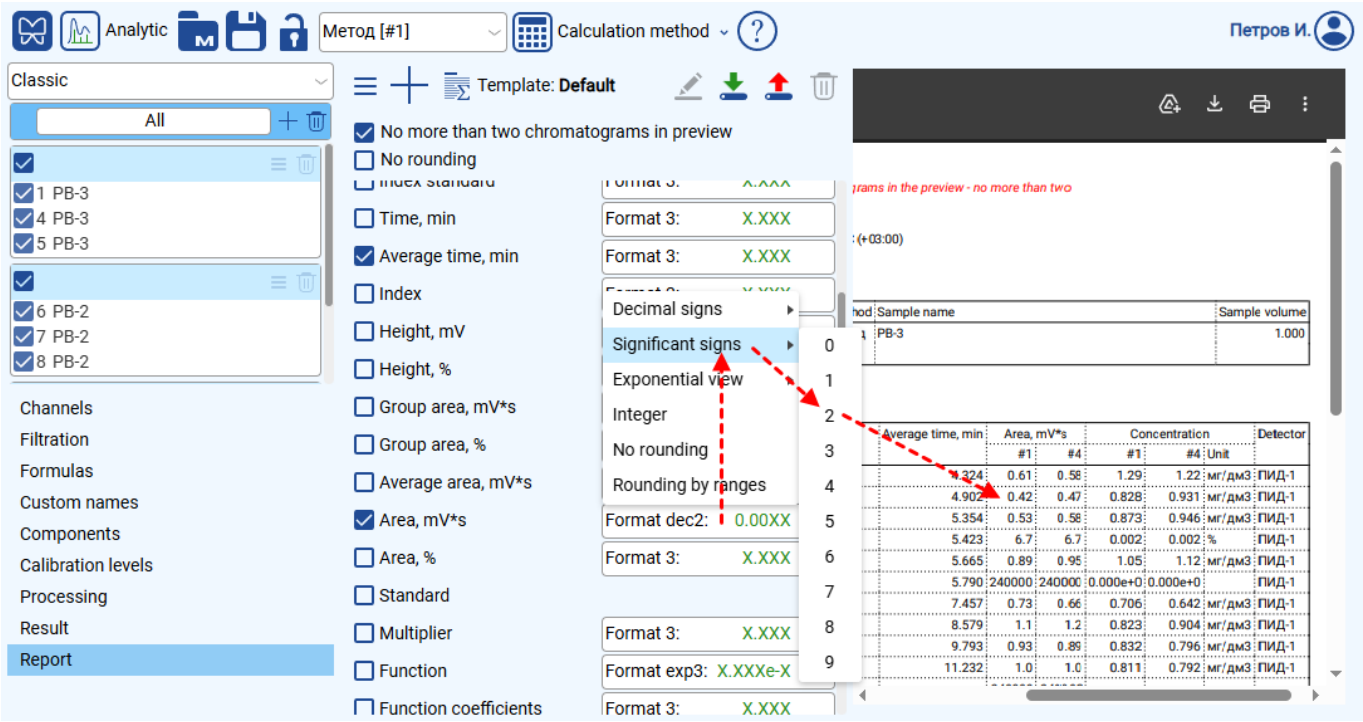


Fig 3.34 – Setting rounding

In addition to simple rounding, you can also set rounding depending on the range of the value the rounded value falls into, for example, concentration.

To do this, in the corresponding menu (picture above), select “Rounding by ranges”. In the dialog that appears, set the ranges of values and the rounding method for each:

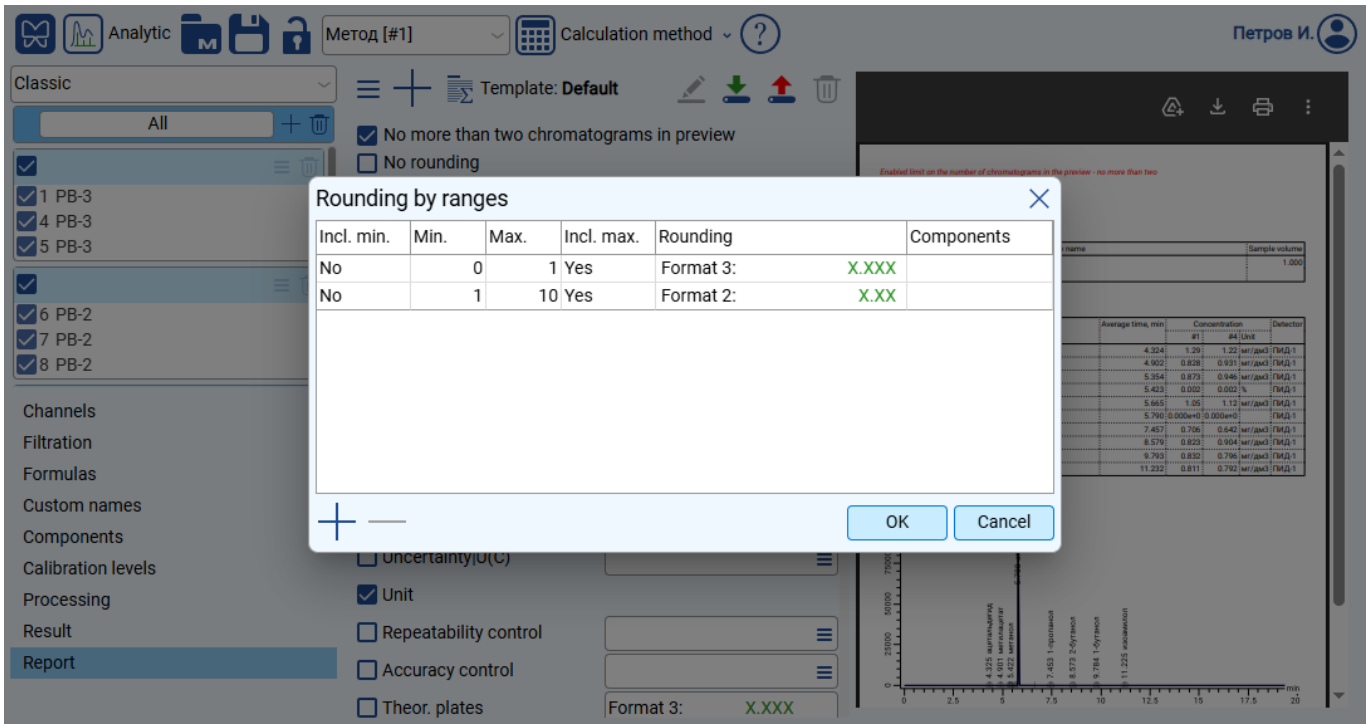


Fig 3.35 – Rounding by ranges

Uncertainty. Some regulations require that an error or uncertainty be attributed to the average result, calculated using simple linear or exponential equations. For this calculation, you can use preset settings by selecting a regulatory document from the list, or create your own if your regulatory document is not in the list. See video below:

{video method_report_uncertainty Uncertainty}

Convergence control. This parameter allows you to calculate the acceptability of convergence (repeatability) and supplement the table of components with the corresponding data. If necessary, you can also display the settings of this calculation in the report.

The standard is given by a simple linear or exponential equation.

You can use preset settings by selecting a regulatory document from the list, or create your own if your regulatory document is not in the list.

{video method_report_repeatability Repeatability}

Accuracy control. The setting type is similar to “Convergence control”. Designed to assess the deviation of the calculated value of the component concentration from the specified (certified) value. To perform such an assessment, concentrations must be specified in the chromatogram sample info.

3.9.8 Calibration

This section displays the calibration of each component in the report.

Section parameters:

Calibration control. Clicking on a parameter will open a dialog where you can select the method of calibration control:

- By relative standard deviation, %
- By R^2
- By accuracy, %

You can add control values for each component individually or for several at once (in this case, leave the "Component" field empty).

These settings can be exported to a file...

...and import from file.

If calibration control is specified, its result can be used in the "Scheduler" for automatically collecting calibration and assessing its acceptability.

In addition to this section, some Application Calculations can evaluate the acceptability of calibration.

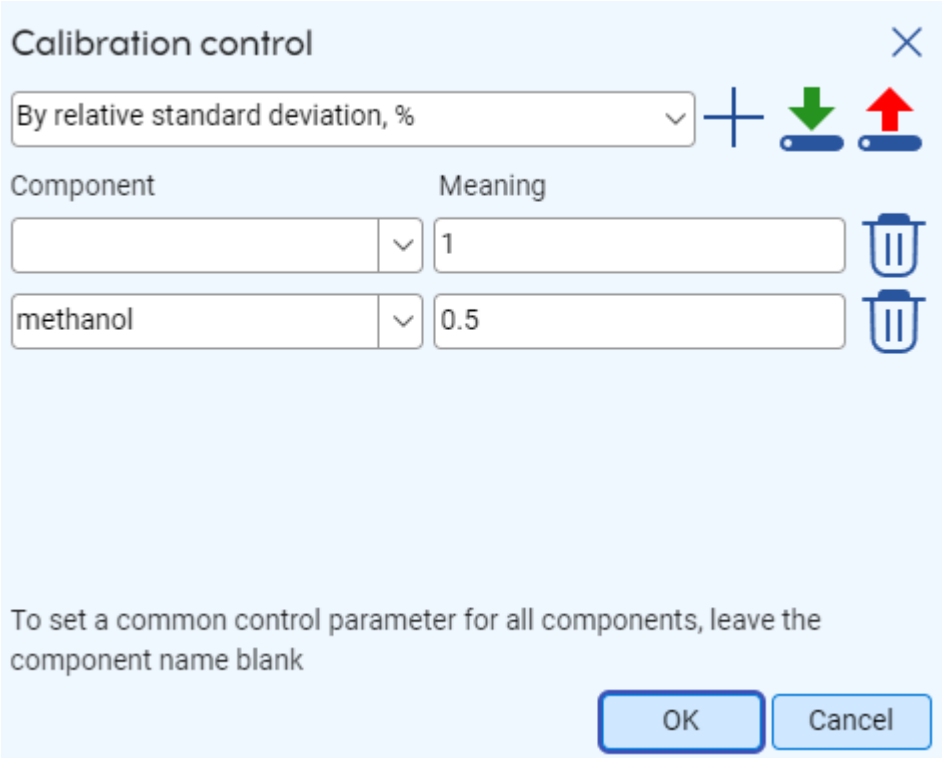


Fig 3.36 – Calibration control settings

Next, specify which columns you want to display in the table, set the size of the graph in centimeters.

To correctly display large tables, you can specify which of them should be moved to the next page of the report.

#	Amount (Q)	Area (S), mV*s	Accuracy, %	Calibration chart
1	1.030	0.609	25.247	
4	1.030	0.577	18.691	
5	1.030	0.482	0.853	
6	4.800	2.338	3.233	
7	4.800	2.226	1.710	
8	4.800	2.254	0.458	
9	9.500	4.514	0.693	
10	9.500	4.413	1.547	
11	9.500	4.478	0.104	

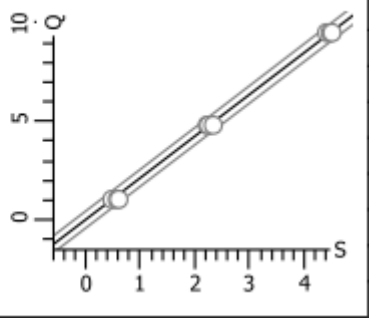


Fig 3.37 – Calibration table in the report

3.9.9 Chromatograms

When this section is included, chromatogram graphs will be added to the report.

Set the height of the graph in centimeters.

Specify which channels to show. By default, all.

Channels will appear in the list if a chromatogram is selected on the left sidebar.

Chromatogram display. This parameter determines the type of graphs. You can display them individually or group them in one image in different colors.

- Each channel.
- Each channel in the range.
- Group by channels.
- Group by chromatograms.

{video method_report_display_chromatograms Report display chromatograms}

Divide into sections, min. If there are many peaks on the chromatogram and they merge, you can **divide** the graph into several parts (they will be located one under the other). Specify the duration of the section in minutes. The parameter is available if the display type is selected – "Each channel".

Range start, min.

Range end, min

These parameters allow you to explicitly specify which part of the chromatogram should be displayed in the report. They are available if the "Each Channel" or "Each Channel in Range" display type is selected".

No, the highest peak. If this option is enabled, the scale will be set for the graph to fully display the **second-highest peak vertically**. It is convenient to enable this parameter to ignore the solvent, usually the highest peak, because of which micro-impurities are not visible.

3.9.10 Audit trail

This section displays a table with the history of chromatogram changes in the report.

The section is added automatically if chromatogram auditing is active.

It can also be added manually as a application calculation. However, if chromatogram auditing is disabled, then adding a section is pointless, it will be empty.

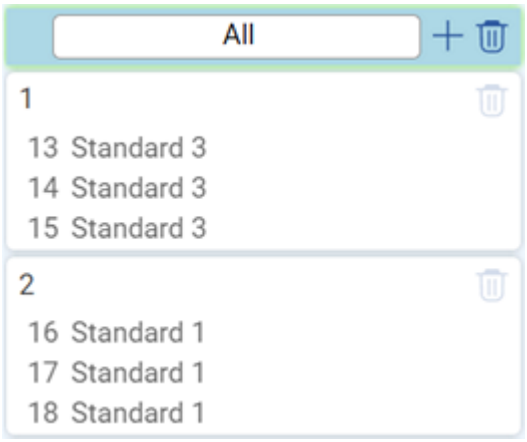
3.9.11 Auto report at the end of the analysis

In order to automatically create a report at the end of the analysis, it is necessary to use the Group report in the "Sequence".

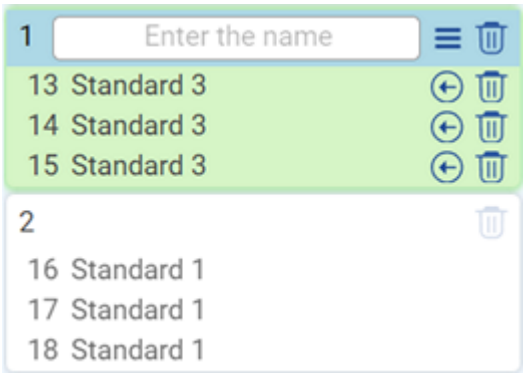
3.10 Calculation

After setting and editing any method parameters (component parameters, processing parameters), the changes should be applied. To do this, click on the "**Calculation method**" button on the upper toolbar.

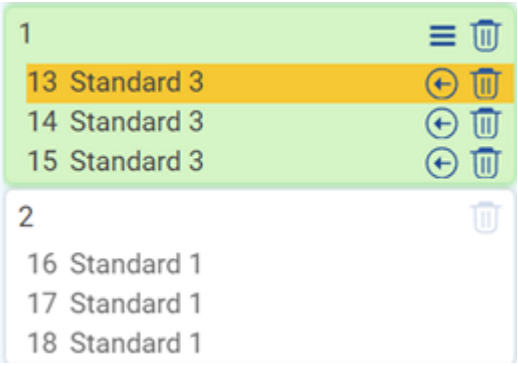
Depending on what is selected on the left sidebar, the calculation will be performed for one or more chromatograms:



All calibration levels are selected.
When performing the calculation, the data in all chromatograms included in the calibration will be recalculated.



The calibration level is selected
When performing the calculation, the data will be recalculated only in those chromatograms that are included in the selected calibration level.



The calibration point is selected.
When performing the calculation, the data will be recalculated only in the selected chromatogram (the chromatogram corresponds to the calibration point).

4 ANALYSIS PROCESSING

You can evaluate the result of the current analysis on the sidebar tab of the same name. When working with multiple chromatograms, use the "Batch Overview" tab.

4.1 Performing analyses

 Set up the sequence of analyses in the Scheduler.

 Run the sequence for execution.

If the sample is injected manually:

- If **preprun** is used, wait for the chromatograph to enter the "Waiting" stage. The device will perform a **preprun**.
- Wait for the chromatograph to reach the "Ready" stage.
- Inject the sample and press the "START" button on the chromatograph.

If the sample is injected by an automatic sampler, the operator is only required to wait for the end of the sequence and begin processing.

4.1.1 General analysis

If you need to take into account the undetectable components, perform actions:

- Add an undetectable component to the method.
- Set the undetectable component concentration in the chromatogram sample info.

{video analysis_general Analysis}

4.1.2 Analysis with an internal standard

If you conduct a quantitative calculation by the internal standard, perform actions:

- Set the links to internal standards in the method.
- Set the internal standard concentration in the chromatogram sample info.

{video analysis_istd ISTD}

4.1.3 Identification

If the retention times of the components have changed on the chromatogram (for example, the operator pressed the "Start" button a little earlier or vice versa later when injecting the sample), the peaks may be unidentified or incorrectly identified. In such situations, it is often impractical to adjust the method. Chromatec Analytic allows you to adjust the times directly in the current chromatogram without changing the method

{video analytic_identification Identification}

4.2 Process parameters

As in the method editor, the “Processing” tab is available in the chromatogram window. However, here the contents of this tab are read-only; process parameters cannot be changed.

In some cases, such as incorrect identification, it may be necessary to adjust the method based on the current chromatogram.

The best thing to do in such a situation is to create a new method!

If creating a new method is currently impossible, for example, there are no calibration mixtures, then the method can be adjusted based on the current chromatogram.

To do this, you need to unlock the processes in the chromatogram. When you click on the corresponding button (in the "Processing" tab), a dialog will appear:

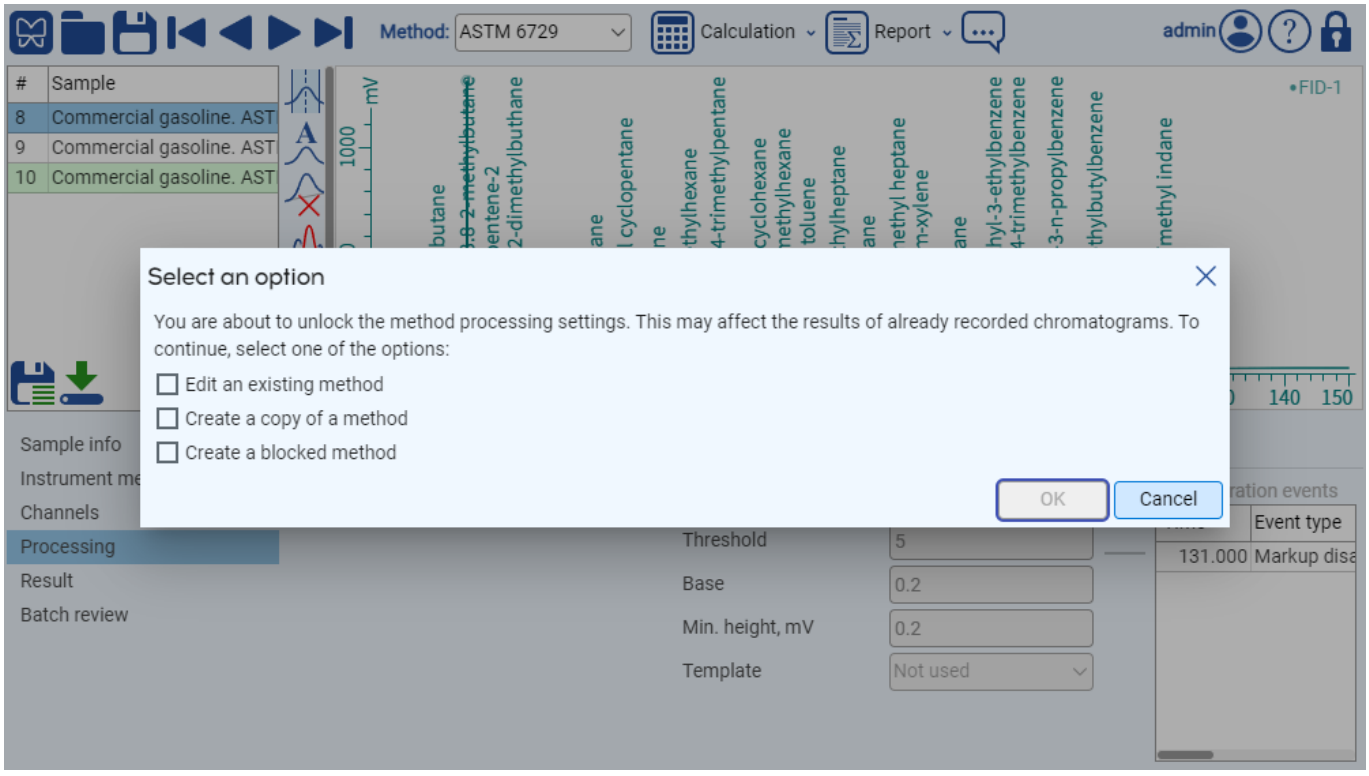


Fig 4.1 – Unlocking processes in the chromatogram

- **Edit an existing method**. You will make changes directly to the method currently applied to the chromatogram. The danger here is that old chromatograms may then produce incorrect results.
- **Create a copy of the method**. The safest and recommended option for making changes.
- **Create a blocked method**. Option to adjust retention parameters based on the current chromatogram. In this case, it will not be possible to change the calibration points in the resulting locked method.

4.3 Batch review

This page provides detailed information on the selected batch.

Two viewing options are available:

- Batch review – applicable for any tasks.
- Batch review V2 – first of all, is focused on working with MSD, but some functions will be convenient for any other tasks.

{video analytic_batch_review Batch review}

4.3.1 Summary table of results

The summary table includes the results of processing all chromatograms of this batch and can be displayed in one of two types:


Line of components – each row of the table corresponds to the chromatogram of the batch. The components are distributed horizontally to the right.


Chromatogram line – each row corresponds to a component. Chromatograms are distributed horizontally to the right.

With a sufficiently large number of chromatograms in the batch and components in the chromatograms, the table, regardless of the chosen style, occupies a significant space in width, which makes it difficult to quickly evaluate the results by any parameter, such as concentration or peak area.

To overcome this disadvantage, you can **click the middle mouse button** on the selected column. In this case, the table will be reduced – only columns with the selected parameters will remain in it. You can also switch to the full view with the middle mouse button.

4.3.2 Results in the summary table

Average and RSD%


In order to display in the summary table the average value of a parameter, or its standard deviation, switch the view to the "line of components".

- Right-click on the column with the parameters of interest.
- Select the "Totals" item (for example, for an area, this item will be called "Area" Totals).
- Select the type of summary data – "Average" or "RSD%".

- The selected parameter will appear at the bottom of the table.

Sum, minimum and maximum


n order to display in the summary table the sum of the values of any parameter within the chromatogram, switch the view to the "chromatogram line".

- Right-click on the column with the parameters of interest.
- Select the "Totals" item (for example, for an area, this item will be called "Area": Totals).
- Select the type of totals – "Sum", "Min" or "Max".
- The selected parameter will appear at the bottom of the table.

{video analytic_batch_review_totals batch review totals}

4.3.3 Chromatogram grid

At the top of the batch Overview page there is a grid of chromatograms. Here you can see the same area on each of the chromatograms of the group corresponding to the component selected in the summary table.

You can change the display of peaks using the buttons on the left sidebar.


Switch the view to "Individual Scale". When this button is pressed, the chromatogram peaks corresponding to the selected component will be displayed in maximum magnification.


Switch the view to "General Scale". When this button is pressed, the chromatogram peaks corresponding to the selected component will be displayed on a single scale for all. This view helps to estimate the change in the size of the peaks of the same component on different charts.

4.3.4 Batch review V2

An alternative to the group's review is available on this page, providing advanced information when working with MSD.

Here in the upper part of the window are located:

- A plot of chromatograms with a peak selected in the table.
- chromatogram of confirming ions for the selected component.
- Graduate schedule of the selected component.


If desired, you can enable the display of the peak of the internal standard for the selected component and its confirming ions.


If desired, you can enable the display of the spectrum for the highlighted peak.

For a pivot table of results, you can also switch the type – components line/chromatograms line.

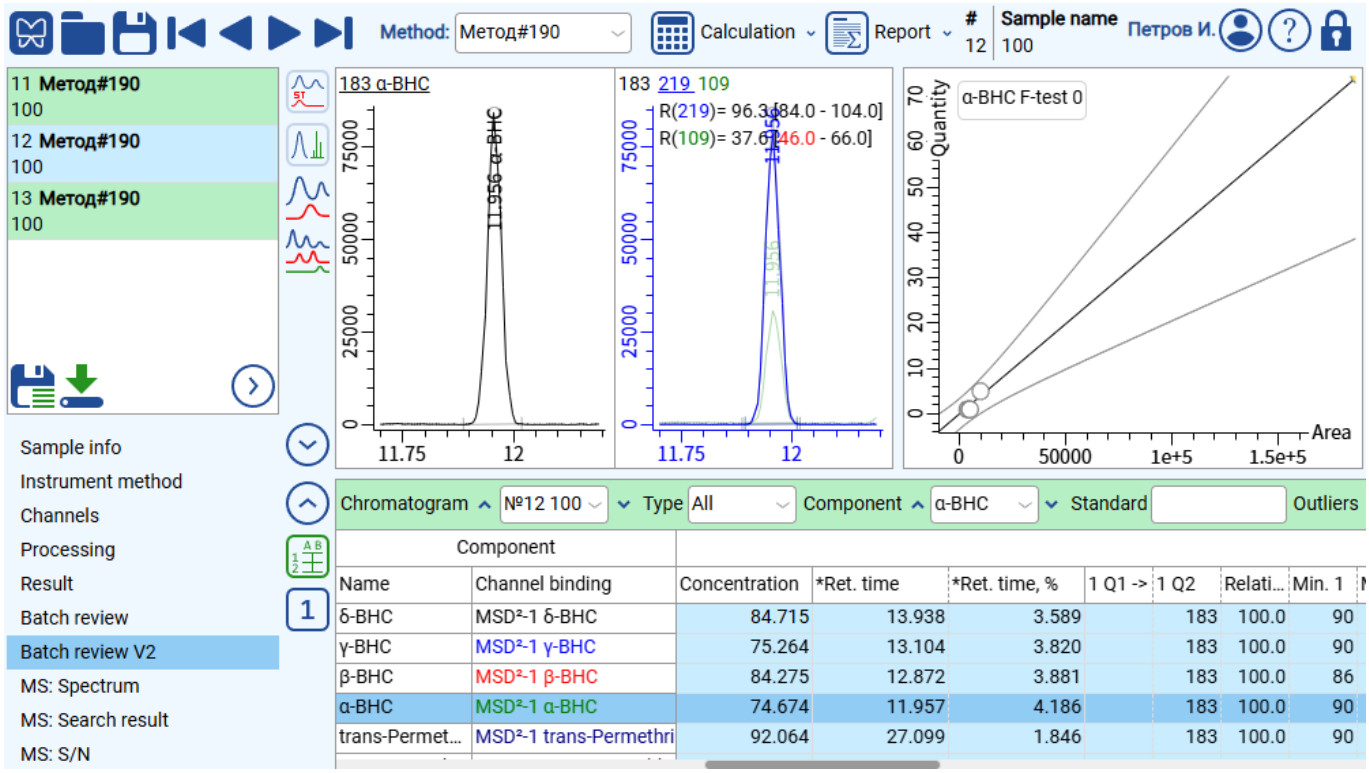


Fig. 4.2 – Batch review V2

Above the summary table is a filter table. Using it, you can choose a chromatogram, component, purpose (all or only calibration). When choosing a filter, only lines and columns corresponding to it will remain in the table.



Fig. 4.3 – The filter of the pivot table

You can also use flags for filtering records according to the criterion of the attitude of ions:

 Turn off outlier filter.

 Display rows that have High/Low outliers.

 Display rows that have High outliers.

 Display rows that have Low outliers.

 Display rows that have no outliers.

4.4 Batch processing

{video analytic_batch_processing Batch processing}

4.5 Qualitative mass spectrometric analysis

The built-in module for qualitative analysis of mass spectrometric data allows:

- search for peaks on the chromatogram in automatic and manual mode;
- subtract the noise signal from the mass spectrum (henceforth – the spectrum) in automatic and manual mode in order to improve the quality of identification;
- identify the spectra obtained by the spectral libraries;
- identify the spectra obtained by the spectral libraries;
- perform MSD calibration – determine the signal-to-noise ratio.

Before you begin working with MS data, install the NIST library and configure library search options.

4.5.1 Working with spectrum

Go to the **MSD:Spectrum** tab. "Chromatec Analytic" workspace is divided into two parts – the chromatogram and spectrum. The spectrum is displayed for the chromatogram point where the marker is located.

The spectrum is displayed for the chromatogram point where the marker is located. On this page, the marker can be set with a simple click in the desired place of the chromatogram.

To obtain a more accurate spectrum, it is recommended to average the spectra of several neighboring points. To do this, use a long press of the left mouse button (more than 0.5 seconds). Such a click causes a marker and allows, without releasing the left mouse button, to select the area in which all the spectra will be averaged. The averaged spectrum will be displayed in the spectrum window.

{video analytic_ms_spectrum Spectrum}

4.5.2 Performing a manual search

Manual search is different from automatic search in that peak search and background subtraction are done manually by the user.

- Place the cursor on the vertex of the peak of interest or select several neighboring points of the top to obtain an averaged spectrum. Averaging gives a more accurate spectrum.
- Right-click and select **Background subtraction** in the context menu.
- Select a section of the chromatogram for background subtraction. This can be done using the mouse while holding down the **CTRL** key.

Background subtraction is not necessary in order to perform the search, but it allows to improve the quality of the spectrum for subsequent identification

You can subtract the background twice by selecting the interval before the peak and after the peak.

{video analytic_ms_search_manual MS manual search}

4.5.3 Performing an automatic search



Go to the **MSD: Spectrum** or **MSD: Search result** tab. Click the **Auto Search button** on the side toolbar.

{video analytic_ms_search_auto MS autosearch}

On the **MSD: Search result** tabs are:

- **Table with retention times and names of detected substances**. To select the peak, you can use both the retention timetable and the chromatogram graph. To do this, it is necessary to select the corresponding peak on the chromatogram. When you hover the cursor over the peak marker, the cursor changes to ↑, after that the line with retention time can be selected by pressing the left mouse button. If a peak is selected on the chromatogram, it is selected in the peak table, and vice versa. If the peak is marked on the current chromatogram, it is sufficient to select the peak itself with the mouse.
- **Table of candidates for each peak**. Each peak has its own candidate table, which is displayed on the screen when choosing a peak.
- **Peak spectrum** (**Obtained spectrum**) and candidate spectrum (**Library spectrum**) placed one above the other for the convenience of visual comparison. Each candidate has its own library spectrum, which is displayed when choosing this candidate.


With this button you can delete the selected search results. Also, selected results can be removed from the list using **CTRL + DELETE**.


Using this button you can delete all unselected search results

Results with a probability greater than that specified in the settings (70% by default) are highlighted in green. If the probability is lower than the specified one (30% default) the color is red.

Fields of candidates table:

Show in the report. If this item is selected near a candidate, the name of the candidate will be displayed above the corresponding peak when the display of inscriptions on the chromatogram is turned on.

Title. The library name of the candidate.

Match. A coefficient of coincidence in direct library search.

R.Match. A coefficient of coincidence in the reverse library search.

Probability. The integral value, which considers the coincidence coefficients in the direct and reverse search, and determines whether the spectrum transferred to the library for identification belongs to the candidate.

Library. The name of the library in which the candidate was found.

4.6 Report

4.6.1 Report creation


To create a report click the Report button on the top toolbar. The report will be created according to the settings, specified in the method.

You can create several report templates and select them from the drop-down list by clicking on the arrow to the right of the "Report" button.

See an example of creating and using templates.

4.6.2 Viewing saved reports

Reports are stored on the server in the data folder. Direct access to this folder is not possible for the user and its review is carried out using the appropriate dialog "Chromatec Navigator".


On the Chromatec Navigator desktop, click on the Reports button. The Report viewing page opens. While there are no reports, there are no folders on this page.


Click on the "Set period" button and specify the beginning and end of the time interval. The table will show only those reports whose creation time falls within this period.


Click this button to go to a higher level (to the parent folder).

{video navigator_report_review Report review}

Chromatec Analytic can create and display reports in the following formats:

- PDF
- HTML
- XLSX
- CSV
- TXT
- JSON

Reports in PDF and HTML format can be printed immediately using standard browser tools.

If the recommended report storage size limit is exceeded, a warning is issued:

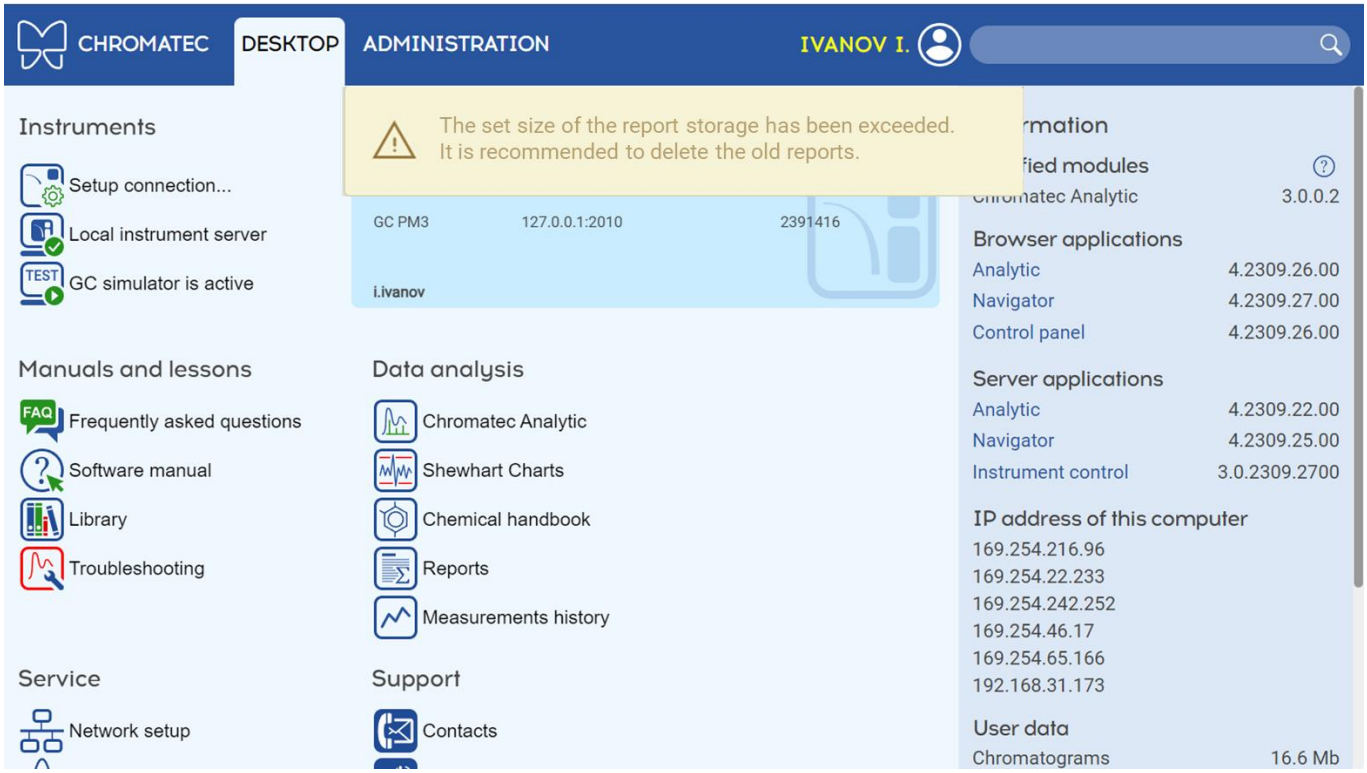


Fig 4.4 – Exceeding the size of the report storage

The report storage size limit is set on the Administration page.

You can download the report to your computer.

If you have the "Delete Data" privilege, you can delete old unnecessary reports.

4.6.3 Reports comparision

You can compare reports in the following formats:

- HTML,
- TXT,
- CSV,
- JSON,
- A4R

In the report overview, select the two you want to compare and click the "Compare reports" in the sidebar button. You can select one report, and after pressing the button you will be asked to select the second one on the disk. The comparison result will open in the window:

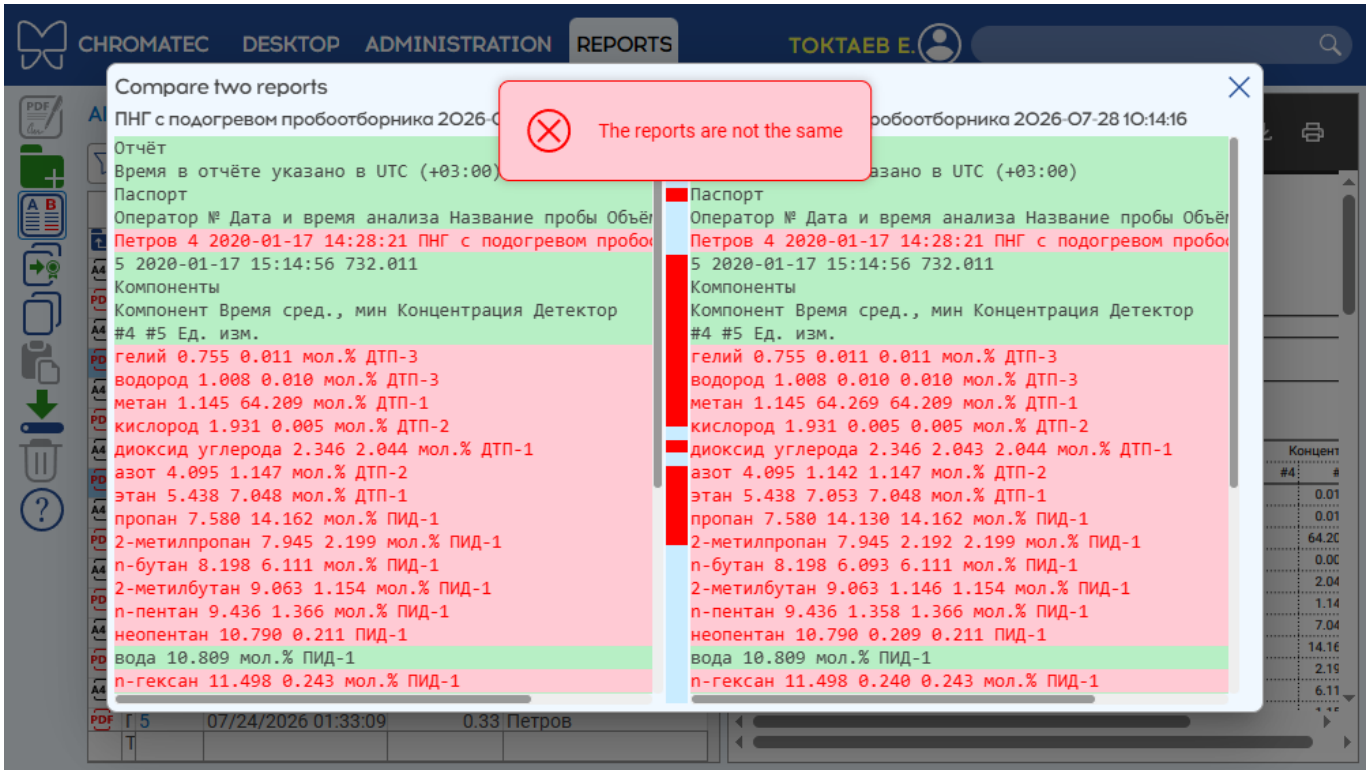


Fig. 4.5 – Result of reports comparision

4.6.4 Digital signature

Reports in PDF format can be digitally signed. With its help, you can protect your report from changes.

A digital signature embedded in a report in PDF format is not qualified. It is based on a self-signed "Chromatec" certificate.