DataApex
Clarity™
CHROMATOGRAPHY SOFTWARE

USER GUIDE

Clarity Software ENG

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Contents

To facilitate the orientation in the **User Guide** manual and **Clarity** chromatography station, different fonts are used throughout the manual. Meanings of these fonts are:

Open File (italics) describes the commands and names of fields in **Clarity**, parameters that can be entered into them or a window or dialog name.
WORK1 (capitals) indicates the name of the file and/or directory.
ACTIVE (capital italics) marks the state of the station or its part.
Chromatogram (blue underlined) marks clickable links referring to related chapters.

The bold text is sometimes also used for important parts of the text and the name of the **Clarity** station. Moreover, some sections are written in format other than normal text. These sections are formatted as follows:

Note: Notifies the reader of relevant information.

Caution: Warns the user of possibly dangerous or very important information.

Marks the problem statement or trouble question.

Description: Presents more detailed information on the problem, describes its causes, etc.

Solution: Marks the response to the question, presents a procedure how to remove it.

1 Installation

Topics covering installation of **Clarity** software, **Colibrick**, **Multicom**, etc. Also the connection between **Clarity** and chromatograph is explained.

1.1 Installing Clarity Software

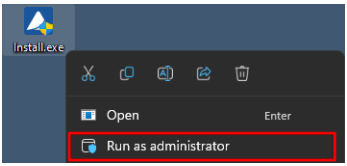
These are the basic steps you have to follow for the First installation of Clarity.

First installation of the software (since version 9.0)

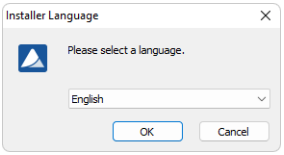
1. Install the software BEFORE connecting any hardware.

   More Info:

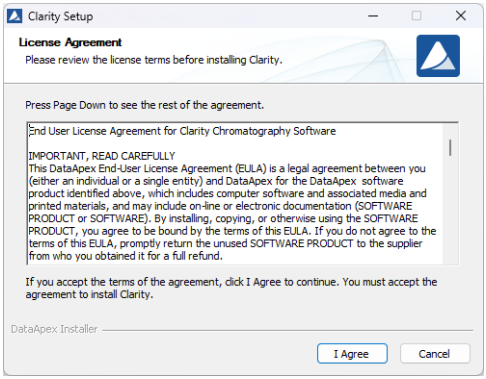
   - The software can be installed by inserting the installation USB and running install.exe or by downloading the installation from the Downloads at our website.
   - On administered systems use „*Run as Administrator*“ from intended User account. Administered systems are managed by an administrator and users using the PC may not have administrator privileges. Insufficient privileges may result in:
     - Clarity not being installed.
     - When installed from Administrator account, the installation directory may be read only for users with limited privileges and the station will be inoperable.



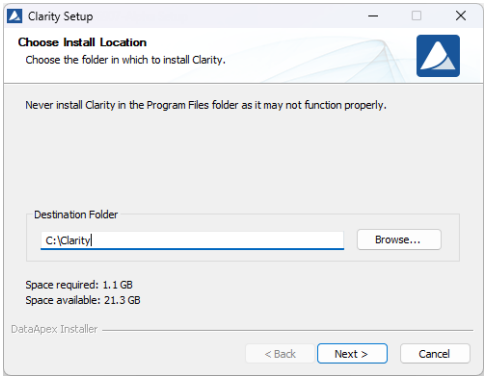
2. Select the language.



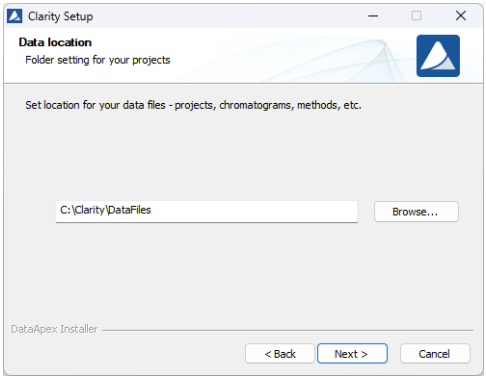
3. Confirm the License Agreement. It is possible to continue only in case you agree with the statement.



4. Choose the destination folder. The user must have Read/Write/Modify access to the installation directory.

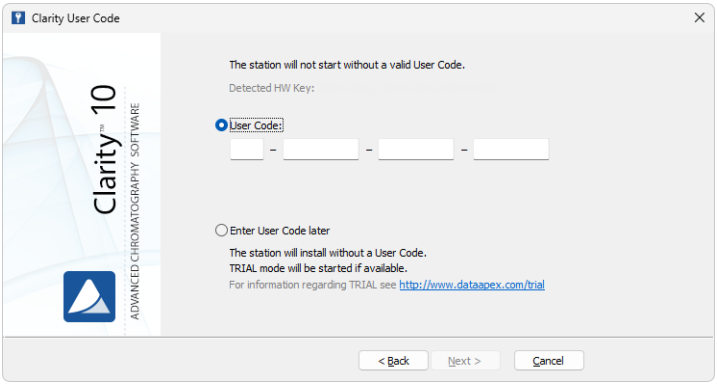


5. Set location for your data files. C:\CLARITY\DataFiles is set by default. Notice that Data location folder name cannot contain following characters / : * ? " < > | and also cannot start or end with a space and cannot end with a dot.



6. Enter the User code corresponding to your hardware key or select *Enter User Code later* to start 30-day Trial.

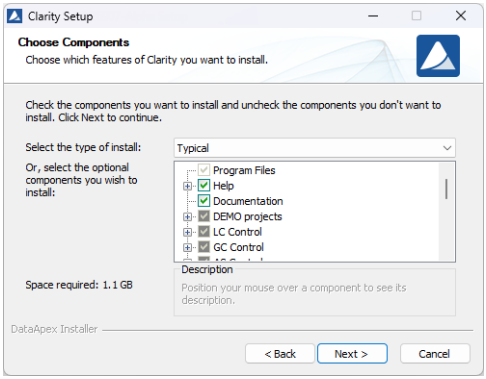
Note: The user code can be found on the back side of the card provided with the Installation USB. Alternatively, you can contact DataApex support to obtain one.



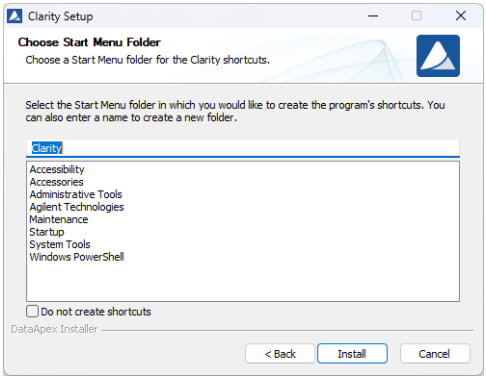
7. Select the type of installation. Make sure that control module for your device is selected to be installed.

Note: In most cases "Typical" should be selected. "Custom"/"Full" installation is necessary e.g., for Agilent and other devices controlled via ICF, DANI devices and few others.

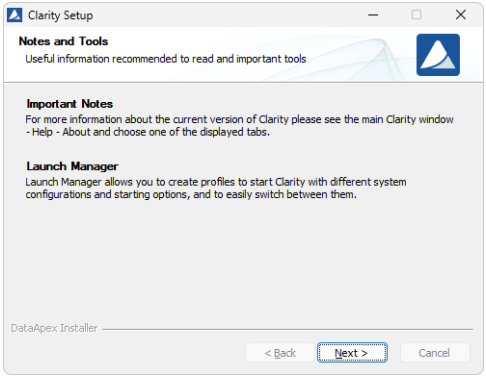
Note: List only contains names of original devices. If you can't find your device, even though it is stated as controlled, it is most likely an OEM version of different device.



8. Select the Start Menu folder for the shortcut or create a new one. After clicking *Install* installation process will start.

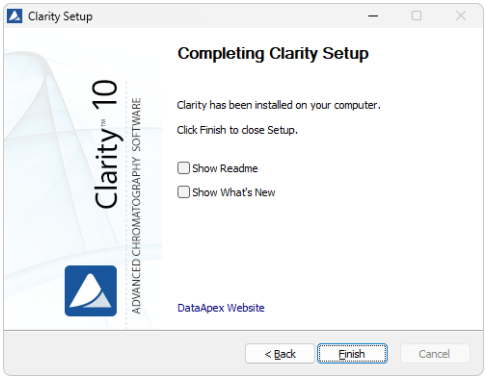


9. Wait for installation to finish. In the end you might be prompted to confirm installation of several hardware drivers.
10. When installation is finished *Notes and Tools window* will be opened.



11. Finally the last window offers to view What's New and Readme.

Note: To run and generate IQ Report start Clarity and use *Help - IQ Report* command in the main window.



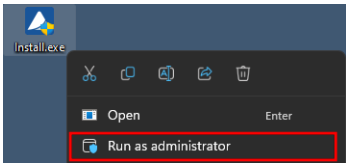
1.2 Updating Clarity Software

These are the basic steps you have to follow to update Clarity.

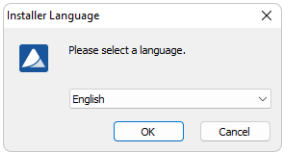
1. Check for the updates: click *Help - Check for Updates...* or download new version of the software from the Downloads at our website.
2. Run the installer.

   More Info:

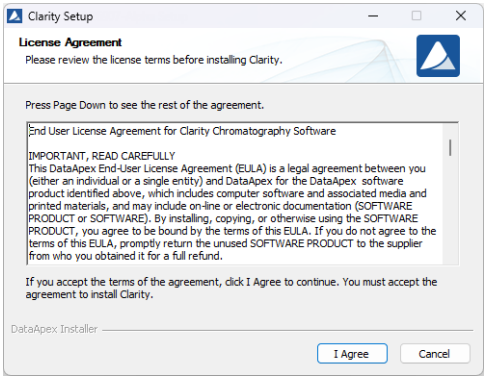
   - On administered systems use „*Run as Administrator*" from intended User account. Administered systems are managed by an administrator and users using the PC may not have administrator privileges. Insufficient privileges may result in:
     - Clarity not being installed.
     - When installed from Administrator account, the installation directory may be read only for users with limited privileges and the station will be inoperable.



3. Select the language.



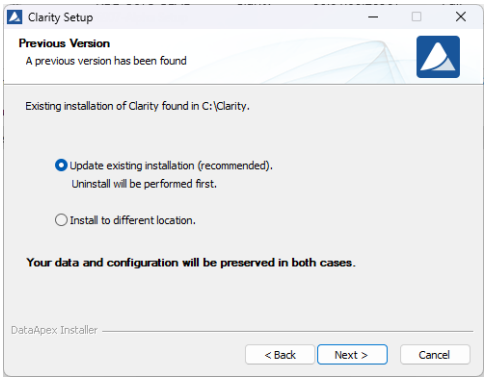
4. Confirm the License Agreement. It is possible to continue only in case you agree with the statement.



5. Previous version of Clarity will be detected. Decide whether to update or preserve this version.

Note: In both cases your data and configuration will be preserved.

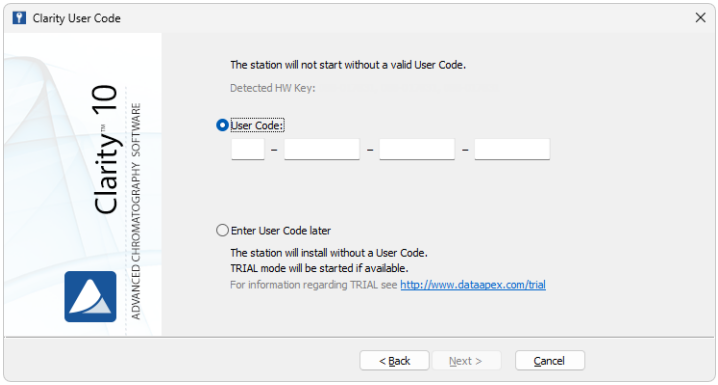
Note: Selecting *Install to different location* will result in presence of two different Clarity version at once (current version will be left as it is and new version will be installed elsewhere).



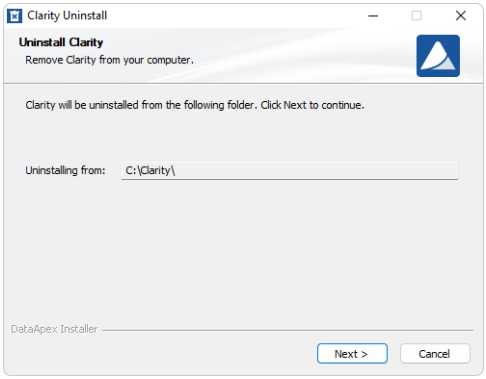
6. If you select to *Update existing installation* it is necessary to confirm the User code (code from current version will be pre-filled).

Caution: Each major version (change of the first version number) since version 9.0 requires new User Code. Make sure that you have a valid User Code for newly installed version before proceeding further. For more information see https://www.dataapex.com/upgrade.

Caution: Downgrading is not supported and might be problematic in some cases.

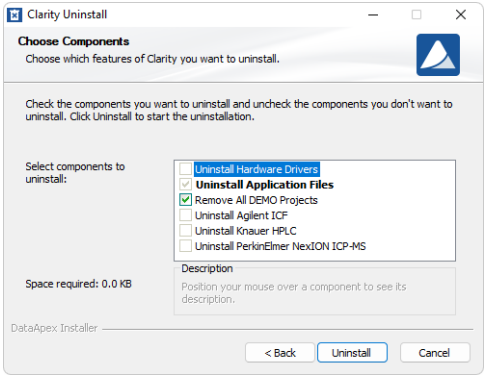


7. Clarity will proceed with uninstallation, following window appears.

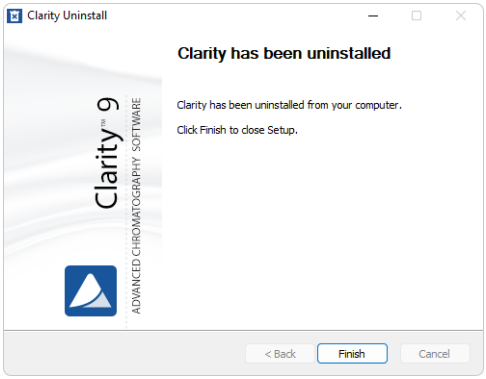


8. Continue to *Choose Components* step and click *Uninstall*.

Caution: When *Remove All DEMO Projects* is selected all files within them will be lost, including any data you saved into their folders. DEMO projects should never be used to store your data.

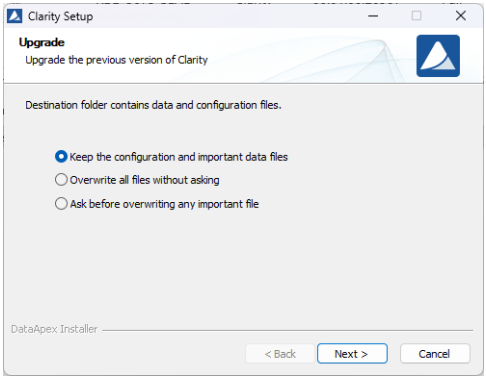


9. Wait for uninstall to finish and click *Finish* in the following window.

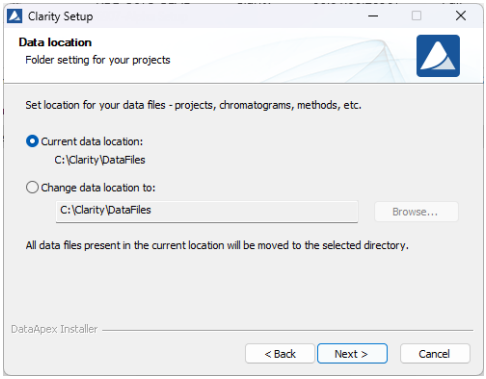


10. Choose what to do with existing data and configuration files.

Caution: It is recommended to select *Keep the configuration and important data files* to preserve all of your settings and data. Other two options might lead to losing important files and should be only used under special circumstances.



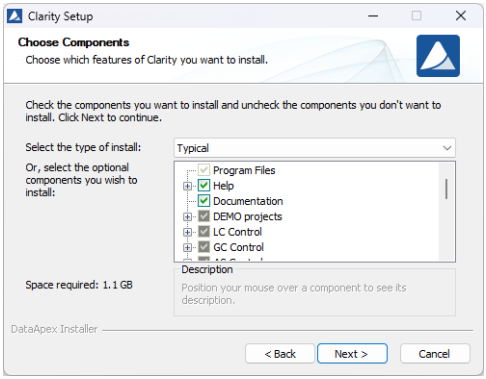
11. Set destination folder for your data files. If data location is changed all data from current version will be moved accordingly.



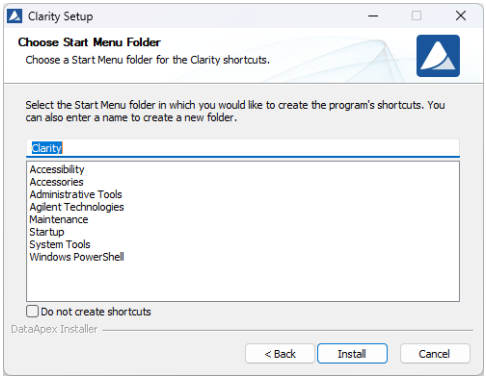
12. Select type of installation. Installation type which was used for current version will be preselected. Make sure that control module for your device is selected to be installed

Note: In most cases "Typical" should be selected. "Custom"/"Full" installation is necessary e.g., for Agilent and other devices controlled via ICF, DANI devices and few others.

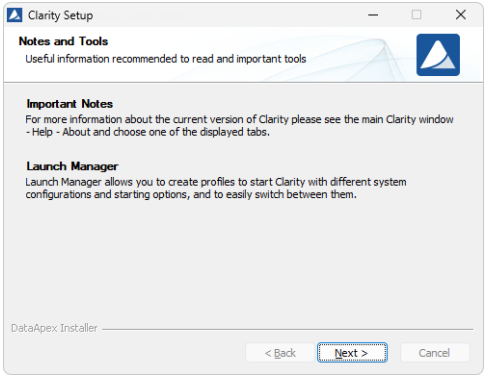
Note: List only contains names of original devices. If you can't find your device, even though it is stated as controlled, it is most likely an OEM version of different device.



13. Select the Start Menu folder for the shortcut or create a new one. After clicking *Install* installation process will start.

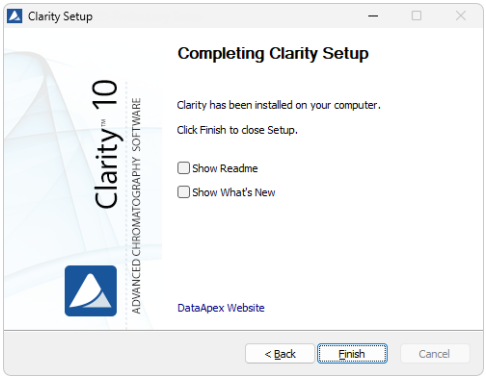


14. Wait for installation to finish.
15. When installation is finished *Notes and Tools window* will be opened.



16. Finally the last window offers to view What's New and Readme.

Note: To run and generate IQ Report start Clarity and use *Help - IQ Report* command in the main window.



Caution: When upgrading from Clarity 6.2 or older to Clarity 7.0 or newer be aware that there is change in the installation structure. The content of the original installation folder is separated to three new subfolders BIN, CFG and DataFiles. The respective files are moved automatically during update to the new locations if you selected *Update existing installation*. In the rare cases this fails, some files may need to be moved manually.

1.3 Installing Colibrick

Colibrick is an external 24-bit A/D converter designed for acquisition of data from any chromatograph. It uses the USB communication channel and it is powered from the PC.

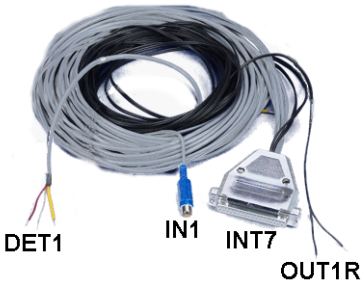
1. First install Clarity.

   More Info:

   - The driver is by default installed in *Typical* installation of Clarity. It can be found in *Hardware* section of *Choose Components* step.
   - The *Colibrick* device is identified by its S/N. If you exchange it by another one later, it will be also necessary to reconfigure it in the *Clarity - System Configuration* dialog.

2. Connect *Colibrick* to a USB port in your computer. It will be detected automatically.

3. Connect the CANNON SUB D 27-pin connector on the (INT7) cable to *Colibrick* back panel.



4. Connect the cables (Starting, Digital output and Analog Signal) to the chromatograph as explained in ***Connecting a chromatograph analogue output to Clarity***.
5. Start Clarity and then add the *Colibrick* channels to specific Clarity instruments as explained in ***Adding a new device***.
6. Check the LED's on the front panel to find out about the status of *Colibrick* and whether it has been installed properly.

More Info:

- Ready (orange) LED status Indicates correct installation.
- Data (blue) LED status Indicates connection to the chromatography data station.
- Digital Input (green) LEDs status
  - LED ON - the input status is High (logical "1") or not connected.
  - LED OFF - the input status is Low (logical "0") or connected to the ground (GND).
- Digital Output (red) LEDs status
  - LED ON - the output status is High (logical "1"), the relay contact is opened.
  - LED OFF - the output status is Low (logical "0"), the relay contact is closed.

1.4 Installing a USB hardware key

Current hardware key with transparent grey casing

Currently supplied RkNDUSB hardware key use HID (Human Interface Device) technology and therefore do not require any additional drivers. These keys can be identified by their transparent grey casing (see image below).

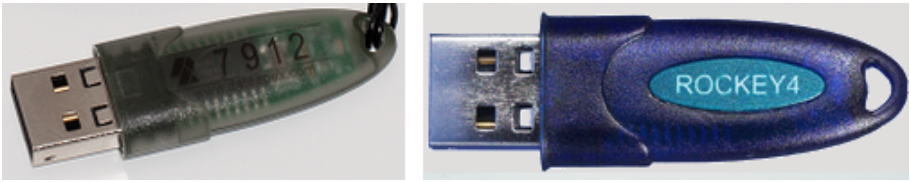
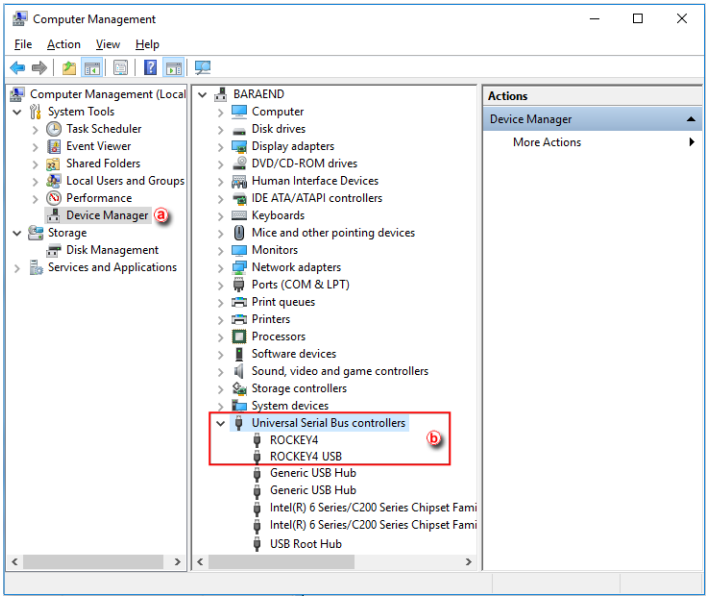


Fig. 1: Current (left) and older (right) hardware key

Older hardware key with blue casing

For older RkUSB key (blue casing) the drivers should be installed automatically during the installation of Clarity. For this reason it is important to install Clarity before plugging the hardware key. If the hardware key is not working properly, follow the procedure below to resolve the issue.

1. Connect the hardware key to a USB port on the computer.
2. Install the Rockey drivers by running INSTDRV.EXE in C:\CLARITY\BIN\HW_DRIVERS\ROCKEY\.
3. Select the Install USB driver option and click on Next to finish the installation.
4. Verify that the driver has been installed correctly. Meaning that the *Device Manager* ⓐ has the item "*Universal Serial Bus Controllers*" - "*Rockey4 USB*" ⓑ .



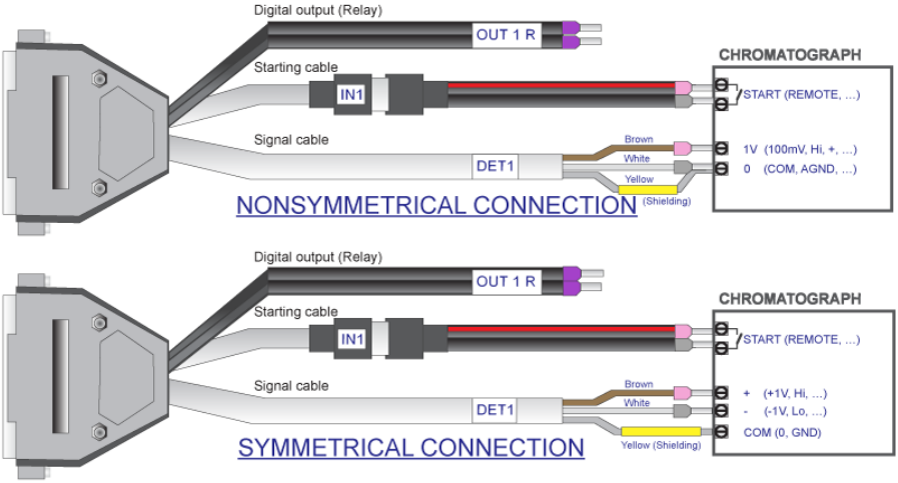
If this does not work, try the following procedure after the installation of Clarity: After connecting the hardware key, Windows will detect a new Plug and Play device and the *Found New Hardware Wizard* will appear.

1. Select "*Search for a suitable driver for my device.*"
2. Select "*Specify a location*" and then select the C:\CLARITY \BIN\HW_ DRIVERS\ROCKEY\folder. The rest of the installation will be carried out automatically.

Note: On Windows 10 and Windows 11, the driver for older hardware key can only be installed if Memory Integrity/Core isolation function of Windows Security is turned off. This function is turned on by default. If an incompatible driver is already installed on the computer, it cannot be turned on. But if it is enabled, the driver installation fails with Error code 39.

1.5 Connecting a chromatograph analogue output to Clarity

The Clarity Station cable (INT7) connects the station to the chromatograph and it is a set of Starting, Digital output and Analog Signal cables connected to a CANNON SUB D 27-pin connector.



1. Install your external A/D converter like *Colibrick* (refer to ***Installing Colibrick***) or an A/D converter card (refer to the specific HW manual).
2. Switch off your chromatograph.
3. Connect the bare wires to the chromatograph depending on your equipment, configuration and the following guidelines.

More Info:

- The **Signal cables** "DET 1" to "DET 4" carry the main signal from the chromatograph to the computer. The connection can be asymmetrical or symmetrical.
- The **Starting cables** "IN1" to "IN4" come in pairs, one part connected to the 27-pin connector and ending on a female RCA connector and the other with a male RCA connector and free leads for connection to a starting contact or a button for a manual start.
- The **Digital Output cables** "OUT 1R" to "OUT 4R" end on free leads and they can be used for synchronizing autosamplers.

Caution: The shielding must be connected. It works not only as the shielding, but also as the analogue ground against which measurement takes place. In the case of asymmetrical output of a detector (only two leads/terminals/pins/screws) the shielding must be connected to the white lead! No lead of the signal cable may remain unconnected.

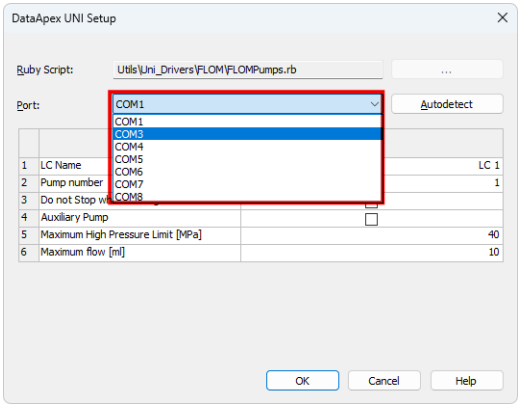
4. Connect the CANNON SUB D 27-pin connector to the A/D convertor.
5. Switch on your computer and your chromatograph.

1.6 Installing Multicom

MultiCOM is a USB to RS232 converter developed for controlling via the RS232 serial interface. It is connected to the PC via the USB port and has 6 serial 9-pin ports. It also has a free USB port for the connection of the *USB hardware key*.

1. First install Clarity. *Multicom* driver is by default installed in *Typical* installation of Clarity. It can be found in *Utils* section of *Choose Components* step.
2. Connect *Multicom* to a USB port in your computer. It will be detected automatically. LED diodes will be turned on one by one.
3. Connect your devices to the *Multicom* RS232 ports.
4. Start Clarity and then add each device to a specific Clarity instrument as explained in *Adding a new device*.
5. Select the appropriate port from the list during the device setup.

Note: When using functions like *Autodetect* and *Check* LED diode of selected port will blink. This can be used to find the desired port number on *Multicom*.



6. Check the LEDs on the top panel to find out about the status of *Multicom* and whether it has been installed properly.

More Info:

Green LED status:

- OFF – not connected to USB, the driver is not installed or *Multicom* is in suspend mode.
- ON (Constant) – idle state, no communication.
- BLINKING:
  - Two short consecutive blinks – only sending data from USB to the COM port.
  - Turned off twice consecutively – only receiving data from the COM port into USB.
  - Constant blinking – both sides are receiving and sending data.

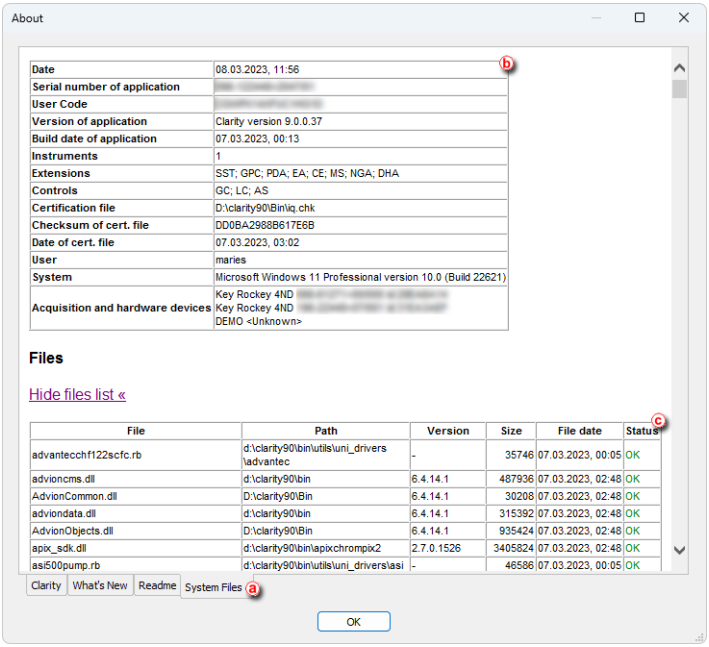
2 Configuring the Chromatography Station

Chapters covering settings in the *System Configuration* dialog.

2.1 Obtaining information about Clarity configuration

To find out information on the supported control modules and Extensions, used A/D converters and purchased Instrument licenses follow this procedure:

1. Open the *About* box: Select *Help - About…* on the *Main* window.
2. Switch to the *System Files* tab ⓐ . Note that it may take a while for Clarity to generate the report.
3. In the first table ⓑ there is info about:
   - Clarity SW version
   - Number of purchased instrument licenses
   - Extensions available
   - The allowed control modules
   - Acquisition and hardware devices
4. Go to the files table ⓒ to find information about the drivers and its status.
   If the status is other than *OK* there may be an issue with the driver. The version of the drivers developed by DataApex should be the same as that of Clarity.

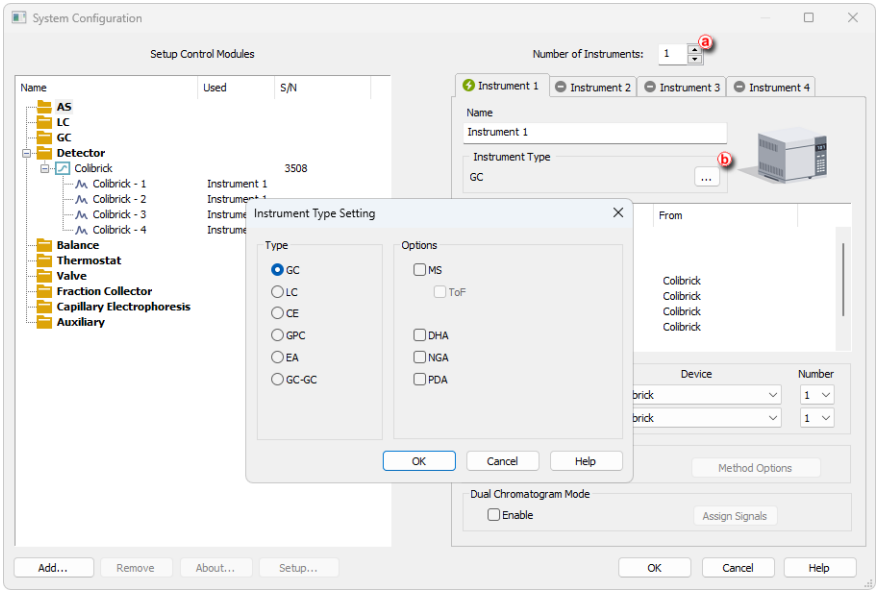


2.2 Setting the number and type of instruments

Before Adding any devices to an Instrument, it is necessary to define the *Instrument Type* and, if applicable, the *Number of Instruments*.

Both settings are configured in the *System Configuration* dialog and depend on the purchased licenses or the intended use (for example Using Offline Instrument for data evaluation). These settings determine which devices can be assigned to individual Instruments.

1. Open the *System Configuration* dialog: select *System - Configuration…* in the *Main* window.
2. In the *Number of Instruments* field ⓐ , set the required number of instruments.
3. Set the *Instrument Type* field ⓑ according to the type of instrument you are using e.g., GC or LC. To be able to assign some of the devices to the *Instrument*, correct *Instrument Type* has to be selected.

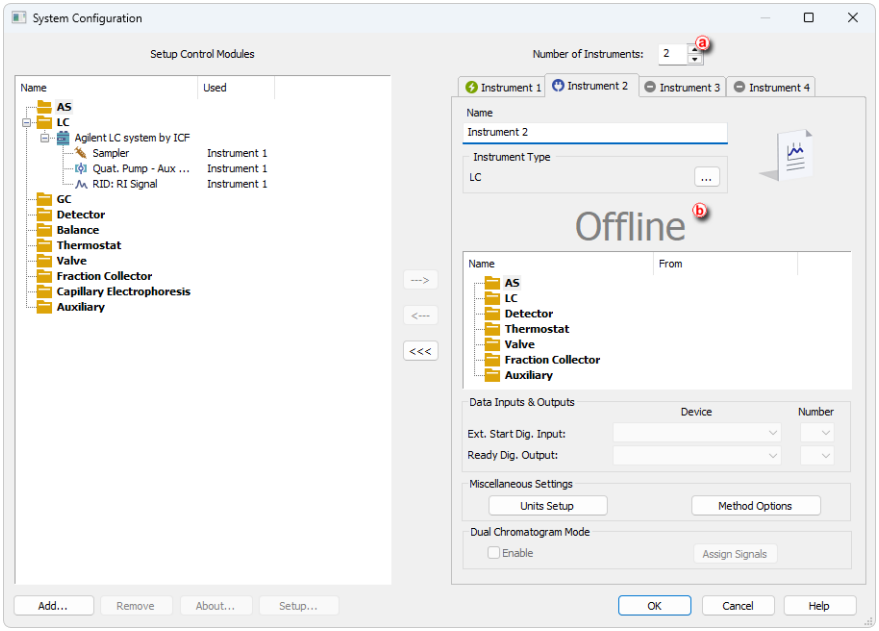


2.2.1 Using an Offline Instrument for Data Evaluation

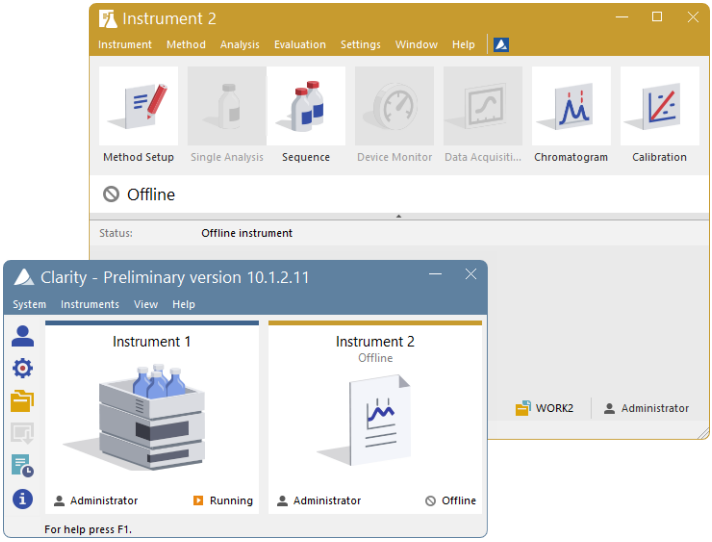
Clarity allows you to use a non-purchased Instrument (*Offline Instrument*) for data evaluation while a measurement is running on another Instrument. The *Offline Instrument* cannot be used for data acquisition, but it can be safely used for opening chromatograms, reviewing results, and preparing reports.

How to set it up and use it

- Open the *System Configuration* dialog from the main Clarity window.



- Increase the *Number of Instruments* ⓐ (for example from 1 to 2).
- A new Instrument tab appears. This Instrument is not licensed for acquisition and is marked as Offline ⓑ .
- Close the *System Configuration* dialog.
- Open the *Offline Instrument* from the main Clarity window.
- Open a project and use the Offline Instrument for data evaluation while the measurement continues on the other Instrument.



Limitations and Recommended Use

When using an *Offline Instrument*, the following limitations must be considered:

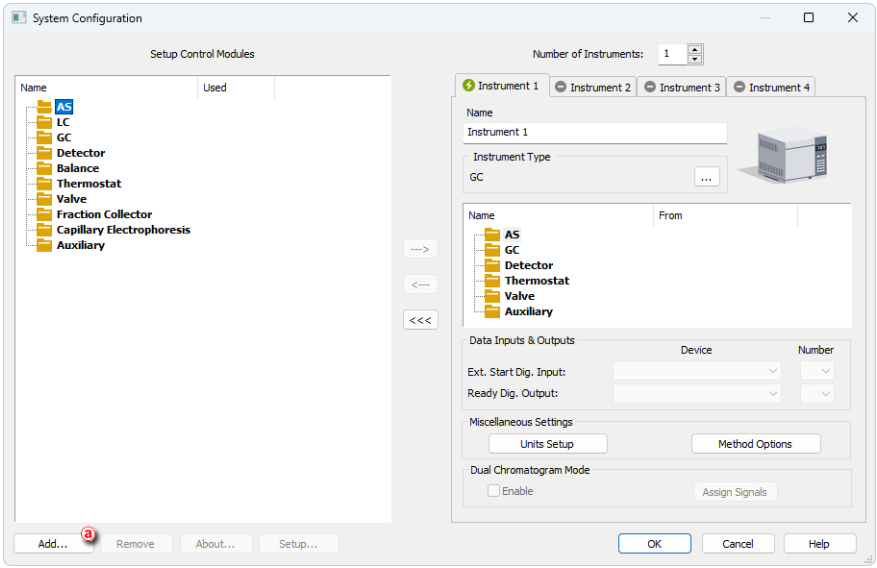
Offline Instrument cannot use devices assigned to a different Instrument.
As a result, methods cannot be prepared or edited on an *Offline Instrument*, because method content depends on the devices available on the Instrument.

Files in use by another Instrument are locked to prevent conflicts.
Any file used by the measuring Instrument (method, sequence, calibration) cannot be edited on the *Offline Instrument* at the same time. This prevents interference with the running measurement. For this reason, an *Offline Instrument* is best used for evaluation of chromatograms from a different project than the one currently being measured, or for read-only work with data that are not actively used.

If users require data evaluation and method preparation from a different computer (for example from an office PC), *Clarity Offline* is a more suitable solution. In such cases, Clarity Offline can be used according to the setup described in the *Clarity in Network* manual.

2.3 Adding a new device

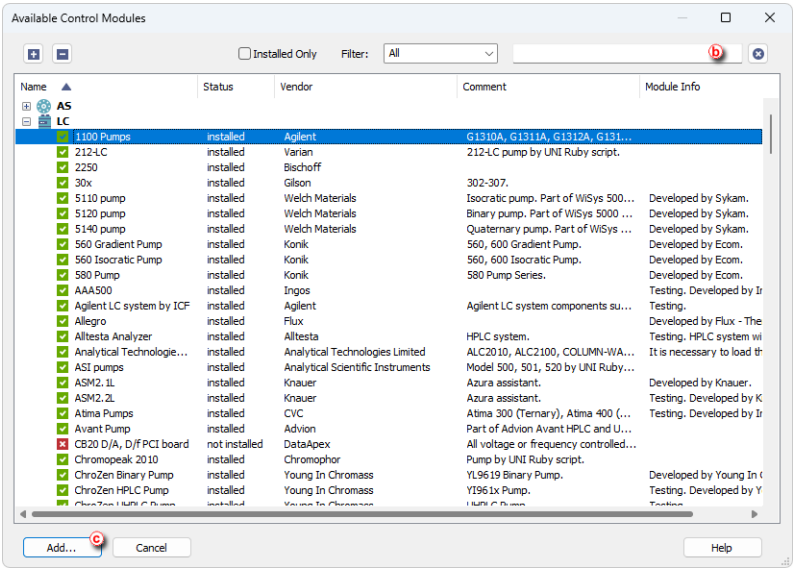
1. Enter the *System Configuration* dialog: select *System - Configuration…* on the *Main* window.



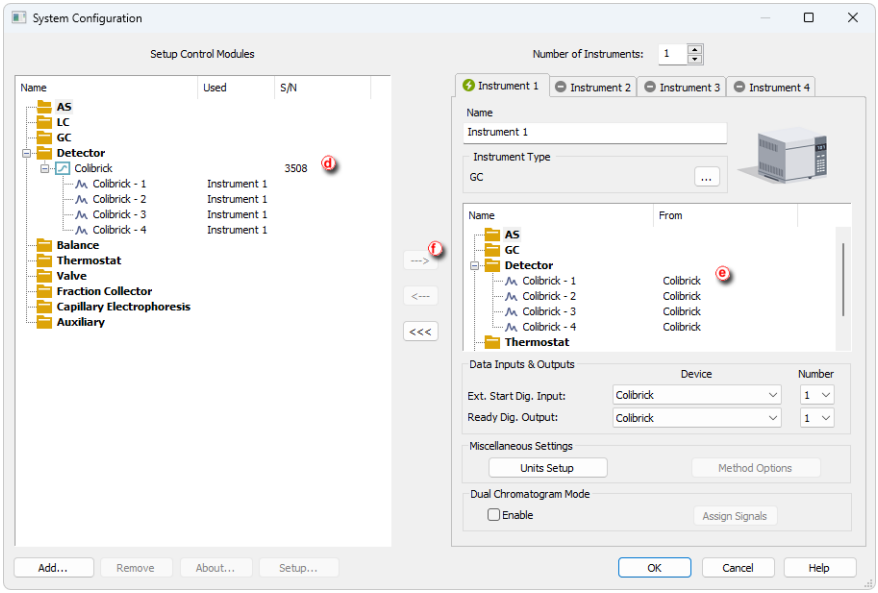
2. If the device you want to add is not in the list, click on *Add* ⓐ and the *Available Control Modules* dialog will open. Here, you can filter the list by typing some text in the filter field ⓑ .

   Note: If the status of the module is *not installed*, double-click the line with this device to see why the module is not installed and how to remedy the situation.

3. Select the device and click on *Add* ⓒ or double-click the line.



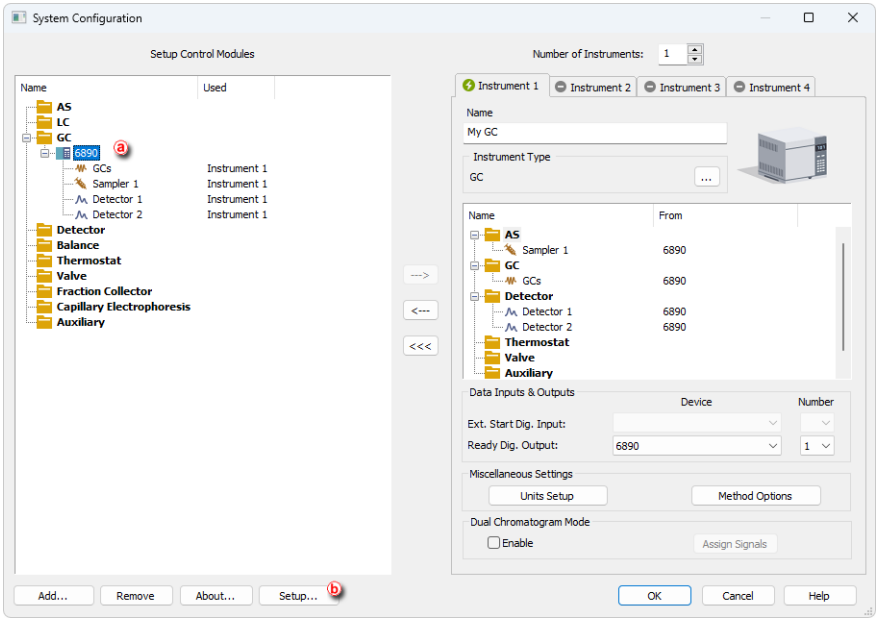
4. Add new devices to the appropriate instrument: drag and drop the device from the left pane ⓓ to the *Instrument* pane on the right ⓔ or select the device and click on ---> ⓕ .



5. If you need to help with configuring a device, go to the topic *Configuring a device*.

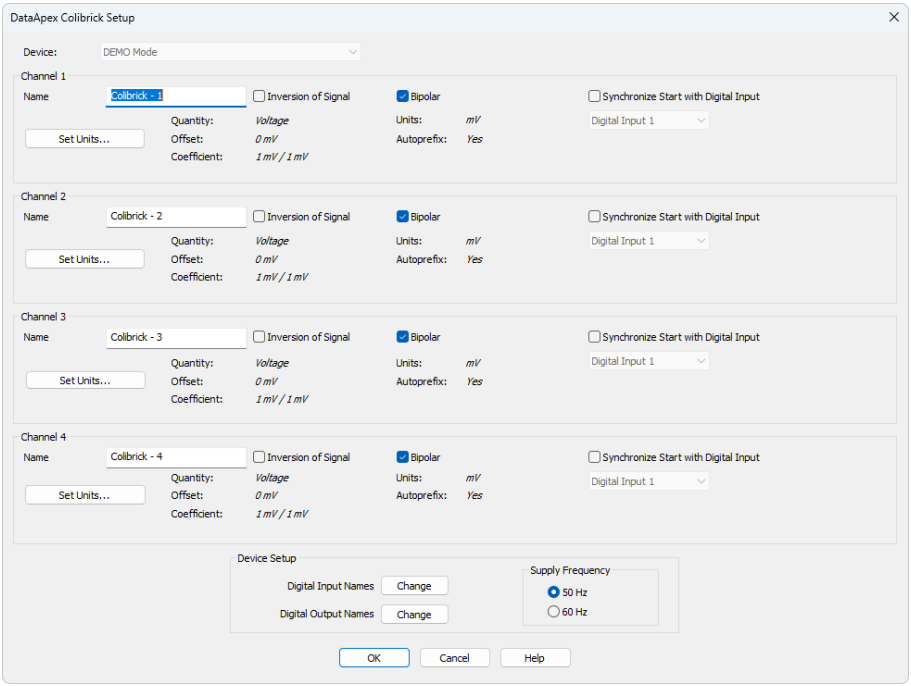
2.4 Configuring a device

1. Enter the *System Configuration* dialog: select *System - Configuration…* in the *Main* window.



2. To configure a device, double-click it or select it ⓐ and click the *Setup...* button ⓑ . A device setup dialog will appear. Setup dialogs are specific to each device.

For more information on how to configure a specific device, go to the specific manual or use the *Help* button.


DataApex Colibrick Setup
Device:
DEMO Mode
Channel 1
Name
Colibrick - 1
Inversion of Signal
Bipolar
Synchronize Start with Digital Input
Quantity:
Voltage
Units:
mV
Digital Input 1
Set Units...
Offset:
0 mV
Autoprefix:
Yes
Coefficient:
1 mV / 1 mV
Channel 2
Name
Colibrick - 2
Inversion of Signal
Bipolar
Synchronize Start with Digital Input
Quantity:
Voltage
Units:
mV
Digital Input 1
Set Units...
Offset:
0 mV
Autoprefix:
Yes
Coefficient:
1 mV / 1 mV
Channel 3
Name
Colibrick - 3
Inversion of Signal
Bipolar
Synchronize Start with Digital Input
Quantity:
Voltage
Units:
mV
Digital Input 1
Set Units...
Offset:
0 mV
Autoprefix:
Yes
Coefficient:
1 mV / 1 mV
Channel 4
Name
Colibrick - 4
Inversion of Signal
Bipolar
Synchronize Start with Digital Input
Quantity:
Voltage
Units:
mV
Digital Input 1
Set Units...
Offset:
0 mV
Autoprefix:
Yes
Coefficient:
1 mV / 1 mV
Device Setup
Digital Input Names
Change
Digital Output Names
Change
Supply Frequency
50 Hz
60 Hz
OK
Cancel
Help

2.5 Connecting Autosamplers (AS)

This chapter describes the most common wiring of autosamplers. The configuration varies depending on the type of chromatograph (GC or LC), sequence mode (*ACTIVE* or *PASSIVE*), and presence of optional control modules in your **Clarity** station.

Typical configurations are:

- AS + GC set - ACTIVE sequence
- AS + LC set - ACTIVE sequence
- AS + GC set - PASSIVE sequence
- AS with Clarity control module - ACTIVE sequence + A/D converter
- AS with Clarity control module - ACTIVE sequence + digital acquisition

All of the aforementioned configurations are described in more detail in the following chapters. If your device configuration does not correspond to any of these cases, contact us at support@dataapex.com.

In an *ACTIVE* sequence, the start is controlled by the station. **Clarity** sends the permission signal to the autosampler and waits until the sampler acknowledges the injection. Data acquisition will be started after the confirmation signal has been sent back to **Clarity** and the permission to another injection is disabled.

In a *PASSIVE* sequence, the start is controlled by the autosampler. **Clarity** waits for an external start signal from the autosampler and only after receiving the signal, it starts the sequence and data acquisition.

The START synchronization between **Clarity** and the autosampler is controlled via cable pins for inputs and outputs, or by serial (RS 232) / USB / LAN port communication.The communication line is defined in the *System Configuration* dialog, which is accessible from the *Clarity* main window through the *System - Configuration…* command. The *System Configuration* dialog operates the communication line via the *External Start Digital Input* and *Ready Digital Output* functions, as described in the following text.

Data Inputs & Outputs group:

- **External Start Digital Input** ① should be set to the device and its specific pin that gives **Clarity** the information about injection being performed. Subsequently, **Clarity** starts Data Acquisition.
- **Ready Digital Output** ② defines the device and its specific pin through which **Clarity** informs other parts of the system that sequence can be run.

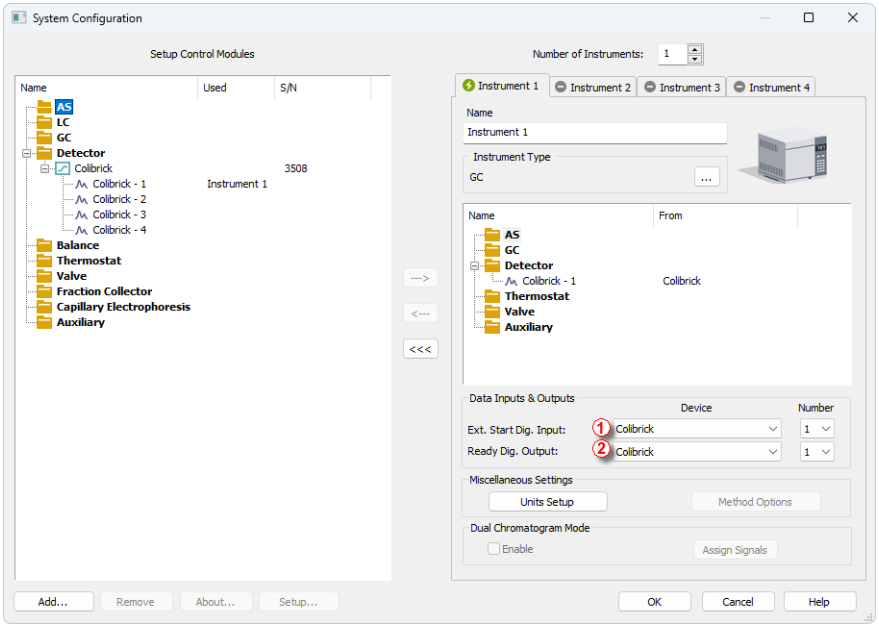


Fig. 2: System Configuration

2.5.1 AS + GC set - Active Sequence

In GC systems, the sample cycle is typically controlled by the GC, as the cool-down time of different systems varies due to the generally used temperature gradient. The sampler is thus synchronized with the GC by a signal wire (READY), allowing the next injection only after the GC gets to the READY state. The autosampler performs the injection and starts the GC using another signal wire (START). Any autosampler that is used in the **Active Sequence** without an **AS Control** module must be synchronized by cable with **Clarity** as well as with the chromatograph. The **IN_n** starting cable should be plugged into the synchronization output (INJECTION) of the autosampler or GC. The **OUT_nR** cable should be connected to the synchronization input between GC and autosampler.

All commonly used autosamplers may be divided into two groups:

- Variant A: Autosamplers started by **closing** the contacts on the input ($\overline{\text{READY}}$).
- Variant B: Autosamplers started by **opening** the contacts on the input (READY).

Variant A - started by closing the contacts

The first diagram shows the wiring of an autosampler that will initiate the injection after its input contact has been closed.

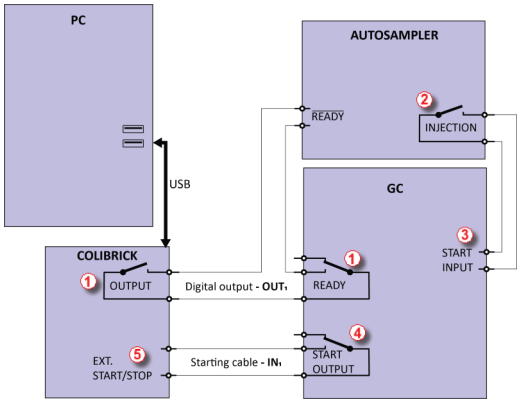


Fig. 3: Wiring of the autosampler - variant A

The injection will start only after the both serially connected contacts (**Clarity** and GC) has been closed ① . After an injection, the autosampler will close the INJECTION contact ② and thus the command to start the temperature gradient program will be given ③ . At the same time, the chromatograph will close the START contact ④ , and thus the command to start acquisition will be given ⑤ .

If the chromatograph does not have a START OUTPUT contact, then the starting cable **IN_n** must be connected directly to the INJECTION output on the autosampler (this way, in fact, parallel to the START INPUT contact of the chromatograph).

To have the contact on the **Colibrick** A/D converter opened in the initial state, it is necessary to set the *Output Initial State* item to *HIGH* in the ***Digital Outputs of Colibrick*** dialog as shown on **Fig. 4** on pg. **33**.. This dialog is accessible from the *Clarity* main window through the *System - Digital Outputs…* command.

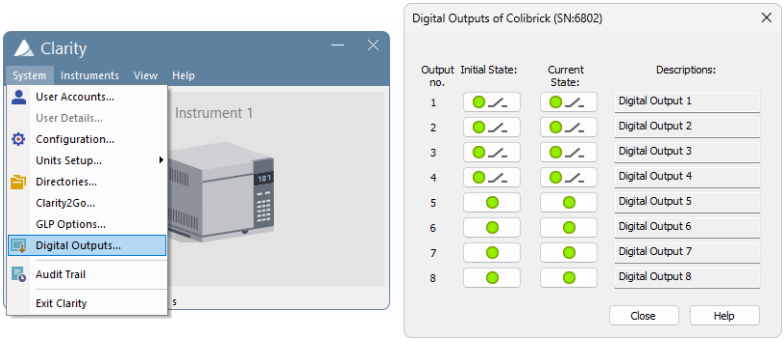


Fig. 4: The Digital Outputs dialog

The start output, mapping of **Clarity** to individual digital outputs of the **Colibrick** A/D converter, can be set in the bottom-right corner of the ***System Configuration*** dialog, see **Fig. 2** on pg. **31**. Use the following settings.

Fig. 5: System Configuration - Data Inputs & Outputs for a GC set

Variant B - started by opening the contacts

In the second diagram, there is an autosampler wiring that conversely waits for output contacts to be opened. This requires different connection (marked by a circle).

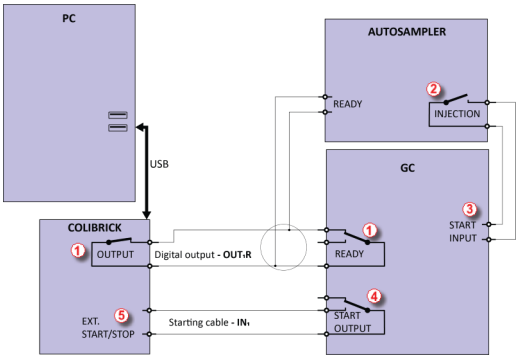


Fig. 6: Wiring of the autosampler - variant B

The **OUTPUT** and **READY** contacts are connected in parallel, and the autosampler will start its operation after both contacts have been opened ① . After an injection, the autosampler will close the INJECTION contact ② and thus the command to start the temperature gradient program will be given ③ . At the same time, the chromatograph will close the START contact ④ and thus the command to start acquisition will be given ⑤ .

If the chromatograph does not have a START OUTPUT contact, then the starting cable **IN_n** must be connected directly to the INJECTION output of the autosampler.

To have the contact on the **Colibrick** A/D converter closed in the initial state, it is necessary to set the *Output Initial State* item to *LOW*.

External Start Digital Input and *Ready Digital Output* settings in the *System Configuration* dialog are the same as for Variant A.

2.5.2 AS + LC set - Active Sequence

In LC systems, the autosampler typically governs the timings. The eventual pump gradient and detector programs are set independently. Any autosampler that is used in the **Active Sequence** without an **AS Control** module must be synchronized with **Clarity** by cables. The **IN_n** starting cable should be plugged into the synchronization output (INJECTION) of the autosampler, and the **OUT_nR** cable should be plugged into the synchronization input (READY) of the autosampler.

The autosampler will initiate the injection after its input contact has been closed ① . After the injection, the autosampler will close the INJECTION contact ② , and the command to start acquisition will be given directly back ③ . When using additional devices (Detectors, LC Pumps, etc.) it is recommended to connect these devices independently to other digital outputs of the A/D converter ④ . Each device will then need a dedicated row in the **Event Table** (**Fig. 9** on pg. **36**.) to be started or stopped by **Clarity**.

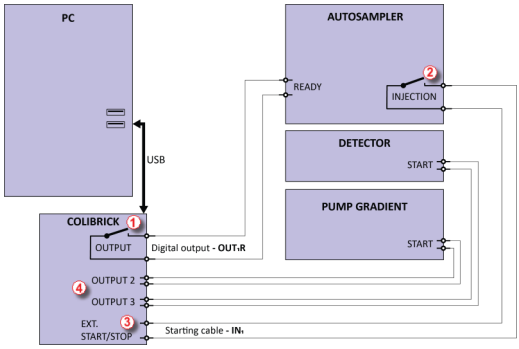


Fig. 7: Wiring of the autosampler in an LC set without the AS Control module

Note: The labels on the input and output contacts may vary depending on the type of the autosampler.

Note: When the detector or pump start inputs are connected in parallel to the **Clarity** start input, make sure to ground the device properly.

The start output, mapping of **Clarity** to individual digital outputs of the **Colibrick** A/D converter, can be set in the bottom-right corner of the *System Configuration* dialog, see **Fig. 2** on pg. **31**. Use the following settings.

Fig. 8: System Configuration - Data Inputs & Outputs LC set

Events to start additional detectors and pumps from **Clarity** must be set in the *Event Table* accessible from the *Method Setup* dialog. In the most typical setup (shown in **Fig. 7** on pg. **35**.) use the setting as displayed in **Fig. 9** on pg. **36**.

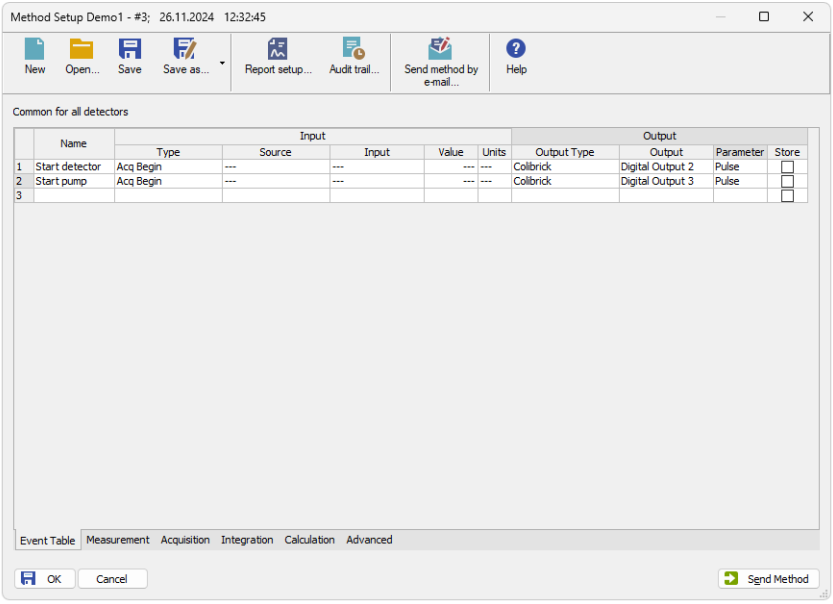


Fig. 9: Event Table for starting detector and pump from Clarity

2.5.3 AS + GC set - Passive Sequence

The autosampler used in the **Passive Sequence** does not need the **OUT$_n$R** digital output cable to be connected. All timings are controlled by the chromatograph and autosampler. **Clarity** performs only one analysis for each start signal received. Synchronization includes only external start of data acquisition in **Clarity** using the **IN$_n$** starting cable.

The sequence must be started in **Clarity** before the autosampler. The autosampler initiates the injection after manual start on the device. The sampler is synchronized with the GC by a signal wire (READY), allowing the next injection only after the GC gets to the *READY* state. After an injection, the autosampler will close the INJECTION contact ① and thus the command to start GC will be given ② . At the same time, the

chromatograph will close the START contact ③ and thus the command to start acquisition will be given ④ .

Caution: It is necessary to set timings in the autosampler and **Clarity** to ensure the next injection will be performed after the previous run is finished.

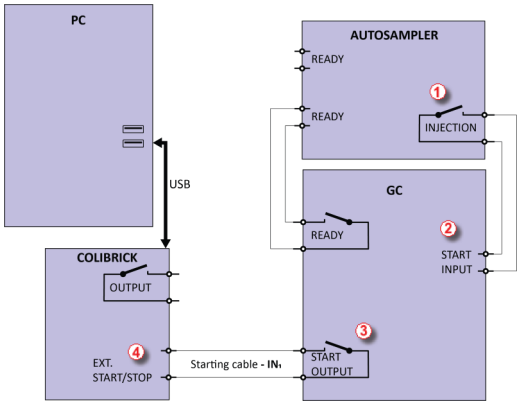


Fig. 10: Wiring of the autosampler in Passive Sequence

Passive Sequence must be used for example in the sets with Headspace autosamplers (without **AS Control** module).

Caution: It is not recommended to use the **Passive Sequence** together with the Control modules.

The start output, mapping of **Clarity** to individual digital outputs of the **Colibrick** A/D converter, can be set in the bottom-right corner of the *System Configuration* dialog, see **Fig. 2** on pg. **31**. Use the following settings.

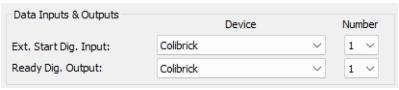


Fig. 11: System Configuration - Data Inputs & Outputs for Passive Sequence

2.5.4 AS with Clarity control module - Active Sequence + A/D converter

When using the optional **AS Control** (p/n **A26**) module, all communication is performed through a separate data cable (usually a serial cable connected to a COM port).

Caution: Refer to the corresponding **Clarity Control** manual (found on your installation media or at www.dataapex.com) for the wiring specific to your instruments.

The following diagram shows a directly controlled autosampler with external digital acquisition by the **Colibrick** A/D converter. In this case the digital output cable **OUT$_n$R** does not need to be connected. For any controlled autosampler in **Clarity**, the

synchronization via starting cable is possible. Some autosamplers, however, do not need the connection of the starting cable, but can send the start of an injection over the communication line.

The autosampler initiates an injection after **Clarity** receives the command sent through a serial cable ① . After the injection, the autosampler will close the INJECTION contact ② and thus the command to start acquisition will be given ③ .

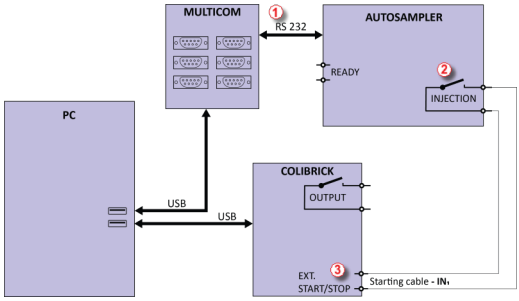


Fig. 12: Wiring of the autosampler with AS Control module + A/D converter

The start output, mapping of **Clarity** to individual digital outputs of the **Colibrick** A/D converter, can be set in the bottom-right corner of the *System Configuration* dialog, see **Fig. 2** on pg. **31**. Use the following settings.

Fig. 13: System Configuration - Data Inputs & Outputs AS + A/D converter

2.5.5 AS with Clarity control module - Active Sequence + digital acquisition

When using optional **AS Control** module in combination with digital acquisition detectors (e.g., the Agilent 6890 module), the connection should be as follows.

All communication with **Clarity** is performed through separate data cables (usually a serial cable connected to a COM port). The autosampler initiates the injection after **Clarity** receives the command sent through a serial cable ① . After the injection, the autosampler will close the INJECTION contact ② and thus the command to start the temperature gradient program will be given ③ . At the same time, the chromatograph will send the command ④ through a serial cable to start acquisition ⑤ .

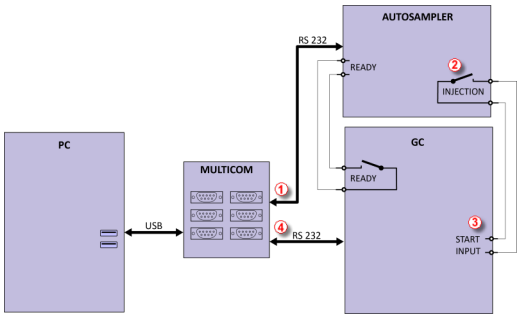


Fig. 14: Wiring of the autosampler with AS Control module and digital acquisition

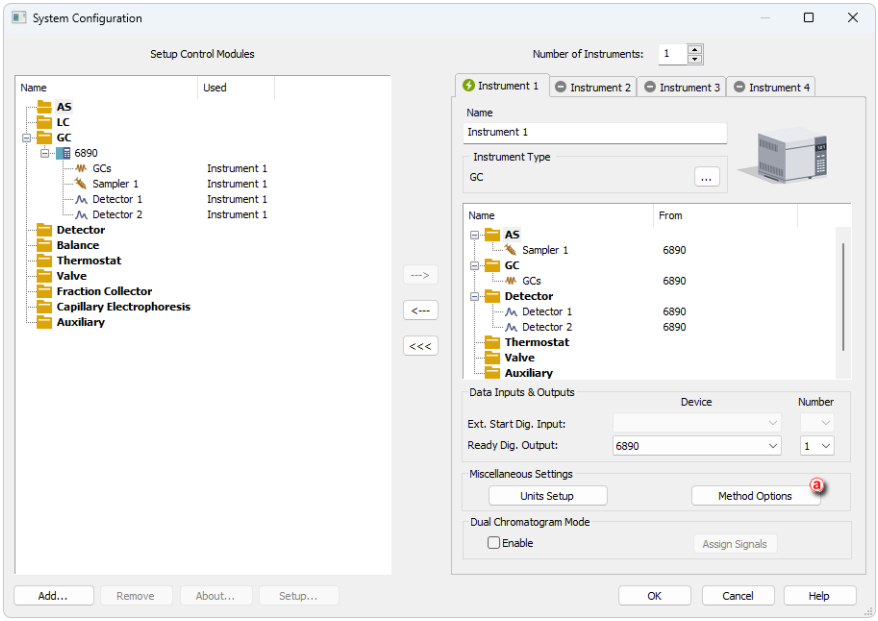
The start output for specific autosamplers can be set in the bottom-right corner of the *System Configuration* dialog, see **Fig. 2** on pg. **31**. Refer to the corresponding **Clarity Control** manual for the wiring to your instruments.

2.6 Setting the options for sending the method to the instrument

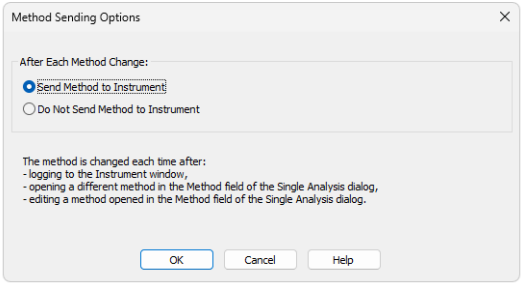
In a default Clarity installation, each time you change the method on Instrument, you need to send it manually to configured devices. Let's describe how to change that behavior so the method will be automatically sent to devices after each time you change the method.

Caution: We do not recommend to set the automatic sending of method on HPLC instruments since you may mistakenly send a method to configured pumps with wrong flow or pressure limits!

1. Enter the *System Configuration* dialog: select *System - Configuration…* on the *Main* window.
2. In the group *Miscellaneous Settings* click on *Method Options* button ⓐ .



3. Choose one of the option of the method sending.



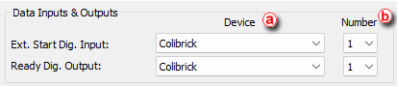
If you select the *Send Method to Instrument* option, the method selected in *Single analysis* window will be sent every time you log into the instrument or this method is modified, or when the sequence is finished.

2.7 Assigning digital input and output to start acquisition

There are basically three means when Clarity decides to start the acquisition:

1. User presses Run button in Single Analysis (user probably did manual injection and notifies Clarity that its time to start)
2. Clarity is outside of run, but one of the controlled detectors starts to provide data marked as run data.
3. Clarity gets the digital input marked as START from device over:
    a. Communication line (LAN, serial (RS-232), USB/GPIB)
    b. Wire as TTL signal (this connection requires an external A/D converter or other device offering digital input to Clarity)

The last case (3) is most typical way and this chapter describes how to assign digital input and output in Clarity for the most common wiring of devices (typically an autosampler). The setting is performed in System Configuration dialog through *Ext. Start Dig. Input* and *Ready Dig. Output* functions.



2.7.1 Data Inputs & Outputs

- Settings are specific for each particular instrument.
- ⓐ : Only devices configured on the Instrument are offered in device list.
- ⓑ : Input number list allows to select input number. Available inputs are specific for particular instrument and correct number depends on actual wiring.

2.7.1.1 External Start Digital Input

The device (in most cases the sampler) provides the injection state to Clarity over its digital output. This may be a real digital output on the device or just a simulated one (Clarity does not distinguish between the two). Selecting a right *Ext. Start Dig. Input* is necessary, because Clarity watches the state of the selected input all the time and reacts on its change.

More Info:

Various devices are providing a lot of different inputs, and these may be used for other reasons, not only for analysis starting. The user needs to select the proper input which will allow the starting. For devices with virtual inputs, and in most cases also samplers with real outputs on the hardware, Start is signaled on output number 1.

After receiving START signal from a sampler, that notifies Clarity about performed injection, Clarity sends instruction to Start Acquisition to other modules (detector, column oven etc.) of the system .

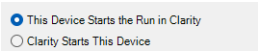
2.7.1.1.1 Possible synchronization issues

Missing start of analysis

Situation could happen when there is configured compact HPLC (without sampler) and external sampler or controlled sampling valve. The sampler or valve lets Clarity

know, broadcasts the analysis start and the HPLC needs to get the information from Clarity, otherwise it will never start running.

For some chromatographs, the settings of the module and its behavior are set in the module's configuration based on the actual wiring, and it is upon the person installing Clarity and setting up the configuration to set the whole system correctly.



For correct option always consider the source of the analysis start first (sampler, sampling valve, Start button on a instrument) and ask a question "What will happen if Clarity does not signal anything? Will the instrument run anyway?"

- If **Yes** - option should be set to *This Device Starts the Run in Clarity*
- If **No** - option should be set to *Clarity Starts This Device*

2.7.1.2 Ready Digital Output

Note: Settings *Ready Dig. Output* in *System Configuration* dialog is relevant only for Active Sequence using sampler without **AS Control** module. Conversely is **not relevant** for controlled samplers used with **AS Control** module (signal over communication line), neither for Passive Sequence.

Ready Dig. Output defines the device and its specific pin through which Clarity informs other parts of the system that injection can be performed. After starting a sequence, controlled modules READY states are verified, Clarity triggers the *Ready Dig. Output* and changes its state, thus broadcasting to other modules of the system that sequence can be run. READY signal is received by the sampler that performs the injection and sends START signal. Then Clarity detects START signal and triggers again *Ready Dig. Output* and change its state, thus preventing the sampler to perform another injection.

Caution: Using the Event Table in Method Setup other actions can be configured changing the parameters of Digital Output. Note, that if the same Digital Output is modified, it may cause conflicts in synchronization. Avoid using these inputs and outputs in the Event Table.

2.7.1.3 Settings Examples

Default assignment of the *Ext. Start Dig. Input* and *Ready Dig. Output* functions can be found in the manual for the corresponding hardware.

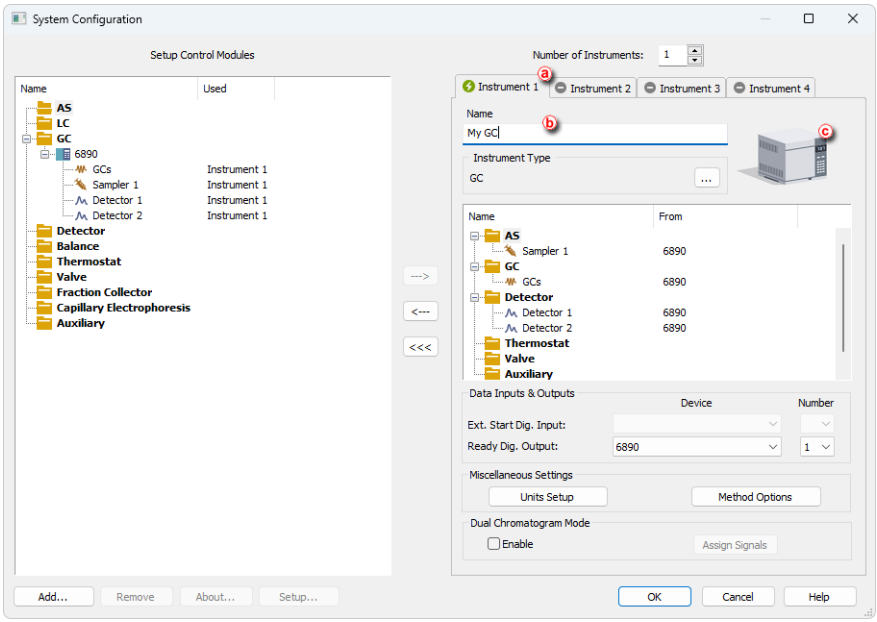
For most common wiring of autosampler see chapter "Connecting Autosamplers (AS)" on page 30 or respective subsections in **Getting Started manual**.

- "AS + GC set - Active Sequence" on page 32
- "AS + LC set - Active Sequence" on page 35
- "AS + GC set - Passive Sequence" on page 36
- "AS with Clarity control module - Active Sequence + A/D converter" on page 37

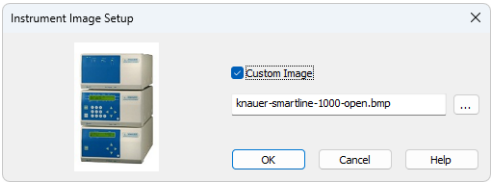
- "AS with Clarity control module - Active Sequence + digital acquisition" on page 38

2.8 Setting a custom image and a name for an instrument

1. Enter the *System Configuration* dialog: select *System - Configuration*…in the *Main* window.



2. Click on the *Instrument 1..4* tab to select the instrument ⓐ .
3. Type the name of the instrument in the *Name* field ⓑ .
4. Click on the image of the Instrument ⓒ to invoke *Instrument Image Setup* dialog.



5. Check the *Custom Image* check-box and then click on ... to select your image. Click *OK* to save your changes.
6. Repeat for every Instrument you wish to change the name or the pictures.

2.9 Tablet mode

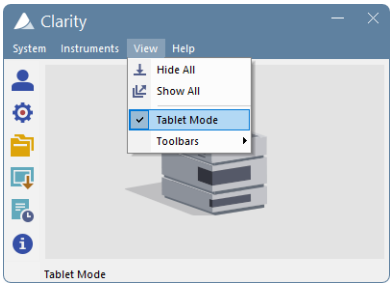
This procedure shows how to activate and use a Tablet mode. The Tablet mode represents a specific windows layout that should simulate a single-window application. It is designed for devices with small displays. The optimum resolution is 1920 x 1080.

In Tablet mode, *Instrument window* is narrower than in standard layout and is positioned on the left side of the monitor, other windows open on top of each other and fill the remaining space on the monitor. Tablet mode allows the use of higher scale in Windows (up to 200 %) which improves work with the software and readability of parameters.

Enabling Tablet mode

1. In *Clarity Main* window menu, click *View* and select *Tablet Mode* item.

   Note: Switching to Tablet mode is possible only when instruments are closed.



2. After logging in to the Instrument, new windows open in tablet layout. *Instrument window* is positioned to the left side of the monitor, other windows open on top of each other and fill the remaining space on the monitor.

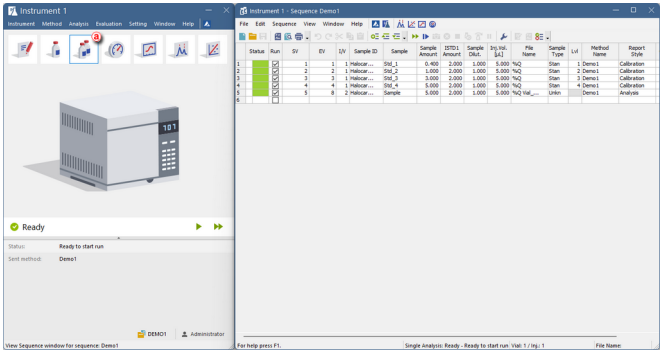
   More Info:

   Instrument window cannot be fully maximized. Its width can be expanded up to a maximum of 50% of the monitor width and is stored.

   Other windows always fill the remaining space of the display.

   Method Setup and *Single Analysis* windows are opened maximized.

   If the scale in Windows is set to more than 100%, some of the icons and analysis status line can break into a new line.



3. Icon of an active window is highlighted by a blue frame in the *Instrument window*ⓐ .

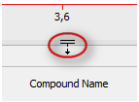
Disabling Tablet mode

1. In Clarity window menu, click *View* and select *Tablet Mode* item (active tablet mode is highlighted by a tick icon).
2. After logging in to the Clarity Instrument, new windows will open in layout used before activating the Tablet mode.

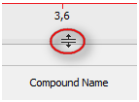
2.10 Adjusting the size of panes

Panes can be adjusted in the Chromatogram and Calibration windows. It applies to horizontal as well as vertical splitters.

Double click on the area next to the border (the cursor changes to) to maximize the pane - double click again to return the pane to its original state.



Move cursor on the border line (the cursor changes to) then click and drag the pane to your desired position (size).



3 User Accounts

Chapters describing how to use User Accounts in **Clarity**, how to restrict some operations for defined users, and how to set shared settings for a group of users. User Accounts allow you to configure the settings for each user (Name, Password, Access Rights, and Digital Certificates) individually, and set the Password Policy for the whole station.

For the procedures on how to set the User Accounts to work in the GLP environment, see the ***Clarity in Regulated Environment*** manual.

The User Accounts can be configured from the *User Accounts* dialog. The proposed workflows regarding User Accounts are as follows:

3.1 Creating User Accounts

1. Open the *User Accounts* dialog: click on or choose *System - User Accounts*.
2. Create one typical *User Account*, that will be used as a template for others. More details can be found in the Creating a new user account topic.
3. Set the *Access Rights* of this user as needed. More details can be found in the Restricting Access topic.
4. Duplicate the created user account by the *Duplicate* command to copy the defined *Access Rights* to the new user. Set the *Name* and *Desktop file* of the new user. If needed, edit also the *Access Rights*. More details can be found in the Duplicating a user account topic.
    a. If you want the appearance of the tables, graphs, user settings, etc., shared between multiple users, set the desktop file to be the same for these users. More details can be found in the Sharing Settings topic.
5. Set the *Password Policy* to comply with your organization policy.
6. Save the *User Accounts* by clicking OK.

3.2 Managing User's Passwords

- When logging for the first time, or when the password expires, the user will be prompted to set a password during logging to Clarity. More details can be found in the Setting a password topic.
    - If it complies with the organization password policy, it is also possible to set a blank password. More details can be found in the Logging without password topic.
- It is also possible to change the user password any time you want. More details can be found in the Changing a password topic.

3.3 Managing User Accounts

- There are two ways how to terminate the User Account in Clarity.
    - Disable the user. The user account is still visible in the list in the User Accounts dialog, but cannot be used for logging in, nor changing its access rights. This is fully reversible as the user that has right to access

User Accounts dialog can *Enable* this account anytime. The user account with the same name as the disabled account cannot be created. More details can be found in the Disabling a user topic.

- Delete the user. After the saving the *User Accounts* dialog after deleting the user, this action is irreversible. The user account with the same name can be created. More details can be found in the Deleting a user topic.

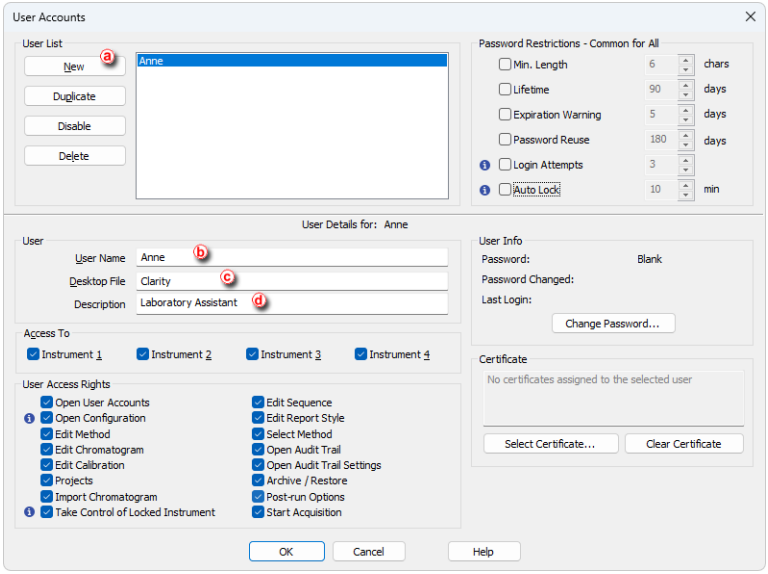
In the *GLP options*, it is possible to disallow the user account deletion and renaming, to ensure traceability and integrity of user accounts.

3.4 Creating a new user account

1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. To create a new user, click the button *New* ⓐ and fill in the new *User Name* ⓑ .
3. Enter the *Desktop File* name ⓒ . If you left the *Desktop File* field empty, a [USERNAME].DSK desktop file will be automatically created.

   Note: This file contains settings regarding the size, location, and visibility of Clarity windows as well as all the modifiable Instrument parameters which are not part of system files.

4. Fill in a user *Description* if you want to. ⓓ
5. Click *OK* to accept the changes.

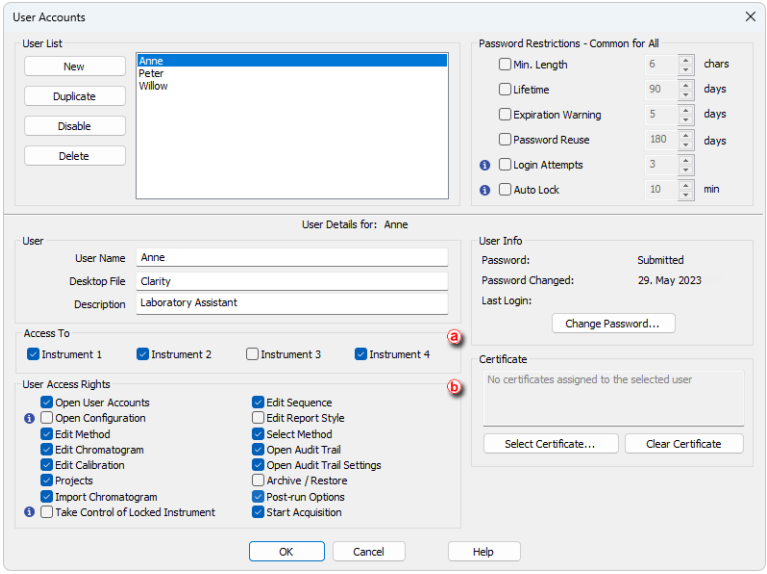


3.5 Restricting access

In Clarity, it is possible to:

- Restrict user's access to instruments
- Restrict user's access to Clarity procedures

1. Open the *User Accounts* dialog: click on or choose *System - User Accounts*.
2. Check the Instruments the user will have access to ⓐ .
3. Check the Clarity procedures the user will have access to ⓑ .
4. Click *OK* to accept the changes.

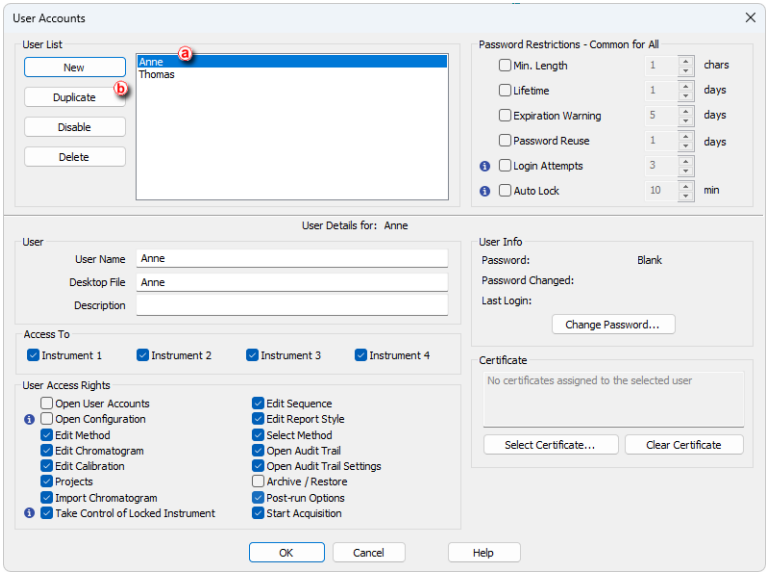


3.6 Duplicating a user account

Once you have set up the *Access Rights* for one account, it is possible to copy it to another new account using the *Duplicate* command.

To achieve this, follow these steps:

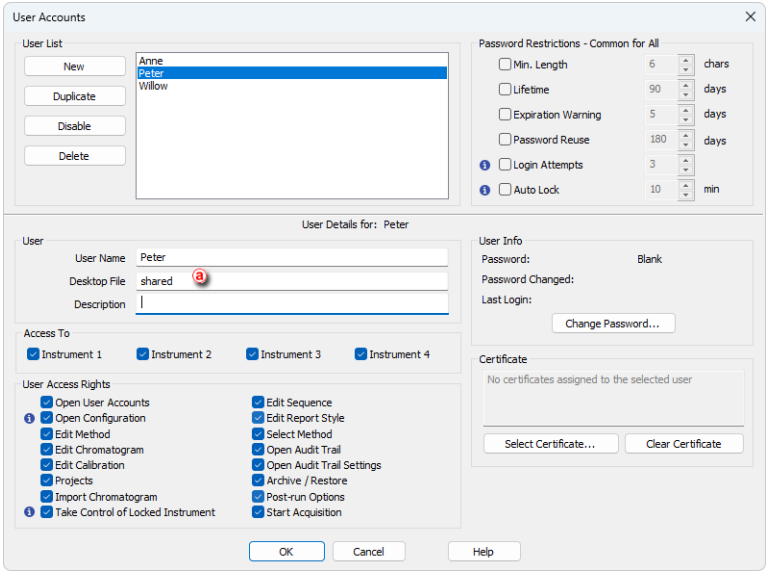
1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. Select the account from which the settings will be duplicated ⓐ .
3. Select the *Duplicate* ⓑ command.
4. Enter the *User Name* of the newly created user account.



3.7 Sharing user settings among users

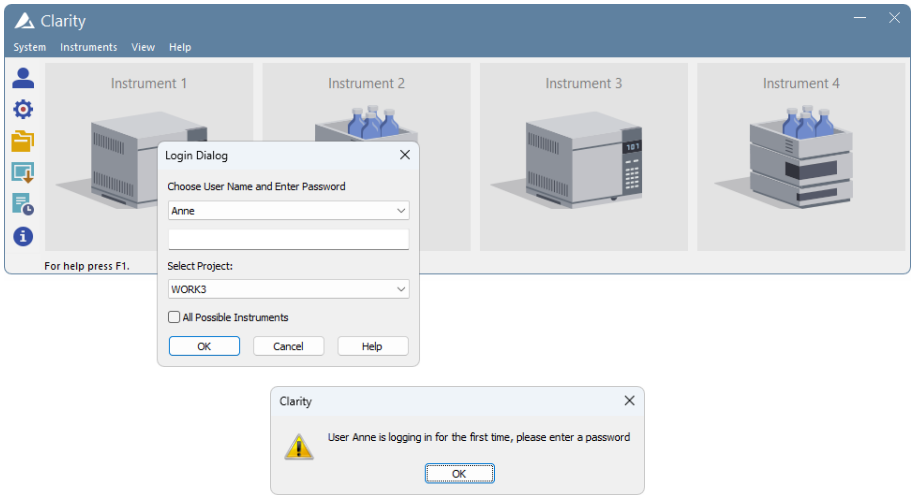
In Clarity, user settings e.g., settings of *User Columns*, the width of columns in tables, customization of toolbars, etc., are saved in the desktop files *.DSK.

1. Open the *User Accounts* dialog: click on or choose *System - User Accounts*.
2. Select the user to have a shared desktop file.
3. Type the name of the desktop file to be shared to the *Desktop File* field ⓐ .
4. Repeat the procedure for every user you want to have the shared desktop setting.
5. Click *OK* to accept the changes.

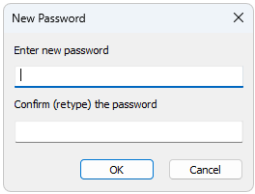


3.8 Setting a password for the first time

1. If the user has been created already and the password was left blank, then the first time you click on any of the instruments in the *Main* window, after selecting the user and clicking *OK* in the *Login Dialog*, you will be asked to enter a new password.



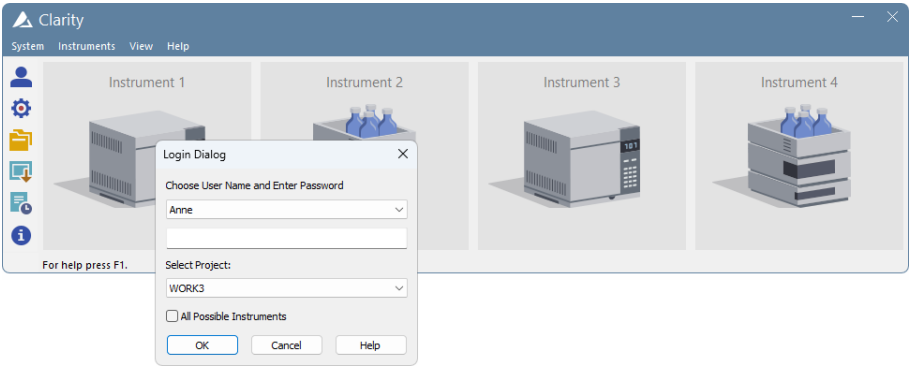
2. Type in and confirm the new password. Then click *OK*.



3. Alternatively or if you are creating a new user, you can follow the same procedure as explained in section ***Changing a user password*** and create a new one.

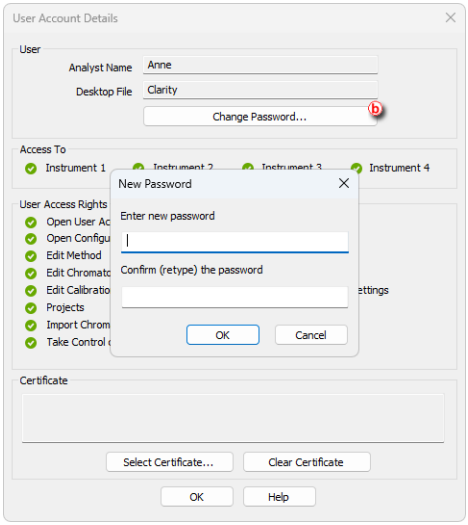
3.9 Logging in without a password

1. Create a new user account without setting up a password as explained in section *Creating a new user account* or remove the password, if it was previously set, in an previously created account as explained in *Changing a user password*.
2. Click on the *Instrument* you wish to open in the *Main* window.
3. Select the user name and click *OK* while leaving a blank password.



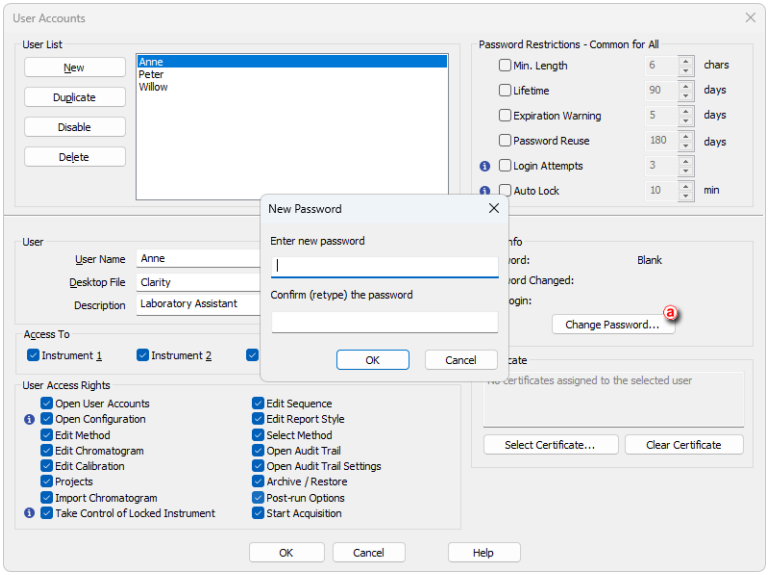
3.10 Changing a user password

1. Open the *User Accounts Details* window by choosing *System - User Details*, select the user, and enter the current password.
2. Click on the *Change Password* button ⓑ and enter and confirm the new password.



Alternatively, if you have access to the *User Accounts* dialog, you can change password by following these steps:

1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. Select the user in the *User List* and then click *Change password* ⓐ .
3. Type the new password, confirm it, and click *OK*.

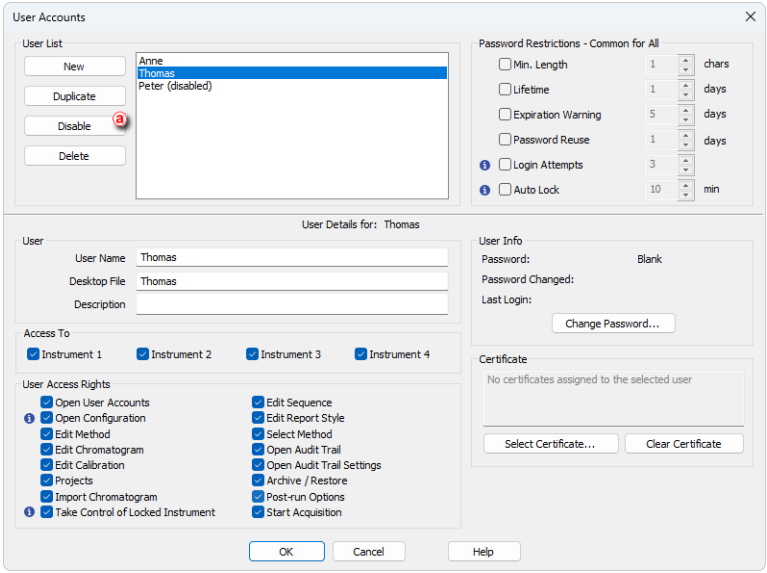

User Accounts
User List
New
Duplicate
Disable
Delete
Anne
Peter
Willow
Password Restrictions - Common for All
Min. Length
6
chars
Lifetime
90
days
Expiration Warning
5
days
Password Reuse
180
days
Login Attempts
3
Auto Lock
10
min
New Password
Enter new password
Confirm (retype) the password
OK
Cancel
User
User Name
Anne
Desktop File
Clarity
Description
Laboratory Assistant
Blank
Change Password...
a
Access To
Instrument 1
Instrument 2
User Access Rights
Open User Accounts
Open Configuration
Edit Method
Edit Chromatogram
Edit Calibration
Projects
Import Chromatogram
Take Control of Locked Instrument
Edit Sequence
Edit Report Style
Select Method
Open Audit Trail
Open Audit Trail Settings
Archive / Restore
Post-run Options
Start Acquisition
Select Certificate...
Clear Certificate
OK
Cancel
Help

3.11 Disabling a user account

It is possible to disable a user account manually in the *User Accounts* dialog. Alternatively, accounts will get disabled automatically if *Login Attempts* are set, and the number of failed attempts was exceeded. It is not possible to log in to a disabled account, but it can be enabled again in the *User Accounts* dialog.

To disable or enable a user:

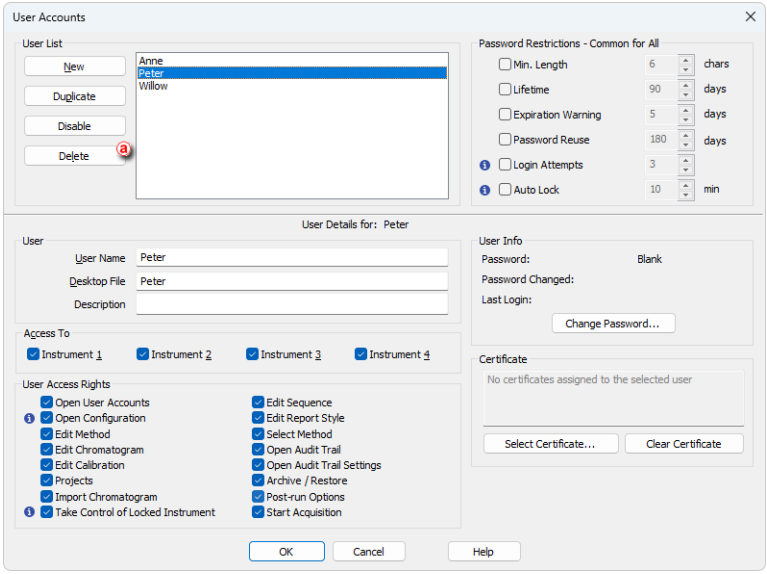
1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. Select the user in the *User List* and then click the *Disable/Enable* button ⓐ .
3. Click the *OK* button to accept the changes.



3.12 Deleting a user account

1. Open the *User Accounts* window: click on or choose *System - User Accounts*.
2. To delete a user, select the user in the *User List* and then click the *Delete* button ⓐ .
3. Click the *OK* button to accept the changes.

Note: It is possible to disable the *Delete* function in the *GLP Options* dialog.



4 Proposed workflow for routine analysis

Below there is description of a procedure that can be used for performing routine analysis of uniform samples. Steps are described in more details in linked topics.

1. Measure typical sample.
2. Adjust the integration of the chromatogram as needed. Details are described in How to integrate chromatogram topic.
3. Save the method including this adjusted integration. Details are described in Saving the chromatogram method as a method file topic.
4. Create model calibration that will be used in calibration cloning. Details are described in Creating model calibration to use in calibration cloning topic.
5. Set the calibration cloning in the sequence, method (and potentially in the calibration). Details are described in Calibrating using clone on first recalibration or Compensating for response drift using bracketing, Improving quantification with the standard addition method.
6. Create a sequence. Do not fill the levels of standard samples and post-run actions.
7. Run the sequence
8. Review the data. In case some minor adjustments are needed adjust the integration.
9. Fill in the Levels and post-run actions to the sequence file.

   Note: If you need to sign the documents and print the report with the signature, do not fill the Print actions in the sequence now. After the recalibration is performed, manually sign every chromatogram and then use Batch dialog - Post-run Options to print the reports with signatures.

10. In *Batch* dialog perform *Complete Processing* of the sequence. Details are described in Reprocessing whole sequence topic.
11. Now you have the sequence recalibrated, reports printed, and possibly other post-run actions performed.

5 Method Setup

Following chapters include useful tips regarding the *Method Setup* and working with method.

5.1 Setting up a method

The method essentially contains information on how the analysis will be performed, how the resulting signal will be processed and what events will be triggered and when.

Any method can be created or edited in the *Method Setup* window. To use the method for measurement it has to be sent to the instrument and for sequence measurement method has to be set at each row.

Method vs. Chromatogram Method

- The sent method specifies the acquisition and processing parameters of created chromatograms and its content is saved to the chromatogram file as "chromatogram method". Processing part of the method can be edited in the chromatogram after the measurement, the acquisition is available as read-only.
- The changes made in the chromatogram do not affect the method file.
- The calibration file is linked to the method and to the chromatogram by its name.

Method Setup window

- The title of the *Method Setup* dialog displays a name of currently opened method. If you make any changes, the method becomes (MODIFIED).
- The upper part of the Method Setup dialog displays a set of icons with which it's possible to create a new method, open existing method, save method, save method as, open *Report Setup*, open method audit trail, send method by e-mail or open help.
- Upon pressing the OK button, method will be saved and *Method Setup* dialog will close.
- Tabs shown in Method Setup window are dependent on devices actually configured on the Instrument, e.g. MS Method, PDA Method, LC Gradient can be only visible when proper instrument type and devices are set.

Send Method

- Only a method that is saved can be sent.
- Pressing the Send Method button will result in two actions:
    - Method will be sent to all connected hardware and thus displayed in the information table of the Instrument window.
    - Method will be set as method for Single Analysis - you can start the single analysis form the instrument window using the icon.

- When measuring sequence, each row can have different method. It is set while creating or editing the sequence tab in the *Method Name* column.

Method Development

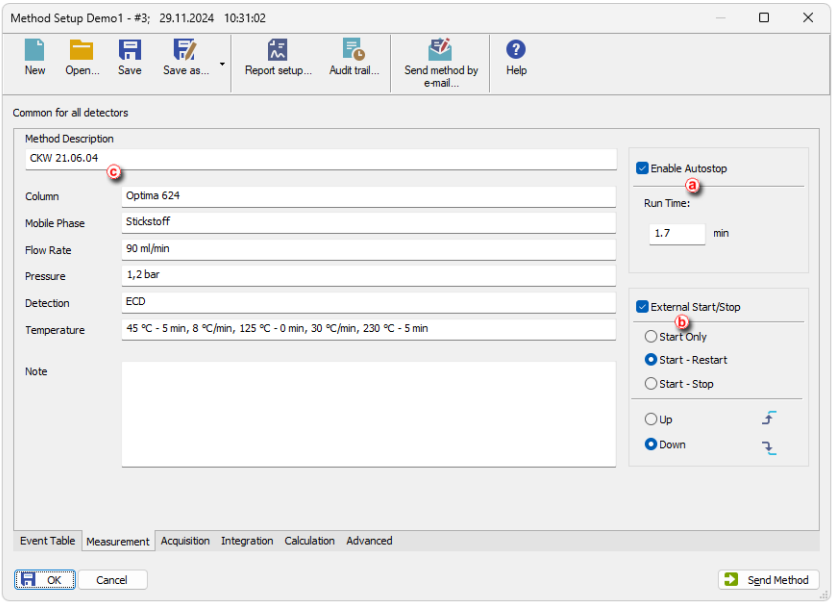
Method currently used for acquisition or present on already locked row of the sequence can't be edited, but can be viewed in read-only mode.

When developing a method, you can configure the following settings among others:

1. **Set the measurement conditions.**

   Here you can disable or enable *Autostop* and set the run time for the analysis ⓐ as well as configure the external signal start and stop settings ⓑ (default setting *Start Only* should be used in majority of applications). *Autostop* can be set within interval 0.2 - 9999 min, such value is not influenced and does not influence any device specific time program settings on different tabs (like *LC Gradient* or *GC*). When time defined in *Autostop* passes, acquisition is finished, chromatogram is created, remaining time from time programs will be spent in so-called *Control* state.

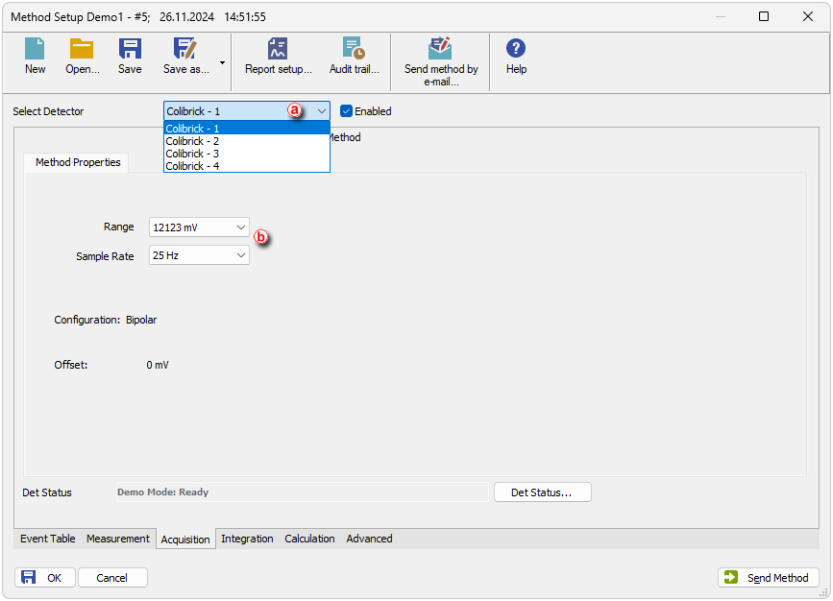
   You can also describe some parameters of the method and add a note ⓒ . Such information is purely informative and do not influence analysis in any way. They are saved into the resulting chromatogram.



2. **Set the Data Acquisition parameters.**

   It allows you to select, enable/disable the detector signals ⓐ and to set measurement parameters e.g., the signal range and sample rate ⓑ . At any time at least one detector has to be *Enabled*.

   Layout of this tab, together with possible parameters to be set, are dependent on the configured devices (control modules) on the Instrument.

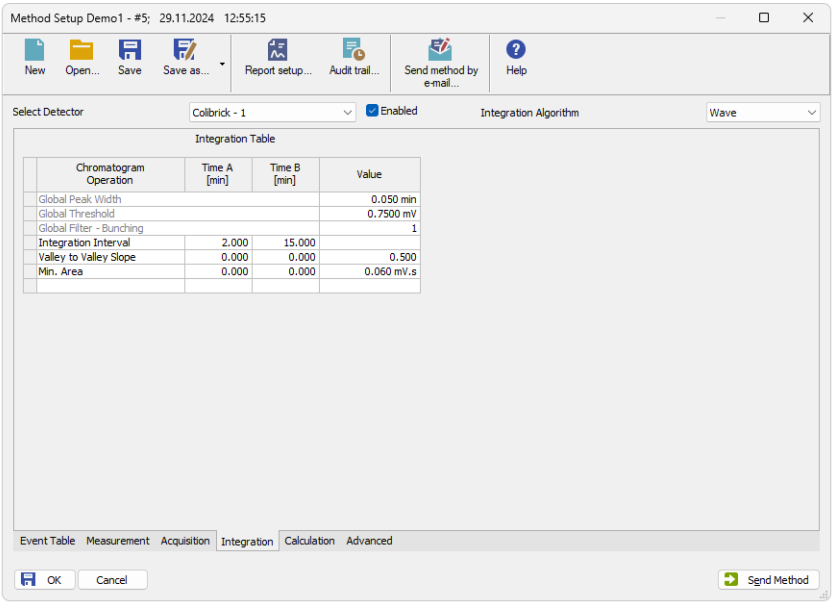


3. **Set the Signal Integration parameters.**

   When using a multi-detector configuration, there is an integration table for each signal, thus every signal can be integrated in a different way.

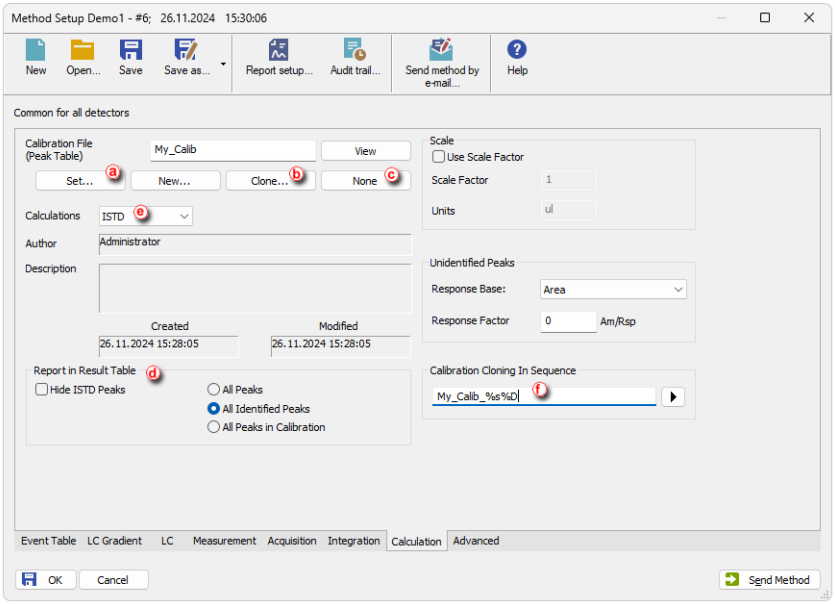
   Every resulting chromatogram acquired with such method will be integrated automatically accordingly the integration tab.

   If you aren't able to edit tab parameters the current detector, it probably isn't *Enabled*.



Note: Integration parameters are often modified manually after the first acquired chromatogram directly in the Chromatogram window. Then you can manually rewrite them into any method in the Method Setup dialog or you can use the *Method - Save as Method* menu command in the *Chromatogram* window to easily copy them into your method. For more details see the chapter **Saving the chromatogram method as a method file** on pg. **99**..

4. **Set the calculation options.**
   - You can create *New...* calibration file or *Set...* the one *created previously* ⓐ and configure the different settings related to it.
   - When calibration file is set, resulting chromatograms will be calibrated according to it and calibration standards will be used to automatically re-calibrate the attached calibration file.
   - *Clone...* ⓑ button will create a copy of a current calibration file. In the following *Save As* dialog you can select the name and location of the new calibration file. The copy will then be linked to the method.
   - If it is desired to have no calibration in the method you can use the *None* button ⓒ .
   - In this tab you can also choose how you want the results to appear in the results ⓓ and set calculation type ⓔ .
   - Name of calibration clone ⓕ must be set here to use calibration cloning in sequences, refer to chapter "Calibrating using clone on first recalibration" on page 141.



5. **Configure the settings in the additional tabs.**

   Method Setup also has tabs specific to currently configured devices, *Advanced* tab, *Aux. Devices* tab, *Aux. Signals* tab (where you can set which signal should be stored) and *Event Table* tab used for configuring what events will be triggered and when e.g. shutting down Clarity after the sequence is finished.

   However, there are some limitations of *Event Table*:

   - It is for specific purposes, not needed for standard analyses.
   - Does not have control against infinite loops.
   - Must be filled per row, Fill Down/Fill Series can't be used here.

Note: For more information on any of the settings above, press F1 in such Clarity window to go the corresponding section of the Help or use the **Clarity Reference Guide**.

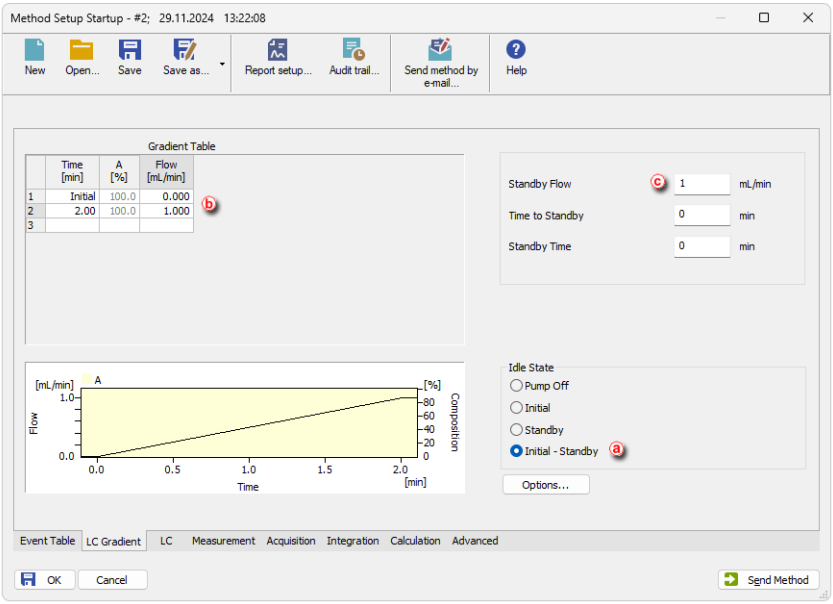
5.2 Setting up a slow flow rate increase and decrease on your LC pump

You can protect your chromatograph column from sudden pressure changes by setting up a *Sequence* together with three different methods, *Startup*, *Shutdown* and *Analysis* to ensure a slow flow rate increase and decrease on your LC pump. This procedure is mainly recommended for pumps controlled by Zebrick D/A converter or UNI Ruby scripts due to less strict pressure limit controls in these control types.

- Set the *Instrument Method Sending* option to "Do not send Method to Instrument", opposite to the topic ***Automatic sending of a method to an instrument after each change***.

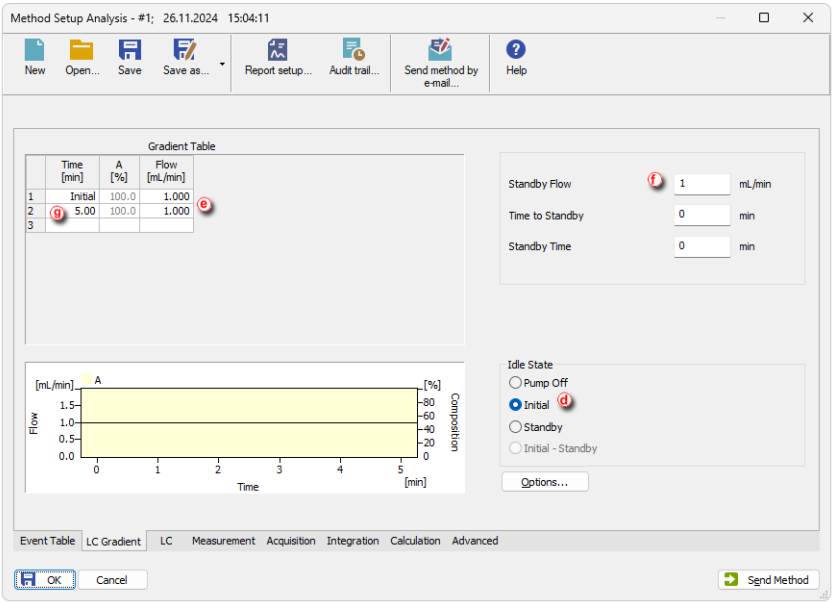
Startup Method

1. From the *Instrument* window open the *Method Setup* window using the *Method - Method Setup* command or the *Method Setup*  icon.
2. Create *New Method* and *Save* it under the name *Startup*.
3. Navigate to the *Method Setup - LC Gradient* tab.
4. Set the *Idle State* to *Initial - Standby* ⓐ .
5. In the *Gradient Table*, ⓑ set the *Initial Flow* to 0 and on the second row set the *Flow* to its *Standby Flow* value ⓒ and the *Time* to obtain the appropriate flow rate increase for your column.
6. Click OK to accept the changes.



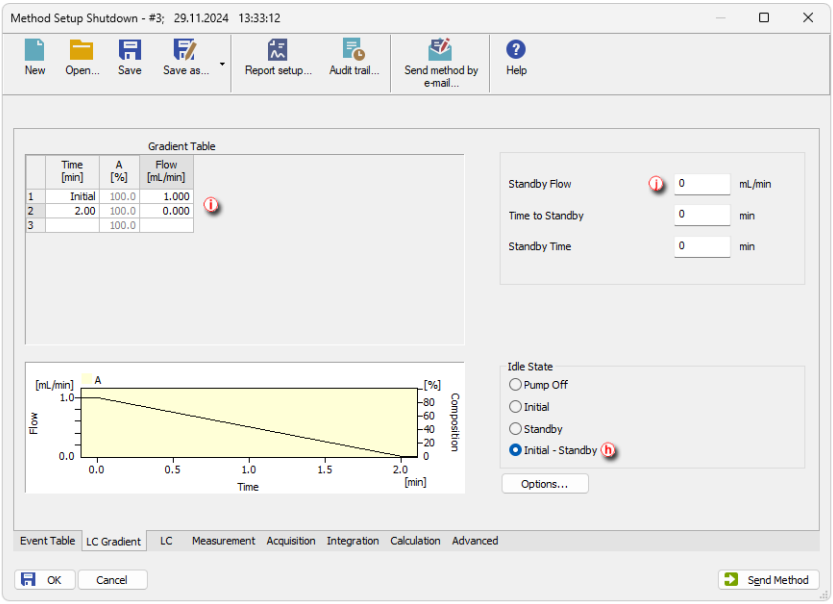
Analysis Method

7. Repeat steps 2 to 6 but this time:
    - Save the *Method* under the name *Analysis*.
    - Set the *Idle State* to *Initial* ⓓ .
    - Set the *Initial Flow*, *Flow* on the second row ⓔ and *Standby Flow* value ⓕ to the value of *Standby Flow* from *Startup* method.
    - Set the *Time* to the total duration of your analysis ⓖ .



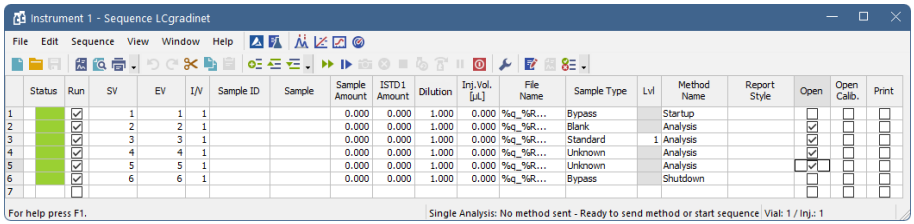
Shutdown Method

8. Repeat steps 2 to 6 but this time:
   - Save the *Method* under the name *Shutdown*.
   - Set the *Idle State* to *Initial - Standby* ⓗ .
   - On the second row, set the *Flow* to 0 and the *Time* to obtain the appropriate flow rate decrease for your column ⓘ .
   - Set the *Standby Flow* to 0 ⓙ .



Sequence

9. Set up a *Sequence* as explained in ***Running a Sequence*** and:
   - On the first row set the *Sample Type* column as *Bypass* and the *Method Name* to *Startup*.
   - On the last row set the *Sample Type* column as *Bypass* and the *Method Name* to *Shutdown*.
   - Set as many rows as you need in between according to the conditions of your analysis or sequence and set the *Method Name* to *Analysis*.



5.3 Event Table

The following chapters contain some useful tips on using the functions of the *Method Setup - Event Table*.

5.3.1 How to make a mark in a chromatogram during acquisition

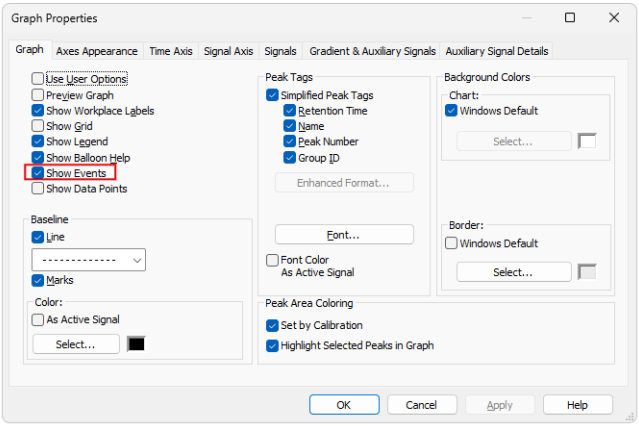
To create a mark in a chromatogram, you can use the *Event Table* tab from the *Method Setup* dialog and any hardware with digital input (such as Colibrick A/D converter) or the Virtual Digital Input Output Loop module. With the proper settings, triggering the digital input is recorded as an event, creating a mark (a vertical line labeled with name and RT) in the *Data Acquisition* and *Chromatogram* windows. The digital input can be triggered by pressing the start button when using HW or by pressing the corresponding Digital Output in the *Device Monitor* when using the Virtual Digital Input Output Loop module.

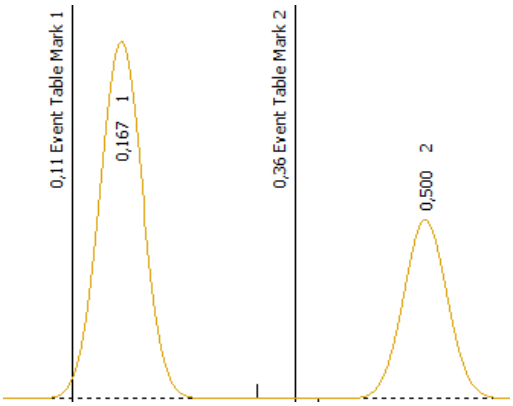
The following settings are necessary:

- HW with a digital input or the Virtual Digital Input Output Loop module configured to an Instrument.
- *Method Setup*
  - *Measurement* tab - *External Start/Stop* enabled and set to *Start Only*
  - *Event Table* tab - set according to the image below, where:
    - Name = the label of the event
    - Source = the module providing the digital input
    - Input = digital input recording the event

	Name	Input					Output			
		Type	Source	Input	Value	Units	Output Type	Output	Parameter	Store
1	Mark	Dig. Input Run	Colibrick	Digital Input 2	Down	---	None			☑
2										☐

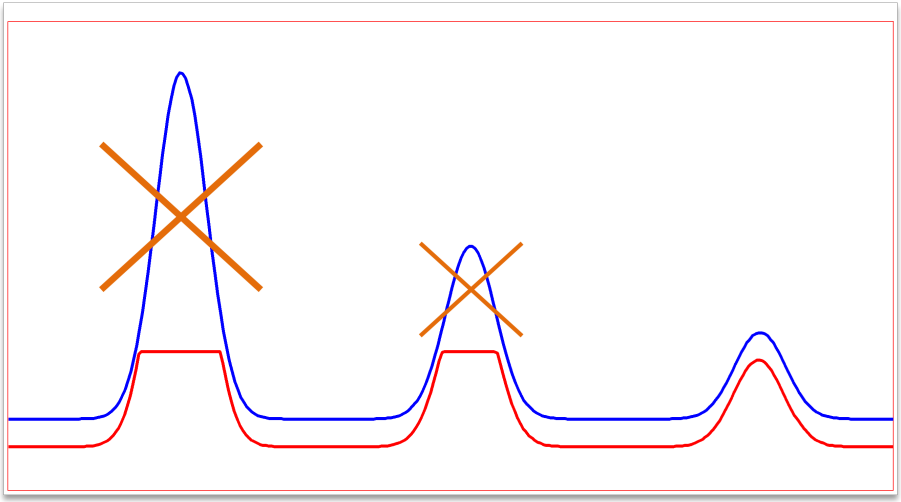
- To display the marks, enable the *Show Events* option in the *Graph Properties* dialog accessible from the *Data Acquisition* and *Chromatogram* windows (the dialog can be invoked by right-clicking the graph area in the respective window and clicking *Properties*...).





5.3.2 Signal out of range indication

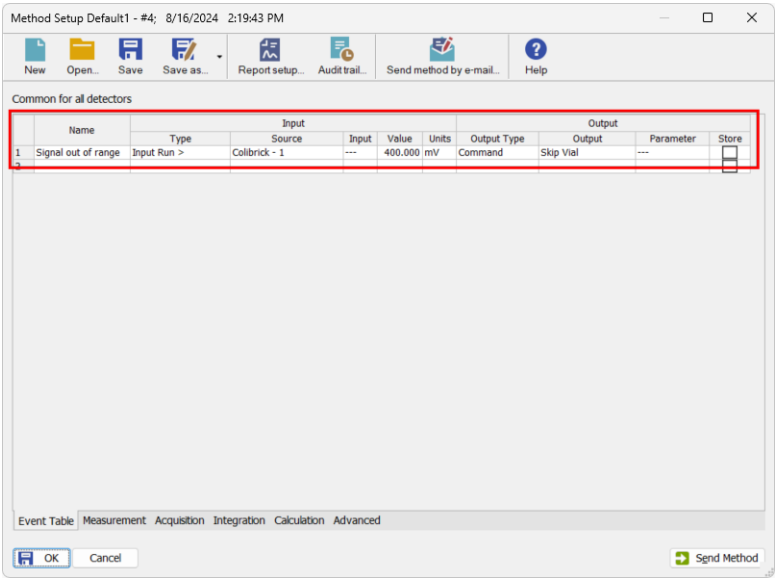
Under specific circumstances, it might occur that a portion of a peak is cut at top. This is caused by the signal being out of range of the current detector or A/D converter:



It is possible to indicate that a signal has reached a value out of the detector range via scheduling an event in the Event table. Such event needs to be triggered by the signal reaching a specific value, that is right below the detector maximum.

For that, set the event according to the following steps:

1. Open the *Method Setup* and prepare the method as necessary (or open an already existing method).
2. Switch to the *Event Table* tab.
3. Fill in the first row of the table:
    a. *Name* (e.g., Signal out of range)
    b. *Type - Input Run >*
    c. *Source* - your detector or A/D converter
    d. *Value* - slightly below the maximum range
    e. *Output Type* and *Output* - based on your requirements, for example *Abort*.

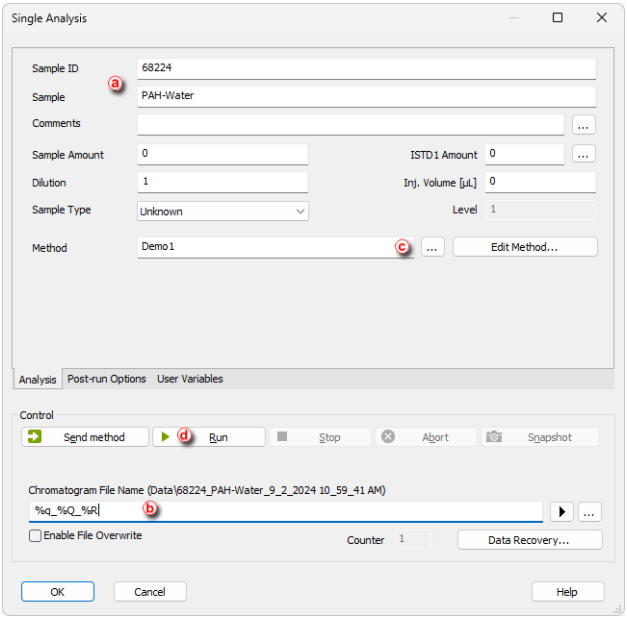


Once the entered input value is surpassed, the specified output event is triggered. Suitable output events also include alarm activation, close a contact, etc.

Note: Solvent peaks typically surpass the detector range. Consider the presence of a solvent peak in the sample before setting output events such as *Abort*, *Skip vial*, etc.

6 Running a single analysis

1. Open the *Single Analysis* dialog by selecting *Analysis - Single* or by clicking the icon in the *Instrument* window.
2. Fill in the sample information in the *Sample ID* and/or *Sample* fields ⓐ .
3. Fill in the *Chromatogram File Name* ⓑ . It is recommended to use variables to do so, for example, *%q* (*Sample ID*) and *%n* (counter) or *%R* (date and time) to prevent file name conflicts. Name preview is displayed above the field. For more info regarding variables see "Chromatogram File Name" in the Clarity Reference Guide.
4. Select the *Method* ⓒ which should be used for measurement. It is also possible to edit it by clicking *Edit Method*.
5. What should happen after analysis like automatic report printing can be set on the *Post-run Options* tab.



6. Start the analysis by clicking the *Run* button ⓓ . Analysis can be triggered also by an *External Start* from the chromatograph. The Instrument will switch to the *RUNNING* state and the *Single Analysis* dialog will close. The state is visible in the status line of the *Instrument* window.
7. It is possible to monitor the analysis from the *Data Acquisition* window, see Pre-evaluating a chromatogram during acquisition for more information.

7 Sequence

Chapters describing how to perform a measurement using *Sequence* and how to work in sequence window efficiently.

7.1 Creating and running a sequence

1. Open the *Sequence* window using the *Analysis - Sequence* command or the icon in the *Instrument* window.
2. Create a new sequence file using the icon ⓐ . or open an already existing sequence ⓑ . If you already have a sequence ready skip to step 12.
3. Save the new sequence using *File - Save As*…. Set the sequence file name and location in the *Save As* dialog.
4. Check the checkbox of the first (empty) row in the *Run* column ⓒ to add it to the sequence. The row will be pre-filled with default data, or with settings from the previous row.
5. Fill in the *Sample ID* and/or *Sample* columns ⓓ .
6. Fill in the *File Name* ⓔ . It is recommended to use variables to prevent file name conflicts, for example, *%q* (*Sample ID*), *%n* (counter), and *%R* (date and time). Hold the mouse pointer over the file name field to see the resulting name. For more information about variables, see "Chromatogram File Name" in the Clarity Reference Guide.
7. The *SV* (Starting Vial) and *EV* (End Vial) rows ⓕ will be pre-filled with numbers corresponding to the sample position in the autosampler tray, if you are using an autosampler. These can be changed as needed; it is also possible to inject from multiple vials in one sequence row.
8. Fill in the volume of the injection in the *Inj. Vol.* column ⓖ .
9. Select the method to be used for the measurement in the *Method Name* column.
10. Tick any of the *Open, Open Calib., Print* etc., columns ⓗ in case you wish to open the measured chromatogram in the *Chromatogram* or *Calibration* windows or print the results after each measurement of a sample.

    Caution: To correctly include chromatographs in the reports, it is necessary to check both the *Open* and *Print* checkboxes. It is also necessary to fill in *Report Style* when *Print* or *Print to PDF* is used.

11. Repeat steps 4-10 for subsequent rows you need to add to the Sequence Table.

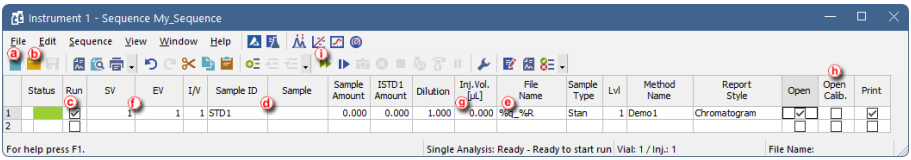
    Note: It is possible to display columns with additional parameters and post-run options by right-clicking the sequence table, selecting the *Setup Columns* command and moving items from the *Hide Columns* to the *Show Columns* list using the *Show* button.

12. Check the validity of the prepared sequence using *Sequence - Check Sequence* or by clicking the icon. In a valid sequence, all rows will show the mark

in the *Status* column. Invalid sequences will issue a warning message describing the cause of the problem.

13. Save the sequence using *File - Save* or the icon.
14. Run the prepared sequence using *Sequence - Run* or the icon ⓘ .

Note: The sequence state will change to the *WAITING FOR INJECTION* or *INJECTING* state, depending on the *READY* state of other controlled modules. The state is visible at the bottom of the *Sequence* window.



7.2 Editing the template for new sequences

Clarity allows you to customize the template from which all new sequences are created. By modifying this template, every newly created sequence will automatically contain predefined parameters, calibration standards, control samples, or any other recurring lines needed for your workflow.

How to edit sequence template:

1. Select *File - Open…*from the *Sequence window* to display the *Open Sequence* dialog.
2. Navigate to the COMMON directory (located in C:\CLARITY\DATAFILES by default) and open the file TEMPLATE.SEQ. (Special templates are available for EA and GPC Extensions)
3. Edit the sequence as needed – including *Sequence Options*, default parameters, calibration standards, control samples, or other recurring rows.
4. Save the template.

Any new sequence created using *File - New* will now use the updated template and automatically include all predefined settings and lines.

The TEMPLATE.SEQ file in the COMMON directory is shared by the entire Clarity station, so any changes apply to all instruments using this directory. It is however possible to set custom locations of the Project directories for each *Instrument* with it own COMMON directory and therefore separate sequence template files. For more information, see chapter "Setting up project directories"

Caution: When importing a sequence file, the TEMPLATE.SEQ settings are ignored. The sequence is created strictly according to the import settings, regardless of any template configuration.

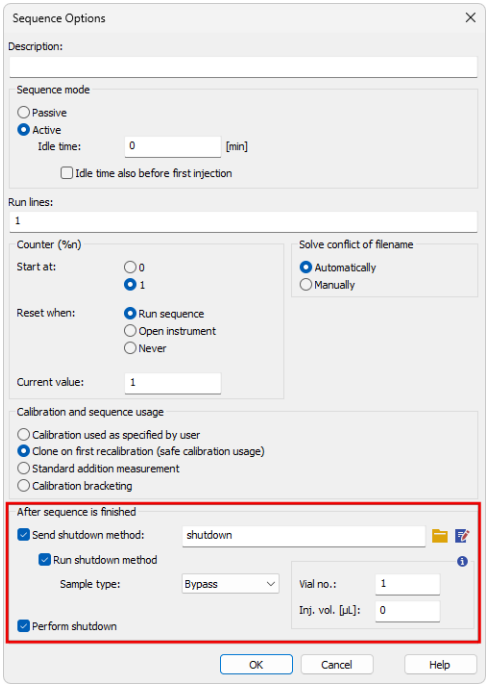
7.3 Shut down after finishing a sequence

After a sequence is finished, it might be convenient to send (and run) a shutdown method and/or perform shutdown. As the behavior of the used (controlled) devices may be quite specific, there are multiple options on how to get them to the desired standby state. For example, some detectors may be able to perform a run with lamps turned off or switch them off after end of a run, while others will not get to the *READY* state without the lamp on. A proper combination of the possible actions needs to be set accordingly.

1. To setup the shutdown parameters, open the *Sequence Options* in the current sequence using *Sequence - Options* or the  icon.
2. Now, you need to decide whether you only need to send the shutdown method to the controlled devices to prepare them for the shutdown (step 3), or if you also need to run the selected method, e.g., for adjusting the gradient (steps 3 and 4). As mentioned in the beginning of this chapter, these settings are highly depended on the individual control module capabilities.
3. *Send shutdown method:* checkbox: Check this checkbox to send the selected shutdown method to the controlled devices. You can select or open/edit the method using the accompanying buttons. This option will only send the selected method to devices.
4. *Run shutdown method* checkbox: Use this option to run the selected method. The resulting chromatogram will be saved to the current project as [SEQUENCENAME - SHUTDOWN - METHODNAME - %R.PRM], where the %R variable stands for the current date and time.

   Note: Use the sample type *Bypass* to omit injection from a vial, or *Unknown* for injection from a specified vial. Valid vial position and injection volume may be required by some autosamplers, even if the injection will not be performed (i.e., when the method is not run or the *Bypass* sample type is selected).

5. *Perform shutdown* checkbox: Use this option to shut down all controlled devices. The shutdown command is sent after completing the run of the shutdown method. Note that the reaction of some devices to the shutdown command may be adjusted in their respective *Setup* window in the *System Configuration*.



Note: The parameters of the *After sequence is finished* section are also executed when the user stops the sequence using the *Stop* command or when the sequence is stopped by an error. If it is necessary to stop the running sequence without sending (and running) the shutdown method, use the *Abort* command.

Note: When a sequence including the shutdown procedure is finished and new rows are added to the sequence, and such sequence is then resumed, the whole *After sequence is finished* will be applied again after the new rows are measured.

7.4 How to run analysis using sequence without autosampler

This section explains how to use a *Sequence Table* to start acquisitions in systems without an autosampler (also applies to a situation with an autosampler that is not directly controlled by the software) and measure a set of samples. In many cases, defining a sequence is more straightforward than performing a multiple *Single Analysis* runs. The sequence table allows you to specify different parameters and measurement conditions for each sample (row) in advance.

Depending on your setup, you can run a predefined sequence of injections either manually or automatically — even in the absence of an autosampler. The exact procedure depends on your hardware configuration and the method used to initiate

data acquisition. Sequence requires external start (individual analysis in sequence cannot be started by *Run* command from Clarity user interface). There are two ways to start an acquisition from the sequence table.

7.4.1 Using sequence for manual injections

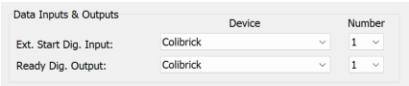
You could define parameters for a series of injections in advance in a sequence table and then inject them one by one manually. When you start the sequence it sends method to the controlled devices and waits for an external start/input. Once initiated, the individual analysis begin — this can for example be achieved by using Run button directly on the device or by activating the synchronization valve via Colibrick, as described below. Each analysis must be triggered individually in this manner.

Note: When the sequence is started, Clarity will be waiting for external start detected as a change in Digital Input state set as *Ext. Start Dig. Input* in *System Configuration* or by a start marker in digitally acquired detector signal data. The start of the measurement can be triggered by a digital input or by the signal from the detector.

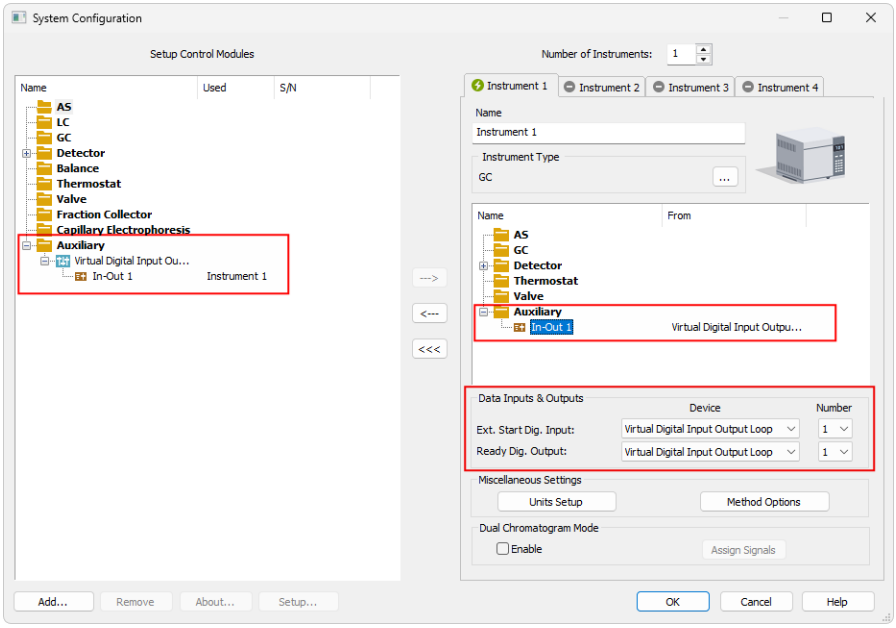
7.4.2 Using sequence for automatic injections without an autosampler

In such case, the sequence must be set to *Active Mode*. This is the default setting and you can activate it via *Sequence - Options* or by clicking the icon. In this mode, the system sends a sequence start command to the sampler to execute the injection (via serial line or digital output configured as a *Ready Dig. Output* in *System Configuration*) and waits for a start signal from the sampler or the detector (received via communication line) or by change in the *Ext. Start Dig. Input*. When no autosampler is used, this process needs to be emulated by directly interconnecting the *Ready Dig. Output* with *Ext. Start Dig. Input*.

In case the A/D converter (Colibrick) is used, the leads for the IN1 and OutR1 on the Colibrick could be directly interconnected.



When no A/D converter is used, the *Virtual Digital Input Output Loop auxiliary device* (requires A24 LC or A23 GC Control license) cold be used to simulate the input/output needed - (those are virtually interconnected). The actual injection triggering depends on the connected hardware.



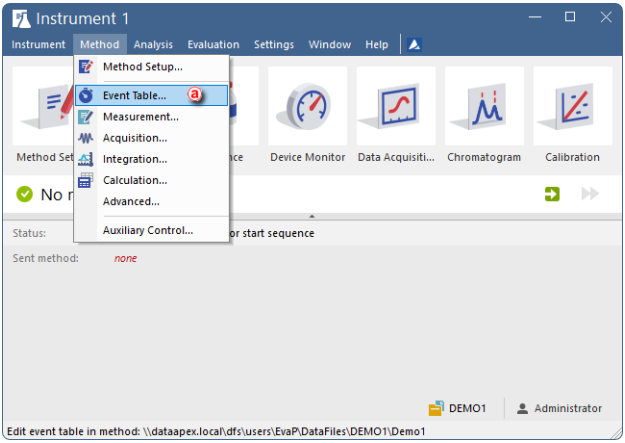
Note: For more detailed info about adding new device (Virtual Digital Input Output Loop) see also "Adding a new device" on page 25.

For analyzers triggered by external contact, but not providing inject marker output signal, the start input could be connected in parallel to the Colibrick Ready Out cable (used typically for EA analyzers or Gow Mac process chromatographs).

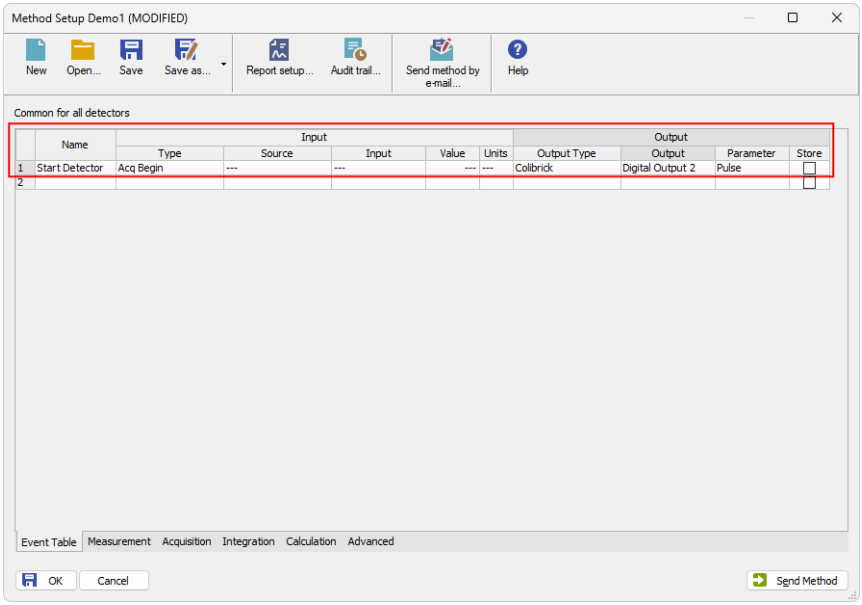
In case the injection is performed by independently controlled valve the injection is then performed during the actual run by switching the valve (or valves) from the Clarity *Event Table*. When the injection valve is controlled through the GC, its switching must be programmed in the GC method Time or *Event Table*.

To set the *Event Table*:

1. Open the *Method Setup* on the *Event Table* ⓐ tab and prepare the method as necessary (or open an already existing method).



2. Fill in the first row of the table as shown in the figure below, and save the method. The example shown illustrates just one of several possible setups. It this example once the acquisition is started Colibrick sends a pulse via its Output 2, triggering a device connected there.



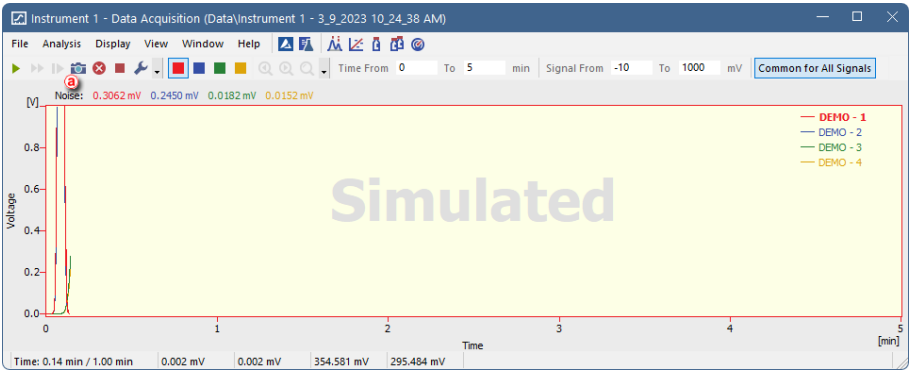
Note: This example of the event table refers to the configuration where the valve is not part of the setup and is controlled via Colibrick. Alternatively, if the valve is instrument-controlled, the output would be connected directly to the valve instead of Colibrick.

8 Pre-evaluating a chromatogram during acquisition

1. Open the *Data Acquisition* window by selecting the *Window - Data Acquisition* command or click the icon in the *Instrument* window.

2. To create a temporary chromatogram, select the *Analysis - Snapshot* option or click the icon ⓐ. Every time you take a snapshot, a temporary chromatogram will be created again from the analysis start up to the moment when you clicked.

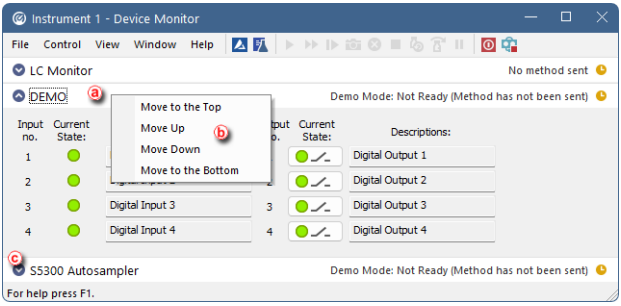
Caution: To preserve a snapshot, it has to be saved under a new name. Otherwise it will be overwritten once the analysis is finished and the final chromatogram is created.



9 Device Monitor

The *Device Monitor* window serves firstly to show the current status of each control module and secondly for direct control of the device. The layout and possible control options greatly vary based on the used control modules.

The window can be personalized. To change the order of individual monitors right click on the module's name ⓐ and choose desired action in the *context menu* ⓑ. The individual monitor panel can be collapsed or expanded using the arrow icon ⓒ in the header of the panel.

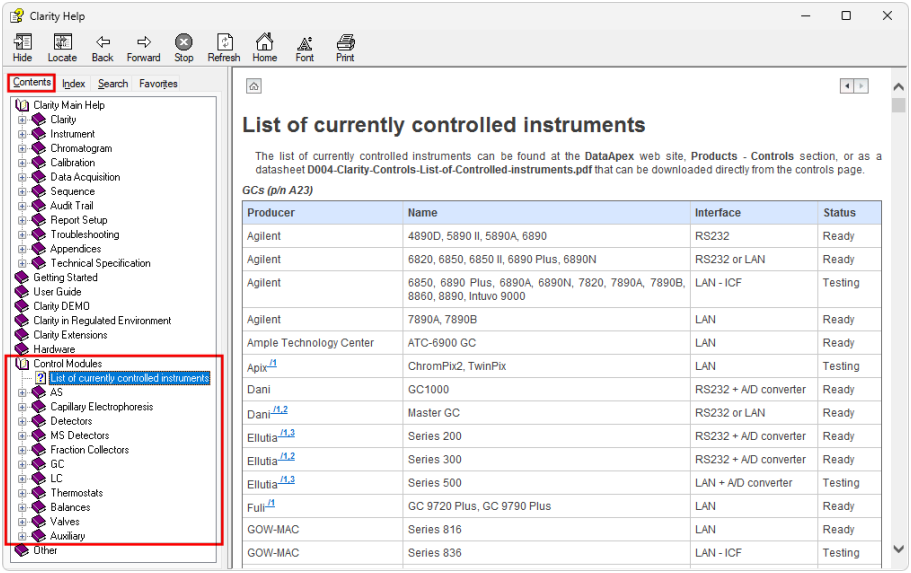


9.1 How to set parameters during run

Besides performing some service commands outside run, in some cases it is possible to perform some actions also during run. This is individual for specific control modules and could be found in the help or manual of respective control module. Control module helps are located at the bottom of the *Contents tab* of **Clarity** help which can be invoked by pressing *F1*. Manuals are available at www.dataapex.com/downloads.

Caution: Manuals are not available for all controlled devices. Control modules developed by third parties are only supplied with help file.

Common actions available for the pumps are described in next chapter.



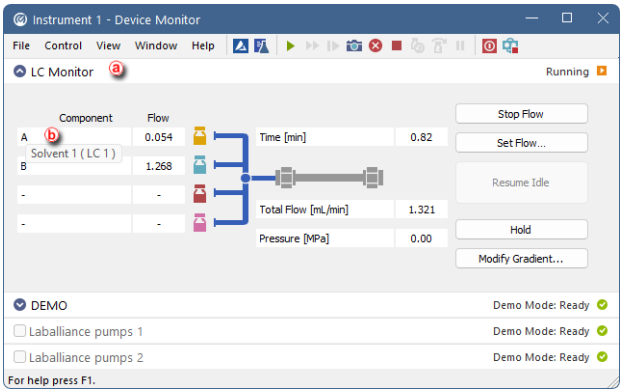
9.2 How to directly control LC gradient pumps during run

To control the configured LC pumps directly from **Clarity**, the *Device Monitor* contains the *LC Monitor* ⓐ section common to up to four pumps (i.e., a maximum of four solvents). Any combination of isocratic and gradient pumps can be used. If more than four pumps are needed, any additional pump has to be added as an auxiliary pump.

Note: The tooltip over each component shows the name of the pump ⓑ .

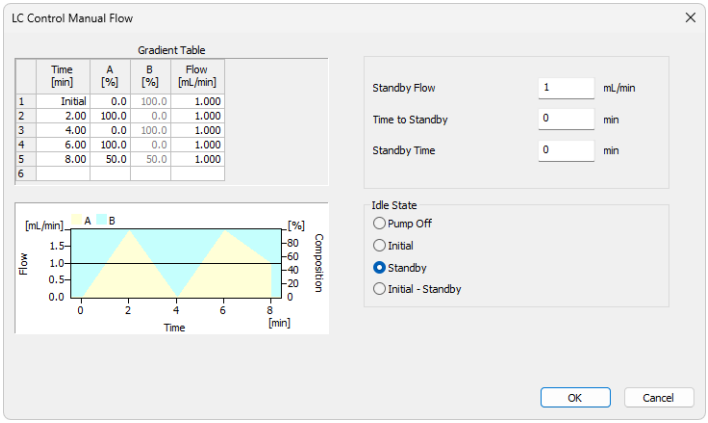
In the *LC Monitor* section of the *Device Monitor*, it is possible to:

- *Stop Flow* (the pump is stopped without stopping analysis) and *Set Flow* (a custom flow rate and composition can be set). Both of these buttons can be used outside or during analysis. Beware that when used during analysis, the gradient from the method cannot be restored and the set flow will be used for the rest of acquisition.
- *Resume Idle* switches the pump to the idle state as defined in *Method Setup - LC Gradient* tab.



Further commands are available for selected pumps (typically those controlled by **Clarity** in real time). They are enabled only during runs with a gradient program.

- *Hold* halts the gradient at its current state. The button changes to *Resume* which can be used to resume the gradient from the point where it was halted.
- *Modify Gradient* invokes the *LC Control Manual Flow* dialog (similar to the *Method Setup - LC Gradient*) which can be used to adjust the gradient for the current analysis. This does not influence the method used for analysis in any way.


LC Control Manual Flow
Gradient Table
Time [min] A [%] B [%] Flow [mL/min]
1 Initial 0.0 100.0 1.000
2 2.00 100.0 0.0 1.000
3 4.00 0.0 100.0 1.000
4 6.00 100.0 0.0 1.000
5 8.00 50.0 50.0 1.000
6
Standby Flow 1 mL/min
Time to Standby 0 min
Standby Time 0 min
Idle State
Pump Off
Initial
Standby
Initial - Standby
[mL/min]
A B
[%]
Flow
Composition
Time
[min]
OK
Cancel

10 Chromatogram Editing

This chapter focuses mainly on adjusting integration. For proposed general workflow see chapter How to integrate chromatogram

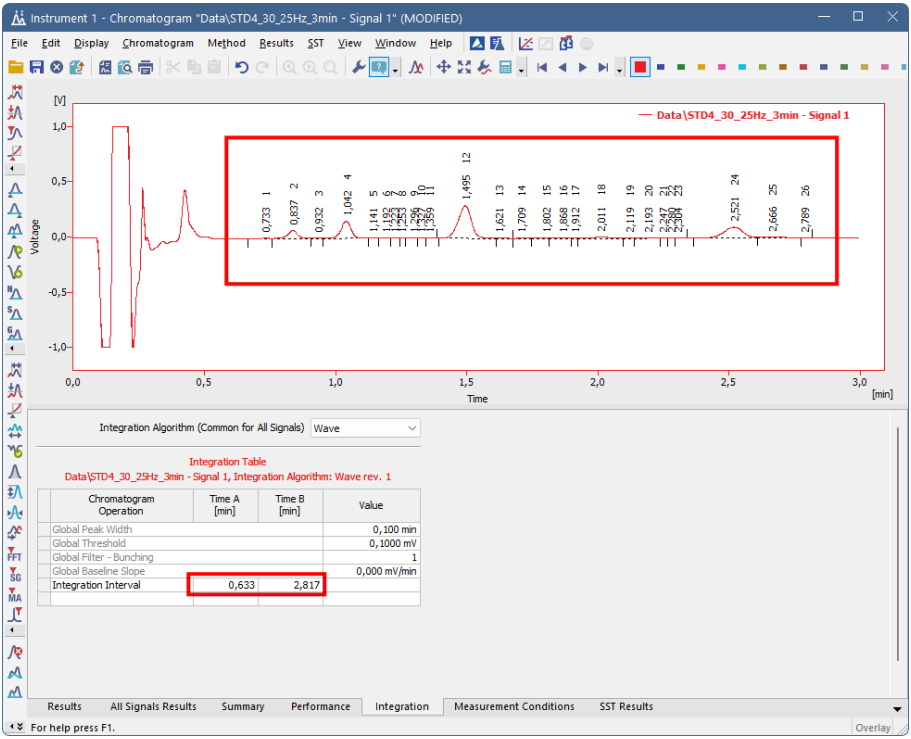
Clarity Tips&Tricks videos covering Integration topics can be found in Clarity Integration playlist.

10.1 How to integrate a chromatogram

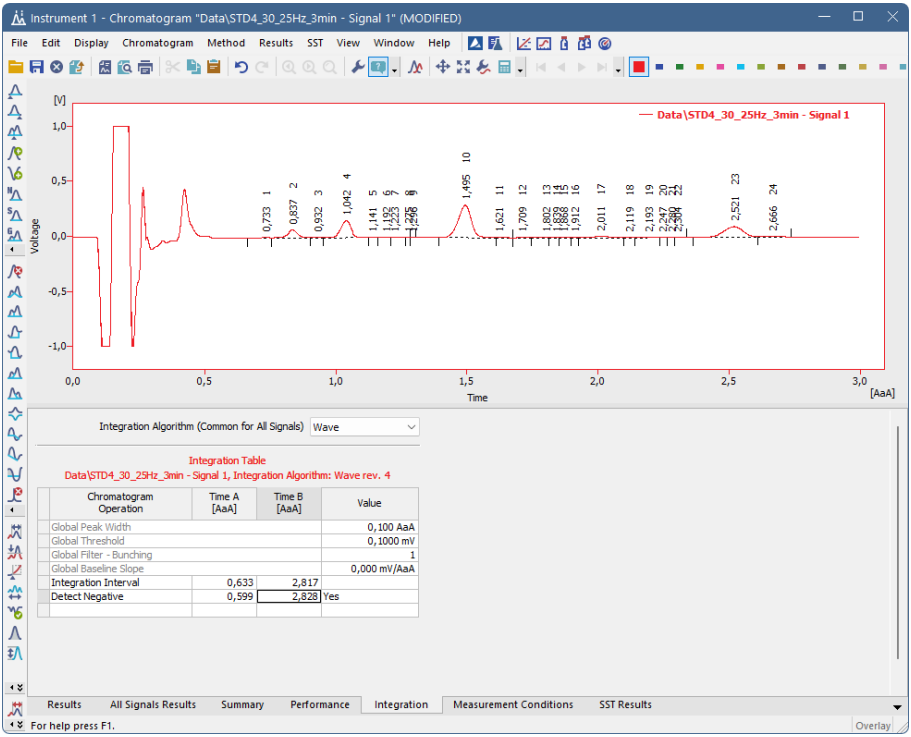
In order to automate the integration of routine samples as much as possible, it is necessary to optimize integration parameters and save them to the method used for measurements. Two integration algorithms (Wave and Legacy) are available, providing slightly different integration procedures. If you cannot achieve satisfactory integration using one of the algorithms, try using the other one. You can select which integration algorithm to use on the *Integration* tab of the *Method Setup* or *Chromatogram* windows.

1. Open one typical chromatogram for your analysis. Before adjusting integration parameters, it may be helpful to optimize the chromatogram display; see Adjusting Display of Chromatogram for details.

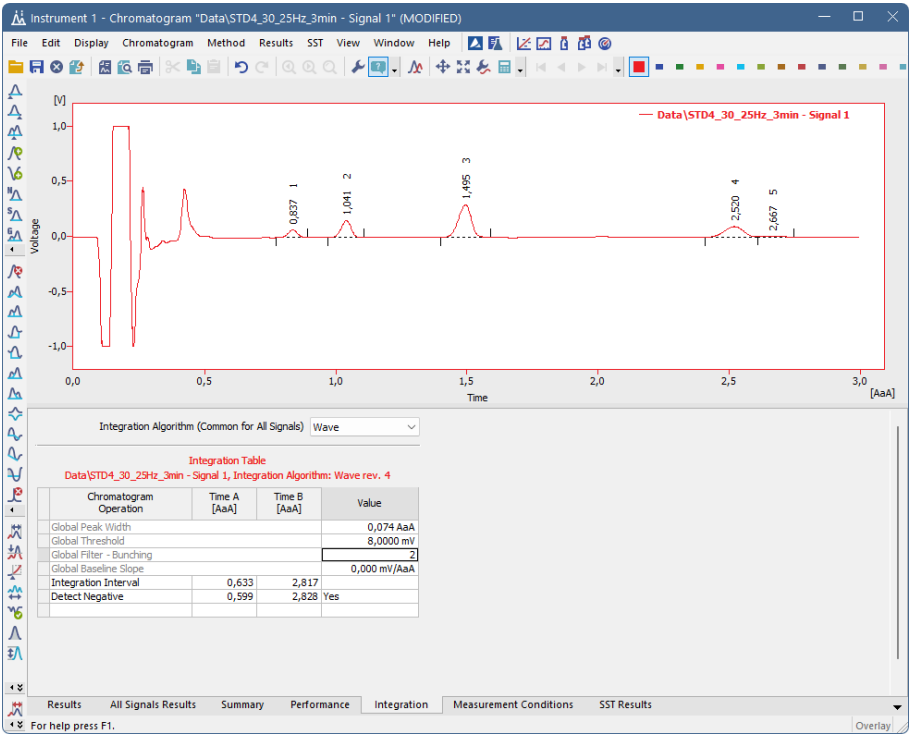
2. Set the *Integration Interval* as needed. More details can be found in the Setting Integration Interval topic.



3. (Optional) Set the *Detect Negative* parameter. This setting has two potential uses: firstly, it can be used when you want to integrate negative peaks; secondly, it may help when the signal has inconsistencies such as dips. This will prevent the integration algorithm from placing peak starts/ends into them.

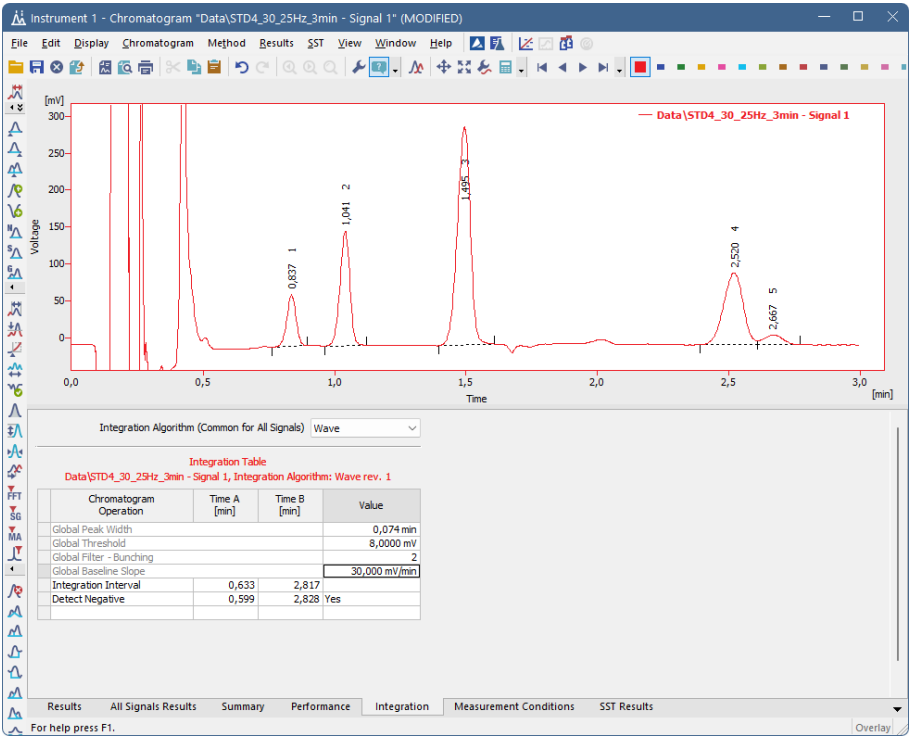


4. Set the *Global Peak Width* parameter. Choose the narrowest peak which should be integrated in your chromatogram and select its start and end. This setting is used for calculation of *Global Filter - Bunching*.
5. Set the *Global Filter - Bunching* parameter. This is a filter which is calculated based on the *Global Peak Width* and sample rate.
    a. Alternatively, for chromatograms with a high noise, it is possible to use other filters - *FFT Filter*, *Savitzky-Golay Filter* or *Moving Average Filter*.
6. Set the *Global Threshold* parameter. This is influenced by the *Global Filter - Bunching* or other filter set previously. Select an interval containing only noise, not peaks. A more detailed description of the global parameters is covered by the topic Modifying Global parameters.



7. Set the *Global Baseline Slope* parameter. Change this parameter after you have all the peaks integrated, it servers to optimize their start/end positions.

Note: The *Global Baseline Slope* option is available only when using the Wave integration algorithm.



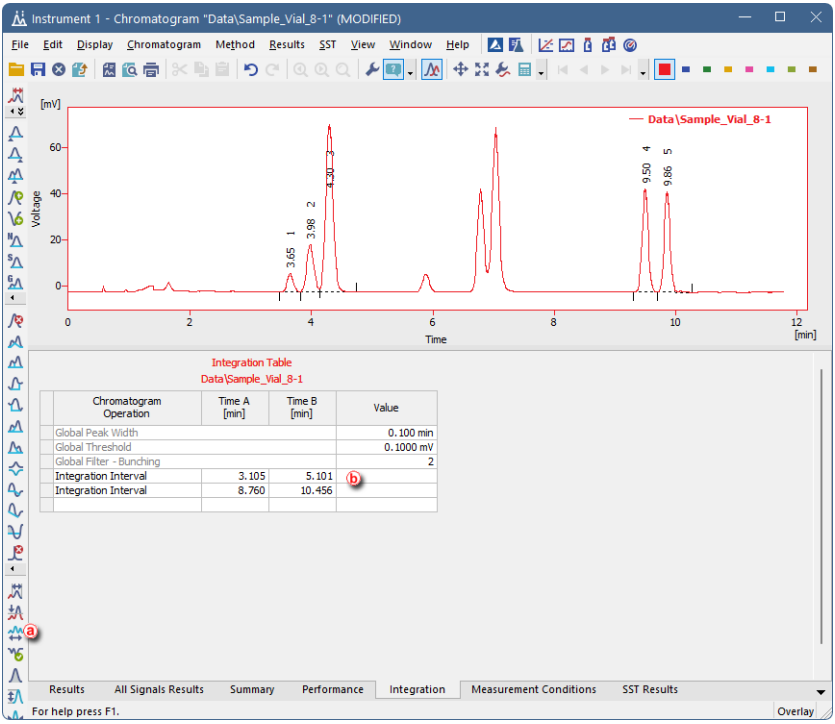
8. If you are still not satisfied with the integration, there are some other options for manual changes.
    a. Try to use some *Interval* parameters such as *Baseline Together*, *Baseline Valley*, *Forward Horizontal* etc..
    b. Or try to use some *Peak* parameters such as *Peak Start*, *Peak End*, *Peak Both*, *Add Positive* etc.

Note: The *Add Positive* operation should be used as the last resort because it is sensitive to retention time shifts. *Peak Start* and *Peak End* should be the preferred parameters as they are defined relative to peak apex.

9. When you are happy with the integration, you can Save chromatogram method as method file and use it for further measurements of similar sample types.
10. If you have already measured some chromatograms and want to use these integration parameters on them you can do it using the Batch - Reprocess by Method.

10.1.1 Setting the integration interval

1. Signal outside of the interval is not integrated, this function is mainly useful for omitting solvent peaks etc.
2. To set the interval on which to apply the integration use *Chromatogram - Integration - Integration Interval* or  icon ⓐ . It is possible to set multiple intervals within a single chromatogram.
3. You can check, modify the interval or delete this operations in the *Integration Table* ⓑ .



Note: If you want to exclude specific interval from the integration refer to ***Remove peak from integration***.

10.1.2 Modifying Global parameters

Peaks are only integrated if they exceed a minimum width (*Global Peak Width*) and height (*Global Threshold*). The *Global Baseline Slope* parameter influences the position of peak starts and ends. These parameters can be applied both globally or locally in a specified interval. It is always recommended to maximally utilize global parameters before using any local ones. *Global Filter - Bunching* works as a smoothing filter, it can to be applied only globally (to the whole chromatogram).

Global Peak Width:

- To adjust the minimum peak width use *Chromatogram - Global Peak Width* or the  icon ⓐ and select the narrowest peak you want to integrate.

Global Threshold:

- To adjust the minimum peak height use *Chromatogram - Global Threshold* or the  icon ⓐ and select an interval containing only noise, not peaks.

Global Filter - Bunching:

- Works as a smoothing filter that automatically averages number of data points in order to preserve at least 30 data points per narrowest peak. It is dependent on the *Global Peak Width* value. To use it, use *Chromatogram - Global Filter - Bunching* or the  icon ⓐ after you are done adjusting the *Global Peak Width* parameter.

Global Baseline Slope:

- To adjust the minimum slope where the peak should start/end, use *Chromatogram - Global Baseline Slope* or the  icon ⓐ and select the point where the peak should start/end.

Note: Available only in Wave Integration Algorithm.

If you are still not happy with the integration suggested by selection from the graph, you can manually modify the parameter values in the *Integration Table* ⓑ .

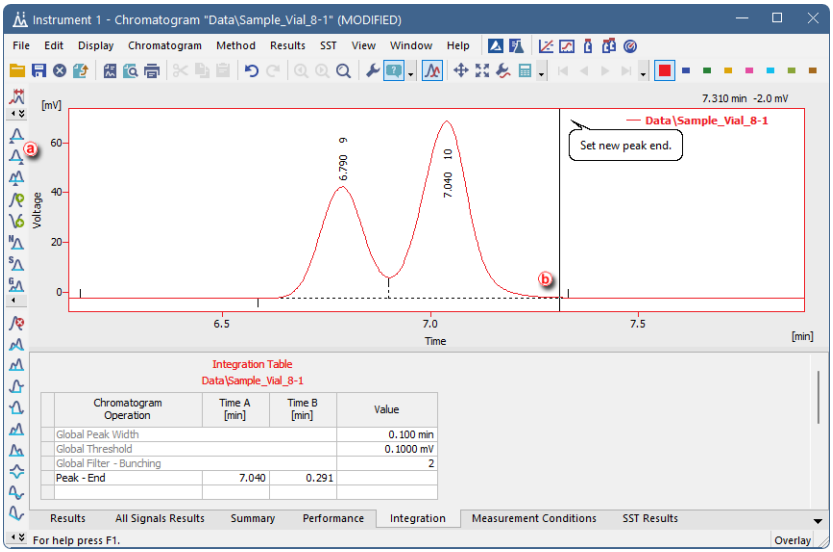
Setting the Local variants of Global parameters:

1. Setting local parameters is similar to the global ones, the only difference is that they are only applied on the selected time interval rather than the entire chromatogram.
2. To set a local parameter, use the *Chromatogram - Integration* context menu and select the parameter you need. Similarly, you can find the icon in the bottom part of the vertical toolbar ⓒ . Select the desired time interval in the graph. A small dialog appears ⓓ , where you can further specify the time interval and mainly select the value of the parameter. You can use the *Suggest Value* button ⓔ to select the value from the graph same as for a global parameter.
3. Again, all values can be further modified in the *Integration Table* if needed.

Note: *Global Filter - Bunching* is a filter that is always applied to the whole chromatogram. To filter data locally, use other filers from the *Chromatogram - Integration* menu.

10.1.3 Modifying the beginning and the end of a peak

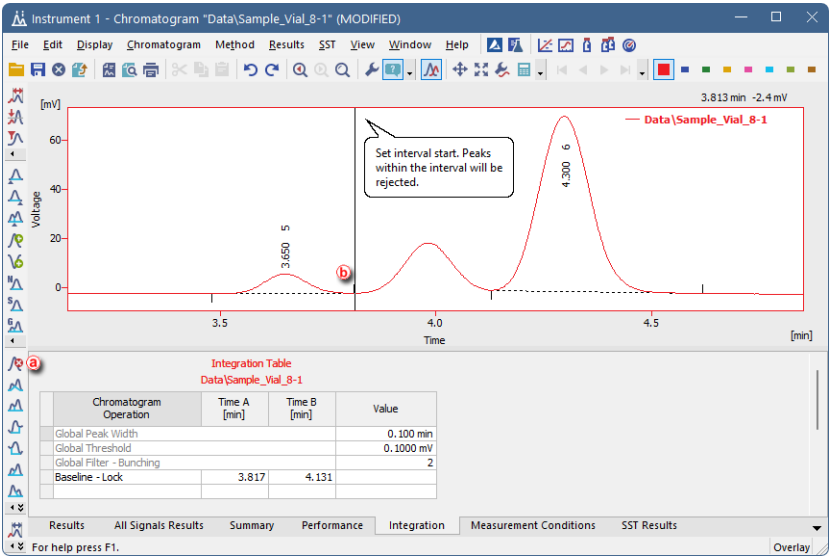
1. To change the position of peak beginning and/or end use *Chromatogram - Peak - Start* and/or *Chromatogram - Peak - End* alternatively use  and/or  icons ⓐ .
2. Set the new beginning ⓑ and/or end by clicking the new position in chromatogram graph.

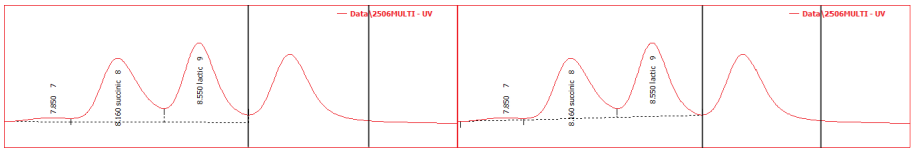


10.1.4 Removing a peak from integration manually

With the introduction of the WAVE integration algorithm, there are now 2 ways to remove the peak from the integration. First one is present also in a Legacy Integration algorithm, the second is exclusive for the Wave IA.

1. Use *Chromatogram - Baseline - Lock* (or icon ⓐ) or *Chromatogram - Peak - Hide*.
2. Click once to mark the start of the interval that should be omitted from integration and click second time to mark its end ⓑ .





Difference between Peak Hide (left) and Baseline Lock (right).

Note the two vertical guidelines marking the beginning and end of the peak. More than one peak can be removed from integration at once.

10.1.4.1 Baseline - Lock

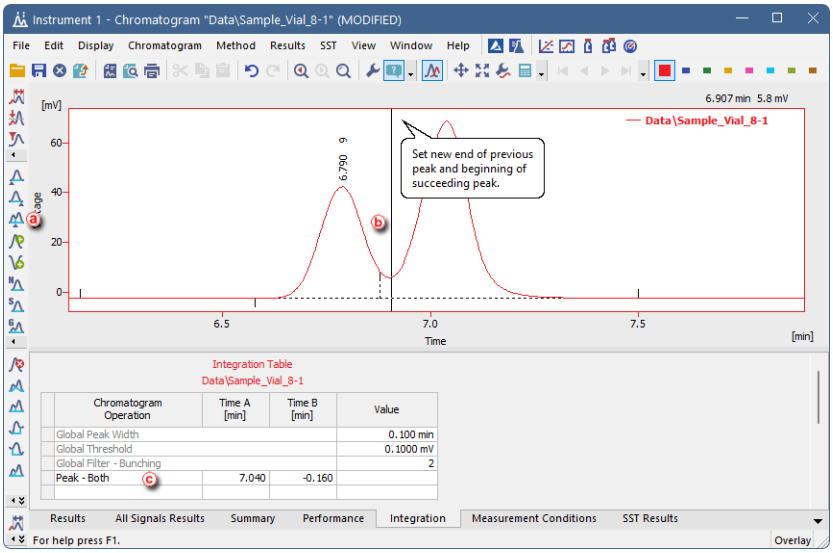
This tool completely removes all peaks that have their maxima within a set time interval. This could affect other peaks with maxima outside the specified window, particularly if they share the same baseline.

10.1.4.2 Peak - Hide (and Show)

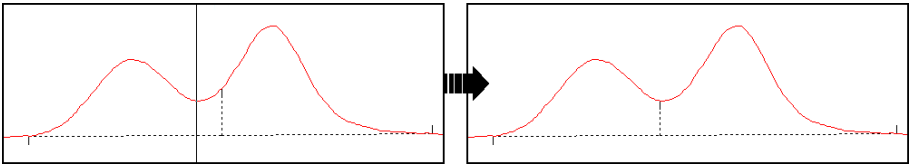
By default, the Wave algorithm might automatically ignore some of the minor peaks identified during integration. However, completely eliminating these peaks could potentially affect the baseline's trajectory. Therefore, these functions offer a flexible way to handle unwanted peaks without completely removing them.

10.1.5 Changing the position of a peak separating line

1. Select *Chromatogram - Peak - Both* or click in the *Peak* toolbar ⓐ .
2. Set the new position of peak-separating line by clicking in the chromatogram graph ⓑ .
3. You can check, modify the position or delete this operation in the *Integration Table* ⓒ .

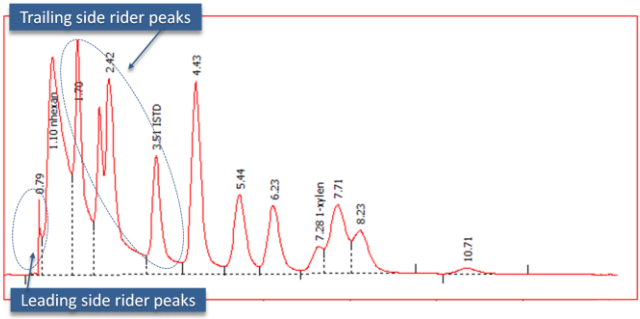


Note the vertical guideline indicating the currently selected peak separator position.



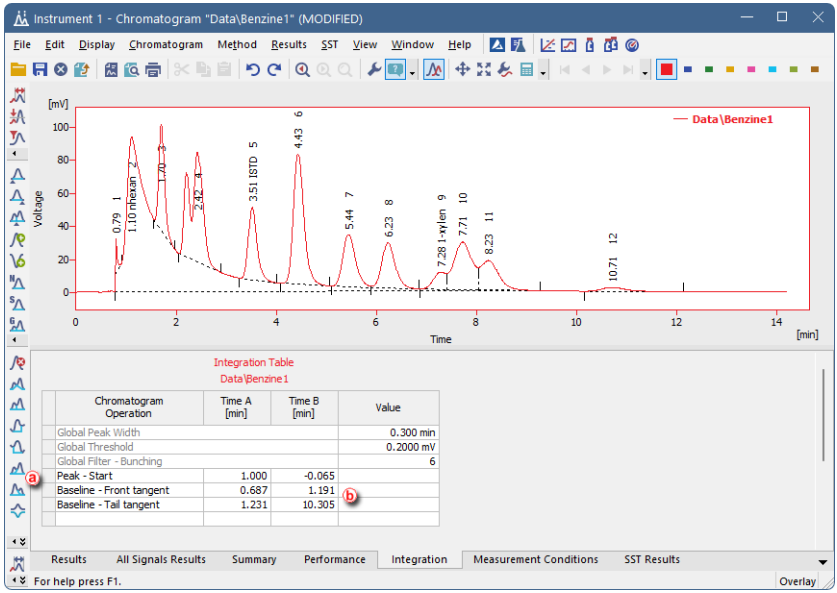
10.1.6 Separating rider peaks by tangent

Rider peaks are small peaks which are not well resolved from a large and asymmetrical neighbor but sit on its leading or trailing side.



1. Select the rider peaks you want to separate on the leading side of the mother peak: use *Chromatogram - Baseline - Front Tangent* or icon ⓐ .
2. Select the rider peaks you want to separate on the trailing side of the mother peak: use *Chromatogram - Baseline - Tail Tangent* or icon ⓐ .
3. You can check, modify the interval or delete this operations in the *Integration Table* (*Baseline - Front tangent* and *Baseline - Tail tangent* rows) ⓑ .

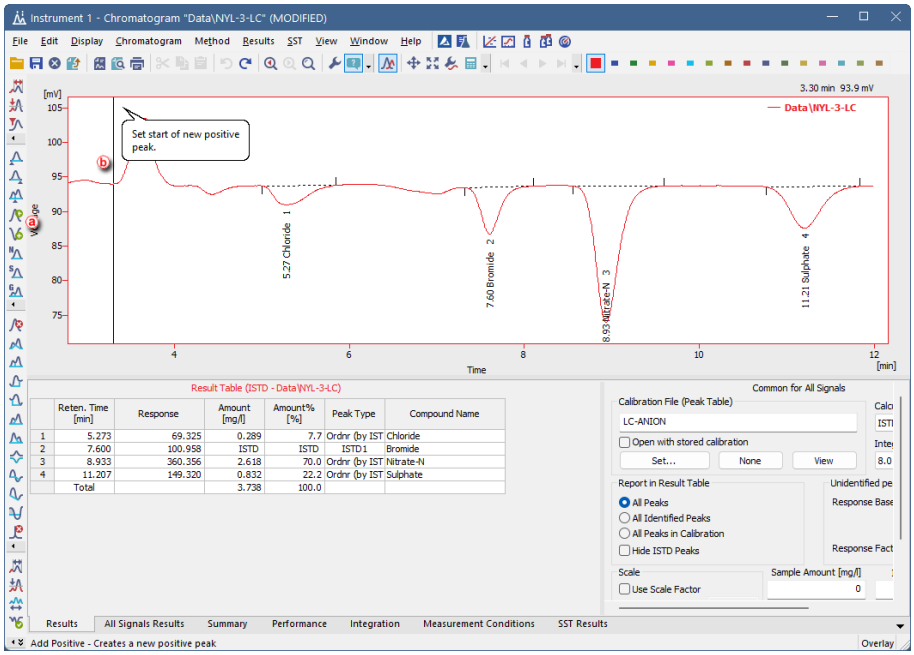
Note: You can also use the *Tangent Slope Ratio* and *Tangent Area Ratio* from *Chromatogram - Separation* menu to set a threshold for the separation of rider peaks based on those two parameters.


Instrument 1 - Chromatogram "Data\Benzine1" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[mV]
Voltage
Data\Benzine1
0.79 1
1.10 nhexan 2
1.70 3
2.42 4
3.51 ISTD 5
4.43 6
5.44 7
6.23 8
7.28 1-xylen 9
7.71 10
8.23 11
10.71 12
Time
[min]
Integration Table
Data\Benzine1
Chromatogram Operation
Time A [min]
Time B [min]
Value
Global Peak Width 0.300 min
Global Threshold 0.2000 mV
Global Filter - Bunching 6
Peak - Start 1.000 -0.065
Baseline - Front tangent 0.687 1.191
Baseline - Tail tangent 1.231 10.305
Results
All Signals Results
Summary
Performance
Integration
Measurement Conditions
SST Results
For help press F1.
Overlay

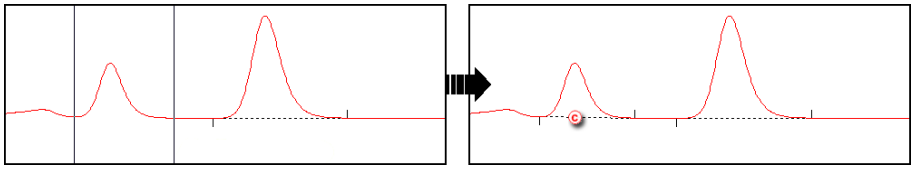
10.1.7 Adding a new peak manually

Caution: Manual addition of a peak should be used as a last resort to finish integration of individual chromatograms. Since the function is based on absolute time, when saved in the method used for acquisition results might be inaccurate if retention time shift occurs.

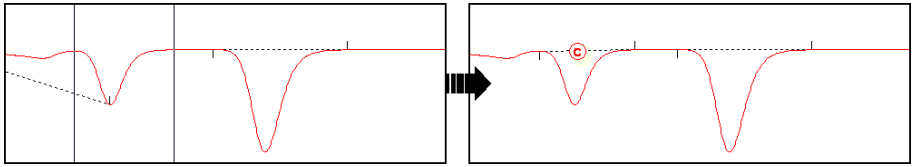
1. Select *Chromatogram - Peak - Add Positive/Negative* (also accessible from context menu) or click and in the *Peak* toolbar ⓐ . Holding Ctrl key while selecting the function will allow you to use it repeatedly.
2. Click in the chromatogram and set the beginning ⓑ and the end of a new peak.



Note the two vertical guidelines marking the beginning and end of the peak. After finishing the operation new peak is added ⓒ .



Add Positive

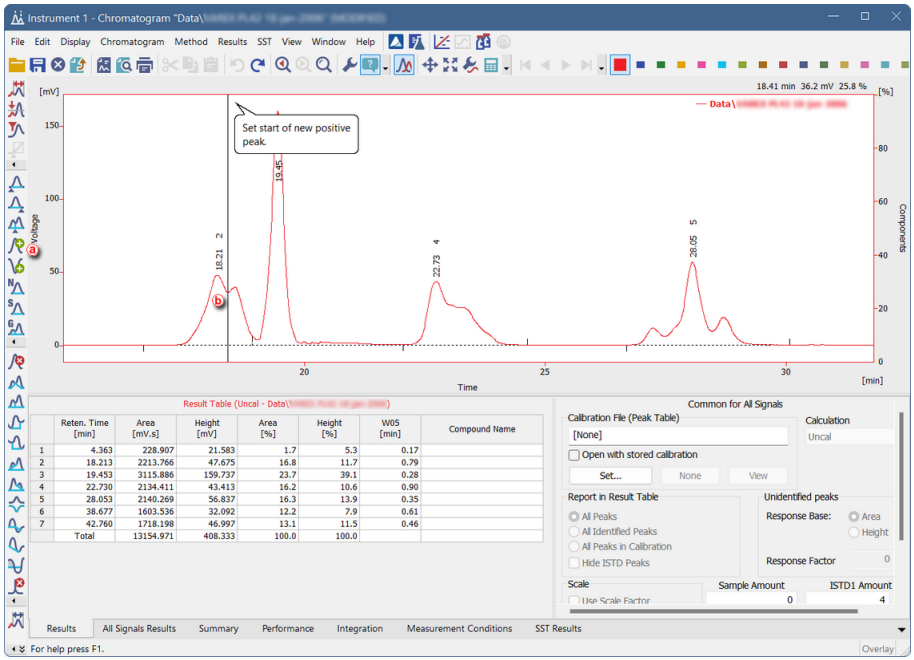


Add Negative

10.1.8 Splitting unresolved peaks using Add positive

The *Add positive* function can be also used for splitting unresolved peaks. Make sure to apply the function on the smaller part of the unresolved peak.

1. Select *Chromatogram - Peak - Add Positive* (also accessible from context menu) or click in the *Peak* toolbar ⓐ .
2. Click in the chromatogram and set the beginning ⓑ and the end of the smaller part of an unresolved peak.



A vertical guideline will appear dividing the unresolved peak.

10.2 Saving the chromatogram method as a method file

Each chromatogram contains saved copy of the method used for acquisition of such chromatogram. However, changes done in *Chromatogram* window (e.g. *Description, Integration Parameters, linked Calibration File*...) are not updated in the original method used for acquisition nor processing. To amend your method accordingly, you can create method from the parameters stored in chromatogram, which is useful after optimizing integration parameters.

1. Open the chromatogram with optimized method.
2. Select the *Method - Save as Method…* to save the method (including the changes made by you) from the current chromatogram as a new method, or for example overwrite (update) your acquisition method.

Note: It is not possible to overwrite any method that is currently in use, for example a method opened on any Instrument.

10.3 Adding or deleting a peak from a group

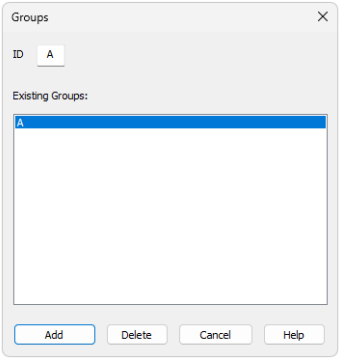
Groups in Clarity are used to combine multiple peaks so they can be evaluated together (by summing their areas, heights, etc.). This is useful when related compounds produce separate but closely eluting peaks that should be treated as one component in quantification and reporting.

It is possible to assign multiple intervals to a single group but peak can belong to only one group, so group intervals must not overlap. If the groups interval overlaps, the interval that was added last takes priority.

Adding a peak to a group

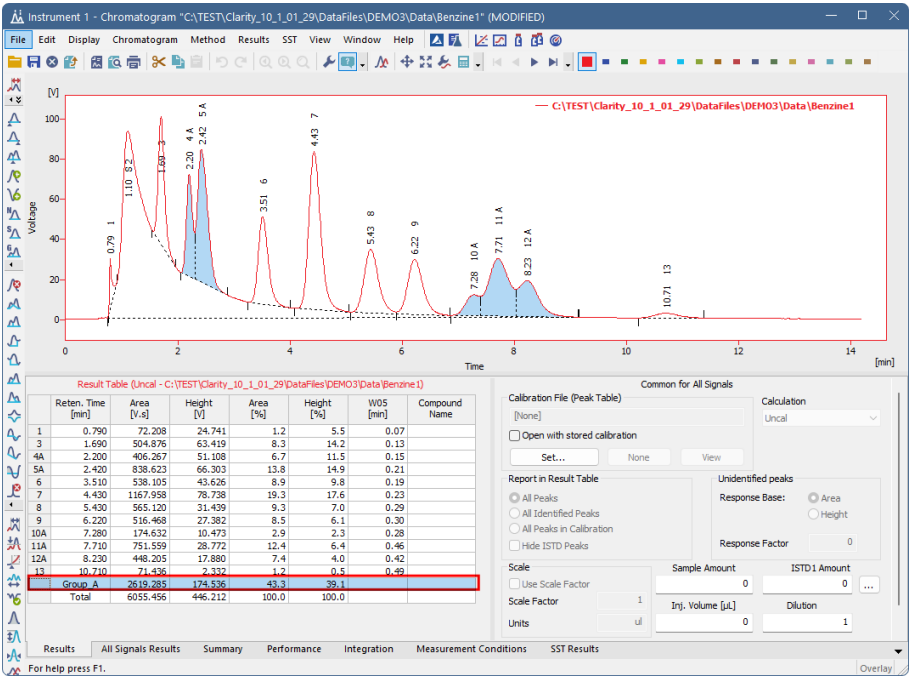
Follow the steps below to add peak to a group:

1. In *Chromatogram* window, open the chromatogram in which you want to group peaks.
2. Use the *Chromatogram - Peak - Peak Groups…* command or the *Group* icon to invoke the *Groups* dialog.



3. Select an existing group from the list or create a new one by entering a letter to *ID*field. A *Group ID* has to be a single capital letter symbol (26 letters of the English alphabet can be used). Entering the *ID* of a group that already has at least one peak highlights that group in the *Existing Groups* list.
4. Click *Add*.
5. The cursor will be locked to the chromatogram graph. Click once to set the start point and click again to set the end point of the time interval. All peaks with a maximum inside of the selected interval will be added to the group.
6. If you want to add an additional peak to a group, select the group in the *Groups* dialog and click *Add*.
7. Same as before, the cursor will lock in the chromatogram graph and you can select another time interval. All peaks with a maximum inside of the selected interval will be added to the group.

New row will be inserted in the *Result Table* that displays the summed values for all peaks in the group. Each peak in the group has its *Group ID* displayed next to its row number. If the *Group ID* option in the *Graph Properties* dialog is enabled, the group's capital letter is shown in the chromatogram at the peak label. When you select the group row in the *Results Table*, the peaks in that group are highlighted in the chromatogram.



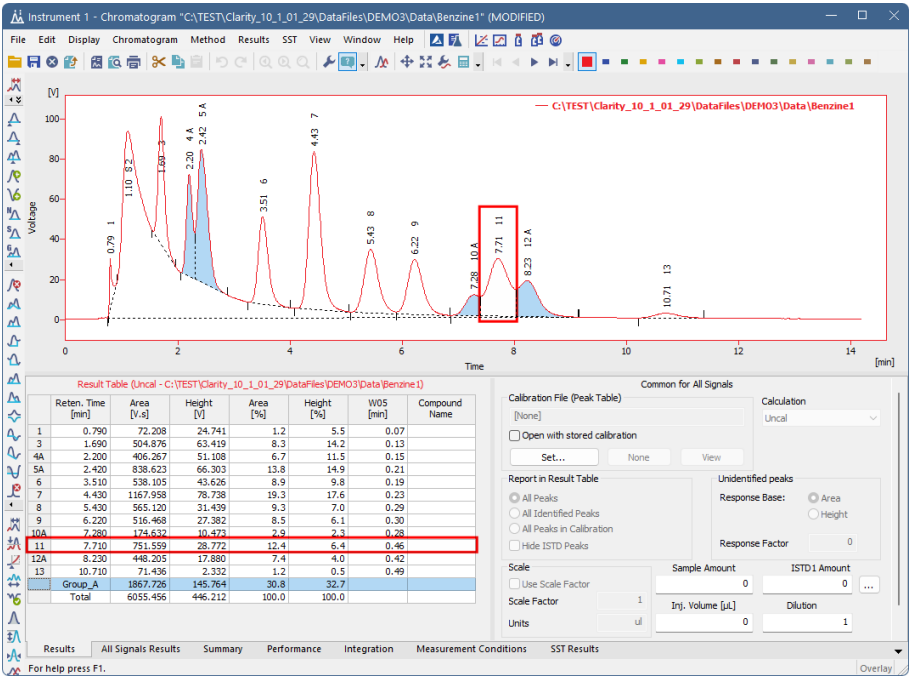
For correct display of results in the *Chromatogram* window that include groups, the groups must also be added into the calibration. For more information, see Adding a group to calibration.

Deleting a peak from a group

Follow the steps below to delete a peak from a group:

1. Use the *Chromatogram - Peak - Peak Groups…* command or the *Group* icon to invoke the *Groups* dialog.
2. In the dialog, select an existing group and click *Delete*.
3. The cursor will be locked to the chromatogram graph. Select the time interval in which the peak you want to delete from a group is located.

Peak is deleted from the group, the change is reflected both in the chromatogram and in the *Results Table*. The values in the *Results Table* are automatically recalculated. Deleting a peak from the middle of an interval provides an alternative to creating two separate intervals.



10.4 Adjusting display of chromatogram

You can customize the appearance of the chromatogram graph using the *Graph Properties* dialog available in the *Chromatogram* window to suit your specific needs. Below are a few useful examples of how you can adjust the display to better highlight the information you care about.

For tips on how to work with multiple signals/chromatograms, see the Working with individual signals of a multisignal chromatogram smoothly topic.

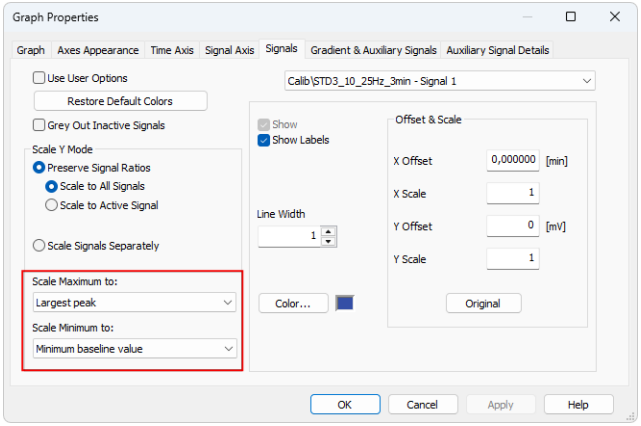
You can open the *Graph Properties* dialog either by right-clicking in the chromatogram graph area and selecting it from the local menu, or via the *Display - Properties...* menu.

Automatically scale the signal Y-axis to the integrated region

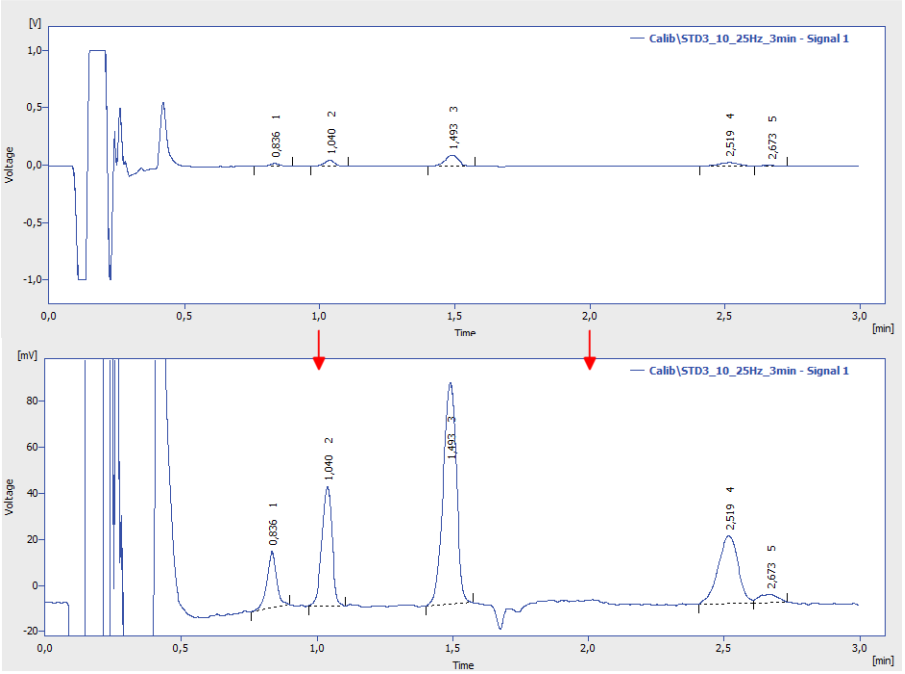
In Graph Properties, go to the *Signals* tab, where you can set how the signal axis is automatically scaled.

If your chromatogram contains a large, unimportant spike that is not integrated, you can improve the visibility of relevant peaks by adjusting the scaling options:

- the *Scale Maximum to Largest Peak*
- the *Scale Minimum to Minimum Baseline Values* (recommended if you do not evaluate negative peaks)



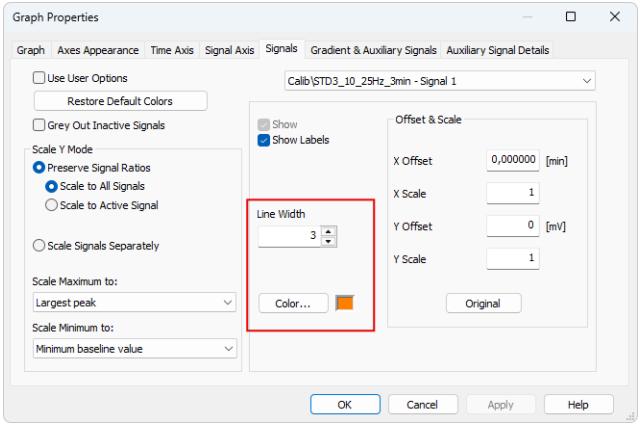
This centers the display on the integrated region, improving visibility of smaller peaks that would otherwise appear tiny due to large, unrelated spikes at the beginning.



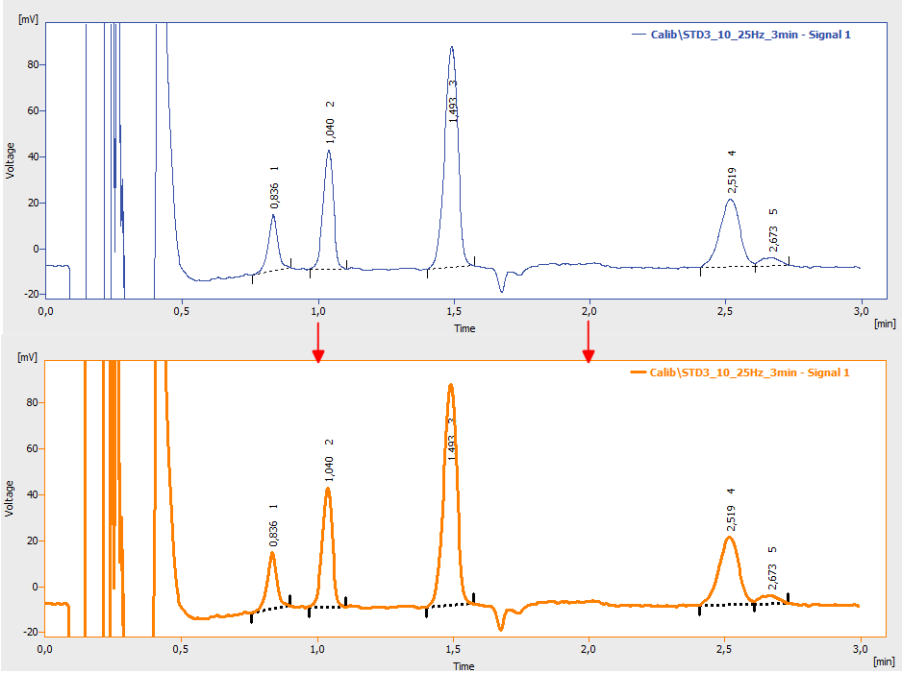
Changing the color and thickness of the signal line

In Graph Properties, go to the ***Signals*** tab. For each signal, you can customize its appearance:

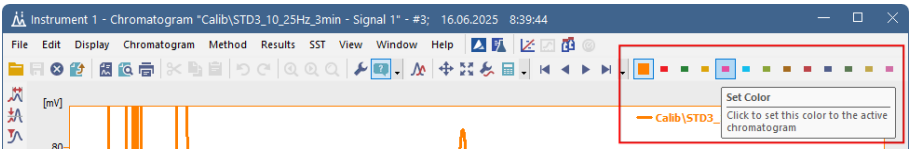
- Click the *Color* button to choose a different color.
- Adjust the *Line Width* value to make the signal line thinner or thicker.



This setting allows you to match your visual preferences and improve readability.



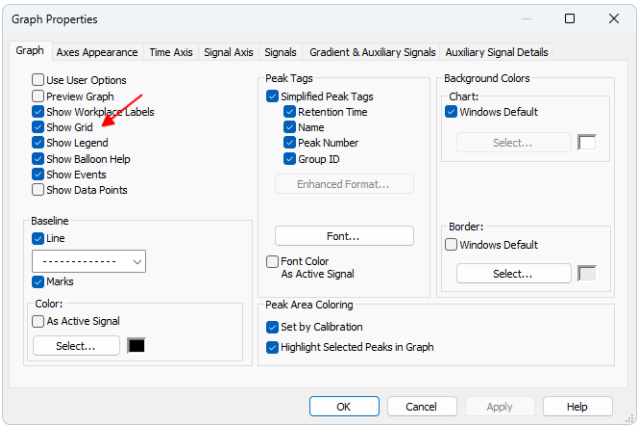
Alternatively, you can change the color of a signal directly from the toolbar: click a color box that is not currently used (i.e., not assigned to any open signal). The selected color will then be applied to the active signal.

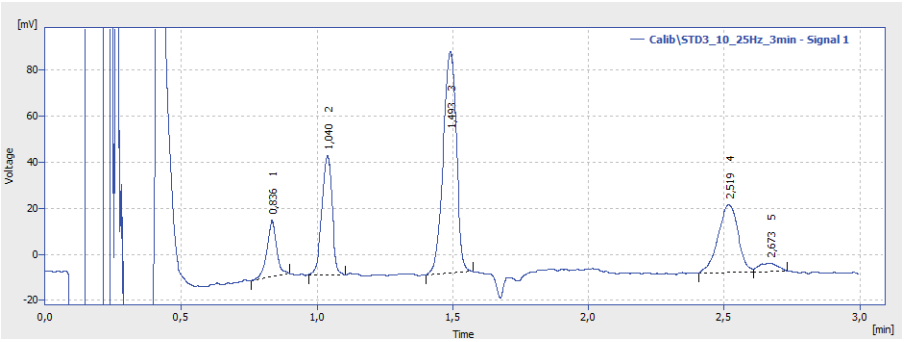


Showing the grid

In some cases, it can be helpful to display grid lines in the chromatogram graph - for example, to better align peaks or assess retention times.

You can enable this option in the *Graph Properties* dialog. Go to the ***Graph*** tab and select the *Show Grid* checkbox.

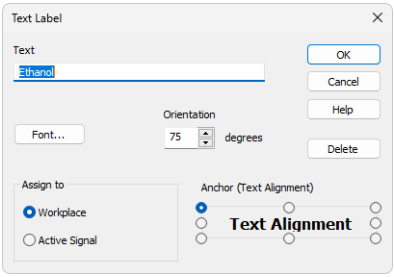




10.5 Adding text and lines to a chromatogram

Adding text label

1. Right-click in the chromatogram graph to invoke context menu and select *Create Label - Text*.
2. "T" will appear next to the cursor, click wherever you would like to place the label. *Text Label* dialog will open.
3. Write the text in the *Text* field.
4. Select the font by clicking the *Font* button.
5. Enter the *Orientation* of the text (0 degrees equals horizontal position).
6. Select the *Anchor point* for the text.
7. Use *Assign to - Workplace*, if you want the text to stay in the same location regardless of the opened chromatogram (labels stored in the desktop file). Or use *Assign to - Active Signal*, if you want the text to shift as the chromatogram signal moves, zooms in and out (labels stored in the chromatogram file). The text will be displayed only when the respective chromatogram signal is active.
8. Click the *OK* button to accept the settings.



9. Click and drag the text if you wish to move it to a different location.
10. Double-click the text to open *Text Label* dialog to adjust the label settings or to delete it.

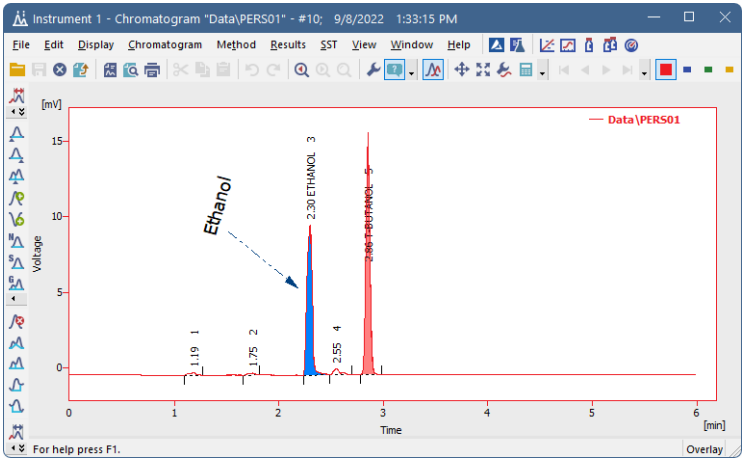
Adding line label

1. Right-click in the chromatogram graph to invoke context menu and select *Create Label - Text*.
2. "L" will appear next to the cursor, click and drag to place the line label. *Line Label* dialog will open.
3. Select whether you want to add an arrow tip at the beginning, end or at both ends of the line.
4. Select the color by clicking the *Color* button.
5. Enter the *Line Width*.
6. Select the *Line Style*.
7. Use *Assign to - Workplace*, if you want the text to stay in the same location regardless of the opened chromatogram (labels stored in the desktop file). Or use *Assign to - Active Signal*, if you want the text to shift as the chromatogram

signal moves, zooms in and out (labels stored in the chromatogram file). The text will be displayed only when the respective chromatogram signal is active.

8. Click the *OK* button to accept the settings.

9. Click and drag the line if you wish to move it to a different location. Alternatively drag one of the ends to change its position.
10. Double-click the line to open *Line Label* dialog to adjust the label settings or to delete it.

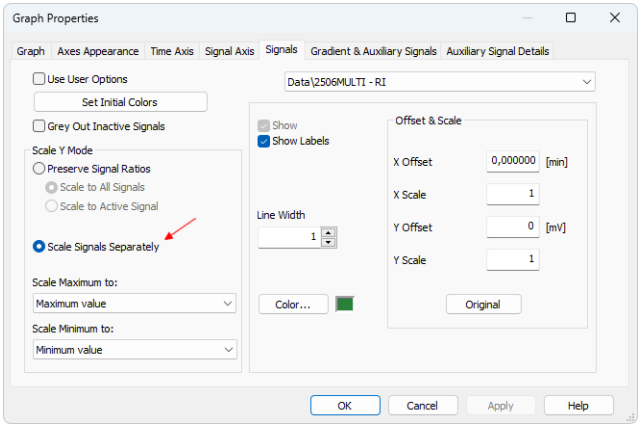


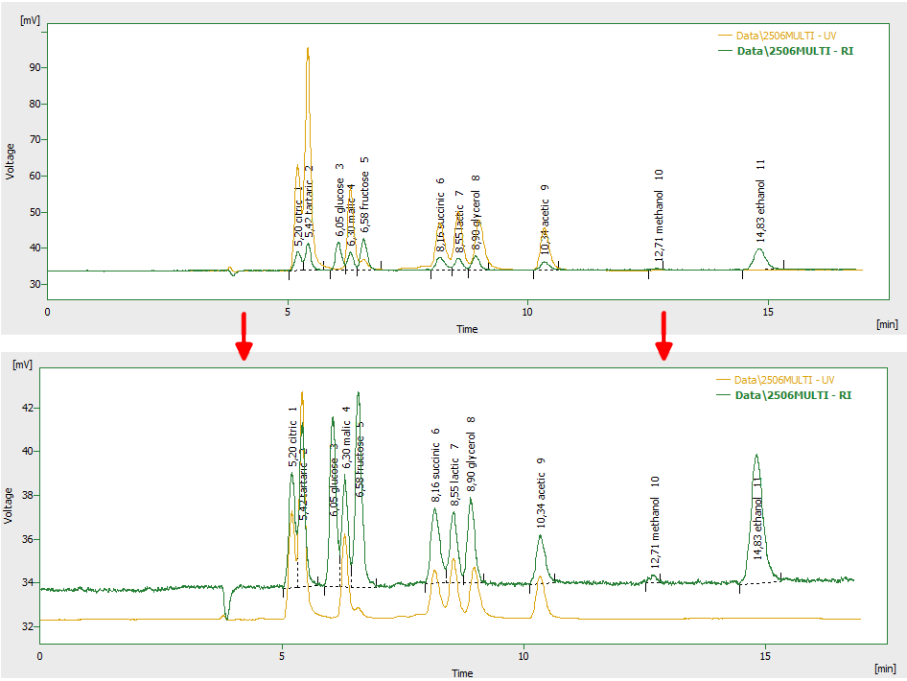
10.6 Working with individual signals of a multisignal chromatogram smoothly

There are some tips on how you can enhance your workflow so that working with multiple signals is more convenient.

Individual scaling of signals

If the peaks differ in height significantly, scale them individually to fit the graph. In the *Graph properties - Signals* tab, select the option *Scale Signals Separately*.

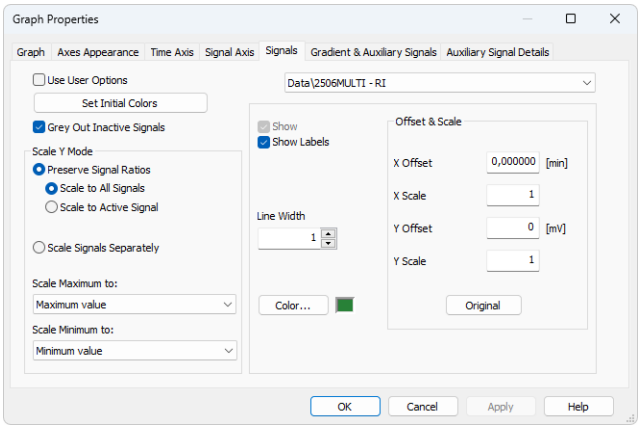

Graph Properties
Graph
Axes Appearance
Time Axis
Signal Axis
Signals
Gradient & Auxiliary Signals
Auxiliary Signal Details
Use User Options
Set Initial Colors
Grey Out Inactive Signals
Scale Y Mode
Preserve Signal Ratios
Scale to All Signals
Scale to Active Signal
Scale Signals Separately
Scale Maximum to:
Maximum value
Scale Minimum to:
Minimum value
Data\2506MULTI - RI
Show
Show Labels
Line Width
1
Color...
Offset & Scale
X Offset
0,000000
[min]
X Scale
1
Y Offset
0
[mV]
Y Scale
1
Original
OK
Cancel
Apply
Help

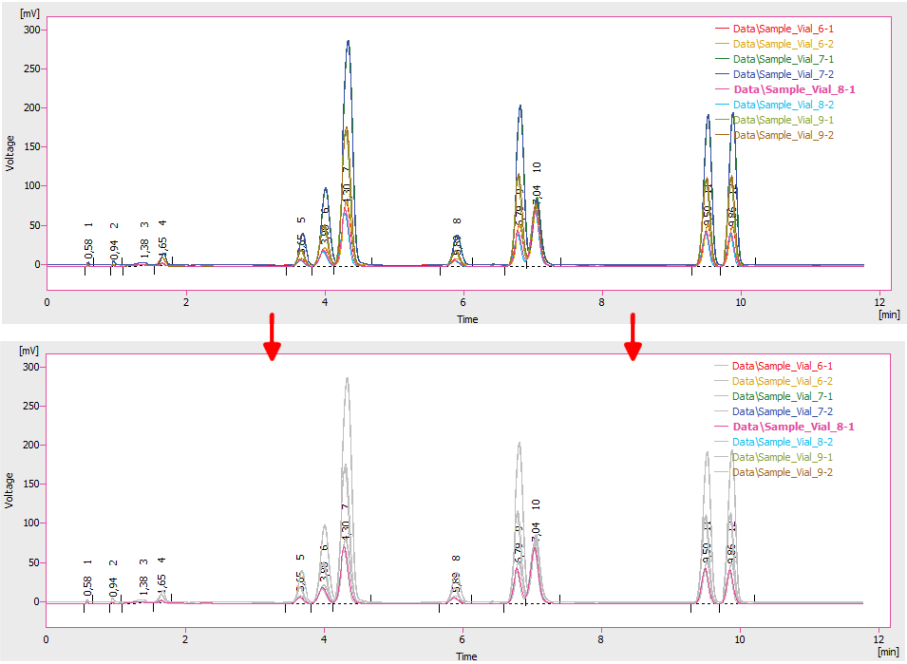

[mV]
Voltage
Time
[min]
Data\2506MULTI - UV
Data\2506MULTI - RI
5,20 citric 1
5,42 tartaric 2
6,05 glucose 3
6,30 malic 4
6,58 fructose 5
8,16 succinic 6
8,55 lactic 7
8,90 glycerol 8
10,34 acetic 9
12,71 methanol 10
14,83 ethanol 11

Graying out

To minimize the distraction by the other signals, it is possible to have inactive signals grayed out.

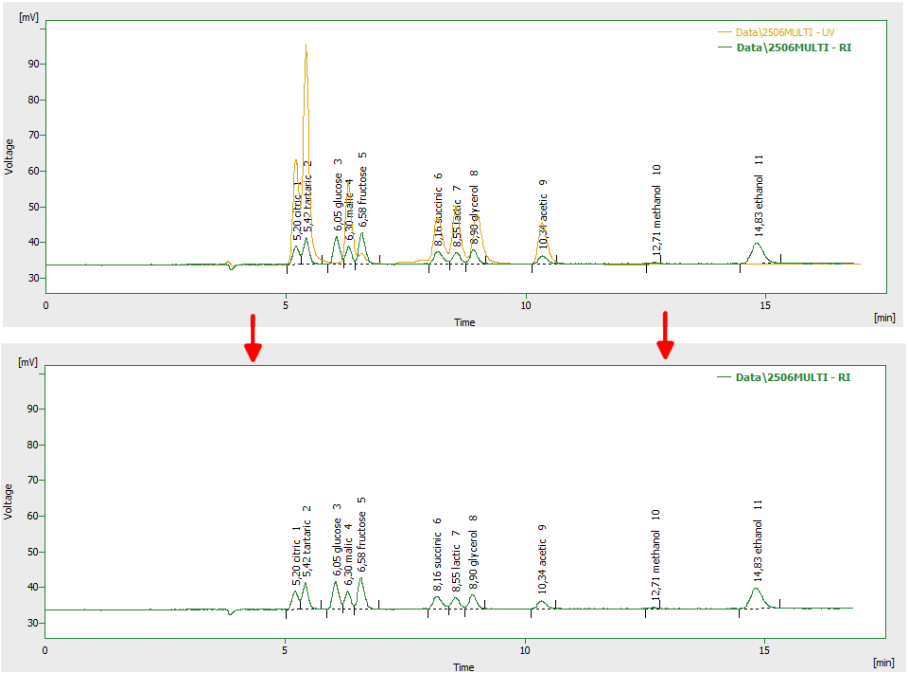
In the *Graph properties - Signals* tab, check the option *Grey Out Inactive Signals*.





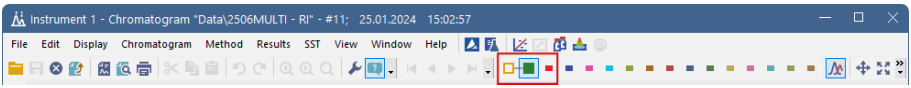
Hiding the signals temporarily

Another option is to hide a signal completely for the session.

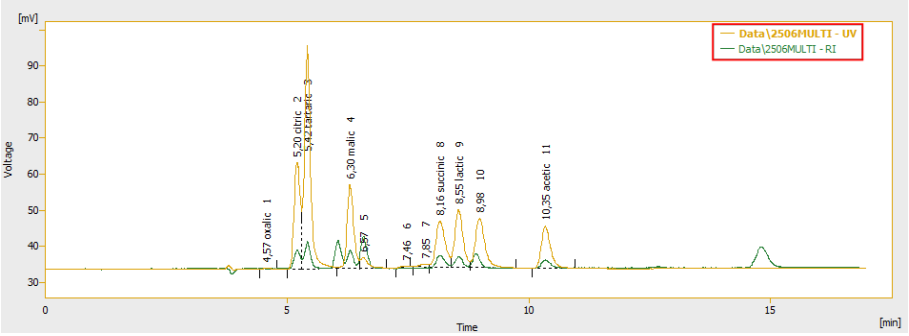


There are more ways how to achieve that:

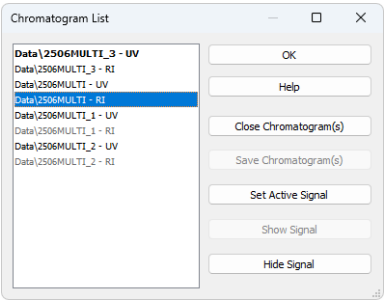
A. Left-click + **CTRL** on the signal color icon in the Toolbar.



B. Double-click + **CTRL** on the name of the signal in the legend.



C. Go to *Chromatogram - Chromatograms...*menu to invoke *Chromatogram List* dialog and select signal(s) to hide.



11 Calibration

The following chapters contain multiple topics which will guide you through the basic principles of using calibrations in **Clarity** and also introduce you to advanced solutions, for example using the *Bracketing*.

Clarity videos covering calibration-related topics can be found in the Clarity Calibration playlist.

The typical workflow for individuals conducting routine analyses should include:

Preparation of the calibration:

1. Create the calibration. For more details, see the Creating a new calibration topic.
2. Add the number of standard levels you use. For more details, see the Adding a new calibration level topic.
3. If necessary, adjust the calibration according to your needs. For more details, see the Adjusting a calibration topic.

For creating a calibration that will serve as model for calibration cloning, check also the Creating a model calibration for calibration cloning topic.

Linking the calibration to chromatograms:

- It is possible to link the calibration to chromatograms directly. For more details, see the Setting a calibration in a chromatogram topic.
- Or it is possible to link the calibration to a method, so all chromatograms measured using this method will have the specified calibration linked. For more details, see the Setting a calibration in a method topic.

Recalibration:

- In most cases, it is efficient to perform the recalibration automatically from the sequence. For more details, see the Recalibrating automatically using a sequence topic.
  We recommend using calibration cloning on the first recalibration if you want to include only the responses from currently measured sequence in the calibration. For more details, see the Calibrating using clone on first recalibration topic.
- It is also possible to recalibrate from previously measured standards. For more details, see the Recalibrating a calibration topic.

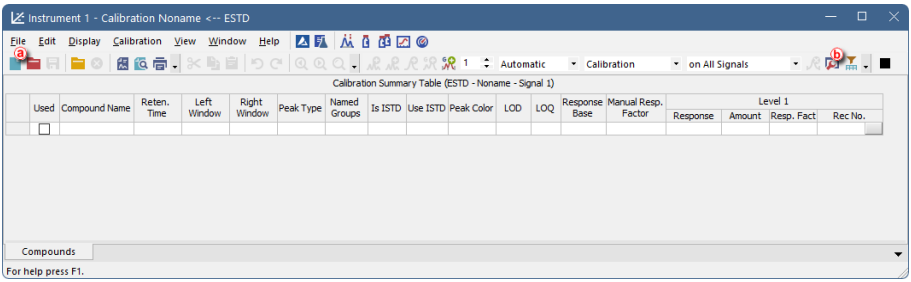
Advanced Topics

Collection of more advanced calibration workflows.

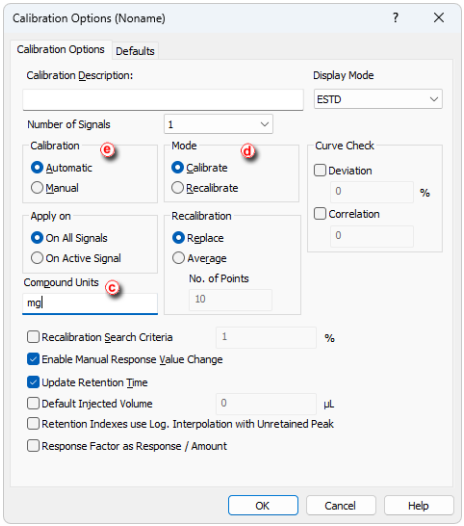
11.1 Creating a new calibration

This chapter covers creating a calibration file. You should have at least one integrated measured standard to be able to fill in the desired peaks into the newly created calibration.

1. Open the Calibration window: choose *Window - Calibration* in the *Instrument* window or click .



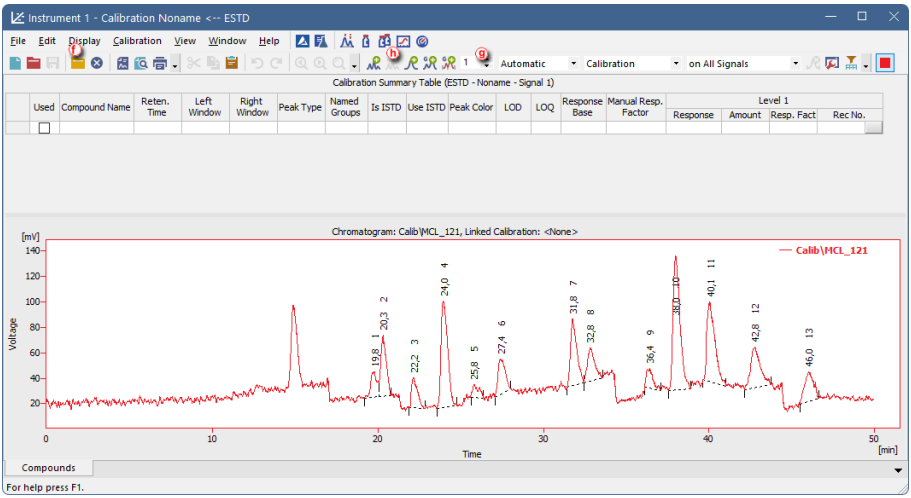
2. Create a new calibration file: select *File - New* or click ⓐ .
3. Open the *Calibration Options* dialog: choose *Calibration - Options…* or click ⓑ .



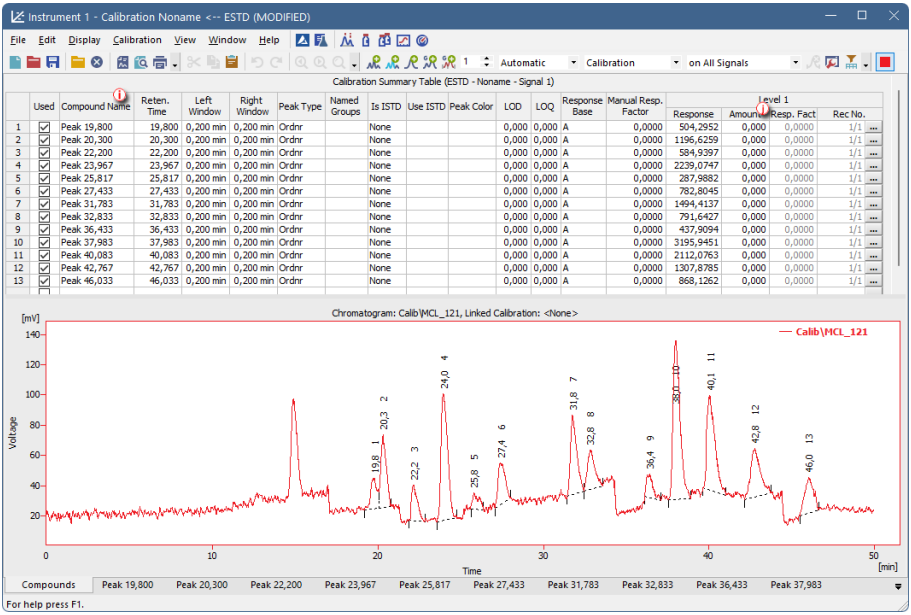
4. Fill in the units in the *Compound Units* section ⓒ to suit your analysis conditions.
5. Set the *Mode* to *Calibrate* ⓓ .

6. Set the *Calibration* option to *Automatic* to add the peaks without modification or *Manual* to modify them one by one ⓔ .
7. Open integrated chromatogram of a standard: choose *File - Open Standard…* or click on ⓕ in the *Calibration* window.
8. Add peaks belonging to the compounds of interest from the chromatogram of the standard to the calibration file.

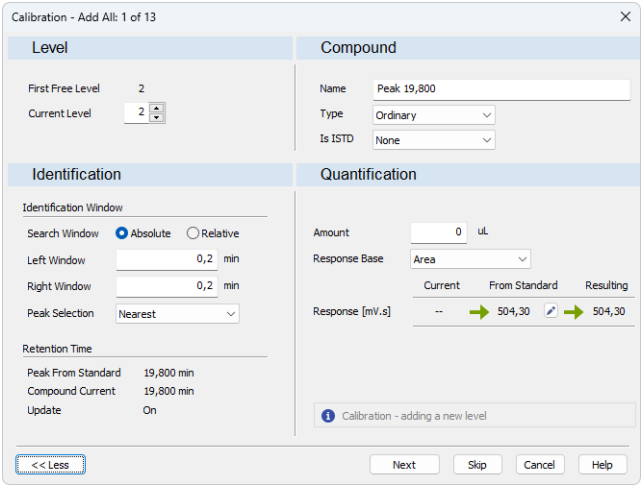
Note: Select *Calibration - Add All* or click on to add all integrated peaks or the Add Peak / Add Group icons to add specific peaks ⓗ . Regardless of the set Current Level ⓖ the peaks will be added to the first free level.



9. If you selected *Automatic* calibration:
   - Name the peaks identified in the *Calibration Summary Table* ⓘ by their retention times by typing the *Compound Name* for each peak. No compound name may be used more than once.
   - Fill in the *Amount* ⓙ for each compound into the *Calibration Summary Table*.



10. If you selected *Manual* calibration: Fill in the Amount, the Compound Name and set any other parameters related to the peak on the *Calibration - Add Peak* window. This window will open once for each one of the peaks processed.

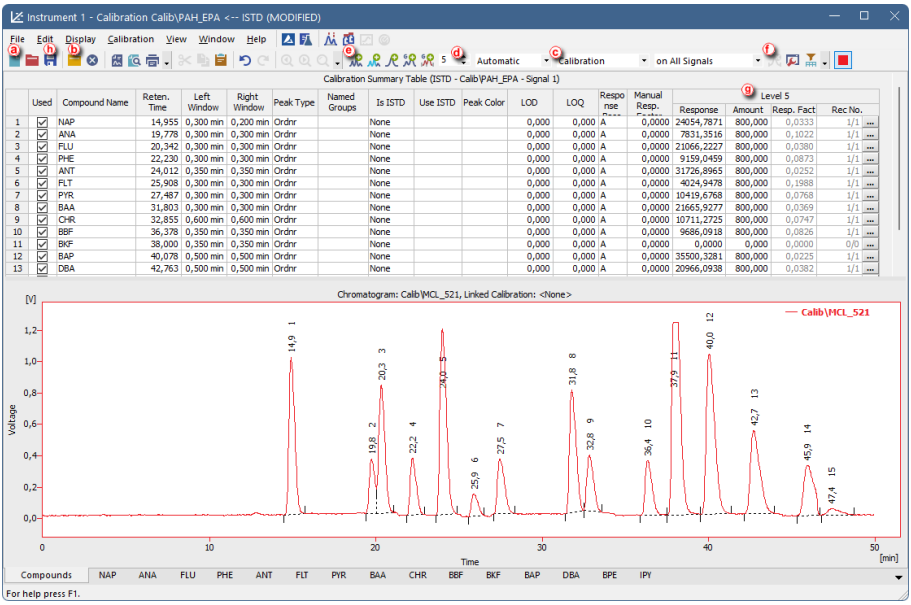


11. Save the calibration file - *File - Save* or click .

11.2 Adding a new calibration level

Here we describe how to add concentration levels to the calibration file to obtain the calibration curve of all compounds. This procedure has to be repeated several times, once for each calibration level to be added.

1. Open the Calibration window: choose *Window - Calibration* on the Instrument window or click icon.



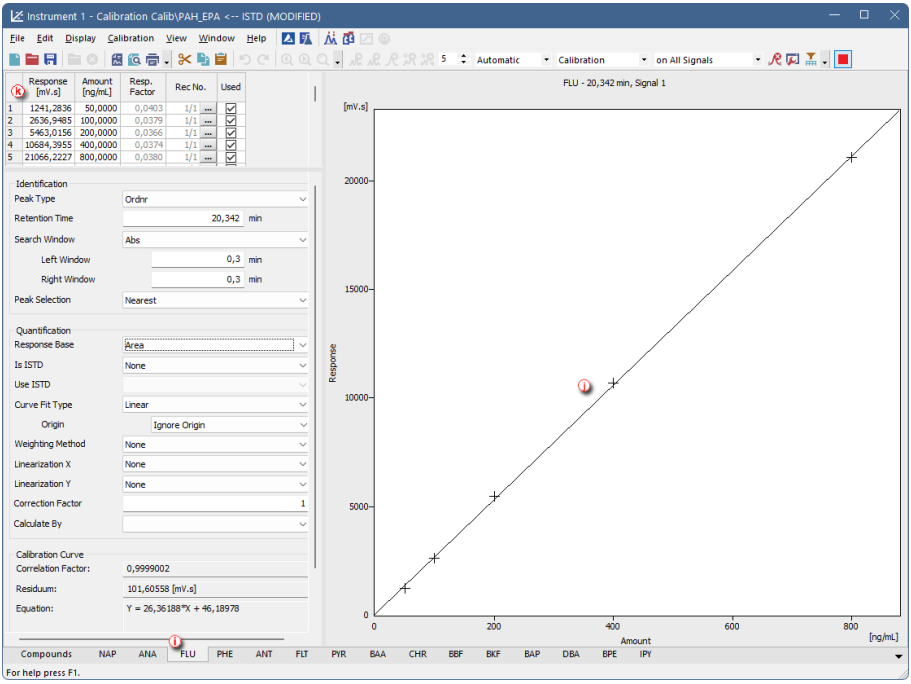
2. Open the calibration file: choose *File - Open…* or click ⓐ .
3. Open calibration standard: select *File - Open Standard…* or click ⓑ .

   Note: Select a measured and qualitatively evaluated chromatogram where all peaks are available, if possible.

4. Check that the *Automatic* option is selected in the first field and the *Calibration* option in the second field of the calibration mode settings ⓒ .
5. The calibration level number is in the *Current Level* field ⓓ set automatically to the first free level.
6. Add all peaks in the chromatogram of the calibration standard to the calibration file: select *Calibration - Add All* or click ⓔ .

Note: In case more peaks than expected emerge in the calibration, the surplus peaks can be deleted by selecting them in the *Calibration Summary Table* and deleting them using *Calibration - Delete Compound* or clicking on ⓕ .

7. Set the amounts of the particular compounds into the *Calibration Summary Table*, into the *Amount* column ⓖ of the respective calibration level.
8. Save the calibration file: choose *File - Save* or click ⓗ
9. Click any tab below ⓘ and you will be able to see the calibration curve ⓙ with all the levels added for one specific compound ⓚ .



11.3 Adding a group to calibration

Here we describe how to add group defined in the calibration standard into the calibration. For more information on how to define a group and add peaks in it, see Adding a peak to a group.

Grouped peaks in the calibration are evaluated together which is suitable for related compounds that produce separate but closely eluting peaks that should be treated as one component in quantification and reporting.

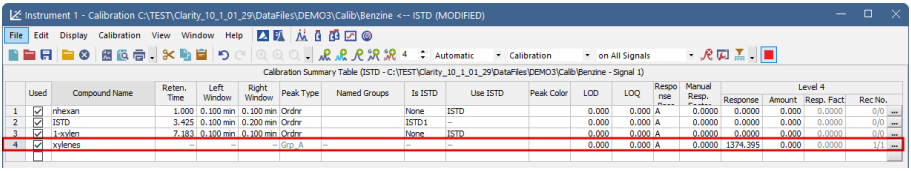
If you only need to sum the amounts of already calibrated peaks for reporting purposes, see Creating a custom result group.

1. Open the *Calibration* window with the desired calibration file and standard file in which at least one group is already defined.
2. Use the *Calibration - Add Group* command or the *Add Group* icon .

   Note: If the calibration standard is hidden (e.g., by resizing the *Calibration* window or expanding the *Compound Summary Table*), the *Add Group* command and icon will not be active.

3. The cursor is locked to the calibration standard graph. Choose the desired group by clicking on it in the graph.

New row will be inserted in the *Calibration Summary Table*. Here you can change the *Group name* in the *Compound name* cell and set other parameters in their respective fields. The group name will be also displayed in the *Result Table* of the *Chromatogram* window if the calibration is linked.



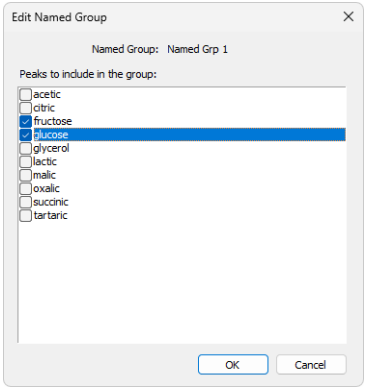
11.4 Creating a custom result group

Here we describe how to add a *Named Group* to the calibration.

Named Groups are used to sum the amounts of already calibrated peaks and report them together. This is useful when legislation requires reporting the summed amount of several compounds (e.g., PAHs in drinking water).

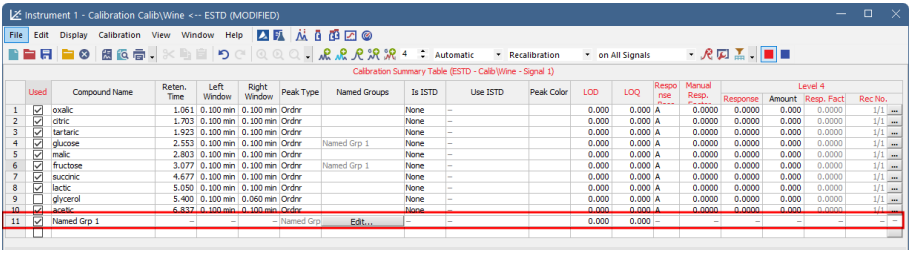
If you need to evaluate related compounds as one component already during calibration, see Adding a group to calibration.

1. Open the *Calibration* window with the desired calibration and standard file.
2. Use the *Calibration - Add Named Group* command or the *Add Named Group* icon to invoke the *Edit Named Group* dialog.



3. Here you can select individual peaks you want to include in a *Named group*. All peaks present in calibration are available for selection and are listed alphabetically. Unlike standard groups, a peak can be part of multiple *Named Groups*.
4. Click *OK*.

New row will be inserted in the *Calibration Summary Table*. The name of the *Named Group* can be set in the *Calibration Summary Table*, the same way as compound names. To edit an existing *Named Group*, click the *Edit...* button in the *Named Groups* column in the selected *Named Group* row of the *Calibration Summary Table*.



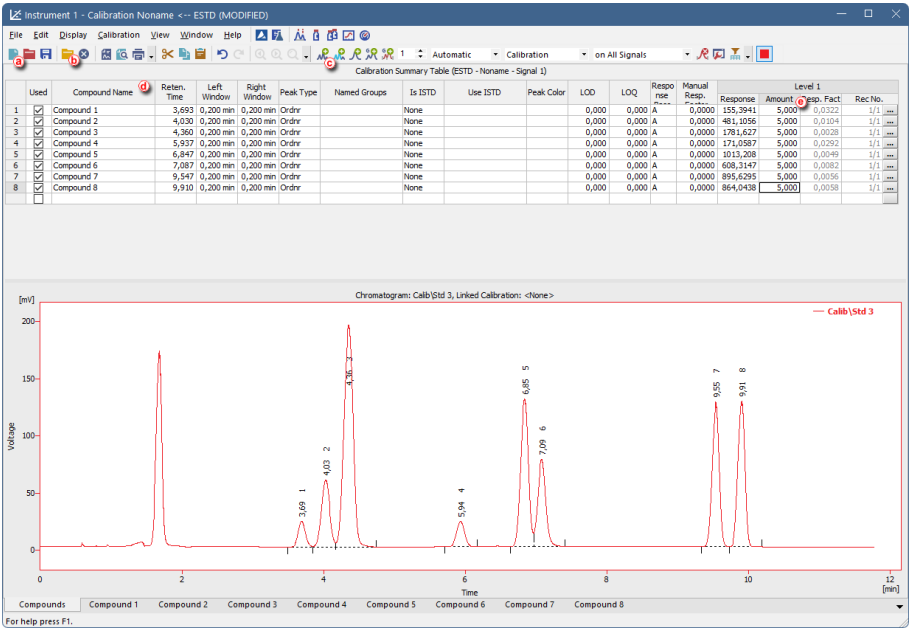
In the *Result Table* of the *Chromatogram* window, *Named Groups* are listed below the *Total* row to indicate that their amounts are not included in the total calculation.

In the *Summary Table* of the *Chromatogram* window, *Named Groups* are not supported.

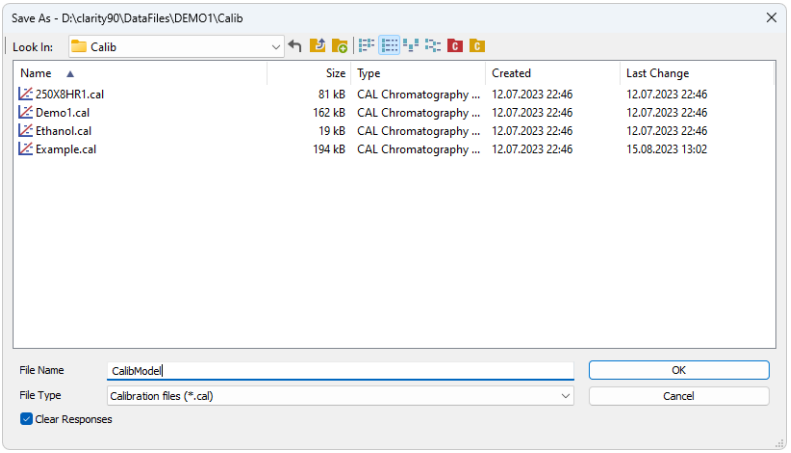
11.5 Creating a model calibration for calibration cloning

This topic will show you how to prepare model calibration to be used during calibration cloning. If you have calibration already created from the previous measurement skip to step 4.

1. In the *Calibration* window, select *New* ⓐ calibration and *Open* ⓑ typical chromatogram as standard.
2. Use *Add All* ⓒ to add the integrated peaks to calibration.
3. Fill in the *Compound Names* ⓓ and the *Amounts* ⓔ for every level that will be used.



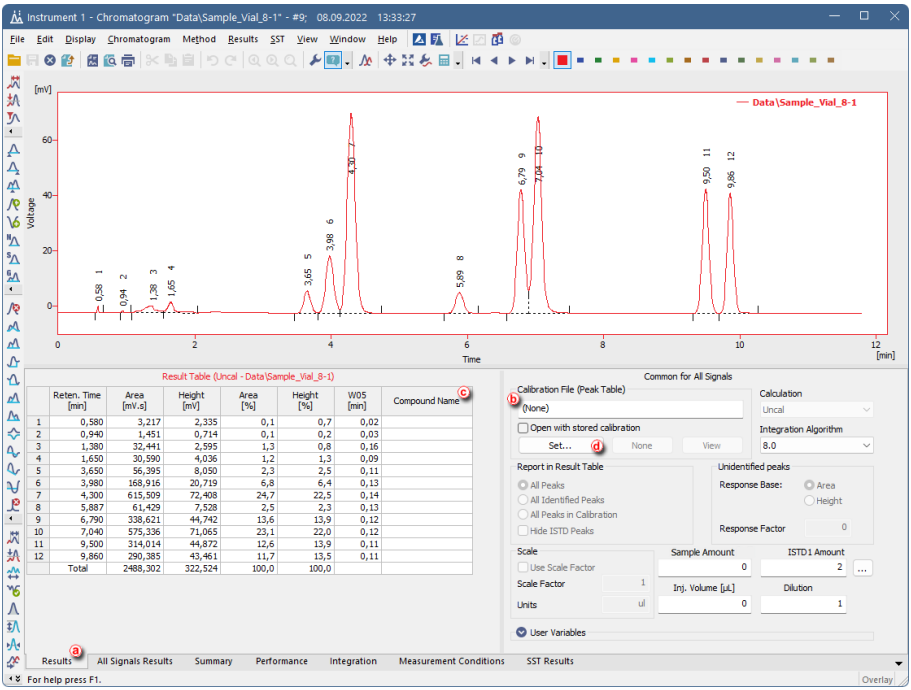
4. Select the *Save As* option. In the *Save As* dialog check the *Clear Responses* checkbox and save the calibration under a new name.



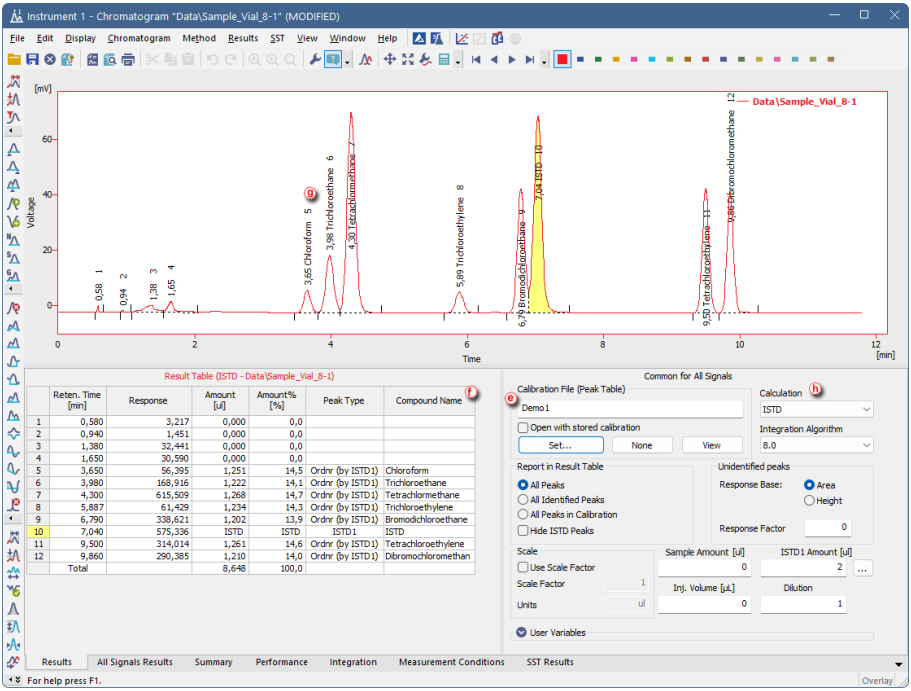
11.6 Setting a calibration in a chromatogram

If the calibration file was not assigned in the method, the measured chromatogram will not have it linked either. Here you will learn how to link a calibration file to a chromatogram.

1. Switch to the *Results tab* ⓐ at the bottom part of the *Chromatogram window*.



2. Check whether the *Calibration File (Peak Table)* field ⓑ is set to *(None)*. If that is the case, then the chromatogram does not have a calibration file linked to it.
3. Also check the *Compound Names* ⓒ in the Result Table section. This column must be empty.
4. To link the calibration file to the Chromatogram, click the *Set…* button ⓓ in the right section of the *Results tab*. You will get a list of all calibrations available in the present project.
5. Select the correct calibration file from the list and click *OK*. The content of the Chromatogram window will change.

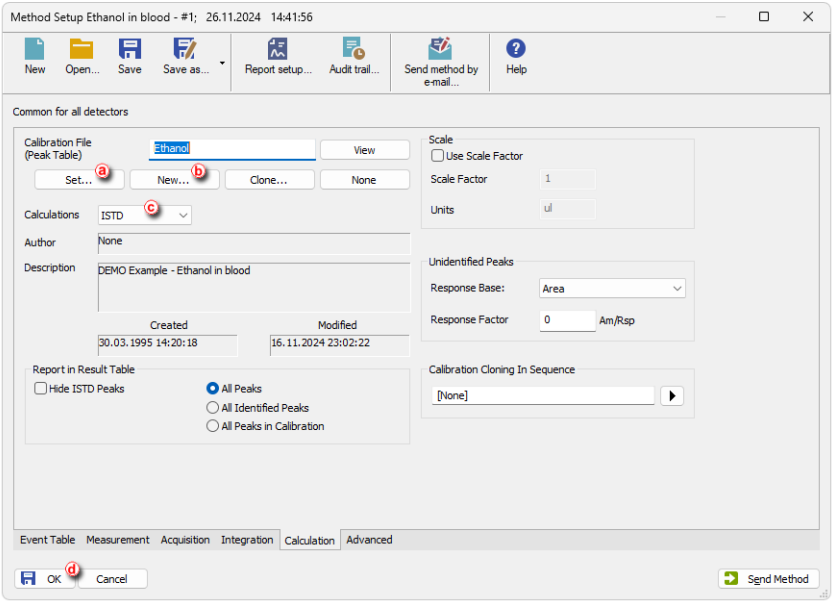


6. Check that the *Calibration File (Peak Table)* field contains the name of the calibration file. ⓔ
7. The *Compound Name* column ⓕ in the *Result Table*, as well as the identified peaks in the graph ⓖ , will now have the names of the identified peaks from the calibration file.
8. Check the *Calculation* field ⓗ to see the type of calculation performed on the chromatogram.
9. Save the chromatogram: select *File - Save* or click .

11.7 Setting a calibration in a method

After the acquisition is performed according to a method, the resulting chromatogram files may be calibrated using a specific calibration. If you need to measure a large number of similar samples, it would be advisable to define a calibration file prior to the acquisition.

1. Open the method from the Instrument window by using the *Method - Method Setup* command.
2. Go to the *Calculation* tab.

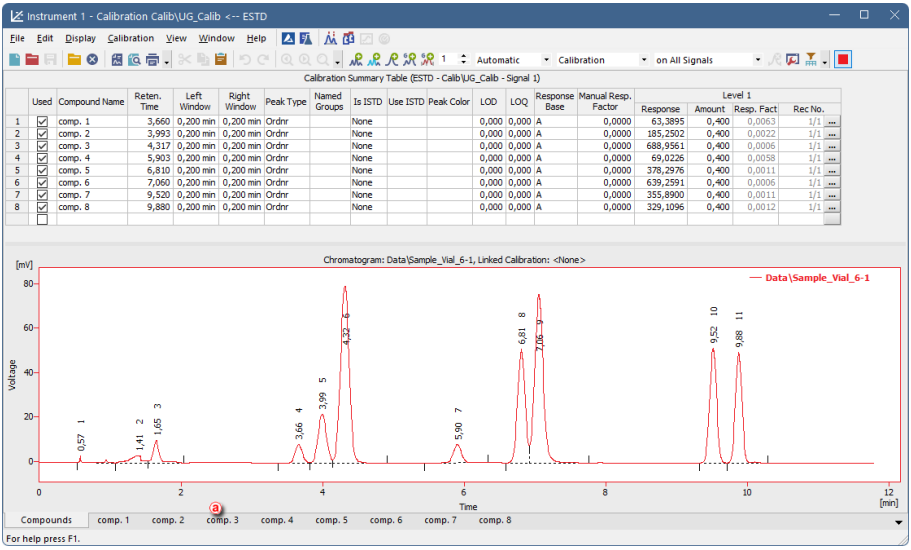


3. Click the *Set…* button ⓐ to select a calibration file for the method, or create a new calibration file by clicking the *New…* button ⓑ .
4. Change the default calibration type in the *Calculations* field ⓒ .
5. Click *OK* ⓓ to save the changes to the opened method.
6. You can modify the calibration file after acquisition. For more info go to *Apply the calibration to a Chromatogram*.

11.8 Adjusting a calibration

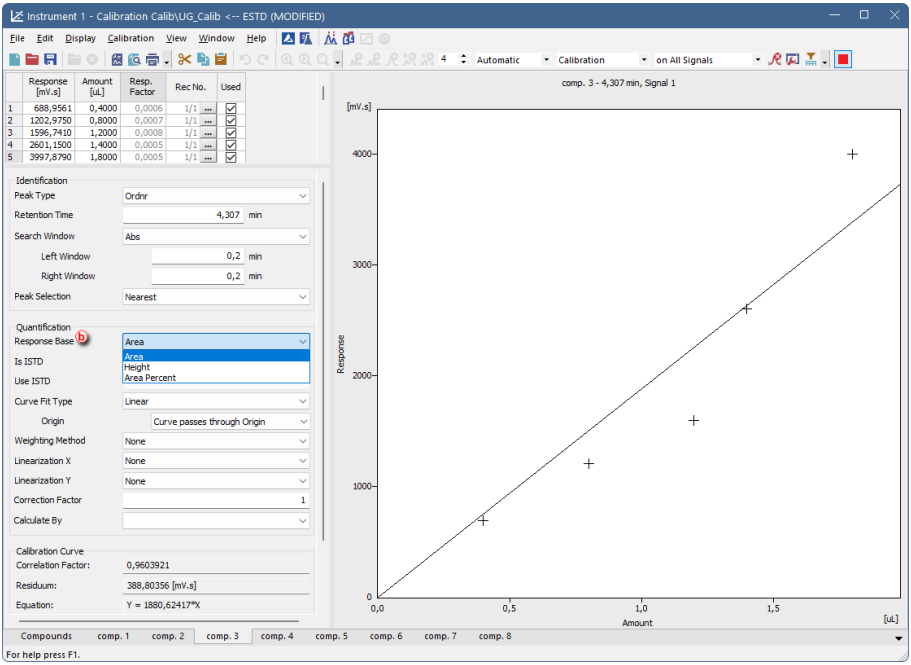
Following articles will describe how to perform some of the most common calibration modifications that can improve your calibration. Using this guide you manage to fit your calibration closer to your analytical application.

Once you added all chromatograms to your calibration and filled ***Amount*** values for all compounds and all levels, you can start to adjust it. Note that the ***Amount*** values are the values you know, because they originate from the concentration levels of your calibration solutions. Further adjustments of the calibration are available on the corresponding ***Compound Tabs*** at the bottom of the window. In our case, the Comp No. 3 ⓐ is edited.



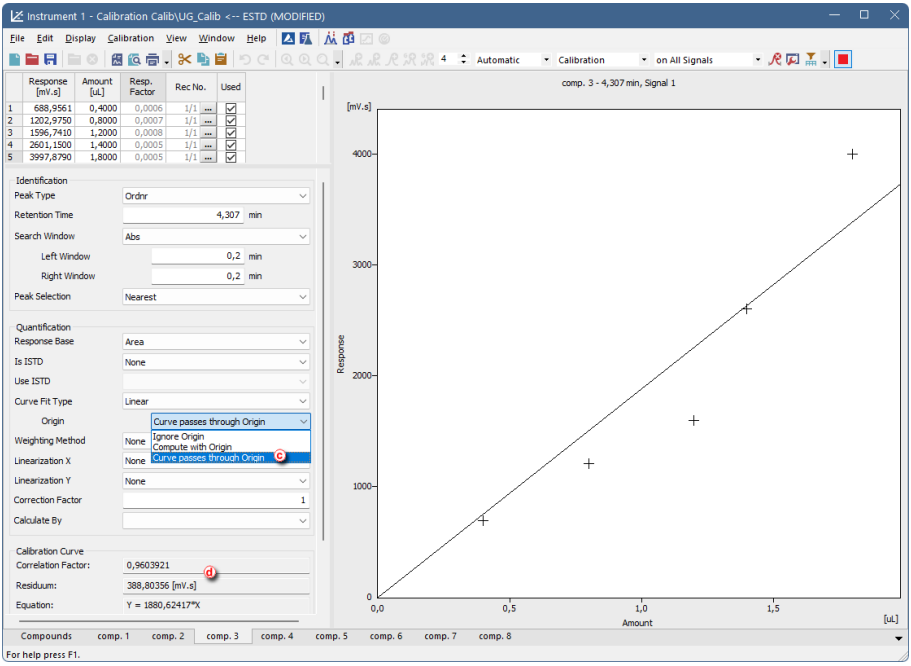
Modifying Response Base

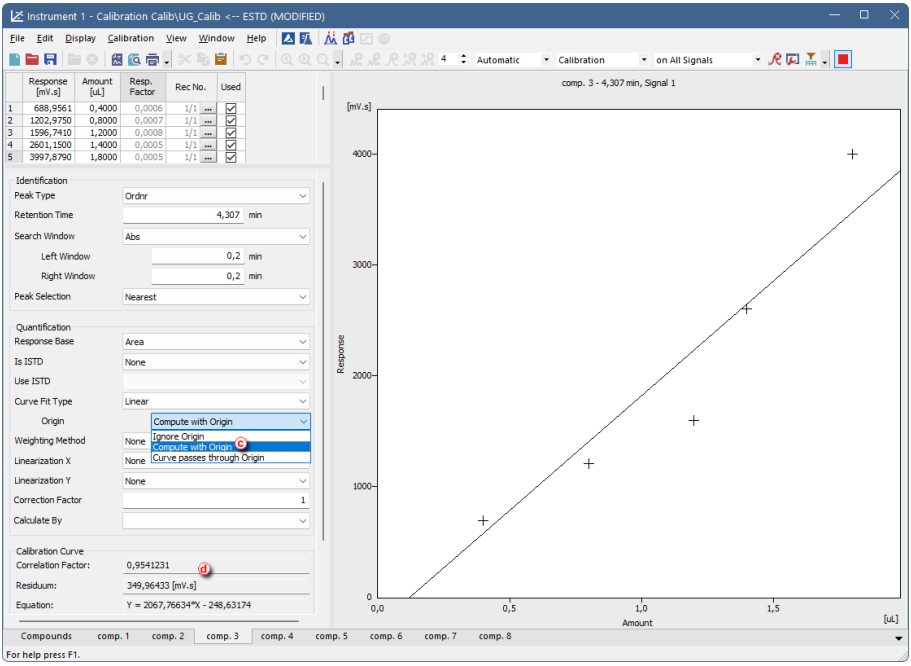
Set the *Response Base* ⓑ to modify whether the calibration curve will be calculated using *Area* or *Height* of the corresponding peak belonging to the specific compound. Changing the *Response Base* can help to create better fitting of the calibration to not well resolved peaks.

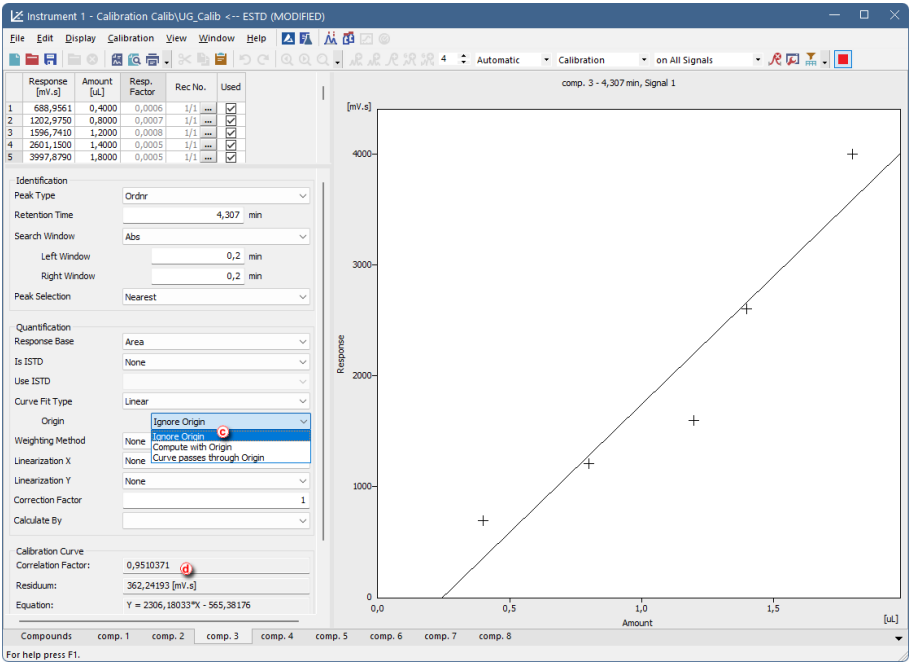


Modifying Origin

Another option how to improve your calibration is setting of *Origin* ⓒ and its incorporation or exclusion in calibration calculations. In **Clarity** there are three available setting options, as described on the following images. There is also demonstrated an effect of the *Origin* setting on calculated *Equation* and *Correlation factor* ⓓ .


Instrument 1 - Calibration Calib\UG_Calib <-- ESTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
on All Signals
Response [mV.s]
Amount [uL]
Resp. Factor
Rec No.
Used
1 688,9561 0,4000 0,0006 1/1
2 1202,9750 0,8000 0,0007 1/1
3 1596,7410 1,2000 0,0008 1/1
4 2601,1500 1,4000 0,0005 1/1
5 3997,8790 1,8000 0,0005 1/1
Identification
Peak Type Ordnr
Retention Time 4,307 min
Search Window Abs
Left Window 0,2 min
Right Window 0,2 min
Peak Selection Nearest
Quantification
Response Base Area
Is ISTD None
Use ISTD
Curve Fit Type Linear
Origin Curve passes through Origin
Ignore Origin
Compute with Origin
Curve passes through Origin
Weighting Method None
Linearization X None
Linearization Y None
Correction Factor 1
Calculate By
Calibration Curve
Correlation Factor: 0,9603921
Residuum: 388,80356 [mV.s]
Equation: Y = 1880,62417*X
comp. 3 - 4,307 min, Signal 1
[mV.s]
Response
Amount
[uL]
Compounds comp. 1 comp. 2 comp. 3 comp. 4 comp. 5 comp. 6 comp. 7 comp. 8
For help press F1.


Instrument 1 - Calibration Calib\UG_Calib <-- ESTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
on All Signals
Response [mV.s]
Amount [uL]
Resp. Factor
Rec No.
Used
1 688,9561 0,4000 0,0006 1/1
2 1202,9750 0,8000 0,0007 1/1
3 1596,7410 1,2000 0,0008 1/1
4 2601,1500 1,4000 0,0005 1/1
5 3997,8790 1,8000 0,0005 1/1
Identification
Peak Type Ordnr
Retention Time 4,307 min
Search Window Abs
Left Window 0,2 min
Right Window 0,2 min
Peak Selection Nearest
Quantification
Response Base Area
Is ISTD None
Use ISTD
Curve Fit Type Linear
Origin Compute with Origin
Ignore Origin
Compute with Origin
Curve passes through Origin
Weighting Method None
Linearization X None
Linearization Y None
Correction Factor 1
Calculate By
Calibration Curve
Correlation Factor: 0,9541231
Residuum: 349,96433 [mV.s]
Equation: Y = 2067,76634*X - 248,63174
comp. 3 - 4,307 min, Signal 1
[mV.s]
Response
Amount
[uL]
Compounds comp. 1 comp. 2 comp. 3 comp. 4 comp. 5 comp. 6 comp. 7 comp. 8
For help press F1.



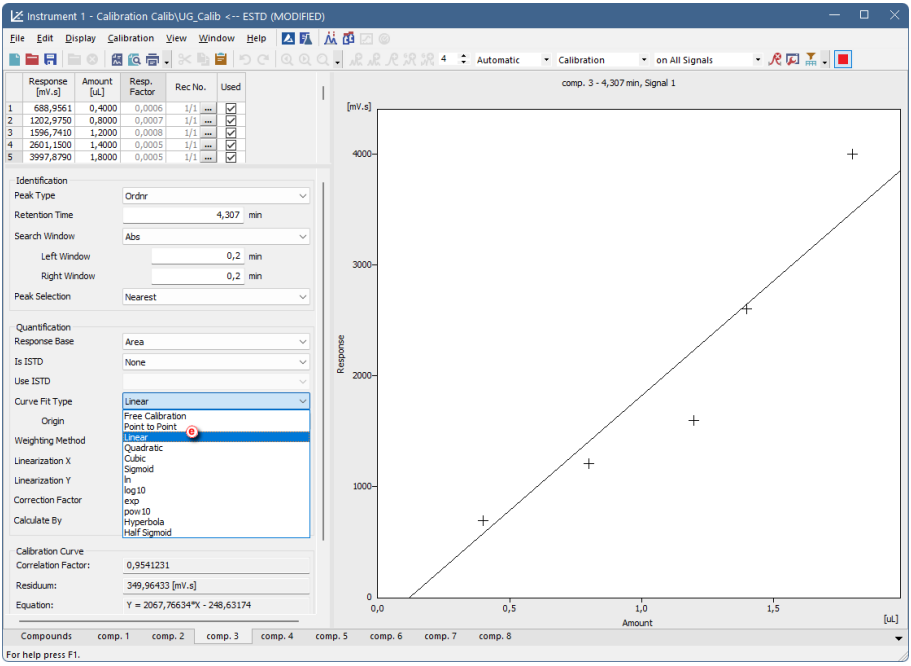
As you can see from the *Correlation factor* ⓓ values, changing the *Origin* setting from the *Curve Passes through Origin* to *Compute with Origin* improved the curve fit. However, the option *Ignore Origin* has proved to be the best match for the used detector.

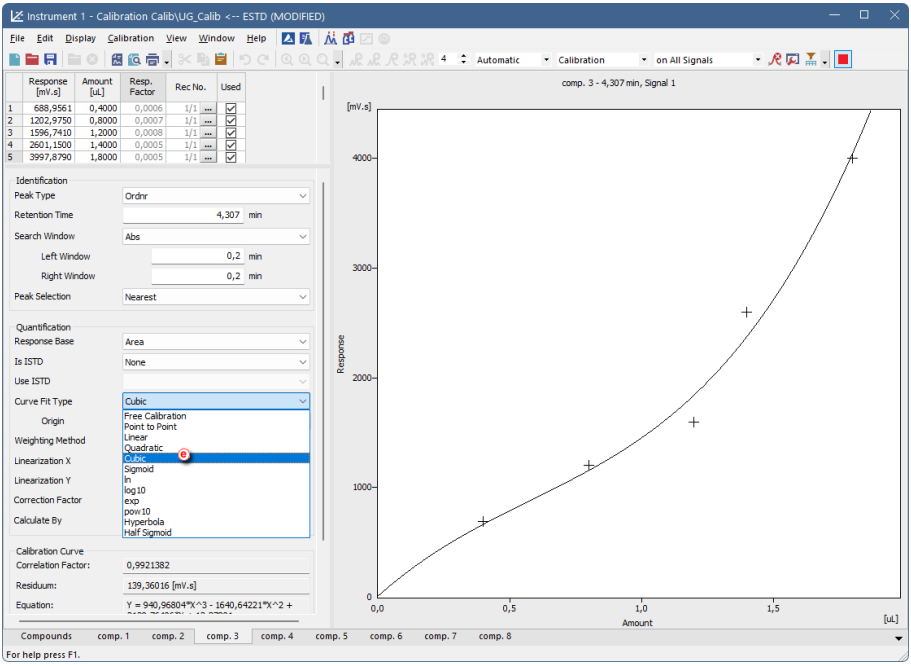
Modifying Curve Fit Type

Following images demonstrate how to modify *Curve Fit Type* ⓔ from *Linear* to *Cubic*. *Cubic Curve Fit Type* is used as an example of non-linear *Curve Fit Types*.

- Linear calibration curve is commonly used for detectors with linear response, such as Flame Ionization Detector (FID) or Refractive Index Detector (RID).
- Non-linear calibration curve is typical for detectors such as Electron Capture Detector (ECD) or Evaporative Light Scattering Detector (ELSD).

When changing *Curve Fit Type* ⓔ pay also attention to the values of the calculated *Equation* and *Correlation Factor*. Increasing value of the *Correlation Factor* indicates better selected *Curve Fit Type* for the measured data.

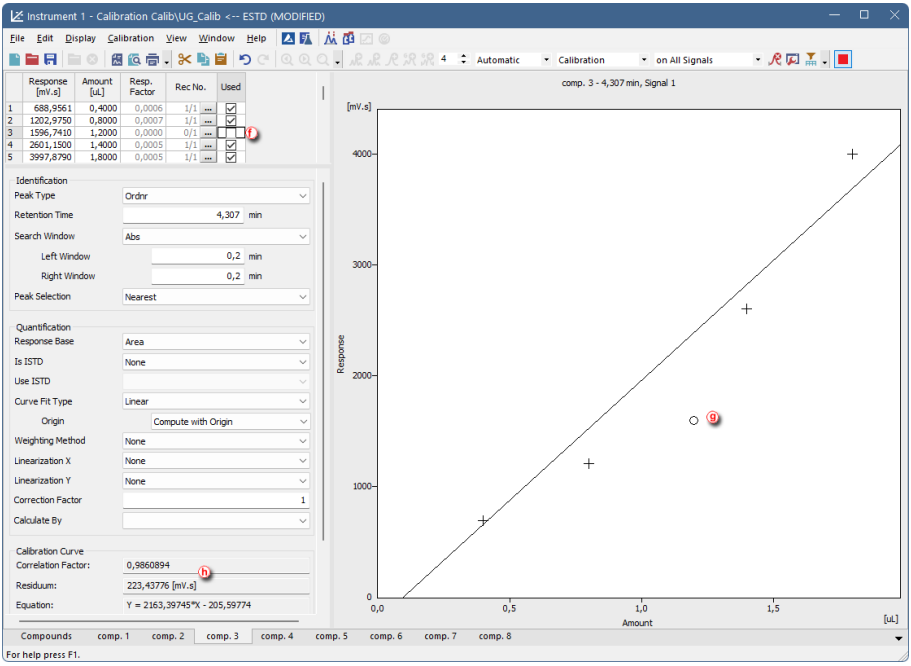

Instrument 1 - Calibration Calib\UG_Calib <-- ESTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
on All Signals
Response [mV.s] Amount [uL] Resp. Factor Rec No. Used
1 688,9561 0,4000 0,0006 1/1
2 1202,9750 0,8000 0,0007 1/1
3 1596,7410 1,2000 0,0008 1/1
4 2601,1500 1,4000 0,0005 1/1
5 3997,8790 1,8000 0,0005 1/1
Identification
Peak Type Ordnr
Retention Time 4,307 min
Search Window Abs
Left Window 0,2 min
Right Window 0,2 min
Peak Selection Nearest
Quantification
Response Base Area
Is ISTD None
Use ISTD
Curve Fit Type Linear
Origin
Weighting Method
Linearization X
Linearization Y
Correction Factor
Calculate By
Free Calibration
Point to Point
Linear
Quadratic
Cubic
Sigmoid
ln
log10
exp
pow10
Hyperbola
Half Sigmoid
Calibration Curve
Correlation Factor: 0,9541231
Residuum: 349,96433 [mV.s]
Equation: Y = 2067,76634*X - 248,63174
comp. 3 - 4,307 min, Signal 1
[mV.s]
Response
Amount
[uL]
Compounds comp. 1 comp. 2 comp. 3 comp. 4 comp. 5 comp. 6 comp. 7 comp. 8
For help press F1.



As you can see, changing the *Curve Fit Type* from *Linear* to *Cubic* increased the *Correlation Factor* from 0.954 to 0.992.

Excluding of Measured Point from Calibration

Clarity also allows excluding any point from calibration. This is helpful in case that the specific measurement went wrong. Following images describe how to do that. Please keep in mind that the excluded point isn't deleted, the point is still part of the calibration, however, it is omitted from calculation of calibration curve. To exclude the selected measurement point from the calibration simply uncheck that measurement in the *Used* ⓕ column. The excluded point in the graph of calibration curve will be changed from cross to empty circle ⓖ and calibration curve *Equation* and *Correlation Factor* ⓗ will be recalculated.

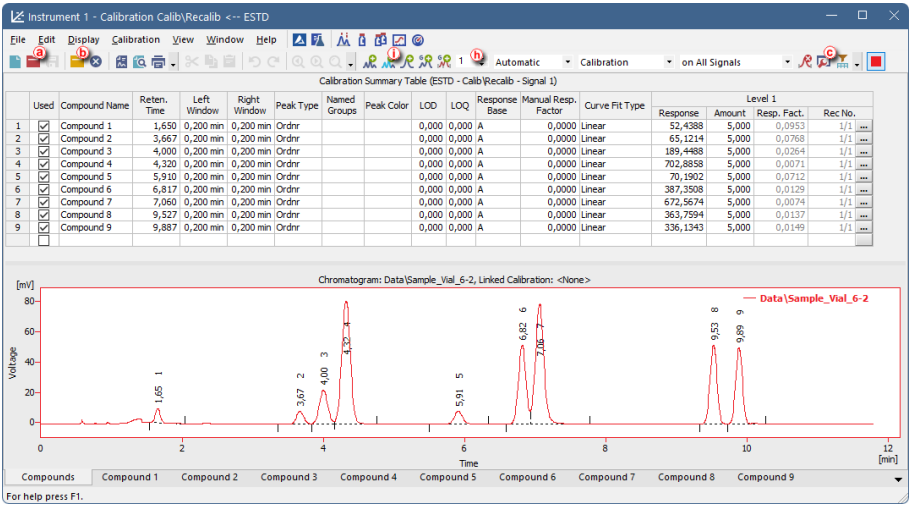


As you can see, excluding the incorrectly measured calibration point resulted in more accurate calibration.

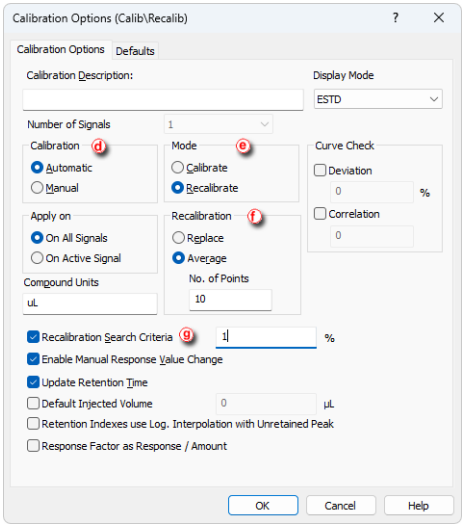
11.9 Recalibrating a calibration

You can modify an existing calibration by reloading peaks within one specific level using the option *Recalibrate*.

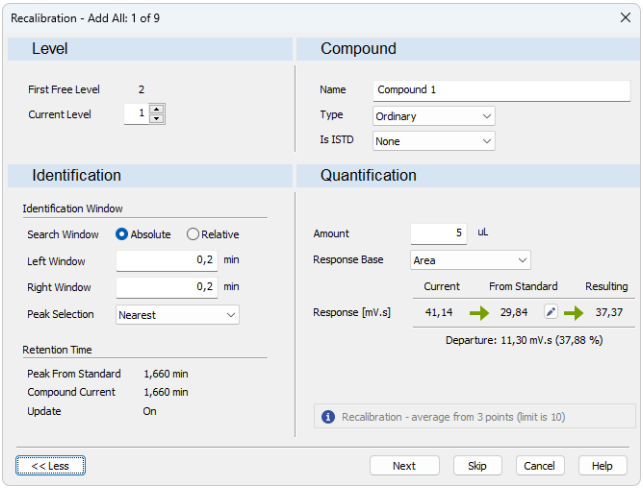
1. Open the Calibration window: choose *Window - Calibration* on the *Instrument* window or click .



2. Open the calibration file: choose *File - Open…* or click ⓐ .
3. Open the calibration standard with which you want to recalibrate: select *File - Open Standard…* or click ⓑ .
4. Open the *Calibration Options* dialog: choose *Calibration - Options…* or click ⓒ .



5. Set the *Calibration* option to *Automatic* to add the peaks without modification or to *Manual* to modify them one by one ⓓ .
6. Set the *Mode* to *Recalibration* ⓔ .
7. Select how and whether the new values will be added in the *Calibration Options* dialog.
    - Choose *Replace* or *Average* option to decide what to do with new response values ⓕ .
    - *Recalibration Search Criteria* defines how much the original and new values can differ for the recalibration to be performed ⓖ .
8. Select the *Level* you wish to recalibrate ⓗ .
9. Add peaks to be recalibrated from the calibration standard to the calibration file on the *Calibration* window using *Calibration - Add Existing* or clicking on ⓘ .
10. If you selected *Manual* calibration:
    - Fill in any parameters related to the peak in the *Calibration - Add All* window. This window will open once for each one of the peaks processed.

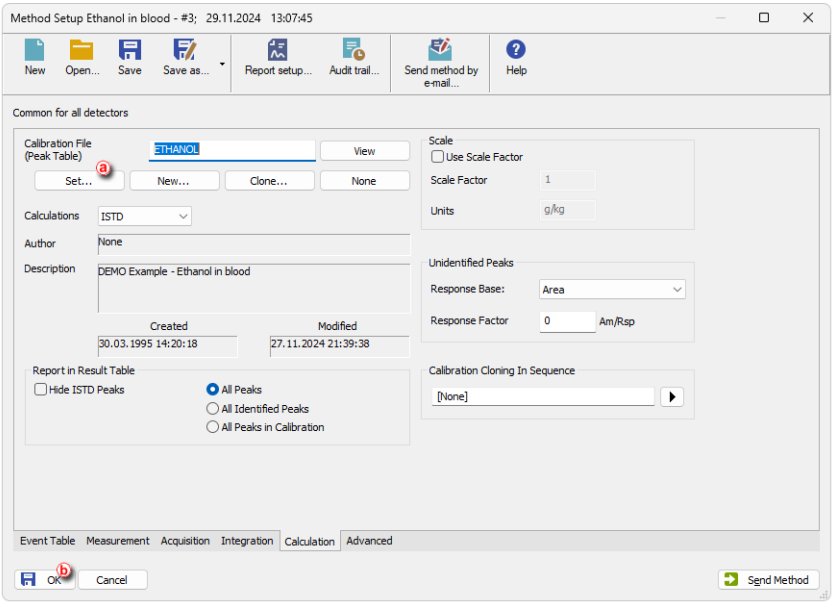


11. Save the calibration file: choose *File - Save* or click on .

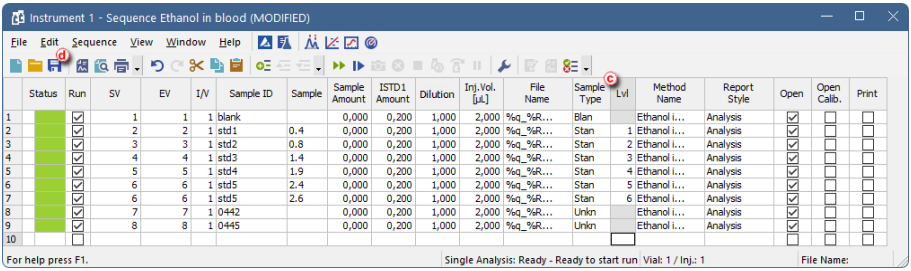
11.10 Recalibrating automatically using a sequence

Here we describe how to add more data to a calibration point from more than one calibration standard chromatogram using a sequence.

1. Open the method file: use *File - Open Method…* on the Instrument window or click in the *Method Setup* dialog.
2. Go to the *Calculation* tab.



3. Connect the calibration file to the method by using the *Set…* ⓐ button.
4. Save the method file - click *OK* ⓑ or select *File - Save Method* or click .
5. Open the Sequence window: select *Analysis - Sequence* or click in the *Instrument* window.



6. Fill in the Sequence Table as described in the section ***Run a sequence***.
7. For the calibration standards, fill in the *Sample Type* and *Lvl* columns ⓒ in the *Sequence Table*.

   More Info:

   The *Sample Type* column for the calibration standard should be set to the *Standard* value, the *Lvl* column for each standard must have a value between *1* and *20*. For a blank sample, select *Blank* in the *Sample Type* column.

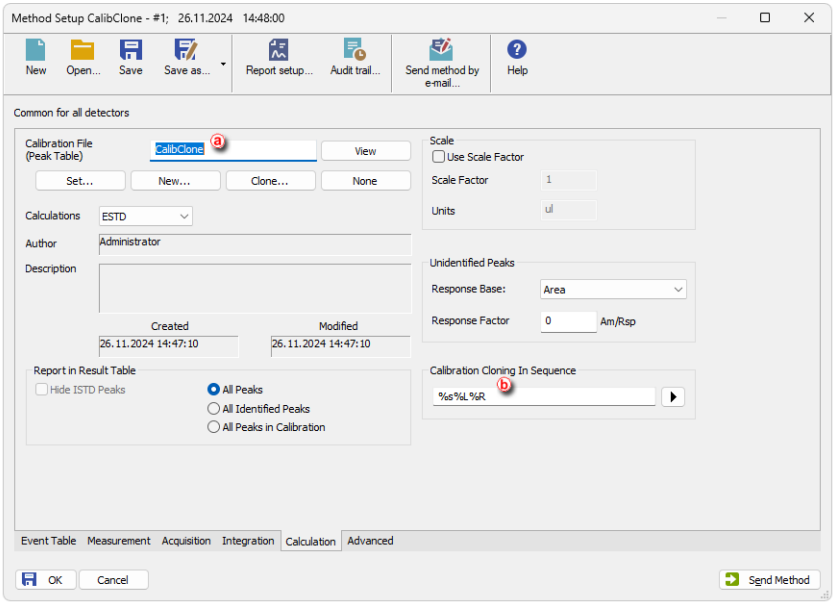
8. Save the sequence file: select *File - Save* or click . ⓓ

The file is now prepared so that the calibration standards measured according to their sequence rows will automatically recalibrate the calibration file.

11.11 Calibrating using clone on first recalibration

Option *Clone on first recalibration* sets the sequence and calibration to the Safe Calibration Usage mode. This option will create a clone (copy) of calibration defined in the method upon completing the first row of the sequence. Cloned calibration is attached to each new chromatogram produced by the given sequence.

1. Open the *Method Setup* dialog - Calculation tab. Select *Method - Calculation* from the *Instrument* window.



2. Click on *Set...* button and select a calibration file ⓐ to be used during cloning at first recalibration.

   Note: This calibration will remain unchanged as newly created clone of the calibration will be used with new responses.

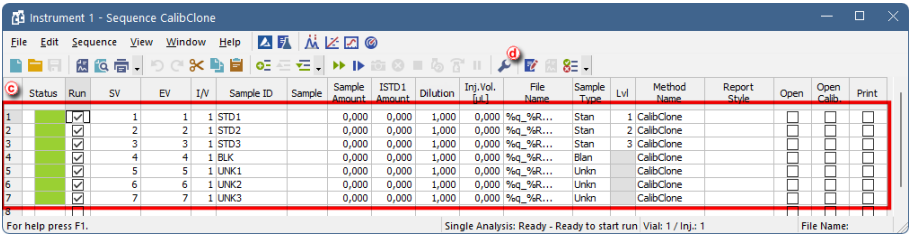
3. Create a custom name for the calibration files in *Calibration Cloning in Sequence* ⓑ as explained in ***Creating customized file names automatically***.

   Note: The name of the final calibration file will match just the content of this field - if you wish to include the name of the template calibration, include the name in this field again (e.g. "test - %s %L %R").

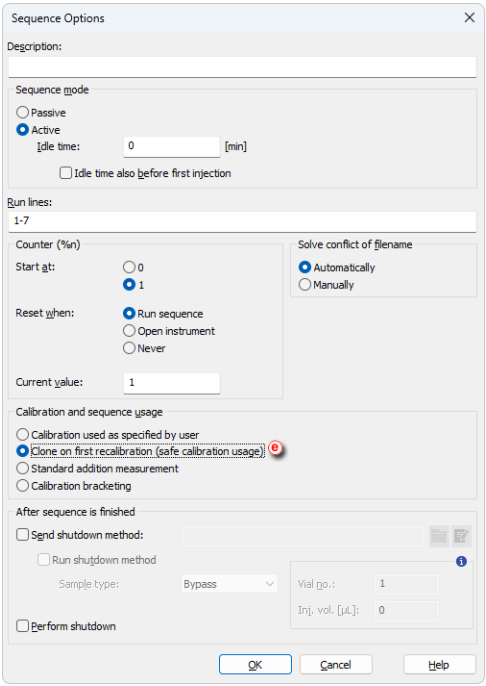
4. Follow the steps in ***Creating and running a sequence*** to create your sequence based on the example below.

   More Info:

   - Set the row/s for the standard/s at the beginning. ⓒ
   - Add a row for a blank, if you wish to.
   - Set the row/s for the unknown samples.



5. Click to open the *Sequence Options* Dialog ⓓ .
6. Select *Clone on first recalibration* ⓔ and click *OK*.



7. Run the sequence as explained in *Creating and running a sequence*.

Note: The measured sequence can be reprocessed using Batch. For more info see the topic Reprocessing whole sequence while using calibration cloning.

11.12 Calibration - Advanced topics

This chapter contains collection of more advanced topics covering calibration usage in Clarity.

11.12.1 Creating a multisignal calibration

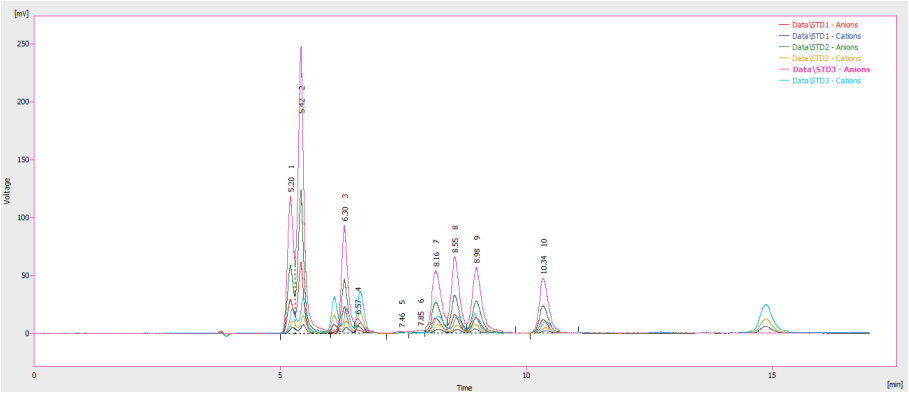
This topic describes how to construct a multisignal calibration in Clarity. Below is an example of creating and constructing a three (concentration) level calibration which provides calculation parameters for calculating results in two-signal chromatograms. This procedure should be utilized when different compounds are detected on each signal. In case all signals detect the same compounds there is no need to use *On Active Signal* option, unless you don't want to quantify all of the compounds on some signals.

Note: For cases there is need to create and construct more than a two-signal calibration, the applied approach remains the same. It varies from the below procedure slightly. These aspects are reflected in the respective steps of this topic.

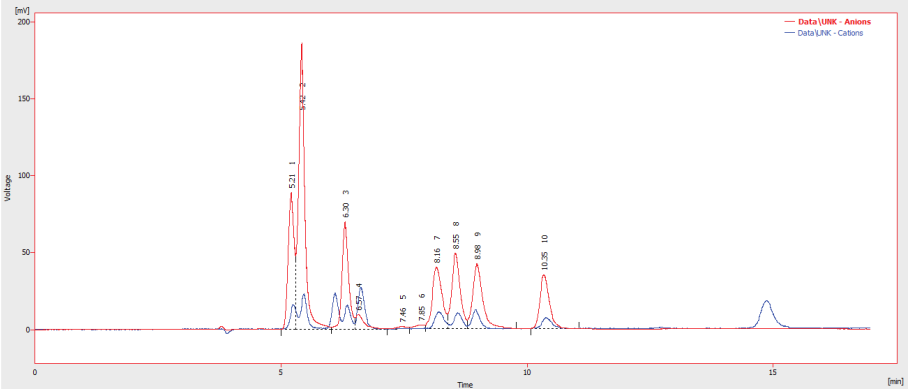
This guide is based on two-signal chromatograms of standards with simulated data (for demonstration purposes it can be said that first signal detects anions and second detects cations) on three concentration levels (5 000 ppm, 10 000 ppm and 20 000 ppm) and one sample chromatogram. All chromatograms used in this guide have been integrated in manner to fit the demonstration purpose.

Prerequisites:

- Integrated chromatograms of standards.

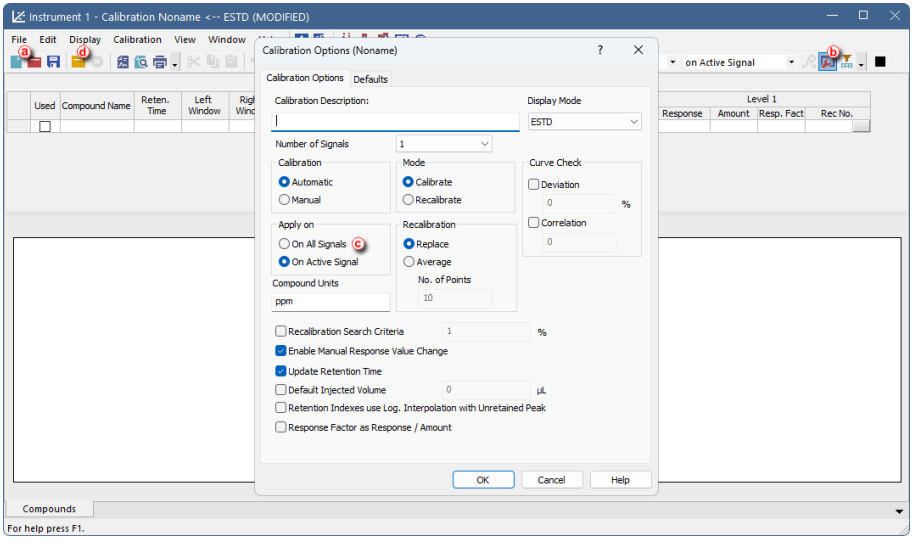


- Integrated chromatogram of sample.



1. Open the Calibration window: select *Window - Calibration* in the *Instrument* window or click .
2. Create a new calibration file: select *File - New* or click ⓐ .
3. Open the Calibration Options dialog: select *Calibration - Options…* or click ⓑ .
4. Set section *Apply on* to option *On Active Signal* field ⓒ .

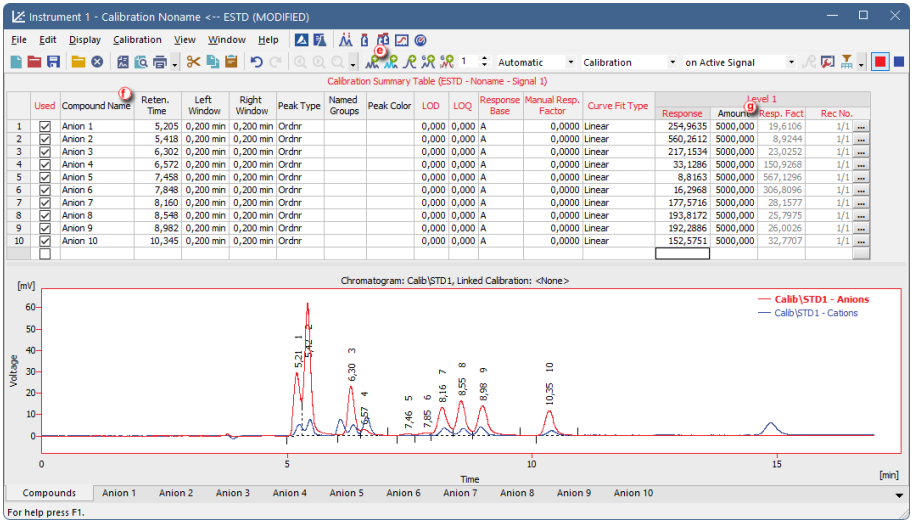
Note: As mentioned in the beginning. If all peaks in the standard chromatogram represent the same compound across all signals it is viable to change the option to *On All Signals*. In such case there is no difference in working with multisignal and single signal calibration.



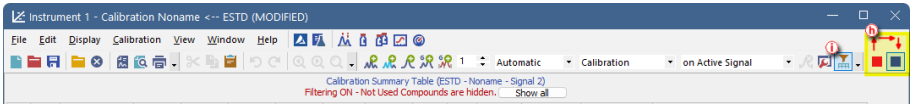
5. Open calibration standard: select *File - Open Standard…* or click ⓓ to open measured and integrated chromatogram with the lowest concentration level where all peaks are available.
6. Make sure the upper toolbar displays *on Active Signal*. It is also recommended to make sure you are currently on the first signal as well (focused red square in right part of the upper toolbar).
7. Fill the *Calibration Summary Table* with peaks from the currently selected signal in chromatogram using the *Add All* icon ⓔ .

   Note: If only some peaks should evaluated it can be done by using *Add Peak* on peaks that need to be included in calibration.

8. Rename automatically pre-filled names of peaks ⓕ .
9. Enter values for given standard into the *Amount* column ⓖ .

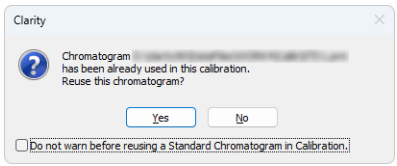


10. Switch to the second signal in chromatogram to make it active ⓗ .
11. Optional: Switch the table filter on using *Filter Not Used Compounds* icon ⓘ . With this option enabled, rows with not *Used* compounds on given signal are hidden, which makes it easier to navigate *Calibration Summary Table*.



12. Fill the *Calibration Summary Table* with peaks from the currently selected (second) signal in chromatogram using *Add All* icon. Dialog will be invoked after clicking *Add All* icon questioning if an already used chromatogram should be reused for this calibration. It is necessary to confirm the reuse by clicking *Yes* button.

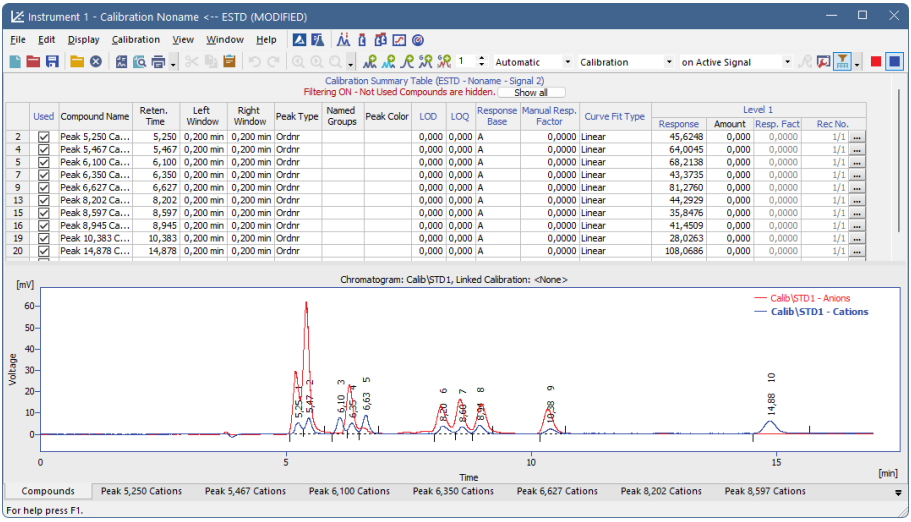
Note: In case of constructing calibration with more than two signals, steps 12 and 14 have to repeated as many times as necessary in order to fill in peaks from all signals to *Calibration Summary Table*.



Note:

This dialog will be invoked multiple times based on number of signals in calibration for calibration with more than two signals. It is possible to switch off invoking of the dialog using the checkbox in the bottom of the dialog.

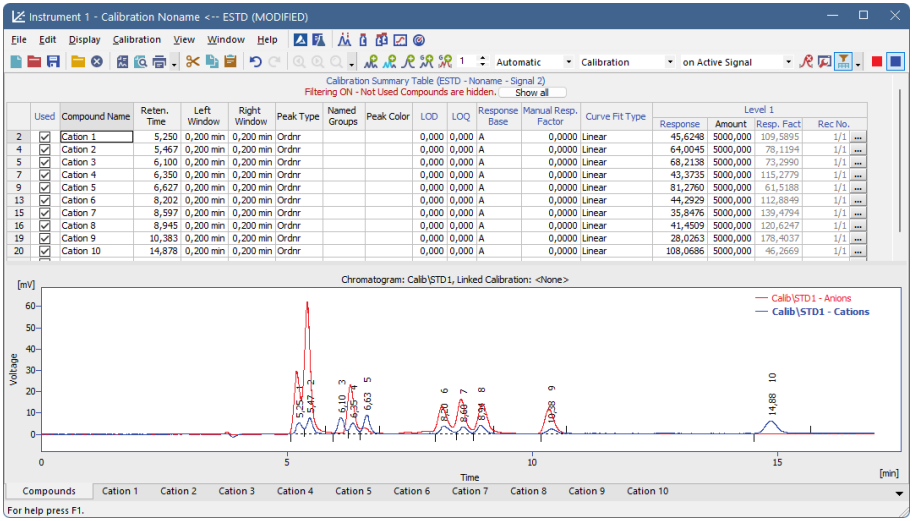
Note: Which signal of chromatogram is active and is being worked with is given by the *Calibration Summary Table* title's color and displayed number of currently active signal.



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 1 Response	Level 1 Amount	Level 1 Resp. Fact	Level 1 Rec No.
2	☑	Peak 5,250 Ca…	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	45,6248	0,000	0,0000	1/1
4	☑	Peak 5,467 Ca…	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	64,0045	0,000	0,0000	1/1
5	☑	Peak 6,100 Ca…	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	68,2138	0,000	0,0000	1/1
7	☑	Peak 6,350 Ca…	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	43,3735	0,000	0,0000	1/1
9	☑	Peak 6,627 Ca…	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	81,2760	0,000	0,0000	1/1
13	☑	Peak 8,202 Ca…	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	44,2929	0,000	0,0000	1/1
15	☑	Peak 8,597 Ca…	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	35,8476	0,000	0,0000	1/1
16	☑	Peak 8,945 Ca…	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	41,4509	0,000	0,0000	1/1
19	☑	Peak 10,383 C…	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	28,0263	0,000	0,0000	1/1
20	☑	Peak 14,878 C…	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	108,0686	0,000	0,0000	1/1

13. Rename the automatically pre-filled names in the *Calibration Summary Table* column.
14. Enter values into *Amount* column. The first concentration level is finished now. It is possible to proceed building up to next levels of calibration.

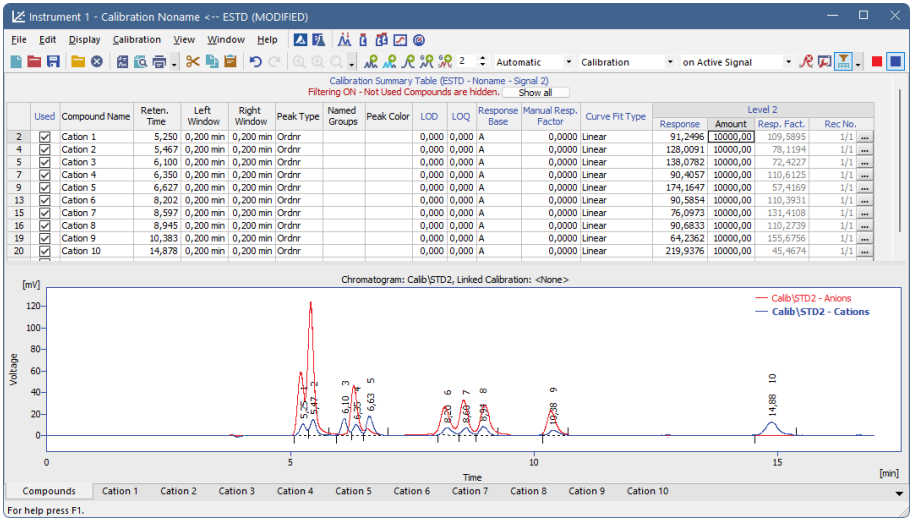
Note: All rows of *Amount* column have to be filled in.



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 1 Response	Level 1 Amount	Level 1 Resp. Fact	Level 1 Rec No.
2	☑	Cation 1	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	45,6248	5000,000	109,5895	1/1
4	☑	Cation 2	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	64,0045	5000,000	78,1194	1/1
5	☑	Cation 3	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	68,2138	5000,000	73,2990	1/1
7	☑	Cation 4	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	43,3735	5000,000	115,2779	1/1
9	☑	Cation 5	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	81,2760	5000,000	61,5188	1/1
13	☑	Cation 6	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	44,2929	5000,000	112,8849	1/1
15	☑	Cation 7	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	35,8476	5000,000	139,4794	1/1
16	☑	Cation 8	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	41,4509	5000,000	120,6247	1/1
19	☑	Cation 9	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	28,0263	5000,000	178,4037	1/1
20	☑	Cation 10	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	108,0686	5000,000	46,2669	1/1

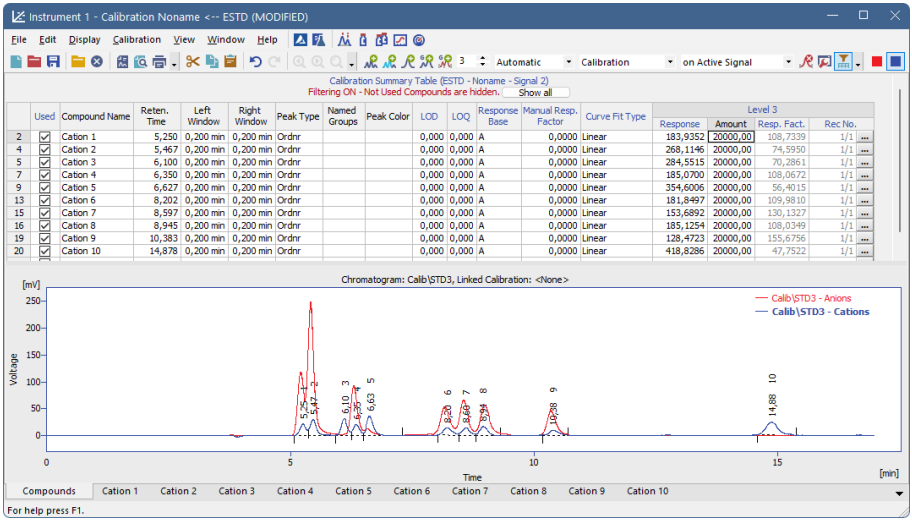
15. Open chromatogram of standard of the next (second) concentration level.
16. Fill the next level of *Calibration Summary Table* with Responses for each signal following the same steps as for Level 1 (Steps 8-16, renaming the compounds is omitted as the names carry over from previous levels).

Note: *Add Existing* can be used instead of *Add All*. This command only adds response for peaks that are preset on first level. This means that extra peaks (or peaks chosen not to be evaluated) that are present in the second (and later) standards, but not in the first one will not be added.



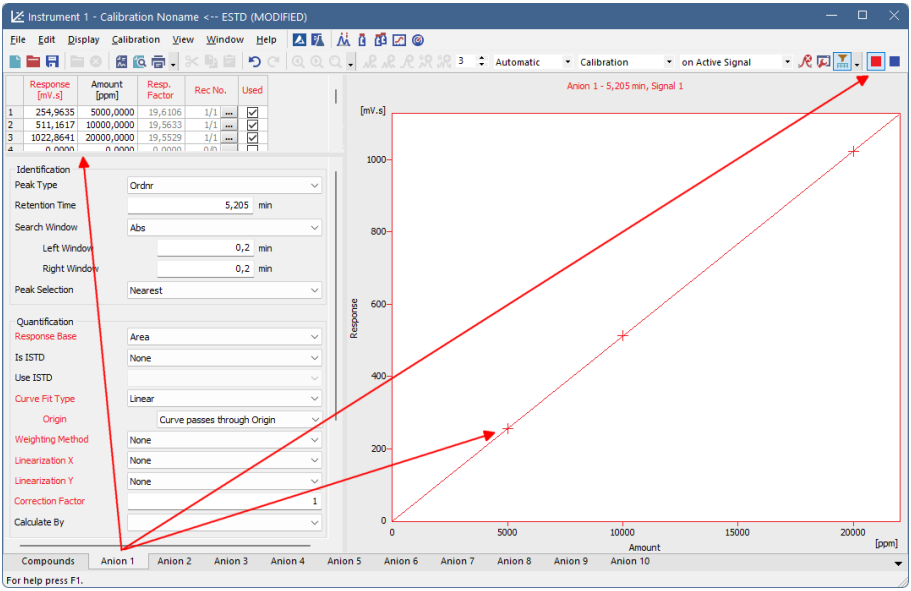
	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 2 Response	Level 2 Amount	Level 2 Resp. Fact.	Level 2 Rec No.
2	☑	Cation 1	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	91,2496	10000,00	109,5895	1/1
4	☑	Cation 2	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	128,0091	10000,00	78,1194	1/1
5	☑	Cation 3	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	138,0782	10000,00	72,4227	1/1
7	☑	Cation 4	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	90,4057	10000,00	110,6125	1/1
9	☑	Cation 5	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	174,1647	10000,00	57,4169	1/1
13	☑	Cation 6	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	90,5854	10000,00	110,3931	1/1
15	☑	Cation 7	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	76,0973	10000,00	131,4108	1/1
16	☑	Cation 8	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	90,6833	10000,00	110,2739	1/1
19	☑	Cation 9	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	64,2362	10000,00	155,6756	1/1
20	☑	Cation 10	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	219,9376	10000,00	45,4674	1/1

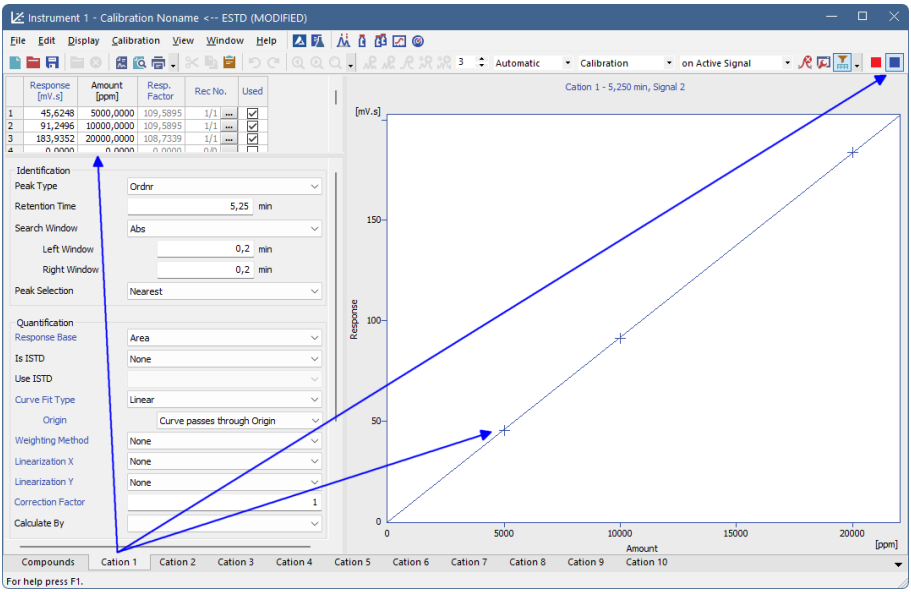
17. Open chromatogram of standard of the next (third) concentration level.
18. Fill the *Calibration Summary Table* in the same manner as for second level (step 18).



	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor	Curve Fit Type	Level 3 Response	Level 3 Amount	Level 3 Resp. Fact.	Level 3 Rec No.
2	☑	Cation 1	5,250	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	183,9352	20000,00	108,7339	1/1
4	☑	Cation 2	5,467	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	268,1146	20000,00	74,5950	1/1
5	☑	Cation 3	6,100	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	284,5515	20000,00	70,2861	1/1
7	☑	Cation 4	6,350	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	185,0700	20000,00	108,0672	1/1
9	☑	Cation 5	6,627	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	354,6006	20000,00	56,4015	1/1
13	☑	Cation 6	8,202	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	181,8497	20000,00	109,9810	1/1
15	☑	Cation 7	8,597	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	153,6892	20000,00	130,1327	1/1
16	☑	Cation 8	8,945	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	185,1254	20000,00	108,0349	1/1
19	☑	Cation 9	10,383	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	128,4723	20000,00	155,6756	1/1
20	☑	Cation 10	14,878	0,200 min	0,200 min	Ordnr			0,000	0,000	A	0,0000	Linear	418,8286	20000,00	47,7522	1/1

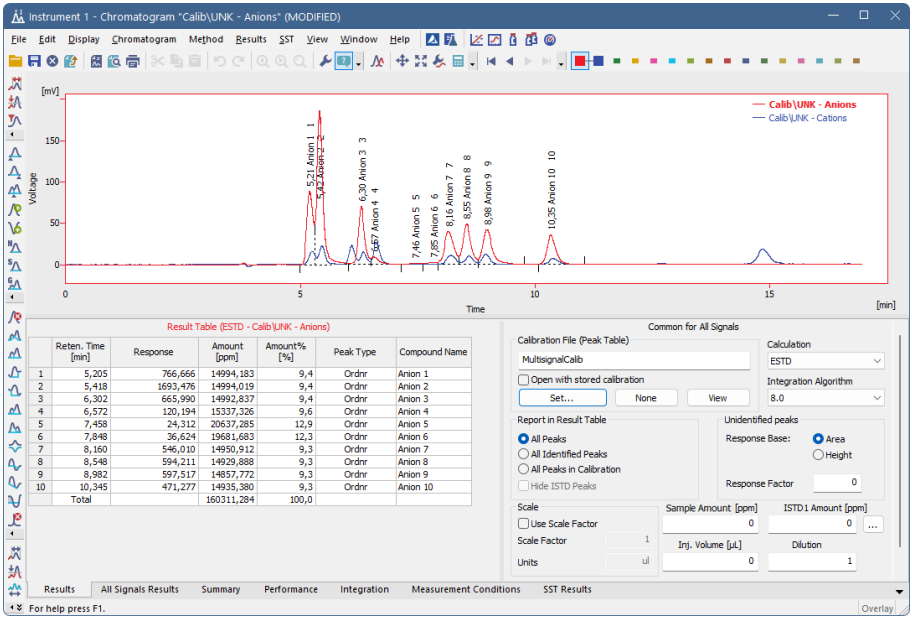
Note: It is possible to review calibration curves for each compound on the respective tabs of individual compounds. Notice that calibration curve are displayed only for valid signal (When filtering is enabled tabs of individual compounds are displayed only on signal where they are used). Signal selection is located in right upper corner of the *Calibration Window*.

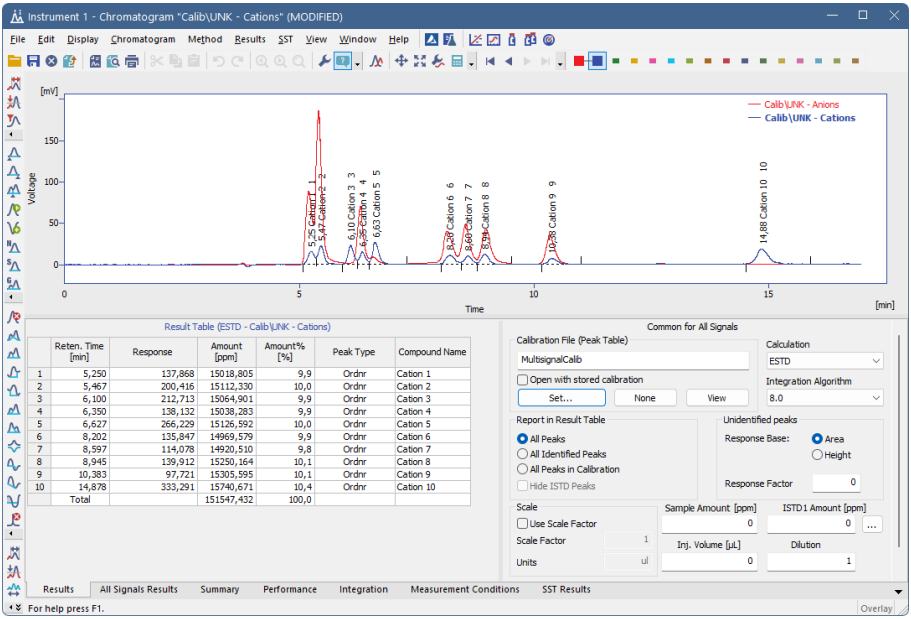


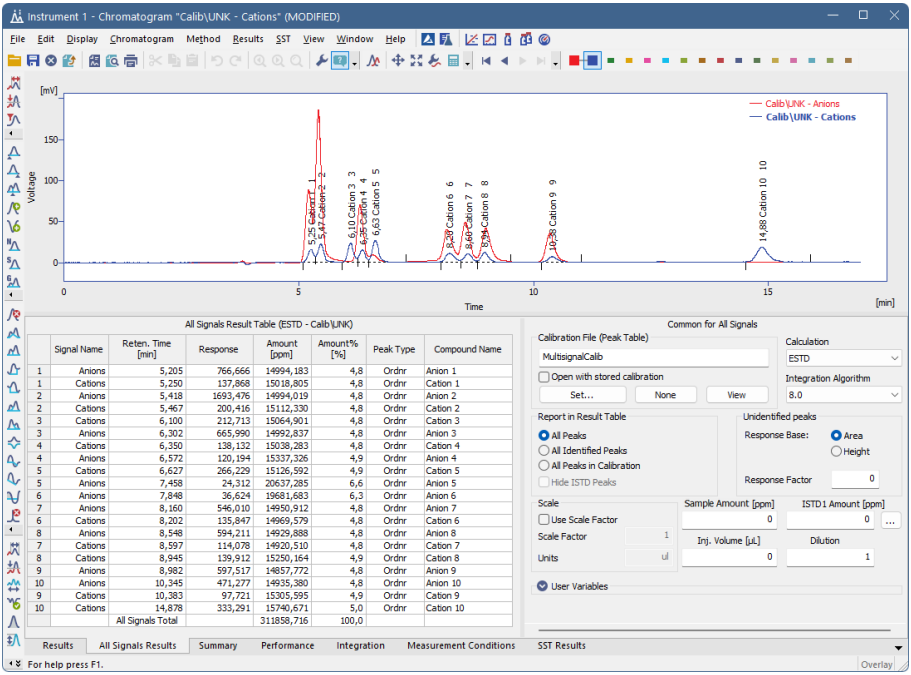


19. When calibration is finished do not forget to save it using select *File - Save* or click on .

20. For calculating result in sample open the **Chromatogram window** select *Window - Chromatogram* on the *Instrument* window or click on  and open chromatogram of sample and link the calibration to chromatogram.
21. Review results on *Results Table* of each individual signal or review results for all signals on *All Signals Results* Table.




Instrument 1 - Chromatogram "Calib\UNK - Cations" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[mV]
Voltage
Time
[min]
Calib\UNK - Anions
Calib\UNK - Cations
5,25 Cation 1
5,47 Cation 2
6,10 Cation 3
6,35 Cation 4
6,63 Cation 5
8,20 Cation 6
8,49 Cation 7
8,94 Cation 8
10,38 Cation 9
14,88 Cation 10
Result Table (ESTD - Calib\UNK - Cations)
Reten. Time [min] | Response | Amount [ppm] | Amount% [%] | Peak Type | Compound Name
1 | 5,250 | 137,868 | 15018,805 | 9,9 | Ordnr | Cation 1
2 | 5,467 | 200,416 | 15112,330 | 10,0 | Ordnr | Cation 2
3 | 6,100 | 212,713 | 15064,901 | 9,9 | Ordnr | Cation 3
4 | 6,350 | 138,132 | 15038,283 | 9,9 | Ordnr | Cation 4
5 | 6,627 | 266,229 | 15126,592 | 10,0 | Ordnr | Cation 5
6 | 8,202 | 135,847 | 14969,579 | 9,9 | Ordnr | Cation 6
7 | 8,597 | 114,078 | 14920,510 | 9,8 | Ordnr | Cation 7
8 | 8,945 | 139,912 | 15250,164 | 10,1 | Ordnr | Cation 8
9 | 10,383 | 97,721 | 15305,595 | 10,1 | Ordnr | Cation 9
10 | 14,878 | 333,291 | 15740,671 | 10,4 | Ordnr | Cation 10
Total | | | 151547,432 | 100,0 | | |
Common for All Signals
Calibration File (Peak Table)
MultisignalCalib
Open with stored calibration
Set... None View
Calculation
ESTD
Integration Algorithm
8.0
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Hide ISTD Peaks
Unidentified peaks
Response Base: Area Height
Response Factor 0
Scale
Use Scale Factor
Scale Factor 1
Units ul
Sample Amount [ppm] 0
ISTD1 Amount [ppm] 0
Inj. Volume [µL] 0
Dilution 1
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
For help press F1.
Overlay



11.12.2 Using Internal Standard (ISTD) in calibration

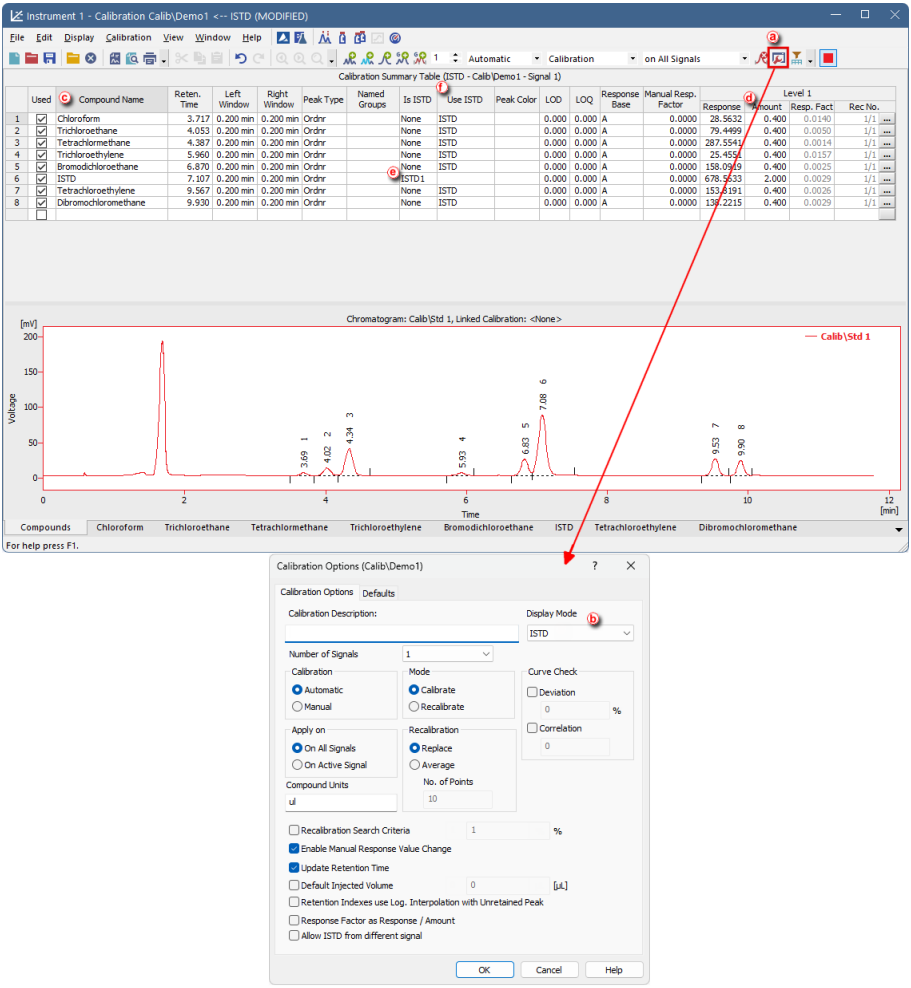
The use of internal standard (ISTD) helps to compensate for non-reproducible injected volume or for analyte losses during sample preparation. A known amount of internal standard compound (which should have similar properties as the analyte, but should not be present in the samples) is added to the standards and samples. The determined analyte amounts are then corrected based on the ratio of the added and detected amounts of the ISTD compound(s).

This chapter provides detailed insights into the differences when creating a calibration with ISTD compared to a standard calibration, as described in Creating a new calibration.

1. In the *Calibration Options* window (accessible via the icon ⓐ in the *Calibration* window), change the *Display Mode* to *ISTD* ⓑ .
2. Open your first calibration standard and add peaks to the Calibration Summary Table as usual.
3. Label the peaks by the compound names in the corresponding column ⓒ and fill in the *Amount* column ⓓ with the amounts of the present compounds including ISTD.
4. In the row corresponding to ISTD, change the type of the cell in the *Is ISTD* column to *ISTD1* ⓔ . The *Use ISTD* column ⓕ now contains the name of the

selected ISTD compound in all the other rows. In compounds tabs, the axes are labeled according to the selected ISTD.

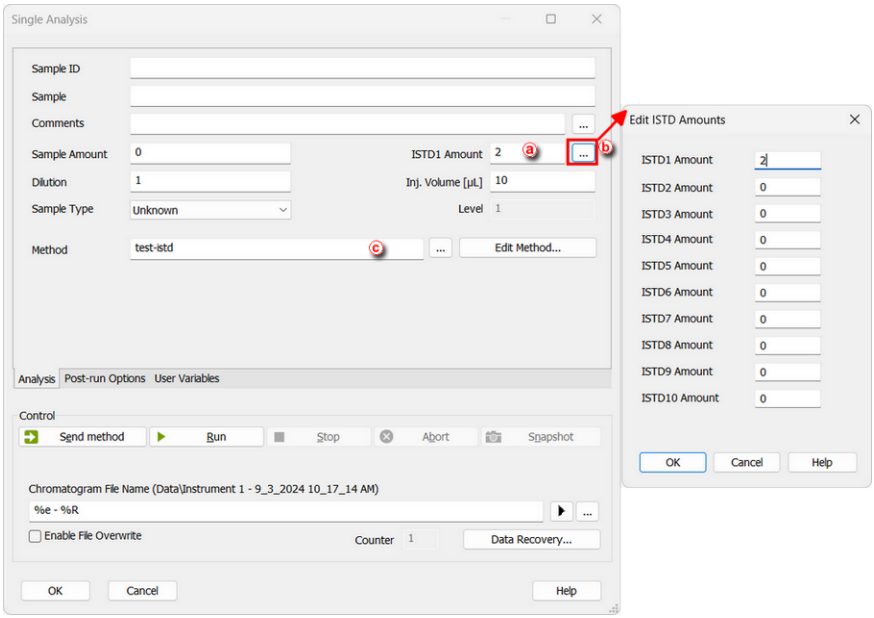
Note: You can set up to 10 compounds as ISTDs in the *Is ISTD* column. When more ISTDs are present, you can specify which one to use for quantification of which compound in the *Use ISTD* column.



5. Now, the first calibration level is set. Continue as usual to set the remaining calibration levels using the measured calibration standards (as shown in Adding a new calibration level). Enter the ISTD amounts according to the mode you plan to work in.

The created ISTD calibration may now be linked to an already measured chromatogram for direct results assessment (see Applying calibration to a chromatogram), and it may be also linked to a method (see Setting a calibration in a method) - this causes that the chromatograms measured using this method will be automatically evaluated using the pre-selected ISTD calibration.

6. To use the ISTD method in single analysis, set the *ISTD1 Amount* ⓐ in the *Single Analysis* window to the desired value. In the case of more than one ISTD compound present, set the amounts in the dialog which opens by clicking the triple dot ... menu ⓑ .
7. Select the previously created method ⓒ . You can *Run Acquisition* ▶ directly from the *Single Analysis* window.



The sequence analysis setup is analogous to the single analysis. The ISTD2–ISTD10 amount columns are not shown by default and can be added via the *Edit - Setup columns...* dialog.

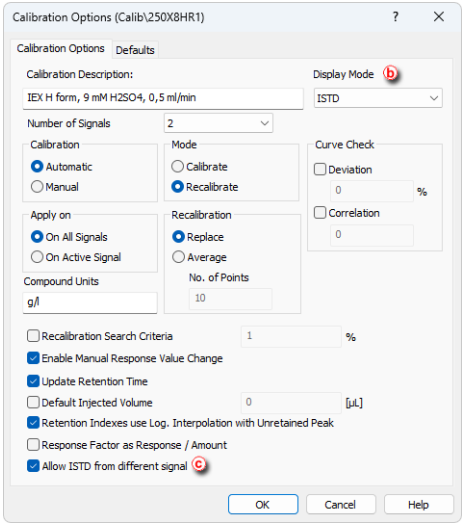
Note: In the case the amount of internal standard is the same for all standards and samples, it is possible to enter zero instead of the amount (which may not be known). In such case, the correction will be based on the ratio of the ISTD peak response in the standards and unknowns. Note that the ISTD amounts must be entered or set to zero both in Calibration and in the Sample Header. A mismatch will be detected and reported as error.

11.12.2.1 Using Internal Standard (ISTD) from different signal in calibration

In analytical workflows involving multiple detectors or multi-signal setups, it is sometimes necessary to measure the internal standard (ISTD) on a different signal than the analytes. This is especially useful in cases where the ISTD is not detectable in the same signal, such as in ICP-MS.

This section describes how to set up a calibration using an ISTD compound measured on a different signal than the analytes.

1. Go to the *Calibration Options* window (accessible via the icon ⓐ in the *Calibration* window).
2. Change the *Display Mode* to *ISTD* ⓑ .
3. Check the Allow ISTD from different signal option ⓒ .
4. Confirm the settings by clicking OK.

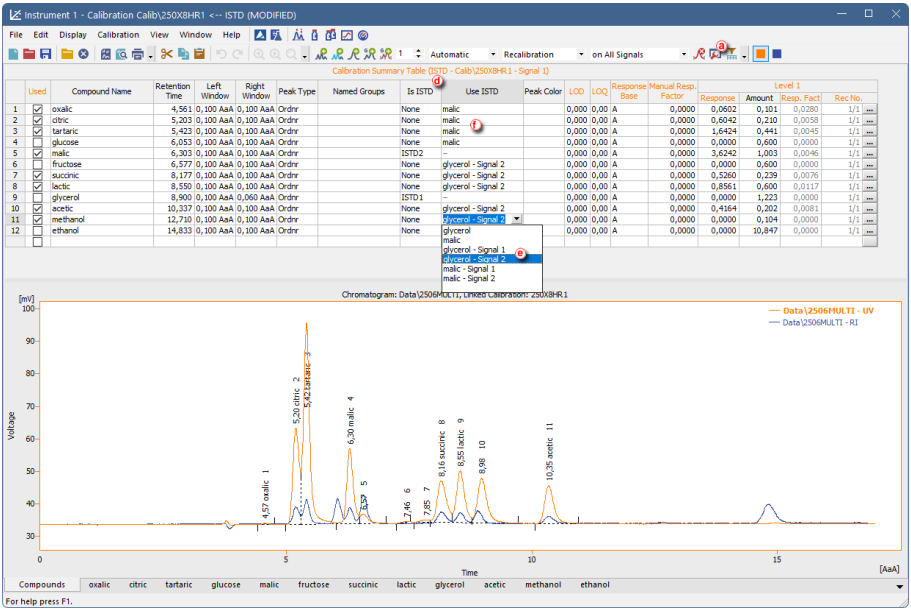


5. Then, fill in the Calibration summary table as described in the Creating a multisignal calibration topic.

In our case, we have a two-signal calibration where Glycerol is detected only on Signal 2, but we want to use it as the ISTD for some compounds also on Signal 1. To contrast the situation, there is a second ISTD – Malic acid – which is detected on both signals, so we want the correction to always use the Malic peak from the same signal as the analyte.

6. Mark both Glycerol and Malic as ISTD in the Is ISTD ⓓ column.
7. In Use ISTD column expand the dropdown menu. There is list of all compounds set as ISTDs, firstly without the identification of the signal, and then again for every signal present.

8. For compounds calculated by ISTD Glycerol, select the Glycerol entry with the Signal 2 identification ⓔ . This means that Glycerol from Signal 2 will be used as ISTD in both signals.
9. For compounds calculated by ISTD Malic, select the Malic entry without signal identification ⓕ . That means the malic from the same signal as the analyte will be used as ISTD.

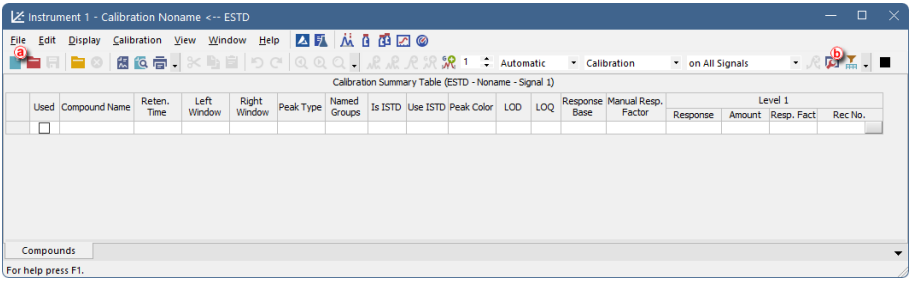


Further work with such a calibration is identical to a standard ISTD calibration - see the Using ISTD in calibration topic for guidance how to measure chromatograms with entered ISTD amounts or topics covering linking calibration to an already measured chromatogram for direct results assessment (see Applying calibration to a chromatogram), or to a method (see Setting a calibration in a method), so the chromatograms measured using this method will be automatically evaluated using the pre-selected ISTD calibration.

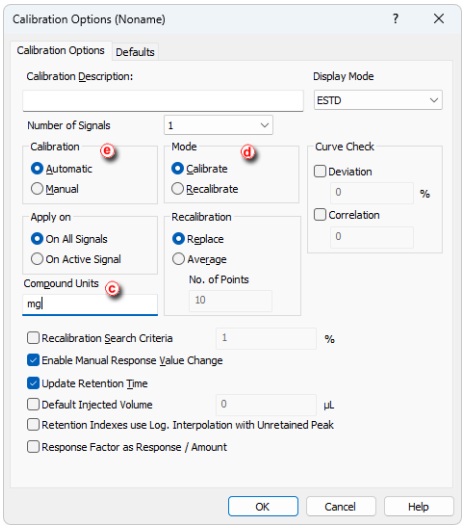
11.12.3 Calibrating with manually entered Response Factors

When using a free calibration, the amounts for each component are calculated using the *Response Factor* instead of a calibration curve.

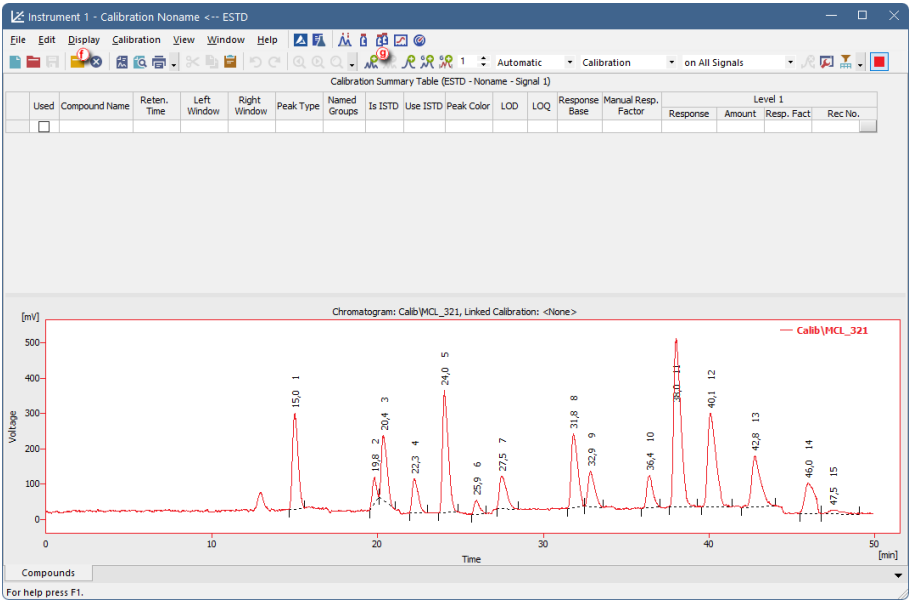
1. Create a new calibration file: select *File - New* or click ⓐ .



2. Open the Calibration Options dialog: choose *Calibration - Options…* or click . ⓑ



3. Check that the *Compound Units* ⓒ are set correctly, *Mode* to *Calibrate* ⓓ and *Calibration* option is set to *Automatic* ⓔ .
4. Open an integrated chromatogram of a standard (containing peaks of compounds of interest with a known concentration): select *File - Open Standard…* or click ⓕ on the *Calibration* window.
5. Add all peaks in the chromatogram of the calibration standard to the calibration file. Choose *Calibration - Add All* or click on ⓖ .

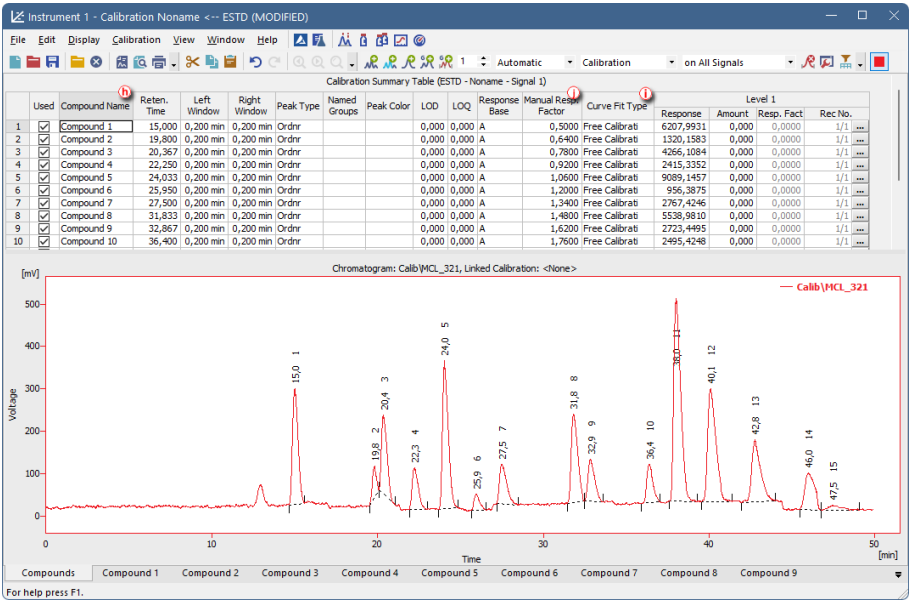


6. Name the peaks identified in the *Calibration Summary Table* ⓗ by their retention times by typing the *Compound Name* for each peak. No peak name may be used more than once.
7. Set the *Calibration Fit Type* to *Free Calibration* ⓘ for each one of the compounds in the *Calibration Summary Table*.

   More Info:

   Right click on the table and select the option *Set Columns...* to add the *Calibration Fit Type* column to the table. Alternatively, you can click on each compound tab at the bottom of the *Calibration* window and set the *Calibration Fit Type* from there.

8. Type in the *Manual Response Factor* for each one of the compounds ⓙ .



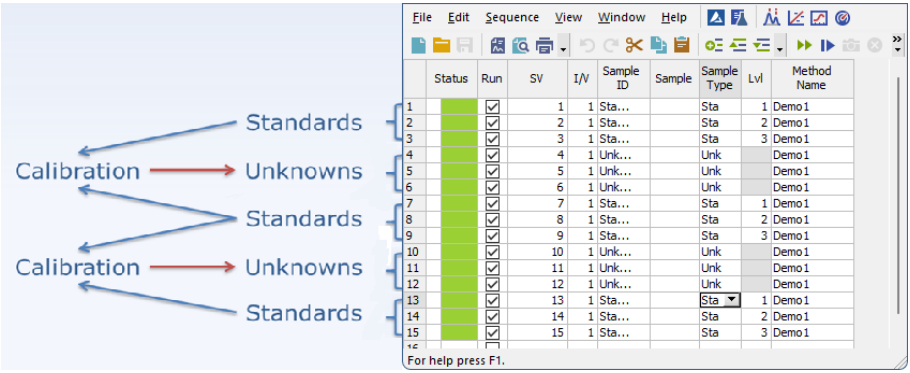
Caution: Calibration curve cannot be constructed when amount is set to zero for all levels. In case calibration curve could not be constructed for one of the compounds, no results are calculated for all of the compounds (as the total amount could be wrong). If you do not want to calculate amounts for all identified compounds, you could use free calibration with zero response factor.

11.12.4 Compensating for response drift using bracketing

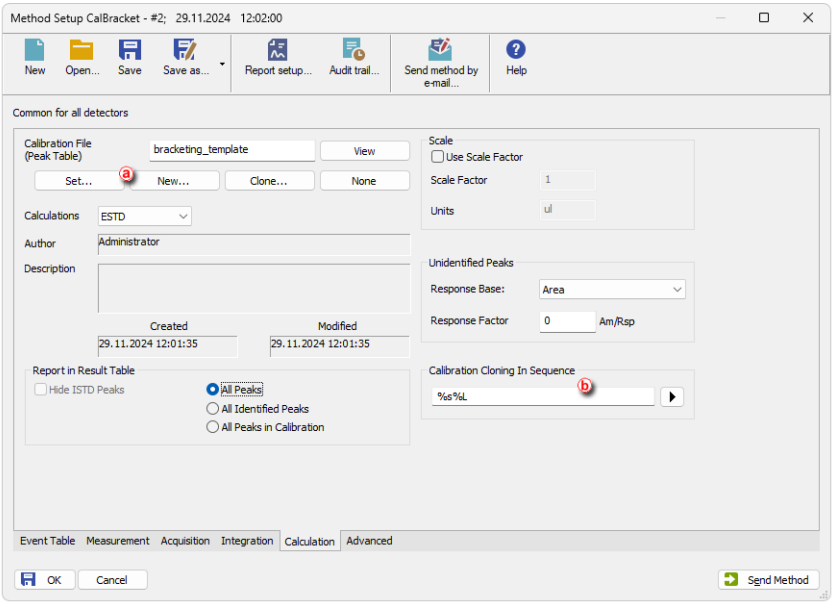
Bracketing is a direct calibration method used to compensate for the variation in instrument response with time. Typical use is for detector response deteriorating or sample containing compounds staining or interacting with the column. Bracketing is not helpful for random variations. Bracketing may be in place when 2 calibration curves measured on the same series of standards have a stable trend and good correlation, but they are not the same.

To use bracketing in sequence, the order of the rows must be standards, then unknowns, then standards again. Usually, two standards are used; more standards could be used if the measuring instrument has a non-linear response. Samples are evaluated by a calibration which is created by averaging the standards before and after the unknown. As every unknown sample series is demarcated by calibration standards it uses a single calibration. Calibration will be cloned from the previous calibration clone whenever an unknown sample or blank follows the calibration standard. The newly cloned calibration file has all responses cleared - apart from the responses from the last series of calibration standards (immediately preceding the current unknown samples).

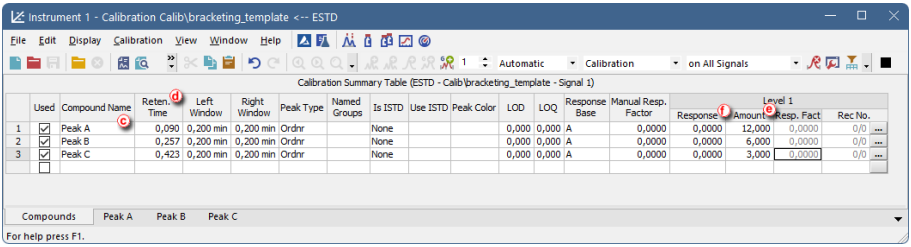
Bracketing in Clarity

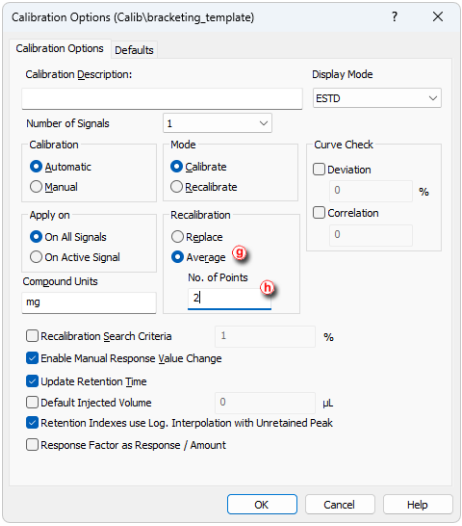


1. Open the method that will be used in the sequence: click *File - Open Method…* from the *Instrument* window.
2. Navigate to *Calculation* tab.
3. Set the template calibration as Calibration File: click *Set...* ⓐ and select the calibration. Note that this calibration will remain unchanged, newly created clone of the calibration will be used with new responses.
4. Set the name of the cloned calibration: set the name in *Calibration Cloning In Sequence* ⓑ. You can use predefined parameters (refer to ***Creating customized file names automatically***).



5. Click *OK* and save the modified method.
6. Open Calibration window and the template calibration: click *Window - Calibration* from the *Instrument* window and *File - Open...* in the *Calibration* window, select the template calibration (in this case bracketing_template.cal).
7. Set *Compound Names* ⓒ , *Retention Time* ⓓ , *Amounts* ⓔ , etc., but no *Responses* ⓕ (you can use previously measured standard to get the Retention Times).
8. Update *Calibration Options*: Set *Recalibration* to *Average*ⓖ and *No. of Points* to 2ⓗ (no more points needed as they would not be applied anyway).
9. Save changes and close the calibration.

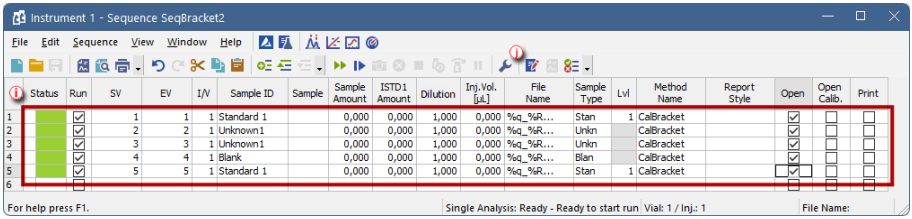




10. Open *Sequence* window and create a new sequence: click *Analysis - Sequence* and then icon.
11. Set the sequence according to the following steps: (for more details about creating the sequence refer to ***Creating and running a sequence***)
    - Set the row/s for the standard/s. ⓘ
    - Add a row for a blank, if you wish to.
    - Set the row/s for the unknown samples.
    - Repeat the row/s for the standard/s.

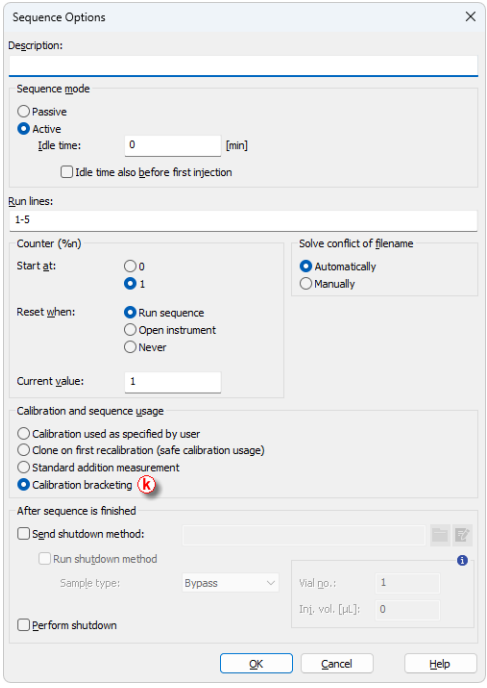
    Note: The sequence must start and end with a row with *Standard Sample Type*.

    - Repeat the previous four steps for every "bracket" of unknown samples you wish to add.



12. Set the sequence to operate in the calibration bracketing mode:
    - Click icon to open the *Sequence Options* dialog. ⓙ
    - Check *Calibration Bracketing*. ⓚ
    - Click *OK*.

Note: If your sequence is using multiple methods, calibration using bracketing is still possible to use but make sure that the Calculation tab is exactly the same for all the methods used in the sequence.



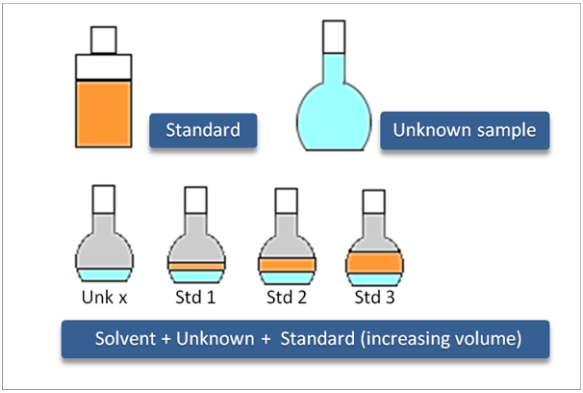
13. Run the sequence (for more details about running the sequence refer to *Creating and running a sequence)* .
14. The results shown while the sequence is running are recalculated at the end of each bracket, when the standard after the unknown sample is acquired. The

calibration used is an average of the two calibrations, before and after the unknown.

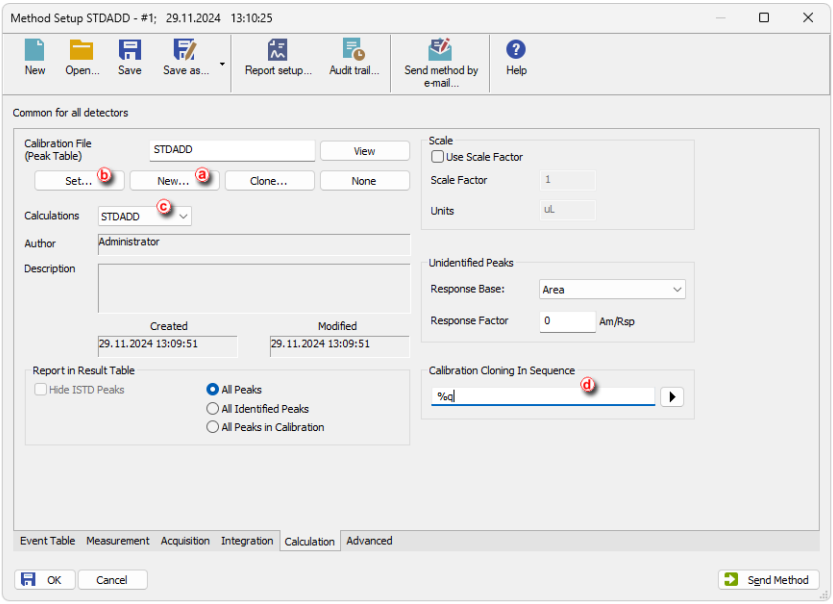
Note: The measured sequence can be reprocessed using Batch. For more info see the topic Reprocessing whole sequence while using calibration cloning.

11.12.5 Improving quantification with the standard addition method

Standard addition is a quantification approach (similar to ESTD or ISTD) useful in case the sample matrix is complex and when it influences responses of analytes. By spiking samples with a series of increasing amounts of the analytes, standard addition calibration curves for each sample are obtained from which the concentrations of unknown samples can be calculated.



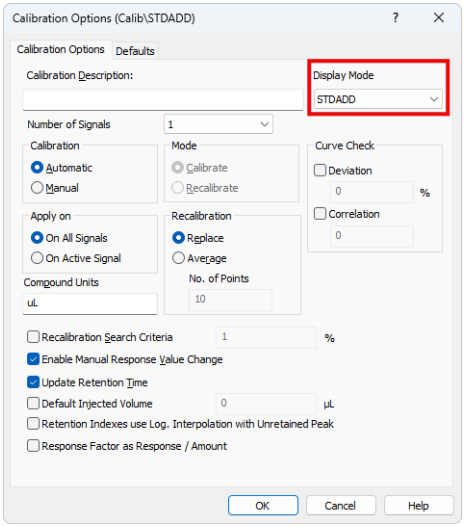
1. Create a new method or open your already prepared method. Go to *Method Setup - Calculation* tab.
2. Create *New* calibration file ⓐ or *Set* your already created Calibration file ⓑ .



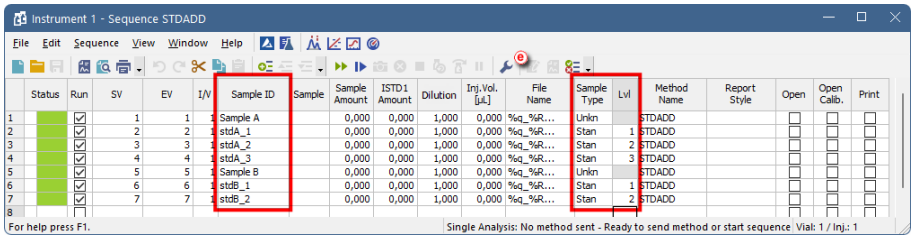
3. Select *STDADD* in the *Calculations* drop-down list ⓒ .
4. Create a custom name for the cloned calibration files in *Calibration Cloning in Sequence* ⓓ and click *OK*.

   Note: Make sure that each of the measured samples will have a unique calibration name; use predefined parameters to achieve that.

5. Open the *Calibration* window by selecting *Window - Calibration* in the *Instrument* window.
6. Open the *Calibration Options* dialog. Choose *Calibration - Options…* or click on . Select the *STDADD* in the *Display Mode* drop-down list and click ***OK***.

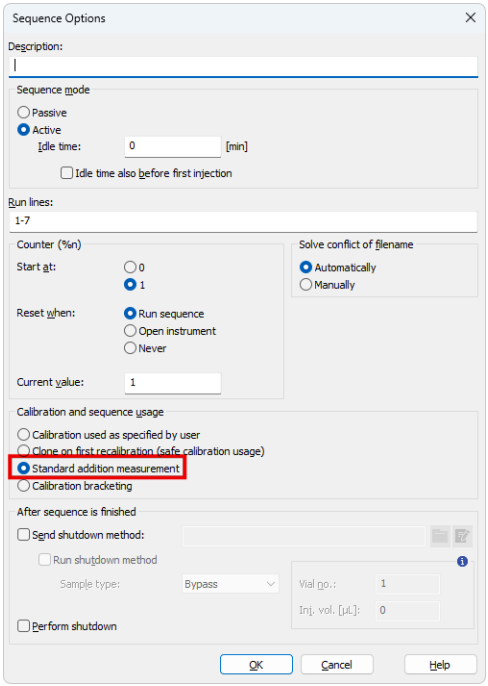


7. Create a new sequence with the given order of the lines:
   - Sample A
   - Sample A with Standard level 1
   - Sample A with Standard level 2
   - Sample A with Standard level X
   - Sample B
   - Sample B with Standard level 1
   - Sample B with Standard level X
   - *continue with the given pattern until desired state*
8. Set the columns as follows: for Unknown samples set *Sample Type* column to *Unknown* and for Standard Addition samples, set *Sample Type* column to *Standard* and *Lvl* column to level corresponding to the added amount in given sample.

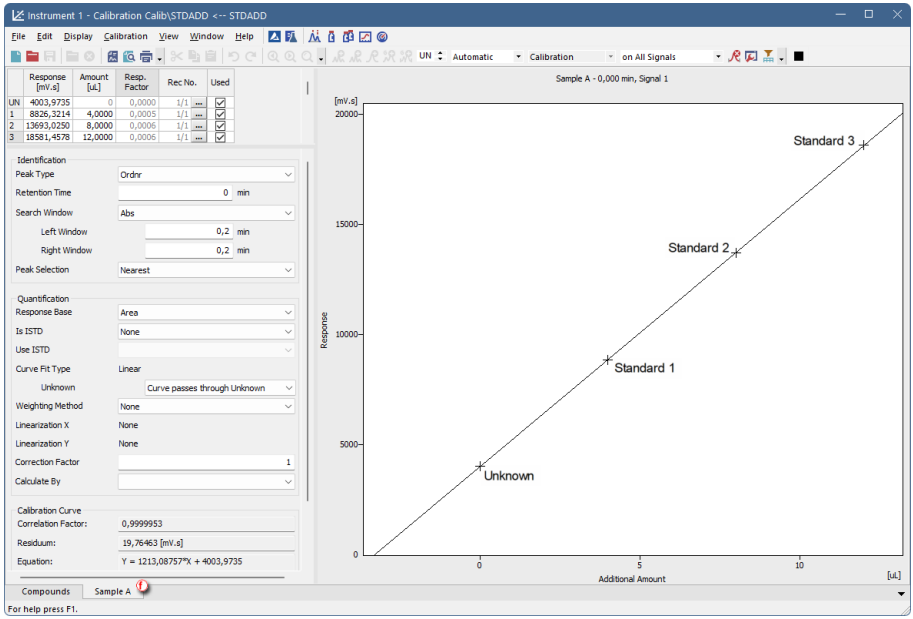


Note: In case you want to use a blank sample too, such sample shall be always put in the sequence before the unknown sample.

9. Click to open the *Sequence Options* dialog and select *Standard Addition Measurement* and click *OK*.



10. Run the sequence and wait until the sequence is finished.
11. Open the *Calibration* window: choose *Window* - *Calibration* in the *Instrument* window or click on .
12. Go to *File* - *Open* and open the cloned calibration file for the desired sample.
13. Click on the *Compound* tab ⓕ to see the calibration curve. Fill in the amounts of the standard samples.



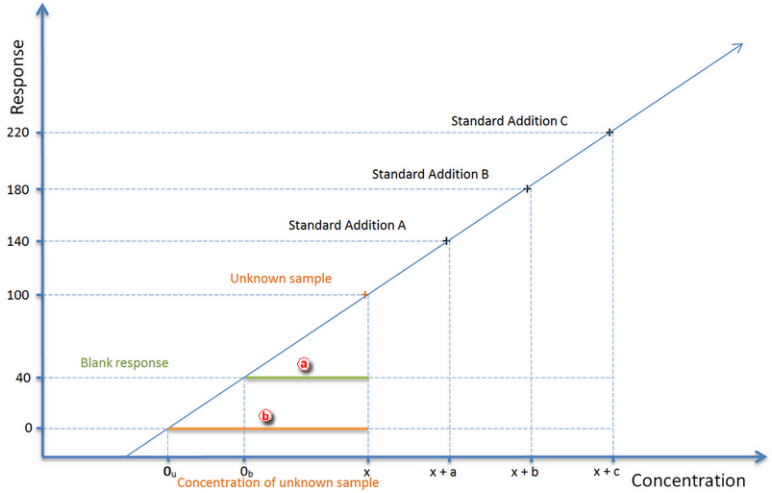
14. Open chromatogram of the desired unknown sample. The Result Table now contains amount of the unknown sample, calculated using Standard Addition.

Note: The measured sequence can be reprocessed using Batch. For more info see the topic Reprocessing whole sequence while using calibration cloning.

11.12.5.1 How the concentration is calculated

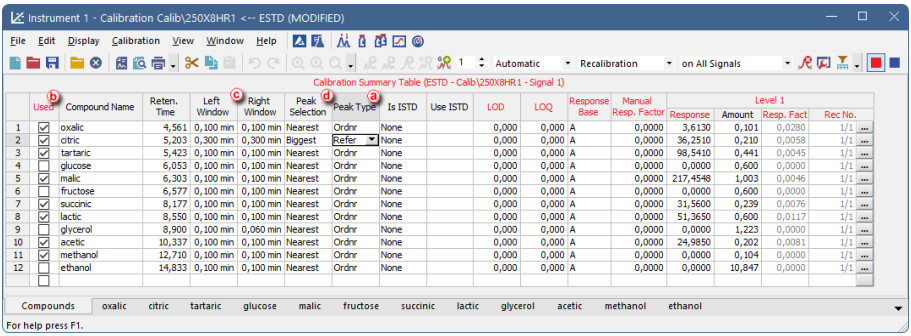
The concentration of an unknown sample is calculated using a calibration curve, which intersects in the point [0,0].

As shown in the picture below, when not using Blank samples the the concentration of an unknown sample equals the orange line (0 response corresponds to 0 unknown sample concentration - 0u), whereas the concentration of the UNKNOWN SAMPLE when using Blank equals the green line (Blank response corresponds to 0 unknown sample concentration - 0b).



11.12.6 Using a reference peak to improve compound identification

A reference peak is a peak used as a reference for recalculating the retention times for the rest of the peaks in a chromatogram. This method allows a better compound identification in those cases where there might be a drift in the retention times in repeated analyses. It is possible to set multiple reference peaks. For ordinary peaks, the expected retention times will be adjusted by linear interpolation between the nearest reference peaks.



1. Open the calibration file: choose *File - Open…* or click on .
2. Select *Refer* on the *Peak Type* column for an easily identifiable compound (i.e. main compound, ISTD standard, any well resolved peak of the matrix) that you will use as a reference ⓐ . To apply the reference peak, *Used* check-box must be checked ⓑ .

3. Edit the Left and Right window values to define the range within which the peak should appear ⓒ. This window may include other peaks if the selected reference peak meets the *Peak Selection* criteria.
4. Select the Peak Selection criteria: biggest, nearest, first or last peak ⓓ.

More Info:

Ordinary peaks are identified by the nearest option by default. For reference peaks the biggest will be set as default. Note that the biggest refers to the selected Response Base, i.e. if the Area is the Response Base, the detected peak may not be the highest one. In specific cases selecting First or Last may be advantageous.

To add the *Peak Selection* column:

- Right click anywhere on the table
- Select *Set Up Columns* to open the relevant window.
- Select *Peak Type* on the right and click on *Show* and then *Ok*.

5. Repeat steps 3 to 5 to add more reference peaks.

Note: In case of multisignal calibration, where compound used as reference does not match the selection criteria on some signal(s), create a variant of the compound only for that signal(s). The name must be different - e.g. Oxalic - UV, Oxalic - RI), copy the rest of the original row, check the used checkbox only for one variant on each signal. Now change the Peak Selection criteria value, or if suitable, change the Peak type to Ordinary, and select other Reference peak on that signal.

6. Save the calibration file: choose *File - Save* or click  .
7. Link the calibration to your chromatogram as explained in *Applying a calibration to a chromatogram*.

11.12.7 Using Calculate By to determine the amount of a compound with no standard available

When no standard of a compound is available and a compound with known response ratio to the unavailable one is present within the sample (this information can be found in respective norm etc.) the *Calculate By* and *Correction factor* can be used to determine its amount in the sample.

1. Open the calibration file.
2. The *Calculate By* and *Correction Factor* are hidden by default. To display them right-click the table, select *Setup Columns...*and in the following dialog move the respective items from *Hide Columns* list to *Show Columns* list.
3. For compound (Chloroform in the example) ⓐ that should be evaulated by another one, select its *Calculate By* field ⓑ and pick which compound to use for the calculation (Trichloroethane in the emxaple).

Note: Only compounds (peaks) already added to the calibration can be selected.

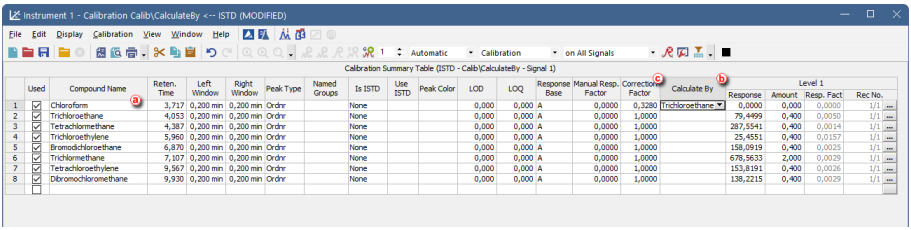
4. Fill the known response ratio to the *Correction Factor* column ⓒ.

Note: The *Amount* filled in the row that will be calculated using calibration curve of another compound will be ignored.

5. The resulting amount in *Chromatogram Results Table* will be calculated according to the calibration curve of compound selected to *Calculate By*, and multiplied by the *Correction Factor*.

Note: A compound marked as *ISTD* should neither be used as a compound that is used to calculate another compound nor as a compound that is calculated using another compound.

In the example Chloroform is calculated based on the calibration curve of Trichlorethane, their response ratio is 0.328.



11.12.8 Normalized Area % Calculation

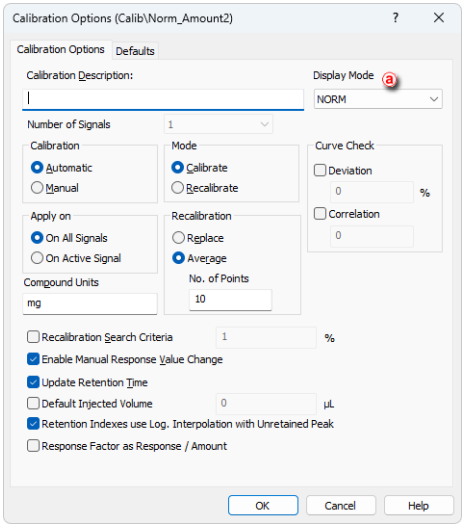
For Normalized Area % calculation no specific settings are necessary, the calculation results are always present in the *Area%* column in the Result table.

11.12.9 Normalized Amount % Calculation

This topic describes how to use Clarity, in order to obtain correct results calculated according to normalization calibration method. The normalization can be achieved by two means. First option is applicable to known response factors specific for each analyte. Second option is to use calibration based on standard sample with known fraction composition. In the latter case, Clarity automatically calculates response factors for all analytes that are subsequently applied in evaluation of the unknown sample. The results are displayed in *Amount%* column in the *Summary Table* and represent percent fraction of each analyte present in the unknown sample.

For both options set the calibration to the NORM Display mode, this ensures that Clarity checks that all the peaks are used for calculations and 100% Amount really corresponds to the whole sample.

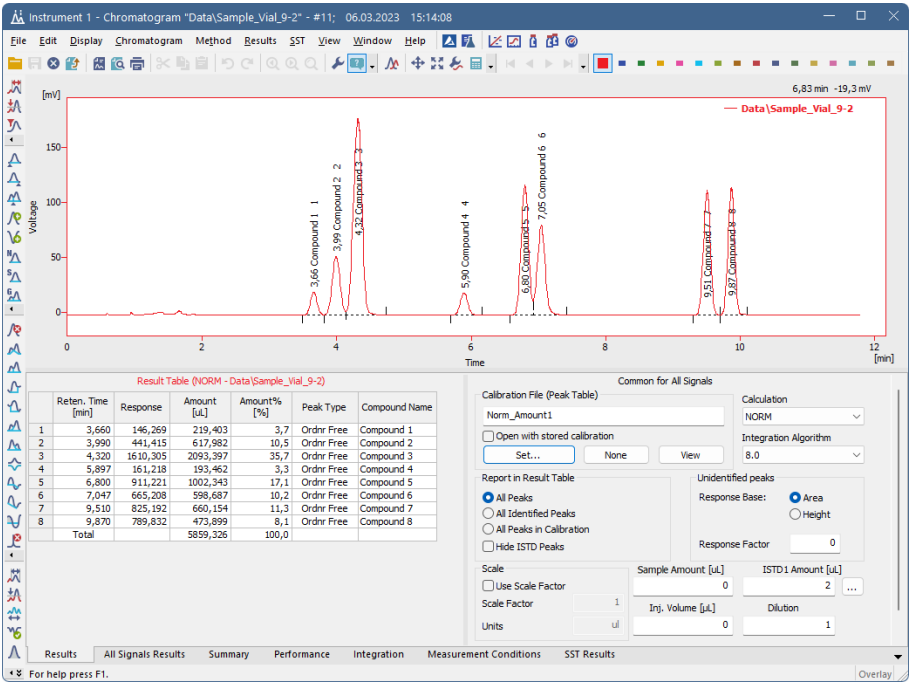
- Set *Display Mode* to *NORM* ⓐ in *Calibration Options* dialog.



A) Application of specific Response Factors

- Use procedure explained in the chapter Calibrating with manually entered Response Factors.

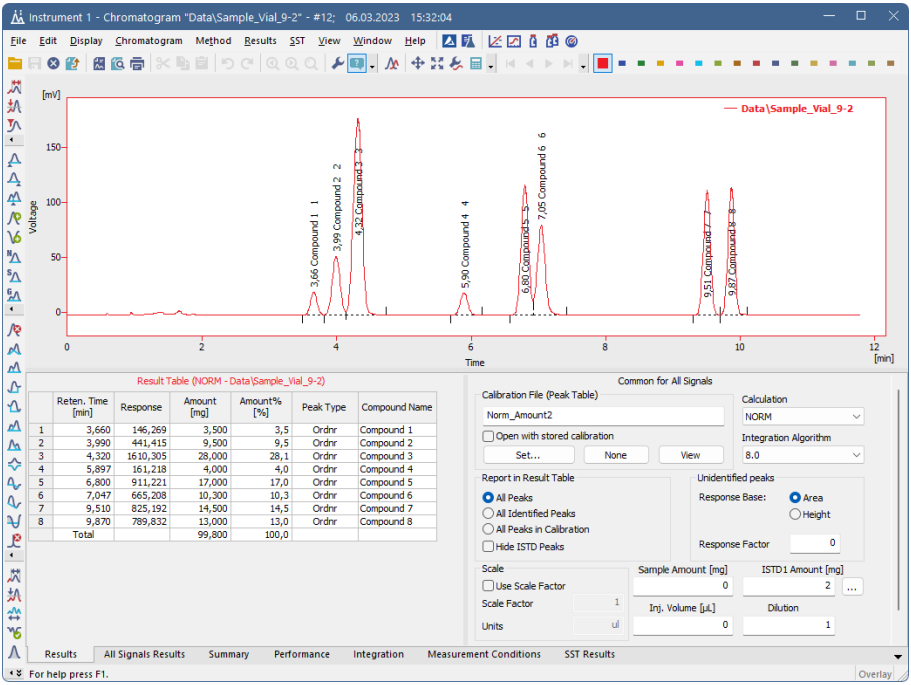
Figure below displays *Result Table* of a chromatogram with linked calibration that was created using the above mentioned method. Note different values in columns *Area [%]* and *Amount%* are caused by various values in *Manual Response Factor* column.



B) Application of automatically calculated Response Factors based on calibration with standard sample with known composition

- Use procedure explained in the chapter Creating a new calibration.

Figure below displays *Result Table* of a chromatogram with linked calibration that was created using the above mentioned method. Note different values in columns *Area [%]* and *Amount%* are caused by calculated values in *Response Factor* column.

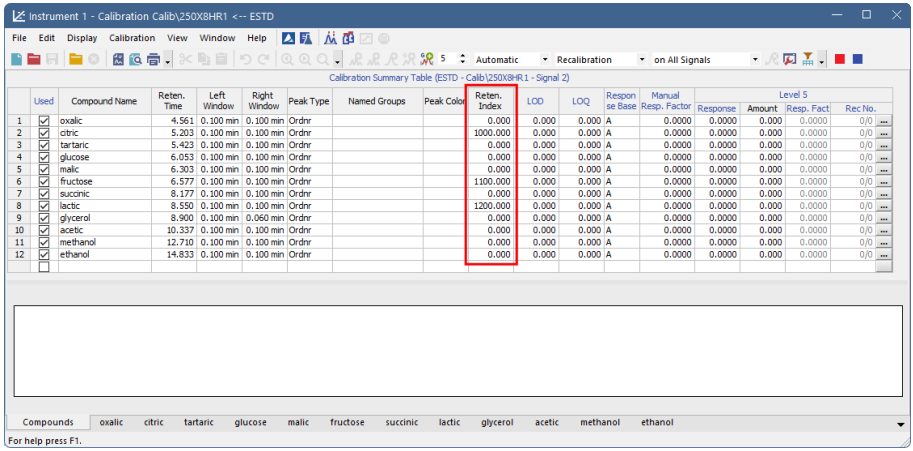


11.12.10 How to use Kováts Retention Indexes

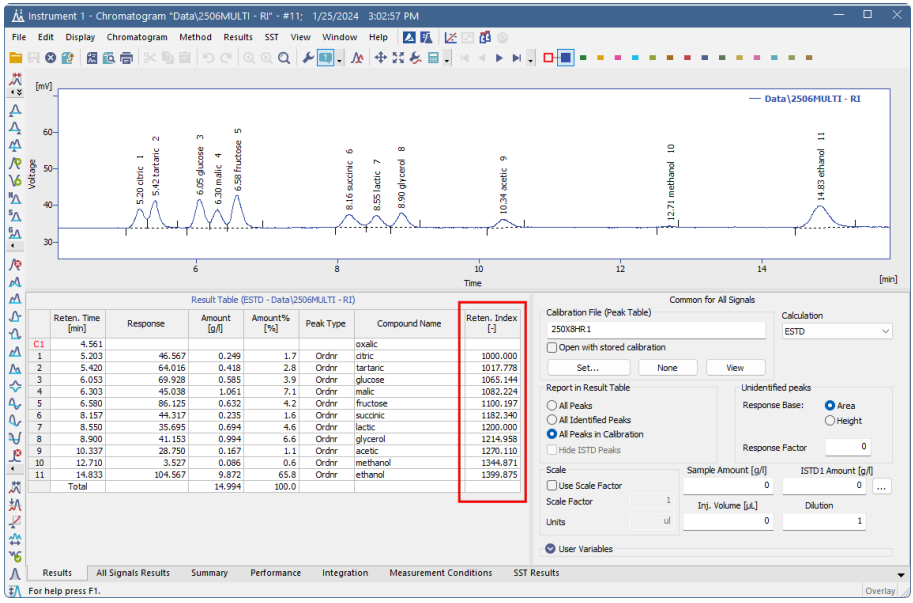
The Kováts Retention Index (*Retention Index* in **Clarity**) is used to convert the retention times of organic compounds into system-independent constants. This allows for the comparison of values measured under different conditions, such as varying column lengths, diameters, and pressures. Consequently, compound identification becomes more feasible. Kováts retention indexes are obtained by logarithmic interpolation of adjusted retention times (or volumes) using *n*-alkene standards.

To set the indexes in calibrations, follow these steps:

1. Prepare your calibration as usual.
2. The *Reten. Index* columns are hidden in the default table layout. To display them, right-click the *Calibration Summary Table* and select the *Setup Columns...* option. In the *Setup Columns* dialog, move the *Reten. Index* item to the *Show Column* list and click OK.
3. Fill in the *Retention Indexes* of the corresponding compounds. The values for the rest of the compounds may remain zero.
4. Save the calibration.

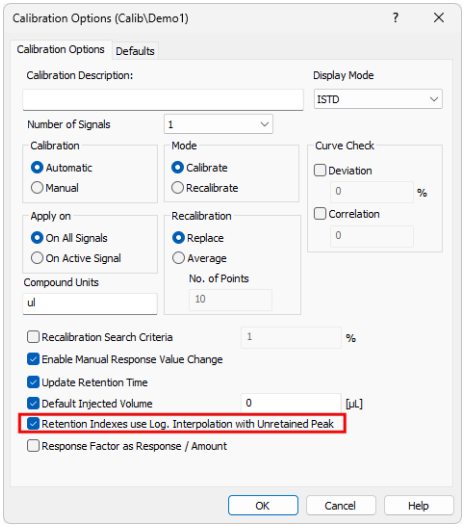


5. Open the desired chromatogram and link the created calibration. Display the *Reten. Index* columns by right-clicking in the *Result Table*, selecting *Setup Columns...*, and moving the *Reten. Index* item to the *Show Column* list in the *Setup Columns* dialog.
6. The *Result Table* will contain the retention indexes calculated according to the calibration.

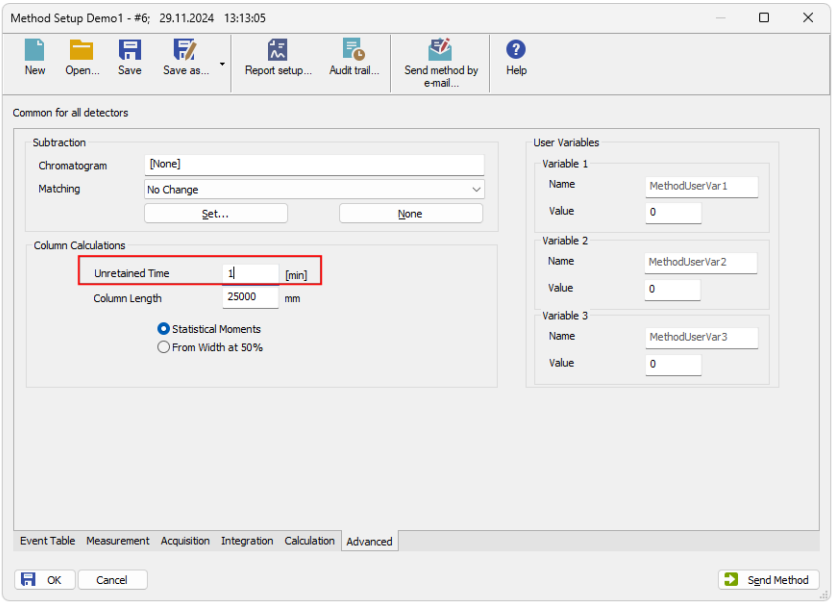


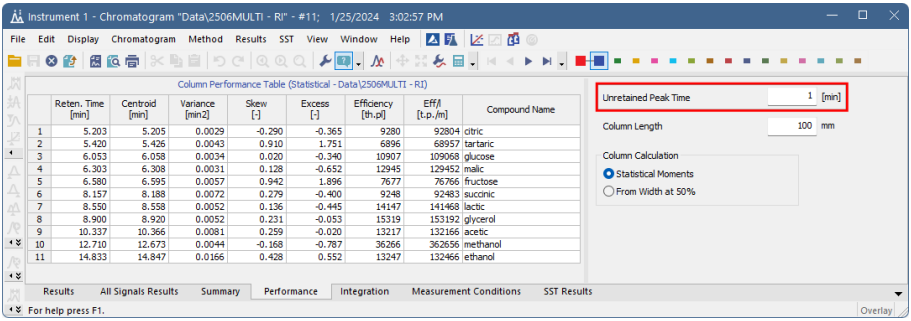
The *Unretained Peak Time* can be used for adjusting the retention times for more precise calculation of retention indexes:

1. In the *Calibration* window, open the *Calibration Options* dialog (using the *Calibration - Options...* command or the icon).
2. Retention indexes are calculated according to the selection of the *Retention Indexes use Log. Interpolation with Unretained Peak* option. If this option is **not** checked, retention indexes are calculated using linear interpolation. If it **is** checked, logarithmic interpolation with unretained peak time is used. Keep this option checked to allow for calculation using the unretained peak time.



3. The *Unretained Peak Time* may be entered in the *Method Setup - Advanced* tab, or directly in the chromatogram on the *Performance* tab.


Method Setup Demo1 - #6; 29.11.2024 13:13:05
New
Open...
Save
Save as...
Report setup...
Audit trail...
Send method by e-mail...
Help
Common for all detectors
Subtraction
Chromatogram
[None]
Matching
No Change
Set...
None
Column Calculations
Unretained Time
1
[min]
Column Length
25000
mm
Statistical Moments
From Width at 50%
User Variables
Variable 1
Name
MethodUserVar1
Value
0
Variable 2
Name
MethodUserVar2
Value
0
Variable 3
Name
MethodUserVar3
Value
0
Event Table
Measurement
Acquisition
Integration
Calculation
Advanced
OK
Cancel
Send Method


Instrument 1 - Chromatogram "Data\2506MULTI - RI" - #11; 1/25/2024 3:02:57 PM
File
Edit
Display
Chromatogram
Method
Results
SST
View
Window
Help
Column Performance Table (Statistical - Data\2506MULTI - RI)
Reten. Time [min]
Centroid [min]
Variance [min2]
Skew [-]
Excess [-]
Efficiency [th.pl]
Eff/l [t.p./m]
Compound Name
1 5.203 5.205 0.0029 -0.290 -0.365 9280 92804 citric
2 5.420 5.426 0.0043 0.910 1.751 6896 68957 tartaric
3 6.053 6.058 0.0034 0.020 -0.340 10907 109068 glucose
4 6.303 6.308 0.0031 0.128 -0.652 12945 129452 malic
5 6.580 6.595 0.0057 0.942 1.896 7677 76766 fructose
6 8.157 8.188 0.0072 0.279 -0.400 9248 92483 succinic
7 8.550 8.558 0.0052 0.136 -0.445 14147 141468 lactic
8 8.900 8.920 0.0052 0.231 -0.053 15319 153192 glycerol
9 10.337 10.366 0.0081 0.259 -0.020 13217 132166 acetic
10 12.710 12.673 0.0044 -0.168 -0.787 36266 362656 methanol
11 14.833 14.847 0.0166 0.428 0.552 13247 132466 ethanol
Unretained Peak Time
1
[min]
Column Length
100
mm
Column Calculation
Statistical Moments
From Width at 50%
Results
All Signals Results
Summary
Performance
Integration
Measurement Conditions
SST Results
For help press F1.
Overlay

12 Batch Processing

This chapter focuses on processing more chromatograms using *Batch* dialog. There are 3 main ways of workflow Reprocessing whole sequence, Reprocessing by Method, and Post-run Options. All will be explained in more detail in this chapter.

Clarity Tips&Tricks videos covering Batch topics can be found in Clarity Batch playlist.

12.1 Reprocessing whole sequence

Reprocessing whole sequence allows recalculation of results for all chromatograms in a sequence after changes to integration, calibration, or calculation parameters. This ensures that all results are consistent and reflect the current evaluation settings before further processing, reporting, or export to external systems such as **LIMS**.

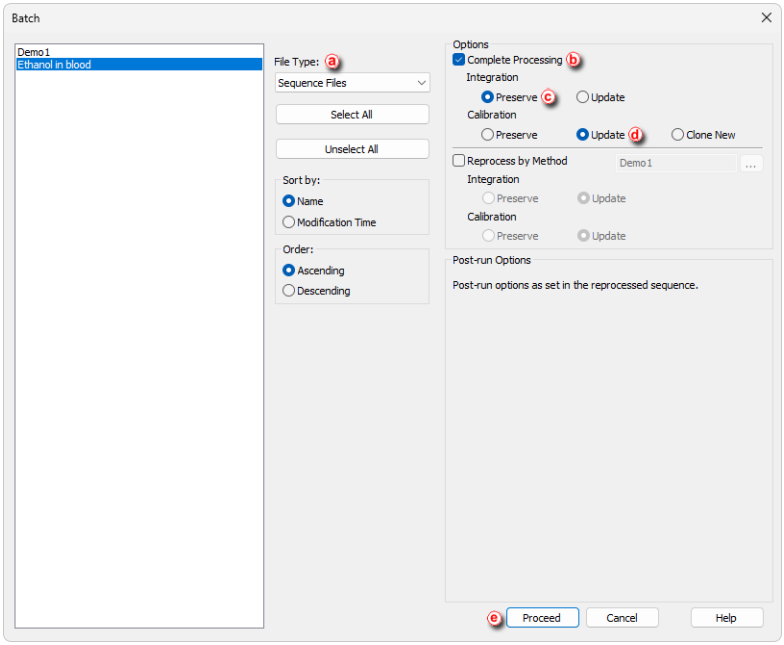
Reprocessing does not modify raw chromatographic data. Only calculated results and derived outputs are updated.

It can also be used with calibration cloning, more in the topic Complete processing with calibration cloning.

The steps below describe a process, where *Integration* is reviewed and if necessary, updated manually in each chromatogram, or sequence is already measured using a method with optimized integration parameters, for more information, see Save chromatogram method as method file.

1. Open the *Batch* dialog by using *Analysis - Batch* in the *Instrument* window.
2. Set *File Type* to *Sequence Files* ⓐ .
3. Select the Sequence you want to reprocess.
4. Check the *Complete Processing* ⓑ checkbox.
5. Under *Complete Processing*, adjust the processing behavior as required:
    - Select *Preserve* ⓒ in the *Integration* to keep manually adjusted integration.
    - Select *Update* ⓓ in the *Calibration* to perform recalibration using updated integration.
6. Click *Proceed* ⓔ to start with the batch processing.

The sequence is processed row by row. All selected recalculations and post-run actions defined in the sequence are performed.



Caution: The operations during *Batch* reprocessing are done row after row, injection after injection. In some situations it is necessary to perform the *Complete Processing* in two steps - first just the recalibrations, second the post-run actions (either using the *Complete Processing* again with the *Integration* a *Calibration* settings set to *Preserve*, or through running the post-process on selected chromatograms only through procedure described in Performing Post-run Options from Batch section). For example, if the sequence is using calibration bracketing the unknowns are measured before second standards set and if the unknowns were reported during the recalibration step, the responses from the second standard set would be missing in the report.

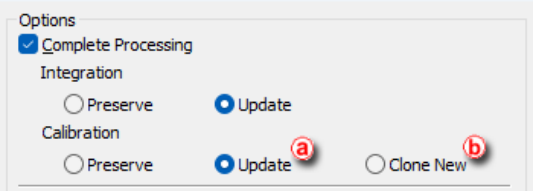
12.2 Reprocessing whole sequence while using calibration cloning

If you are using any kind of the calibration cloning in the sequence the reprocessing whole sequence is similar to regular reprocessing described in the previous topic.

Please refer to the Calibrating using clone on first recalibration, Compensating for response drift using bracketing or Improving quantification with the standard addition method topics to learn more about Calibration Cloning in Clarity.

The difference from the standard Reprocessing procedure described in Reprocessing whole sequence topic is shown below.

- In the *Batch* dialog you have additional option for calibration behavior, the meanings of options are:
  - If you select Update ⓐ in Calibration part of Options section the calibration (s) that are currently linked to measured chromatogram (s) will be recalibrated (new cloning is NOT performed).
  - If you select Clone New ⓑ in Calibration part of Options section new calibration(s) will be created as if the sequence was run again (new clone(s) are created and linked to chromatograms).



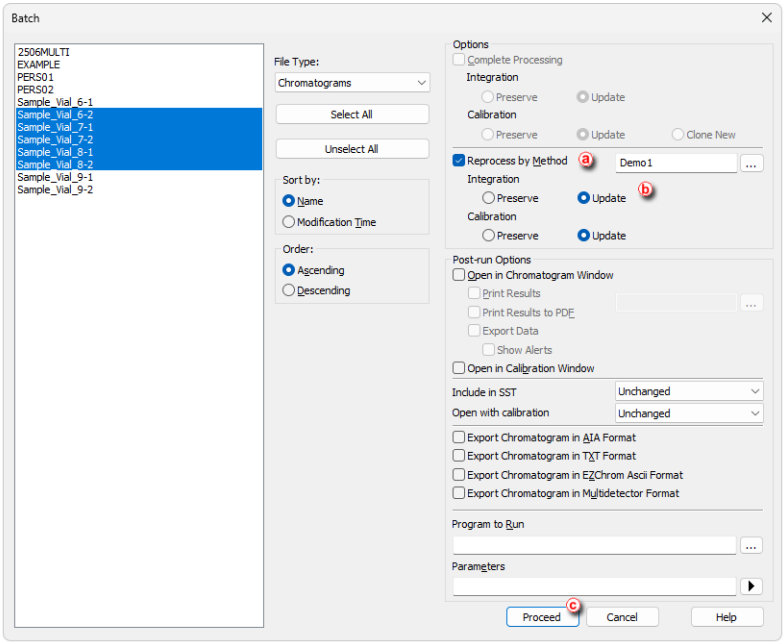
12.3 Reprocessing by selected method

Reprocessing by method is suitable for applying Integration parameters to previously measured chromatograms after these parameters were saved to the method by Save chromatogram method as method file. You can also changed the link to the calibration file without the calibration being reprocessed.

Note: If the Sequence file is selected to be reprocessed by method, all currently linked chromatograms will be reprocessed. No recalibration is carried out, when *Calibration - Update* is selected only links to calibration are changed without any changes to the calibration file itself.

1. Prepare your method with desired integration and linked calibration.
2. Open *Batch* dialog by menu *Analysis - Batch...* from the Instrument window.
3. Select chromatograms you want to reprocess (Alternatively, select sequence(s), depending on your *File Type*).
4. Select *Reprocess by Method* ⓐ and define your created method.
5. Select *Update* ⓑ Integration in case you want to change integration parameters as set in the defined method.
6. Click on Proceed ⓒ .

Note: *Reprocess by Method* can be combined with *Post-run Options* if you are sure that changes in chromatograms do not have to be reviewed before exporting/printing.



Now your chromatograms are reprocessed, with linked calibration file and amended integration parameters from the used method.

12.4 Performing Post-run Options from Batch dialog

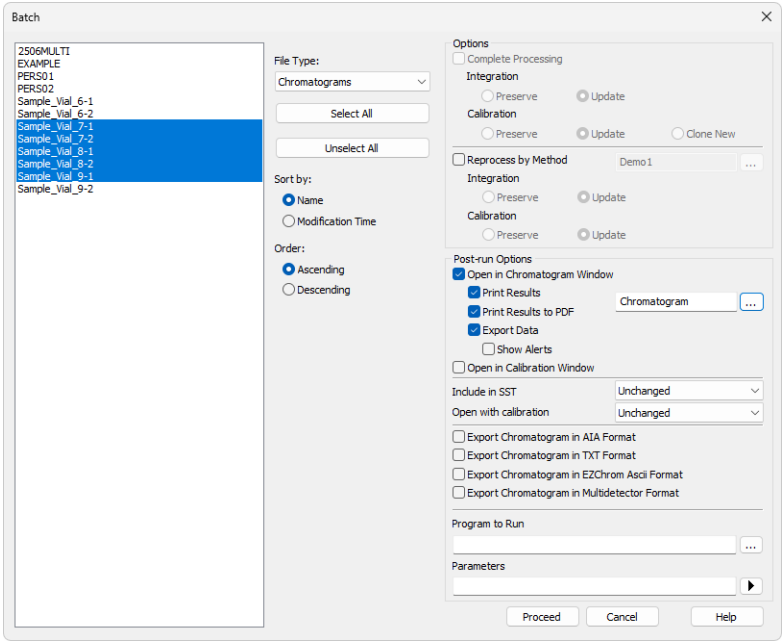
This procedure is useful if you need to *Print* or *Export* more chromatograms at once, e.g. after all of them were reviewed and signed.

1. Navigate to *Batch* dialog by clicking *Analysis - Batch* in *Instrument* window.
2. Select chromatogram(s)/sequence(s) that you want to print reports for (when sequence file is selected, all chromatograms that are currently linked in it will be reported). Which files are displayed is based on *File Type* drop-down menu.
3. Select *Open in Chromatogram Window* to be able to select *Print Results* and/or *Print Results to PDF* and/or the *Export Data* (or select any other option).
4. Select report style you would like to use by clicking ... button.
5. (Optional) change *Open with Calibration* to *Stored*, this will ensure that data will be printed in the state they were saved in last time.

   Note: By default chromatograms are opened with *Linked* calibration. If the calibration was changed after saving chromatograms the results might be influenced.

6. Click *Proceed*.

Note: It is also possible to process data before printing them by using *Complete Processing* or *Reprocess by Method* options. When *Complete Processing* is selected, the post-run options are governed by settings in reprocessed sequence. For more info see chapter regarding Batch dialog for more info.



13 Results and Calculations

This chapter describes how to define and use custom calculations in Clarity. Custom calculations are useful for extending the *Result Table* or *Summary Table* with user-defined formulas, allowing you to evaluate data in ways not covered by standard calculations.

13.1 Comparing the results from several chromatograms

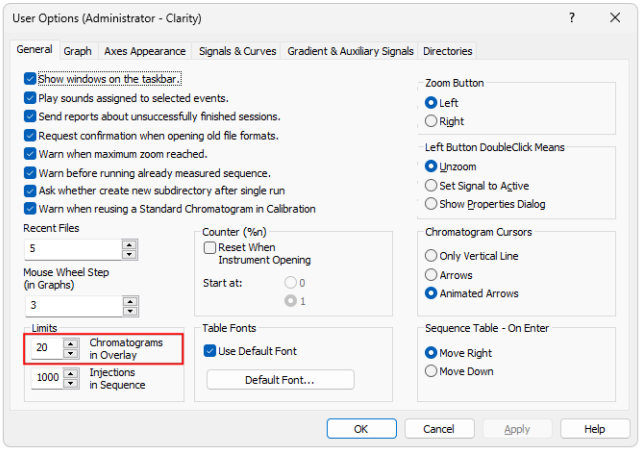
Clarity provides two complementary ways to compare results from several chromatograms:

- *Overlay mode*, which displays multiple chromatograms simultaneously in a single graph.
- *Browse Through Chromatograms*, which allows reviewing them one by one in sequence.

Both approaches can be used to evaluate differences between chromatograms, verify results, and prepare data for reporting or further processing.

13.1.1 Comparing chromatograms using Overlay mode

The default maximum number of chromatograms that can be open in Overlay mode is 20. If your workflow requires comparing a larger number of chromatograms (for example, when producing a summary report), this limit can be changed in the *User Options* dialog, accessible from the *Instrument* window by using *Setting - User Options...*.

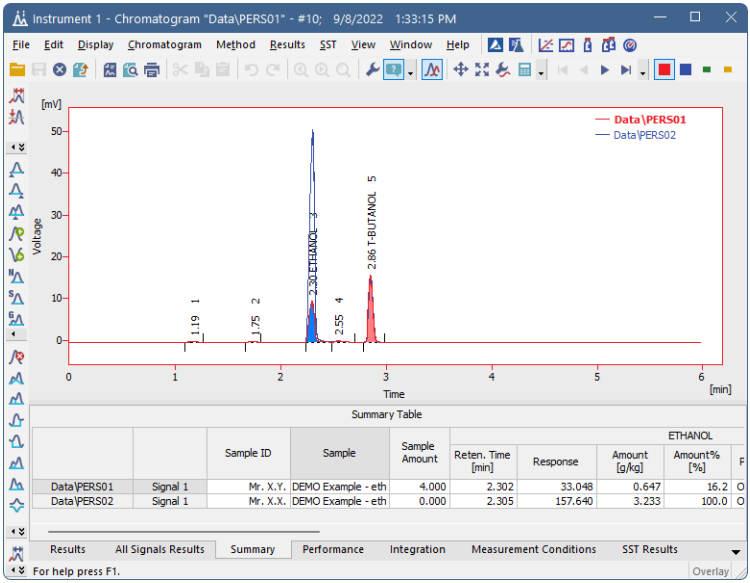


To view chromatograms in *Overlay mode*, follow these steps:

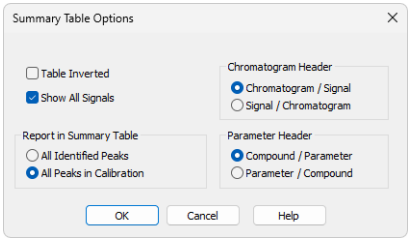
1. Open the chromatograms using *File - Open Chromatogram...*.
2. In *Open Chromatogram* dialog select desired chromatograms and click *Open in Overlay*.

3. Click on the *Summary* tab in the lower part of the window to display the *Summary Table*. In the rows you can see chromatograms and signals with measured values and in the columns there are identified peaks from all calibrated chromatograms.

Caution: *Summary Table* is based on calibration, meaning only calibrated peaks will be present in it.



4. Right click on the *Summary Table*to access options for adjusting its layout or content, including the *Inverted* view, which switches the table from a horizontal format to a vertical one for easier inspection of individual results.
5. To see all signals, select the *Show All Signals* checkbox in the *Summary Table Options* dialog accessible from the pop-up menu of the *Summary Table*. By default, only signals containing calibrated peaks are visible in the *Summary Table*.



Note: It is also possible to compare parameters from different chromatograms and check if they fall within set limits by using the SST Extension.

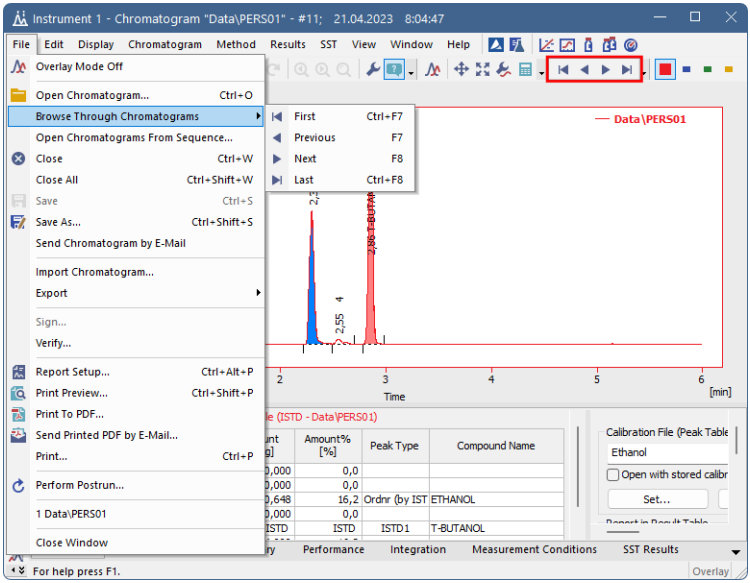
13.1.2 Comparing chromatograms by browsing them sequentially

In addition to *Overlay mode*, Clarity also allows reviewing multiple chromatograms one after another using the *Browse Through Chromatograms* function. This method is useful when you want to visually inspect each chromatogram individually, especially when working with large batches.

To use this feature, the *Overlay mode* must be disabled.

To browse chromatograms, follow these steps:

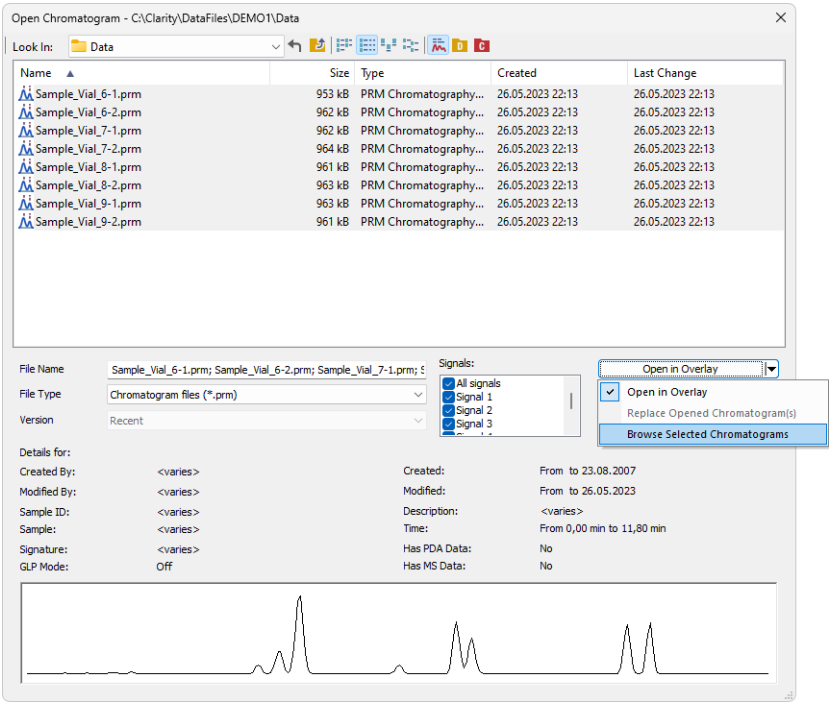
1. You can browse the chromatogram by using *File - Browse Through Chromatograms* or by using the navigation controls in the toolbar. By default, Clarity browses the folder of the currently open chromatogram.



2. In the *Open Chromatogram* dialog, select the chromatograms you want to review. You can also filter the list by typing simple wildcard patterns (*, ?).

Caution: Using *%variables* when creating chromatogram file names is strongly recommended, as it ensures that useful information, such as sample name, injection number, or date, is included automatically. This makes it much easier to search, sort, or filter chromatograms when browsing through them.

3. When you have the desired files selected, you can open them by using *Browse Selected Chromatograms*.



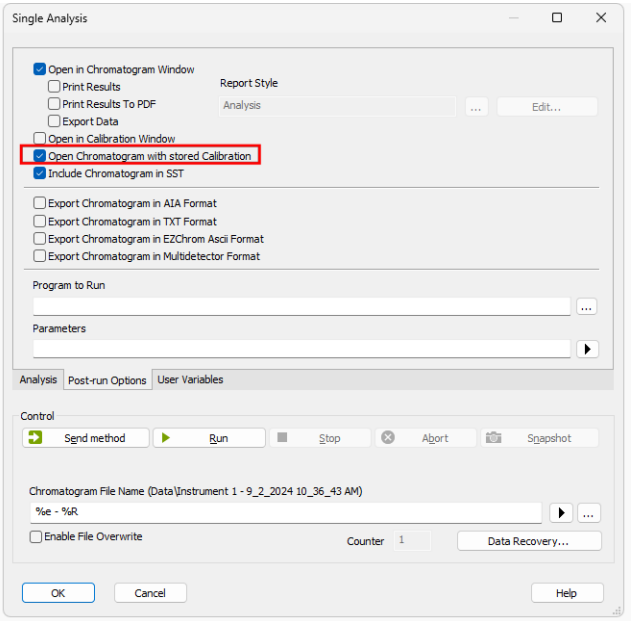
13.2 How to display older results when linked calibration is modified

Clarity does not store any results in the chromatogram, the result table is always calculated from the actual state of the calibration file referenced in the *Calibration Table (Peak Table)*, i.e. *Linked* calibration. Any changes in this calibration will be immediately reflected in the displayed results. Each time a chromatogram is saved the current state of the linked calibration is stored (i.e. *Stored* calibration) in the chromatogram history (just values needed to calculate the results, not a complete calibration). Chromatogram opened with a version from history (i.e. opened with *Stored* calibration) will display results as they were at that time.

In case the calibration file is reused for some time, opening the chromatogram with linked calibration will show changed results due to changes in the linked calibration. To avoid this, two approaches are possible:

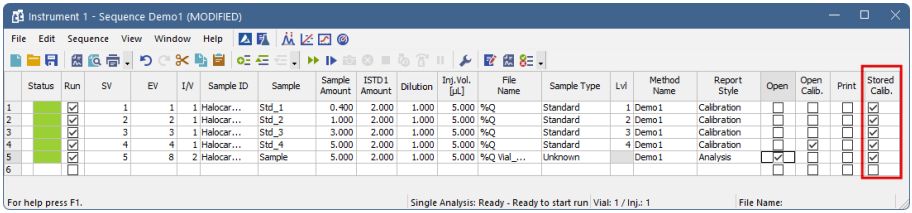
1. Make a copy of the calibration file so each series of measured chromatograms will be linked to a separate calibration file. This has advantage in case some amendments to the calibration will be necessary later, as the amendments will affect only the related chromatograms. Such procedure could be automated from sequence. For more information regarding this procedure, see the chapter **"Calibrating using clone on first recalibration"** on pg. **141**..

2. Using the *Open with stored calibration* option. Such option is accessible from multiple dialogs, depending on whether Single Analysis or Sequence is measured (automated approach) or this option can be selected upon opening the chromatogram.
    - In the *Single Analysis* dialog - *Post-run Options* tab, select the *Open Chromatogram with stored Calibration* option.



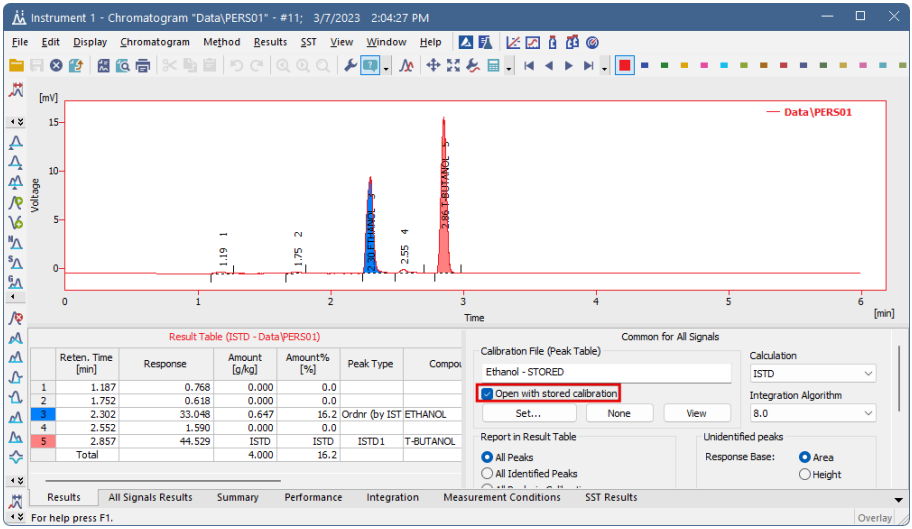
    - In the *Sequence* window select checkbox in the *Stored Calib.* column. By default, *Stored Calib.* column is hidden. To show it, right mouse click in the sequence table and choose *Setup Columns...*. From the *Setup Columns* dialog, choose *Stored Calib.* from the left list and click on the *Show* button - it will be added to the show list. Once you click the *OK*

button, you will return to the *Sequence* window and the new *Stored Calib.* column will be added.



- In the *Chromatogram* window select *Open with stored calibration* option. This will open the chromatogram with the most recent point from history and show the results according to the stored calibration. Any changes in the linked calibration will not affect those results. To open the chromatogram with the stored calibration this way it is necessary to re-open the chromatogram using the *Open Chromatogram* dialog - re-opening the *Chromatogram* window is not sufficient.

  Note: This setting is only applied and saved to the currently opened chromatogram. It will not be transferred to the next (different) opened chromatogram.

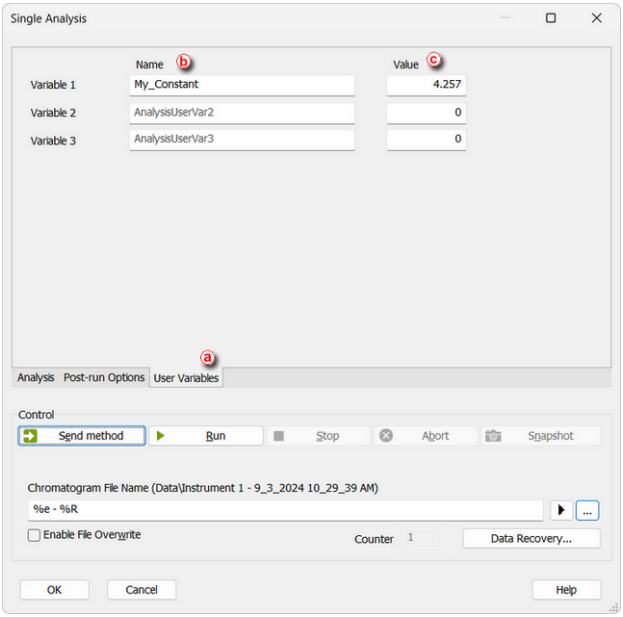


13.3 User Variables

This topic describes how to set up *User Variables*. *User Variables* let you define custom numeric values that can be reused in *User Columns* formulas, making calculations more flexible. *Analysis User Variables* are set in the *Single Analysis* or *Sequence* window and *Method User Variables* are set in the *Method Setup* window.

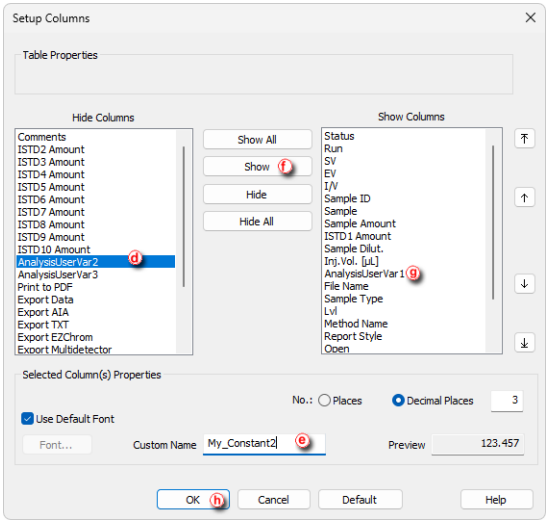
A) Setting of Analysis User Variables in Single Analysis window

1. In *Single Analysis* dialog navigate to the *User Variables* tab ⓐ .
2. Define *Name* of the variable ⓑ . If the field is left empty, default name *AnalysisUserVar1-AnalysisUserVar3* will be used.
3. Define numerical *Value* of the variable ⓒ .

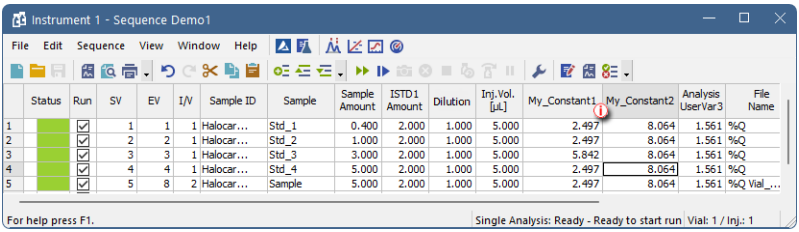


B) Setting of Analysis User Variables in Sequence window

1. In *Sequence* window the *AnalysisUserVar1 - AnalysisUserVar3* columns are hidden by default.
2. To display them right-click on the *Seqeunce Table* and use *Setup Columns...* command.
3. Select the variable in the *Hide Columns list* ⓓ , fill its name ⓔ and click *Show* ⓕ (item will be move to the *Show Columns* list ⓖ).
4. Repeat the previous step if more variables are needed then click *OK* ⓗ .

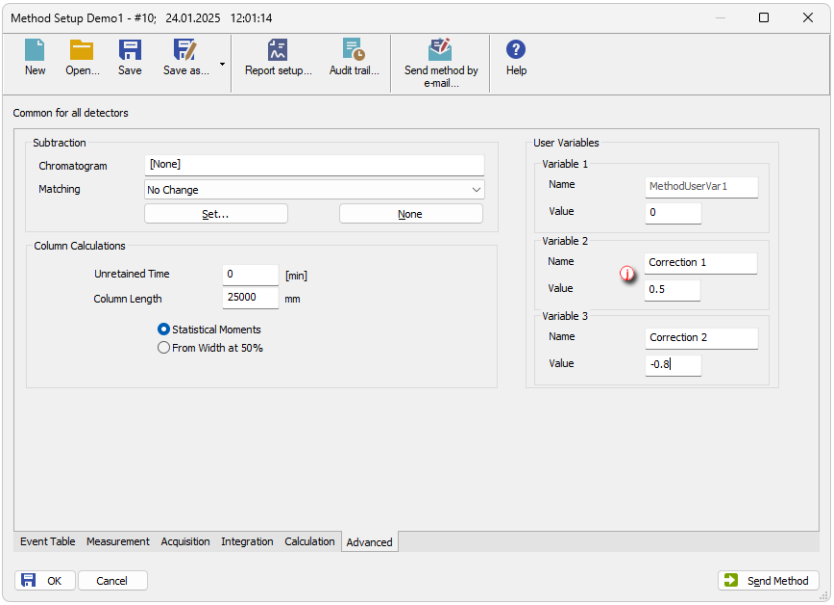


5. Defined *Custom Name* of the variable is used directly in the column header ⓘ . Fill in the values for each row (different values can be used).



C) Setting of Method User Variables in Method Setup window

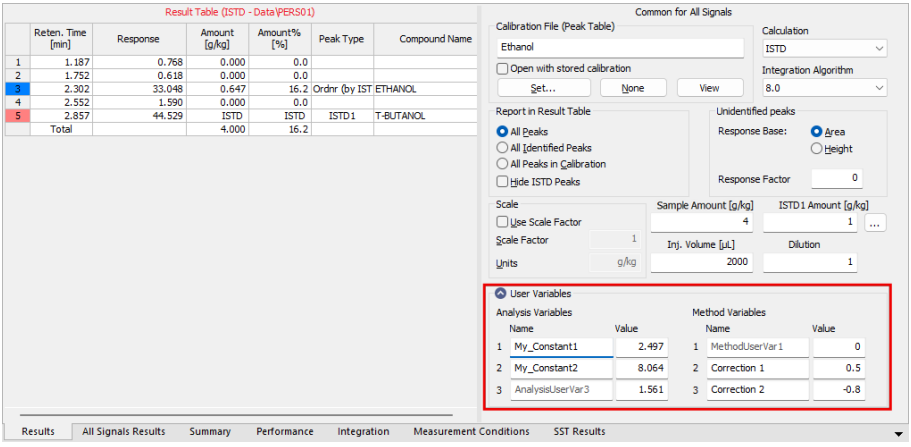
1. In the *Method Setup* dialog navigate to *Advanced* tab
2. Define *Name*, numerical and *Value* of the variables that should be used ⓙ . Default name *MethodUserVar1-MethodUserVar3* is used when the *Name* is empty.



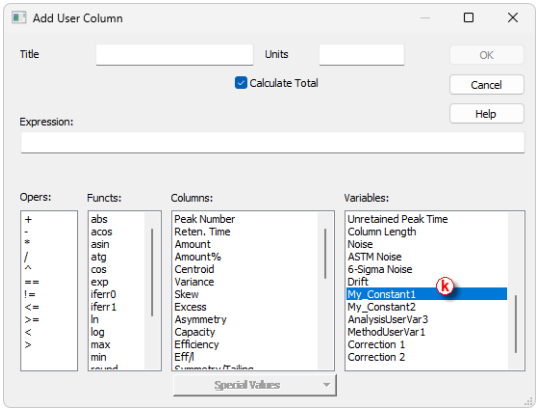
D) Setting of User Columns with User Variables

Analysis and *Method User Variables* are also editable directly from *Chromatogram* window on *Results* tab in *User Variables* section (it is collapsed by default and must be expanded by clicking the arrow symbol).

Variables can be modified in the same manner as in the previous cases.



Note: To use variables in custom calculations add *User Column* as described in chapter "User Columns" and while formulating the *Expression* select the desired variable from *Variables* list ⓚ .



13.4 Custom Calculation in Result Table

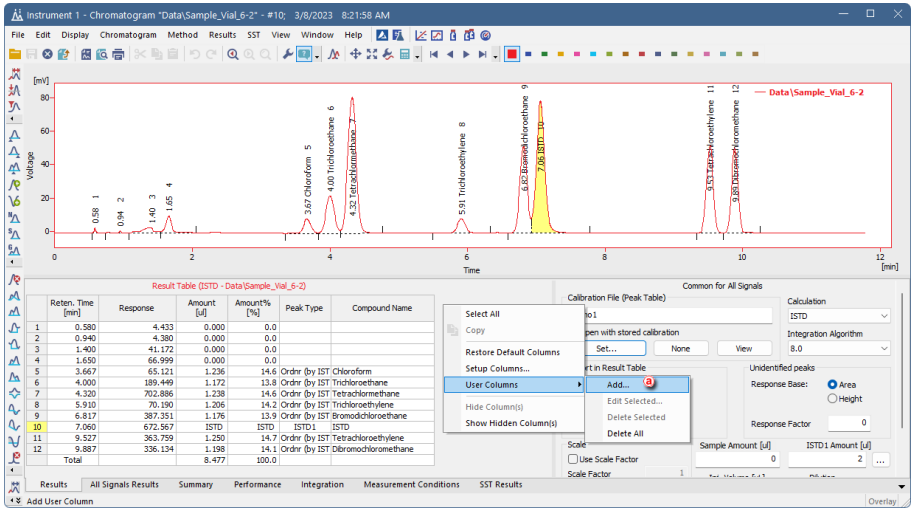
This topic describes how to create custom calculations in the *Result Table* using *User Columns*.

Note that majority of calculations require chromatogram to be calibrated. Without it the necessary values are not available.

Caution: *User Columns* are stored in .DSK files. If the station is used by multiple users it is recommended to set shared .DSK file as described in chapter "Sharing settings among users".

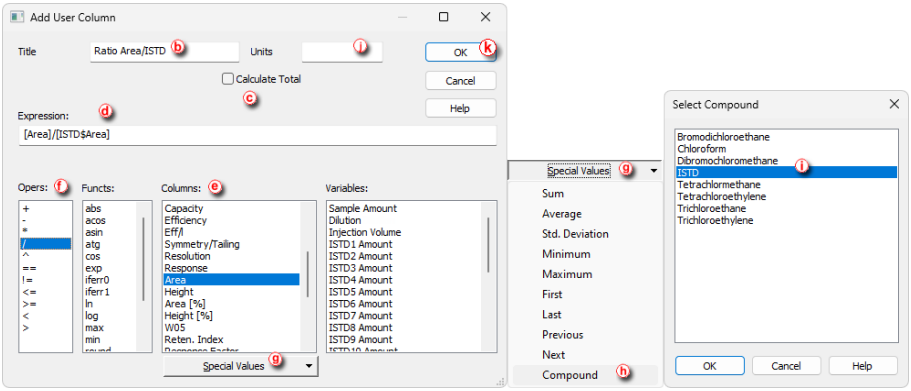
How to add User Columns to Results Table

1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Right click on the *Result Table* and select *User Columns - Add...* ⓐ , the *Add User Column dialog* will be opened.



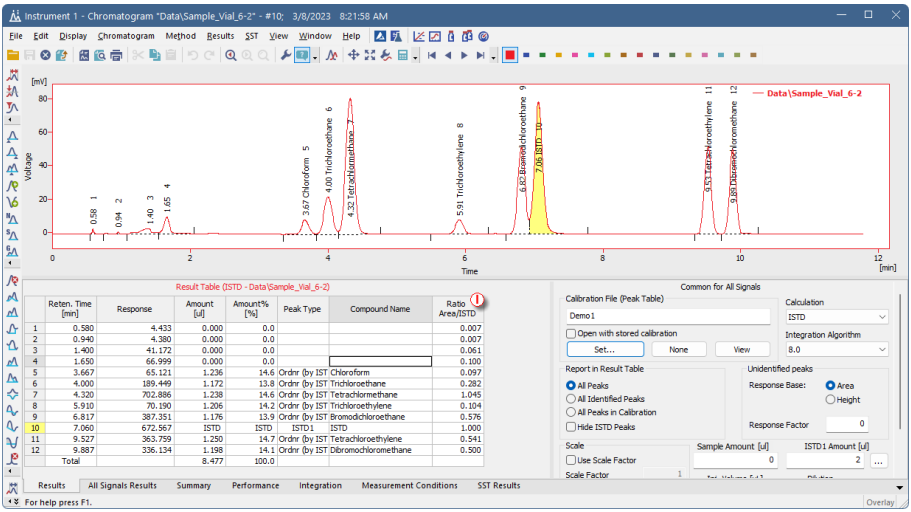
3. Fill in the *Title* ⓑ of the new column. In our case *Ratio Area/ISTD*.
4. Check/Uncheck *Calculate Total* ⓒ (depends on whether sum of calculated values has a meaning).
5. Fill in *Expression* ⓓ line , which presents the user's defined calculation. In our case:
    - In *Columns:* ⓔ list double-click *Area*.
    - In *Opers:* ⓕ list double-click */*.
    - In *Columns*:list select *Area*, then click on *Special Values* ⓖ , select *Compound* ⓗ , choose *ISTD* ⓘ and click *OK*.
6. Fill in appropriate *Units* ⓙ based on the formula.
7. Click *OK* ⓚ in the *Add User Column* dialog.

Note: It is possible to fill *Expression* by typing if you know the correct syntax.



8. New *User Column* is added to the *Result Table* ⓘ .

Note: You can edit existing *User Columns* by right-clicking into them and selecting *User Columns - Edit Selected...*.



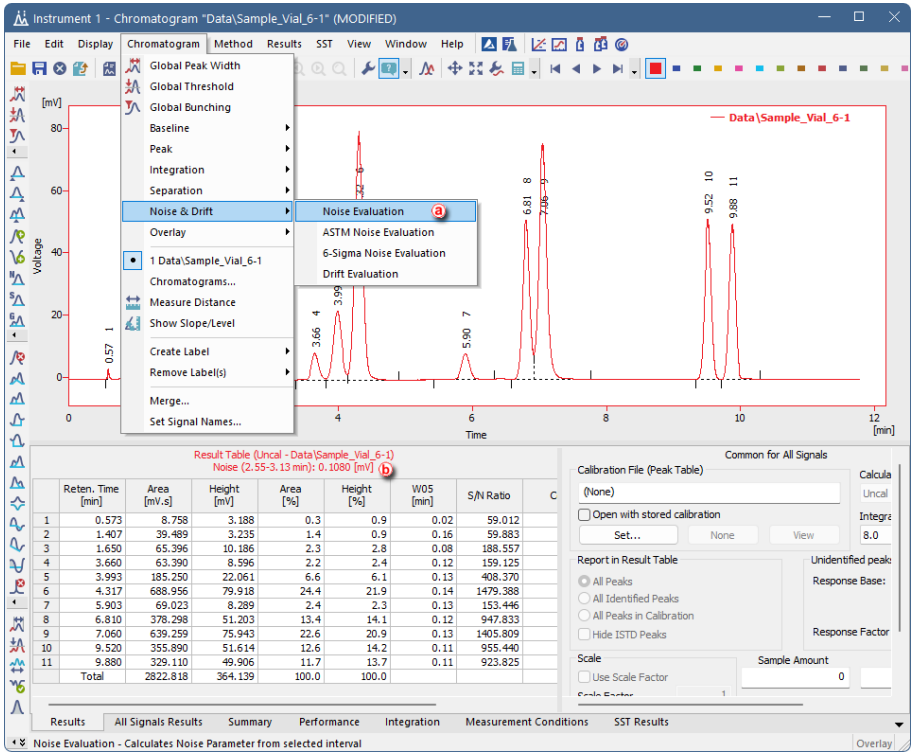
13.4.1 Signal to Noise Ratio Calculation

This article describes how to calculate Signal to Noise Ratio using *User Columns* calculations with *Variables*.

13.4.1.1 Noise Parameter Evaluation

At first *Noise* value has to be evaluated. This value is subsequently used to calculate the *Signal to Noise Ratio*.

1. Open measured chromatogram in the *Chromatogram* window
2. Use *Chromatogram - Noise & Drift - Noise Evaluation* ⓐ and select the interval for noise calculation. The same result can be obtained from the *Integration Table* after selecting the *Evaluation - Noise* operation and inputting the desired interval manually.
3. The value of the evaluated Noise Parameter is shown in the *Result Table* header ⓑ .
4. For the same chromatogram such value is stored as a *Noise* variable in the *Edit User Columns - Variables* ⓔ .



13.4.1.2 Calculating Signal to Noise Ratio

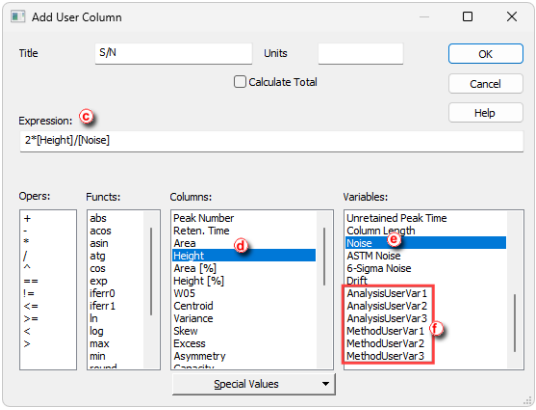
Signal to Noise Ratio is important parameter used for method validation. Most commonly used generic formula for Signal to Noise = 2*Peak Height/Noise.

For such calculation, two possible approaches exist:

- The *Noise* is determined from the same chromatogram within area with no peaks. The *Noise* variable ⓔ can be used directly in the formula entered in the *Expression* ⓒ edit box. In that case the resulting formula will be for example 2*

[Height]/ [Noise], where both parameters are determined from the same chromatogram.

- The *Noise* is determined from other chromatograms (e.g., by measuring blanks and evaluating the *Noise* in the area of expected peak). In the *Edit User Column* dialog in the *Expression* ⓒ edit box use the [Height] ⓓ from the Columns section for peak height and enter the calculated *Noise* value as a constant. The resulting formula will be then e.g. 2*[Height]/0.1080, where the number 0.1080 is the calculated *Noise* parameter. Alternatively, the calculated *Noise* parameter could be stored as a *Method User Variable* or as an *Analysis User Variable* ⓕ to simplify changes of the value - this variable can be then used instead of entering the numerical value in the *Expression* edit box.



Note: In the *Expression* edit box, variables are treated as numbers, therefore operators and numbers can be used to modify the formula. The resulting formula can be e. g. 2* [Height]/ [Noise] or 2* [Height]/ [UserVariableNoise] (where the [UserVariableNoise] represents user variable to which the Noise value determined from chromatogram blank is stored) or 2*[Height]/0.1080 (where the 0.1080 represents the actual Noise value determined from chromatogram blank).

Note: Setting the *Analysis User Variable* or the *Method User Variable* is described in the section **User Variables on pg. 190**.

13.4.2 How to calculate Relative Retention Time

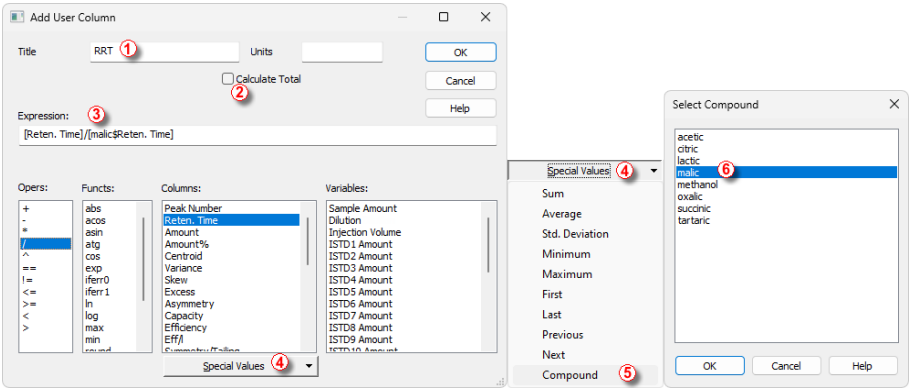
This chapter describes how to calculate Relative Retention Time (RRT). In Clarity, there are basically two ways how to achieve that. In the first one, there is peak in the chromatogram that you want to use for the calculation. In the second approach, you fill in the time for an Unretained Peak and then use it for the calculations.

13.4.2.1 Relative Retention Time calculation based on an existing peak

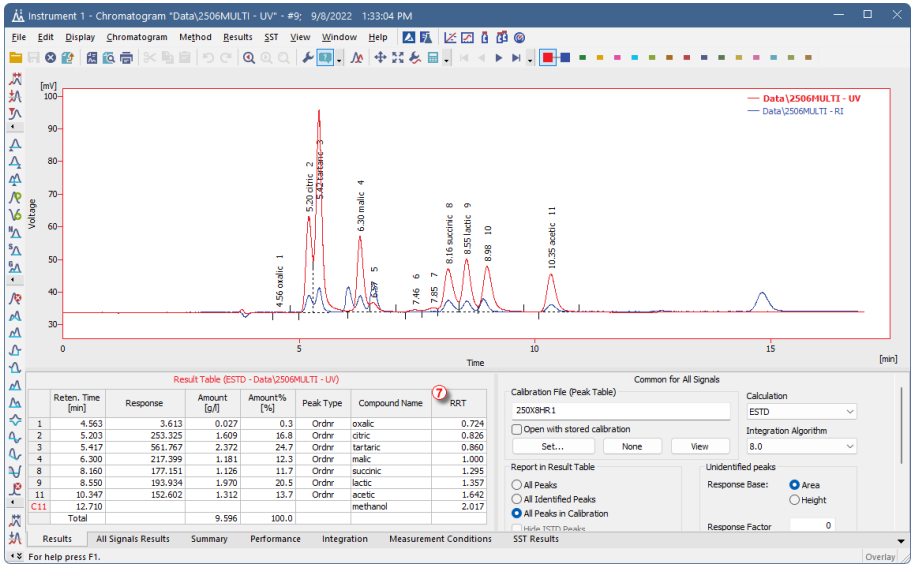
1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Add a *User Column* as described in chapter "User Columns".

3. Fill the *Title* for the new column - e.g., *RRT* ① .
4. Uncheck *Calculate Total* ② .
5. Enter "*[Reten. Time]/[malic$Reten. Time]*" formula to the *Expression* field ③ , where "malic" represents your compound which should be used for calculation of RRT. You can either use items from the *Columns:* list or type them manually.

Note: To insert *[malic$Reten. Time]* select *Reten. Time* in *Columns:* list, click *Special Values* ④ , in the drop-down list select *Compound* ⑤ , and in the following dialog, select the compound ⑥ you want to use for calculation of RRT (the list is based on the used calibration file).



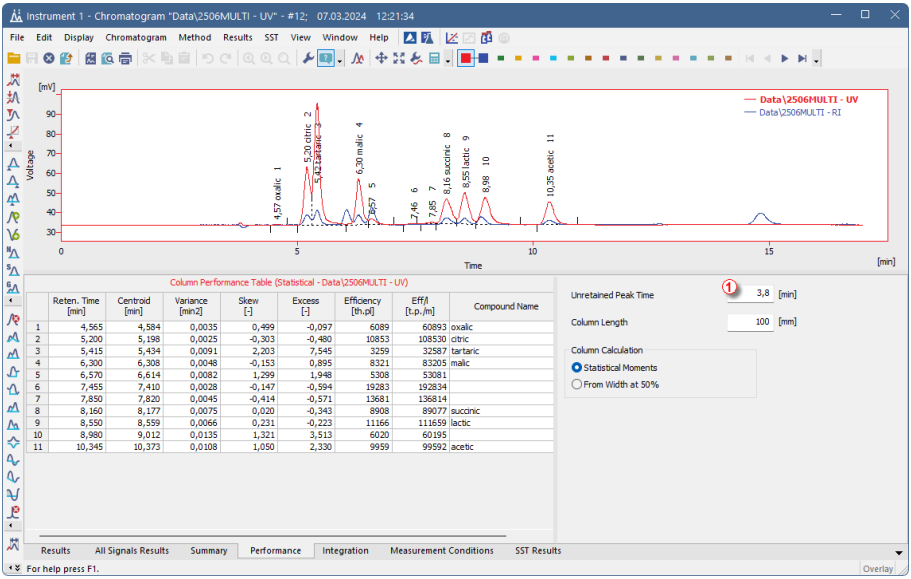
6. Close the *Add User Column* dialog using *OK*
7. A new *RRT* column ⑦ is displayed in the *Result Table*.



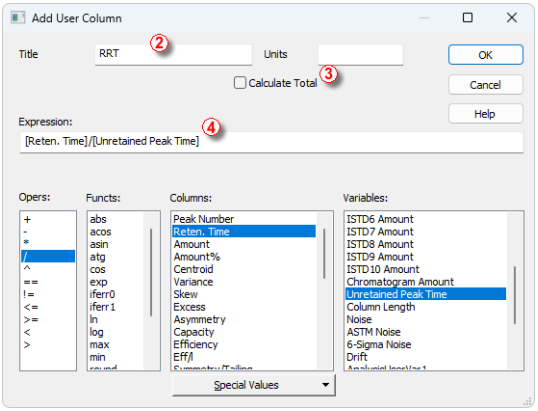
Note: You can do a quick check that the calculation is correct: look at the *malic* compound, the RRT shoud be *1*.

13.4.2.2 Relative Retention Time based on the Unretained Peak variable

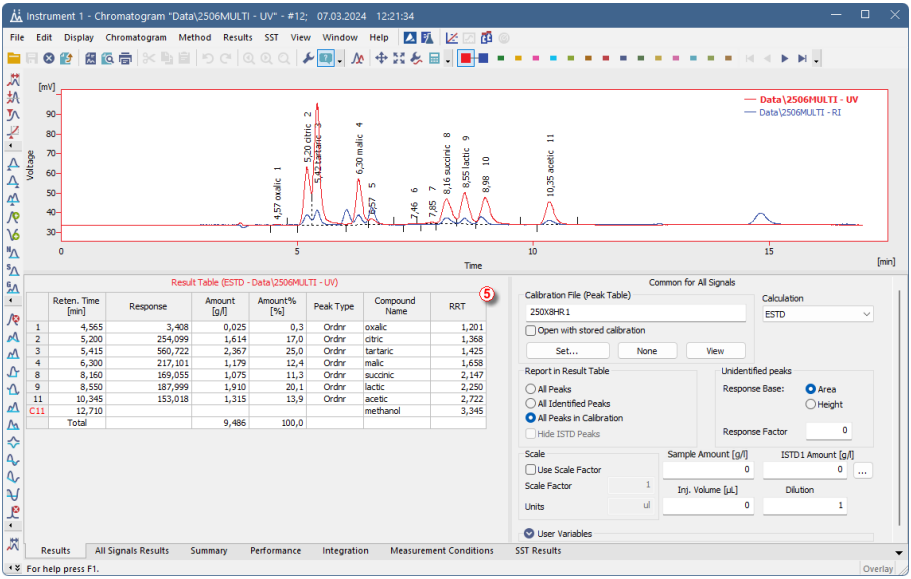
1. Open the chromatogram you want to work with and switch to the *Performance* tab.
2. Fill in the *Unretained Peak Time* as you need ① .



3. Go to the *Results* tab.
4. Add a *User Column* as described in chapter "User Columns".
5. Fill the *Title* for the new column - e.g., *RRT* ② .
6. Uncheck *Calculate Total* ③ .
7. Enter "*[Reten. Time]/[Unretained Peak Time]*" formula to the *Expression* field ④ . You can either use items from the *Columns:* and *Variables:* lists or type them manually.



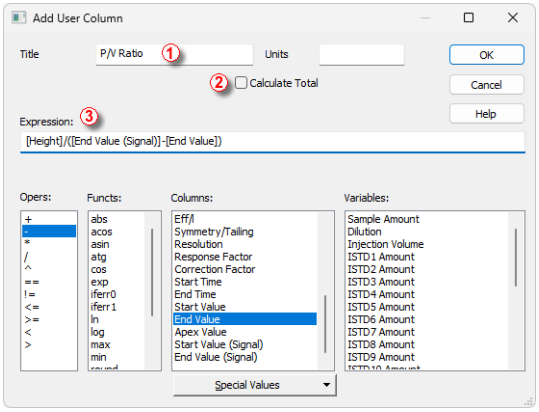
8. Close the *Add User Column* dialog using *OK*.
9. A new *RRT* column ⑤ is displayed in the *Result Table*.



13.4.3 How to calculate Peak to Valley Ratio

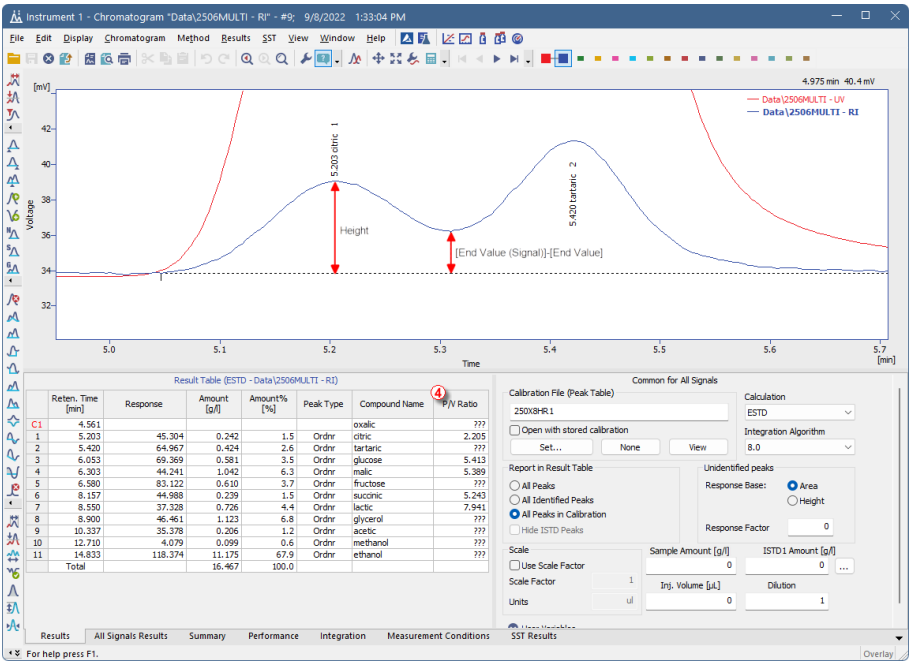
This chapter describes how to calculate Peak to Valley, which is a ratio of signal height in peak apex and signal height in the end of peak. This ratio is used for e.g., impurity determination.

1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Add a *User Column* as described in chapter "User Columns".
3. Fill the *Title* for the new column - e.g. *P/V Ratio* ① .
4. Uncheck *Calculate Total* ② .
5. Enter "*[Height]/([End Value (Signal)]-[End Value]*)" formula to the *Expression* field ③ . You can either use items from *Columns:* list or type it manually.
6. Close the dialog by clicking *OK*.



7. New *P/V Ratio* column ④ is displayed in the *Result Table*.

Note: Value is only valid for peaks, where peak end is not on the baseline.

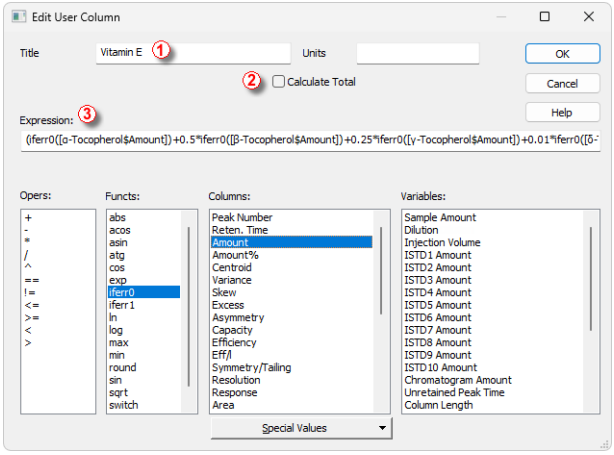


13.4.4 How to handle not-found compounds in your calculations

If any compound is missing from a chromatogram, its amount is not calculated. In any equations within *User Columns*, where this amount would be used, the calculations would produce ??? (invalid result). In such cases, the *iferr0* function can replace the

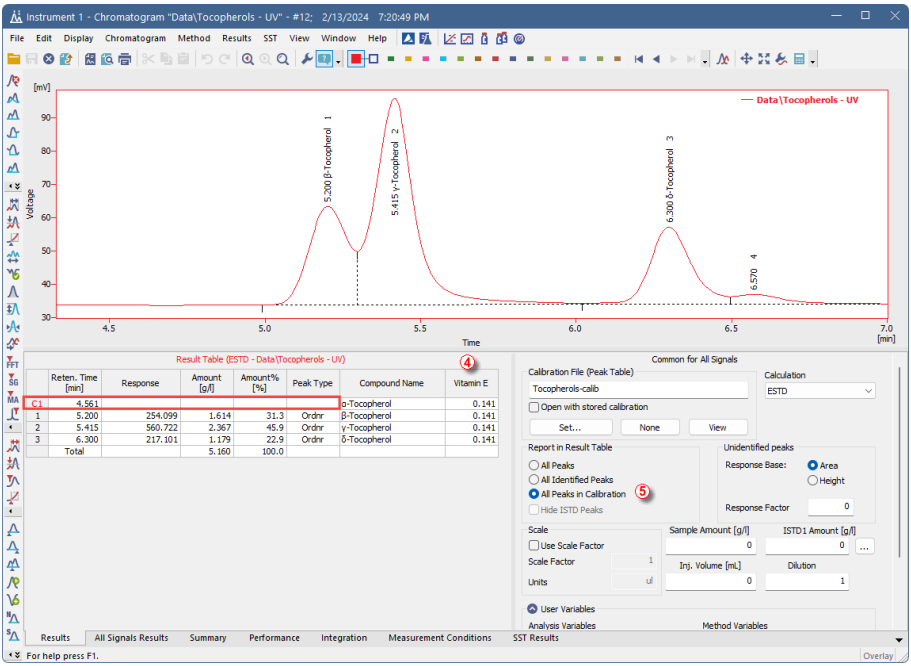
missing value with 0 (analogically, the *iferr1* function replaces the missing value with 1). This functionality can be used in situations, when a substance is present in multiple chromatogram peaks, possibly even in different ratios. *User Columns* can be used to determine its total content. The *Expression* (equation) would then contain the Amounts of compounds in the chromatogram. However, some of the compounds may not be present in the evaluated chromatogram. The following case scenario shows how the *iferr0* function can be used. The goal is to calculate the content of Vitamin E in different Tocopherols.

1. Open a chromatogram you want to work with and switch to *Results* tab.
2. Add a *User Column* as described in chapter "User Columns".
3. Fill the *Title* for the new column - e.g. *Vitamin E* ① .
4. Uncheck *Calculate Total* ② .
5. Enter the formula for calculating the vitamin E content, e.g., "*([α-Tocopherol$Amount]+0.5* [β-Tocopherol$Amount]+0.25* [γ-Tocopherol$Amount]+0.01*[δ-Tocopherol$Amount])/10*" to the *Expression* field. You can either use items from the *Columns:* list with *Special Values* or type it manually.
6. Apply the *iferr0* function on the items that may be missing from the result table. The resulting function will look like the following: *(iferr0 ([α-Tocopherol$Amount])+0.5*iferr0 ([β- Tocopherol$Amount])+0.25*iferr0 ([γ-Tocopherol$Amount])+0.01*iferr0([δ-Tocopherol$Amount]))/10* ③ .
7. Close the dialog by clicking *OK*.



8. The new *Vitamin E* column ④ is displayed in the *Result Table*.
9. In the case that any of the compounds is not found in the chromatogram (such as here, in the case of α-Tocopherol), the Amount is not calculated. The *iferr0* function replaces the not-found Amount with zero in further calculations.

Note that the *All Peaks in Calibration* ⑤ option is selected. Otherwise, the missing compound would not be present in the *Result Table*, and the calculation would not be possible.



13.4.5 Calculating percentage content of a compound in a solid sample

This is a standard procedure used across various chromatography applications - a known amount of a sample is dissolved in a known volume of a solvent and the goal is to determine the percentage content of the compound in the sample.

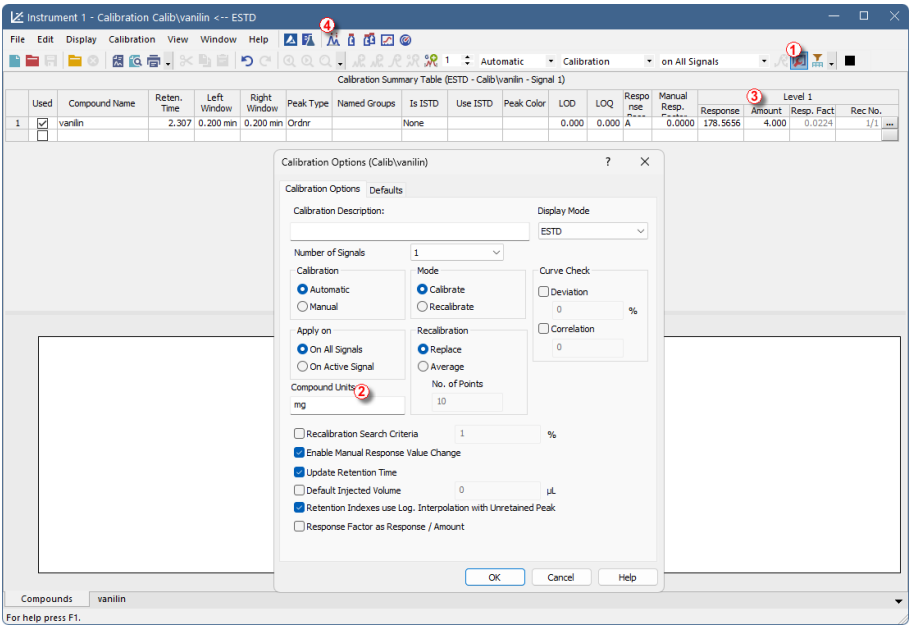
1. Open your calibration/create a new one in the *Calibration* window.
2. Click the  icon to open *Calibration Options* dialog ① .
3. Specify used unit for the amount in *Compound Units* field ② . Confirm changes by clicking *OK* button.

Note: Fill the unit used for the total amount of sample. In our specific case sample was weighted and *mg* is used. Set units are used in the *Chromatogram* window for further calculations.

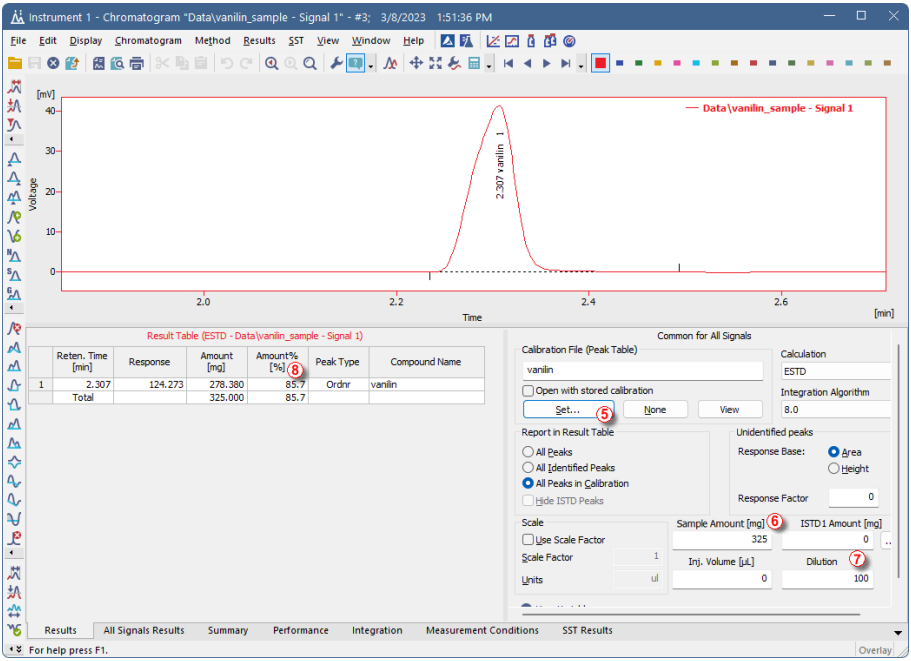
4. Fill corresponding *Amount* for each compound as concentration ③ .

Note: That means amount divided by the volume of solvent used to prepare the standard solution. In our example *400 mg* of **vanilin** was dissolved in *100 ml*, thus the *Response* from the standard chromatogram corresponds to *4 mg/ml* which is the value entered in the *Amount* field in the calibration.

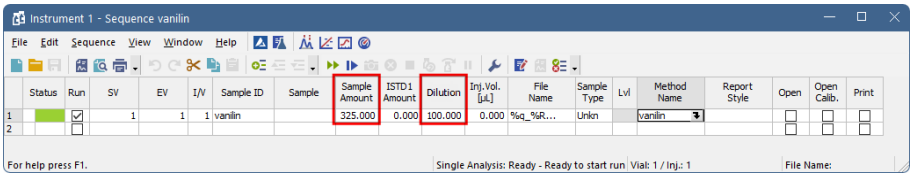
5. Save the calibration and open *Chromatogram* window ④ .



6. Open chromatogram(s), assign each chromatogram prepared calibration using the *Set...* button ⑤ .
7. Fill the amount of the sample that had been used ⑥ . *Sample Amount* refers to the mass of the sample used. Units are automatically copied from the *Calibration Options* (see step 3). The entered amount replaces the *Total* value in the *Amount* column of the *Result Table*. In our example: *325 mg* of sample had been used.
8. Fill the dilution that had been used ⑦ . *Dilution* refers to the solvent volume that has been used to dilute the sample. Dilution multiplies the values in the *Amount* column of the *Result Table*. In our example: *325 mg* of sample had been diluted by *100 ml* of solvent.
9. Column *Amount%* in the *Result Table* now displays the percentage amount of the compound in the sample ⑧ .



Note: It is possible to automatize this process. Calibration can be linked to the used method so it is automatically linked. *Sample Amount* and *Dilution* can be pre-filled in *Single Analysis* or *Sequence* windows.

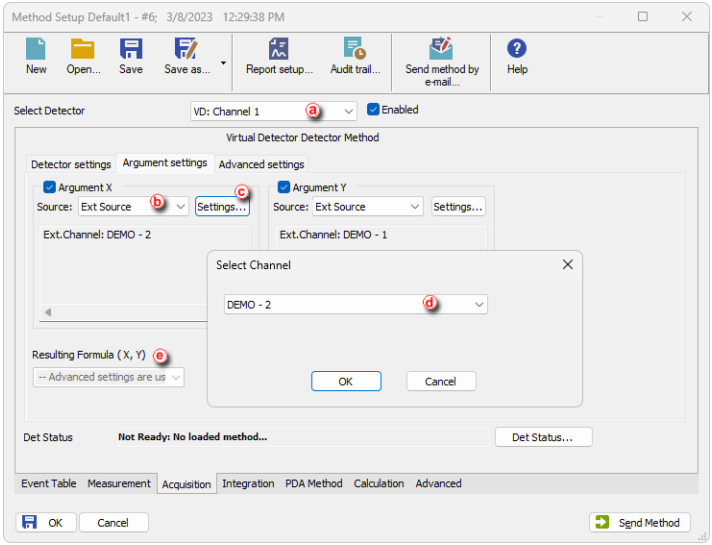


13.4.6 Confirming the identity of a compound by using the signal ratio

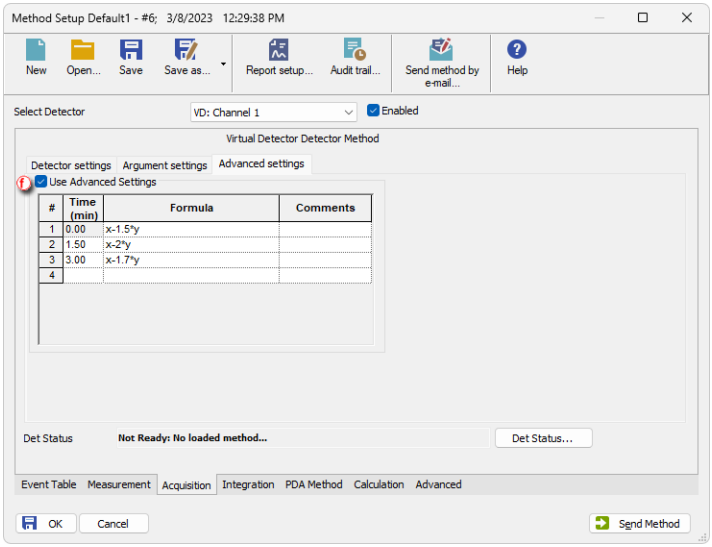
The identity of a compound can be confirmed by using a dual wavelength detector in conjunction with the Virtual Detector and checking if the signals ratio is constant with the following procedure. Prerequisite to this is a know signal ratio for used wavelengths. With correct comparison formula the Virtual Detector signal should result in flat line when the peak is pure compound, impurities with different signal ratio would be represented as response change on the Virtual Detector signal.

1. Add the Virtual Detector as well as your dual wavelength detector to the instrument, if not already present, based on chapter *Adding a new device*.
2. Open the Method Setup dialog and navigate to *Acquisition* tab.

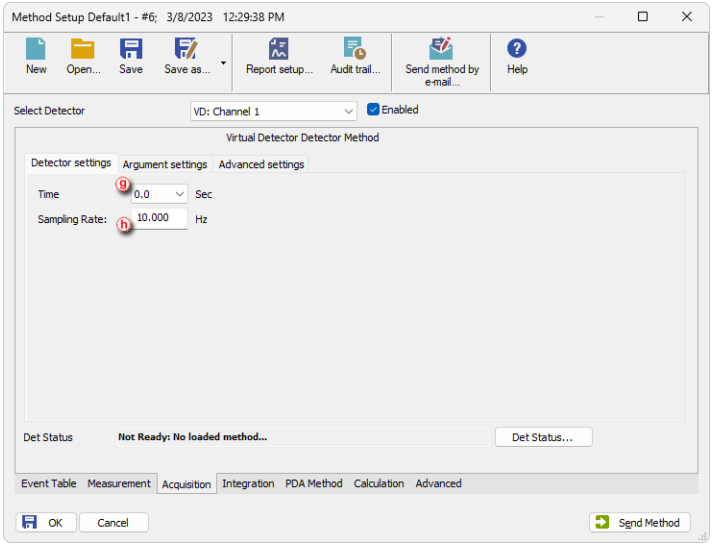
3. Select *VD: Channel 1* in the *Select Detector* drop-down list ⓐ .
4. On the *Argument settings* tab, tick the *Argument X* checkbox, select an *Ext. Source* ⓑ , then click on the *Settings* button ⓒ , select the appropriate detector *Channel* ⓓ and click *OK* .
5. Repeat the same steps for *Argument Y* and select the second channel from the detector.
6. If want to use the same signal ratio for entire analysis you can fill in the *Resulting Formula* field ⓔ with the proper formula. If you need multiple formulas for different times skip this step and continue with the next one.



7. To set multiple formulas for different time intervals navigate to the *Advanced settings*, check the *Use Advanced Settings* ⓕ checkbox and fill the time table as needed.



8. On the *Detector settings* tab, set the *Time* to 0 ⓖ to avoid distortion and fill *Sampling Rate* ⓗ equal to the actual detector sample rate.



Method prepared this way can be used to check compound identity as mentioned in the beginning of this chapter.

13.5 Custom Calculation in Summary Table

This topic describes how to create custom calculations in the *Summary Table* using *User Columns*.

Note that majority of calculations require chromatogram to be calibrated. Without it the necessary values are not available.

Caution: *User Columns* are stored in .DSK files. If the station is used by multiple users it is recommended to set shared .DSK file as described in chapter "Sharing settings among users".

How to add User Columns to Summary Table

The main difference between *Result Table* and *Summary Table* is the information represented in columns. In the *Result Table*, calculations are performed for multiple compounds (peaks) within a single chromatogram, while in the *Summary Table* the same calculation is performed for one compound across multiple opened chromatograms.

Because of this, a *User Column* in the *Summary Table* may not display the same values as an identical formula in the *Result Table*.

Below are the steps to set up *User Columns* in *Summary Table*:

1. In the *Chromatogram* window, switch to *Summary* tab.
2. Right click on the *Summary Table* and select *User Columns - Add...*, the *Add User Column dialog* will be opened.
3. Here you can fill in the appropriate *Name*, *Expression* and *Units* of the *User Column*. Unlike in *Result Table*, you can not check *Calculate Total* and select individual compounds from *Special values* when adding *User Columns* to *Summary table*.
4. Click *OK* in the *Add User Column* dialog.
5. New *User Column* is added to the *Result Table*.

14 Data Reports

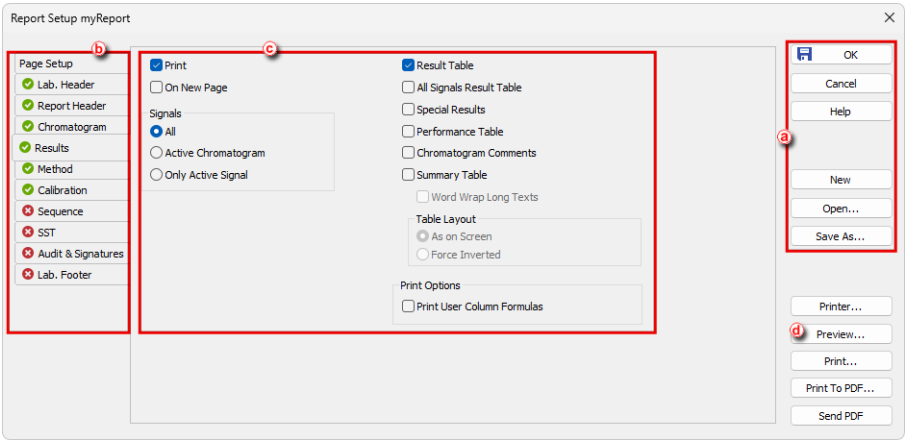
Following chapters describe how to create a report, adjust it and print.

14.1 Setting up a report style for printing

It is possible to select what information and how you want to have printed in the report. You can create different report styles and store them in different *.STY files.

To see an example on how to set up a style to obtain a specific layout see chapter *Creating a report (example)*.

1. From the *Instrument, Calibration, Chromatogram* or *Sequence* windows, select *File - Report Setup*. From the *Method Setup* window click the *Report Setup* button.
2. Click the *New* button if you wish to create a new report style or click the *Open* button ⓐ to open existing report style. Name of currently opened style is included in the window header.
3. Select the tab corresponding to the section you wish to modify ⓑ .
4. Click and drag the tabs to a new position if you wish to change the order in which they will be printed in the report. Tabs can also be moved via context menu which is invoked after right-clicking on them. The first two (*Page Setup, Lab. Header*) and last two (*Audit & Signatures, Lab. Footer*) tabs have fixed position.
5. Select options you would like to include in that section. ⓒ
6. Click *Preview* ⓓ to see the result preview and repeat steps 3.-5. if you wish to modify anything.
7. Click *Save As* to save the report style under a new name or *OK* to accept the changes to the current style. ⓐ



14.2 Printing or previewing a report

The report may include information about methods, calibrations, chromatograms etc. It is possible to setup what information you would like to include in the report as explained in *Setting up a report style*.

Caution: While setting reports it is necessary to pay attention to several crucial settings bellow:

- The information on the report will vary depending on which window we open it from, even if we use the same report style.
  For example, the Chromatogram tab in the Chromatogram Report Setup refers to the chromatograms opened in that specific window. Same tab in the Calibration Report Setup refers to the calibration standard opened in the Calibration window if any. In the Instrument window it will refer to the chromatograms produced after the last run or analysis.
- Only opened chromatograms will be printed. For this reason when setting up automatic printing from *Single Analysis*, *Sequence*, *Batch* windows etc. *Open in Chromatogram Window* option must always be used as well.
- If you set up the report to be printed automatically it is always necessary to specify *Report Style* to be used.

Note: It is also possible to report multiple already measured chromatograms at once using the *Batch* dialog. See Post-run Options from Batch topic for more info.

For more info regarding reports see the **Clarity Reference Guide**.

To *Print* a Report:

1. Select *File - Print* in the *Instrument, Calibration, Chromatogram* or *Sequence* windows. In *Method Setup* click *Report Setup* icon and in the following dialog click *Print...*.

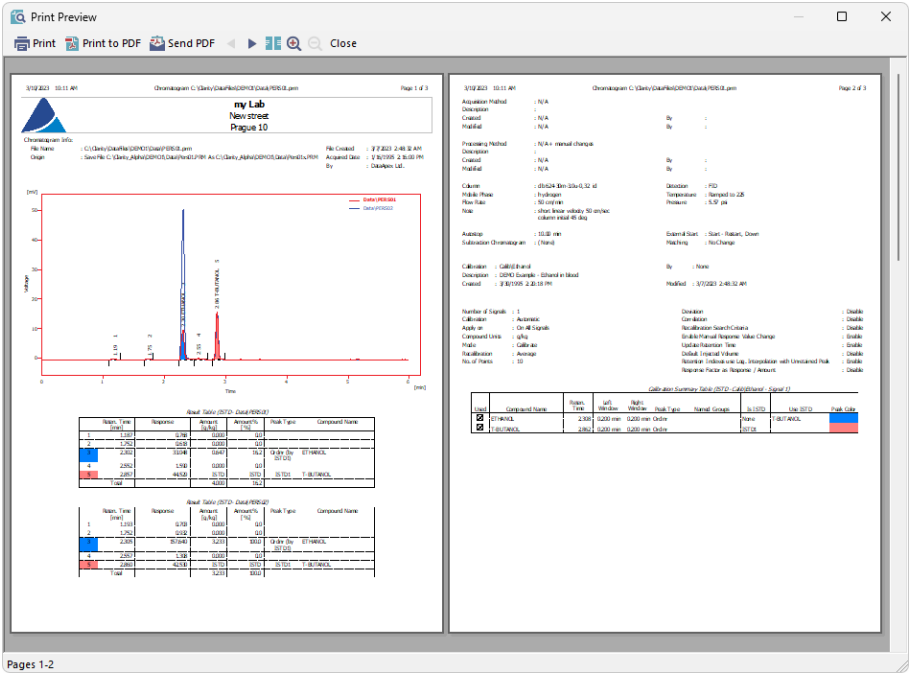
2. *Print* dialog will open for you to setup your printing options and confirm the printout.

To *Print to PDF*:

1. Select *File - Print to PDF* in the *Instrument, Calibration, Chromatogram* or *Sequence* windows. In *Method Setup* click *Report Setup* icon and in the following dialog click *Print to PDF*.
2. *Print to PDF* dialog will open for you to enter file name confirm the saving of the file.

To display *Print Preview*:

1. This feature is useful while preparing your own report style to check whether the outcome is as needed.
2. Select *File - Print Preview* in the *Instrument, Calibration, Chromatogram* or *Sequence* windows. In *Method Setup* click *Report Setup* icon and in the following dialog click *Preview...*.
3. *Print Preview* dialog will open. From there you can browse or print the report.

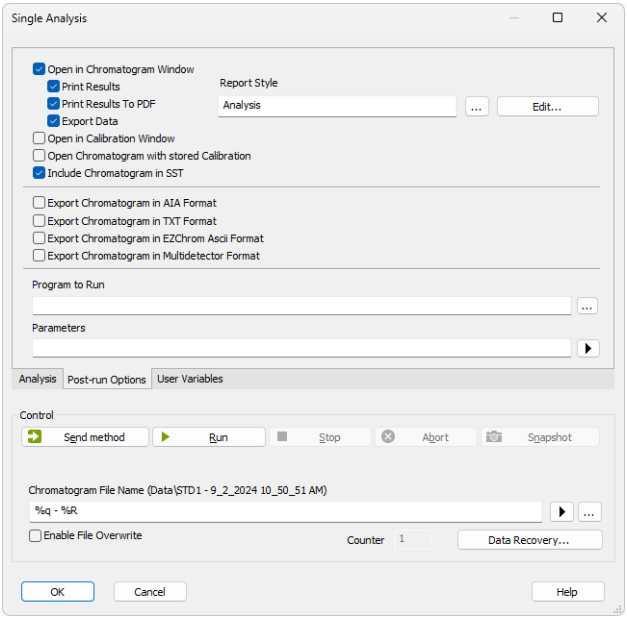


Automatic report generating after analysis is finished:

By default generated reports are placed next to the original files, to change it use *Setting - User Options* in the *Instrument* window. Navigate to *Directories* tab and specify your custom path.

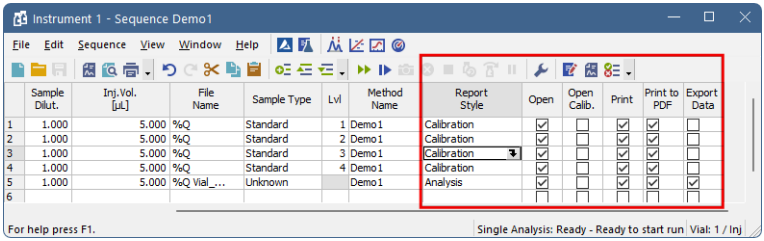
Single Analysis

1. Navigate to *Single Analysis - Post-run Options* tab.
2. Check options *Open in Chromatogram Window*, *Print Results* and/or *Print Results to PDF*.
3. Select *Report Style* by clicking ... button.
4. It is also possible automatically export data, to do so check *Export Data* option. What should be exported can be set by using *Setting - Export Data* in the *Instrument* window.



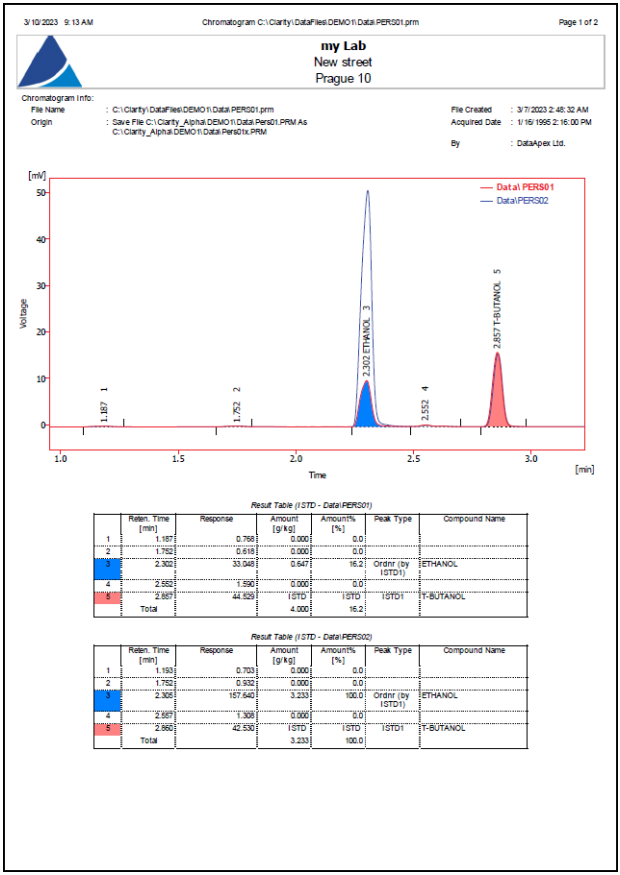
Sequence

1. Procedure is similar to the single analysis. In *Sequence* window some of the required columns are hidden by default, to display them right-click the sequence table and use *Setup Columns* in the following dialog move desired columns to the *Show Columns* list.
2. Check checkboxes in columns *Open*, *Print* and/or *Print to PDF* on rows where report should be generated.
3. Select *Report Style* for each row where report is generated. It is possible to modify specif report style by selecting its cell and clicking .
4. It is also possible automatically export data, to do so check *Export Data* option. What should be exported can be set by using *Setting - Export Data* in the *Instrument* window.



14.3 Creating a report style (example)

This is an example on how to setup a new report style to obtain the results shown in the picture. Beware that tables are printed as on screen, if e.g., calibration table is to wide to fit on one page you can adjust the column width in *Calibration* window.



3/10/2023 9:13 AM Chromatogram C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm Page 1 of 2

my Lab
New street
Prague 10

Chromatogram Info:

File Name : C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm
Origin : Save File C:\Clarity_Alpha\DEMO1\Data\Pers01.PRM As C:\Clarity_Alpha\DEMO1\Data\Pers01x.PRM

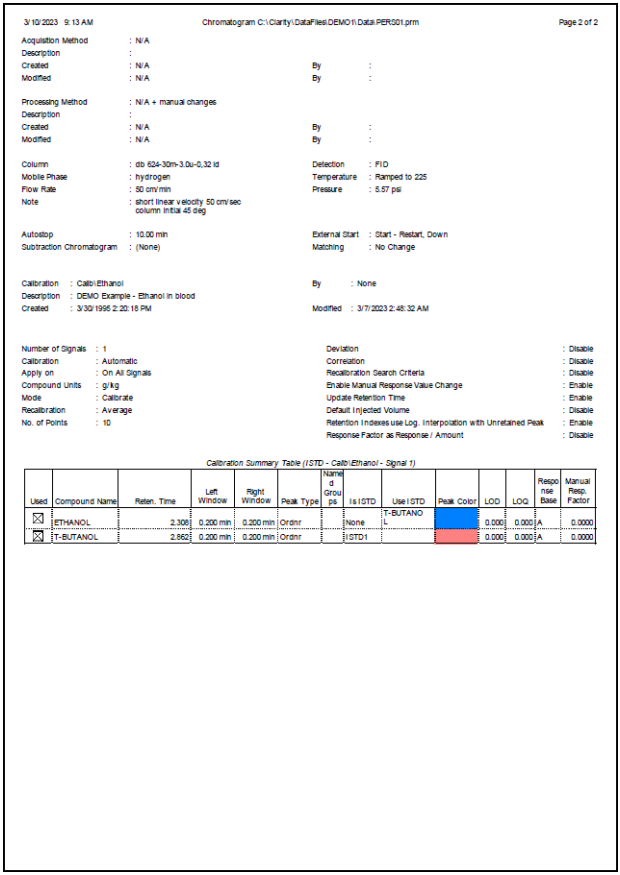
File Created : 3/7/2023 2:48:32 AM
Acquired Date : 1/16/1995 2:16:00 PM
By : DataApex Ltd.

Result Table (ISTD - Data\PERS01)

	Reten. Time [min]	Response	Amount [g/kg]	Amount% [%]	Peak Type	Compound Name
1	1.187	0.768	0.000	0.0		
2	1.752	0.618	0.000	0.0		
3	2.302	33.048	0.647	16.2	Ordnr (by ISTD1)	ETHANOL
4	2.552	1.590	0.000	0.0		
5	2.857	44.529	ISTD	ISTD	ISTD1	T-BUTANOL
	Total		4.000	16.2		

Result Table (ISTD - Data\PERS02)

	Reten. Time [min]	Response	Amount [g/kg]	Amount% [%]	Peak Type	Compound Name
1	1.193	0.703	0.000	0.0		
2	1.752	0.932	0.000	0.0		
3	2.308	157.640	3.233	100.0	Ordnr (by ISTD1)	ETHANOL
4	2.557	1.309	0.000	0.0		
5	2.868	42.530	ISTD	ISTD	ISTD1	T-BUTANOL
	Total		3.233	100.0		



3/10/2023 9:13 AM Chromatogram C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm Page 2 of 2

Acquisition Method : N/A
Description :
Created : N/A By :
Modified : N/A By :

Processing Method : N/A + manual changes
Description :
Created : N/A By :
Modified : N/A By :

Column : db 624-30m-3.0u-0.32 id Detection : FID
Mobile Phase : hydrogen Temperature : Ramped to 225
Flow Rate : 50 cm/min Pressure : 5.57 psi
Note : short linear velocity 50 cm/sec column initial 45 deg

Autostop : 10.00 min External Start : Start - Restart, Down
Subtraction Chromatogram : (None) Matching : No Change

Calibration : Calib\Ethanol By : None
Description : DEMO Example - Ethanol in blood
Created : 3/30/1996 2:20:16 PM Modified : 3/7/2023 2:48:32 AM

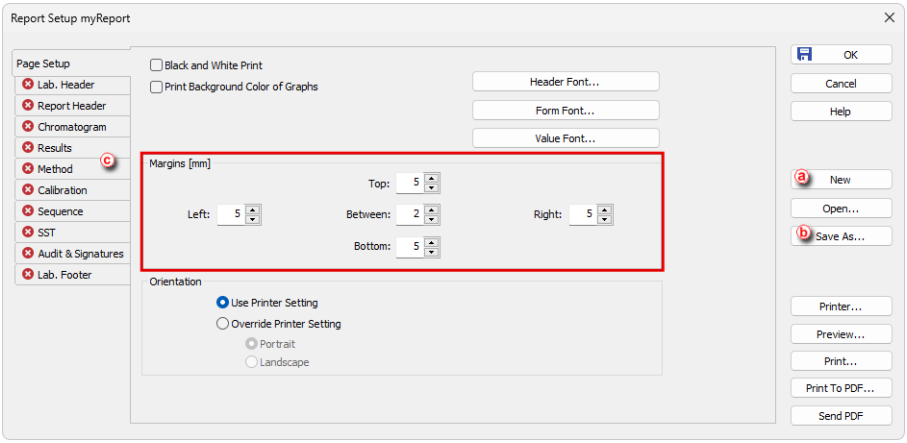
Number of Signals : 1
Calibration : Automatic
Apply on : On All Signals
Compound Units : g/kg
Mode : Calibrate
Recalibration : Average
No. of Points : 10

Deviation : Disable
Correlation : Disable
Recalibration Search Criteria : Disable
Enable Manual Response Value Change : Enable
Update Retention Time : Enable
Default Injected Volume : Disable
Retention Indexes use Log. Interpolation with Unretained Peak : Enable
Response Factor as Response / Amount : Disable

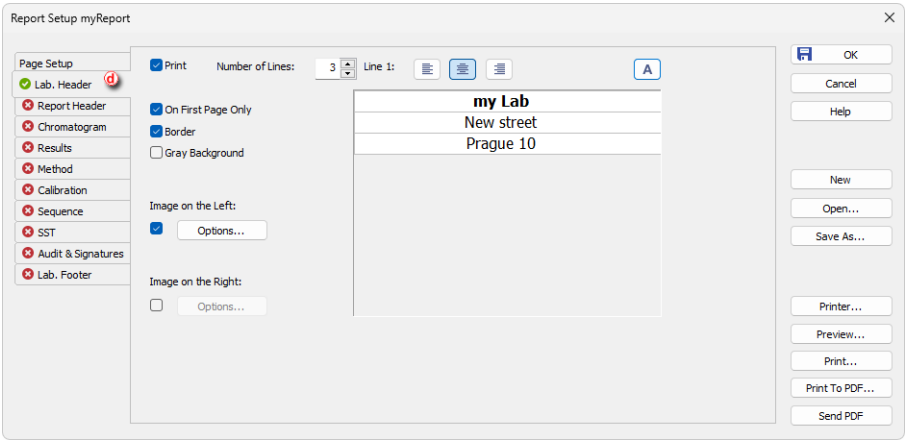
Calibration Summary Table (ISTD - Calib\Ethanol - Signal 1)

Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Response Base	Manual Resp. Factor
☒	ETHANOL	2.306	0.200 min	0.200 min	Ordnr		None	T-BUTANOL		0.000	0.000	A	0.0000
☒	T-BUTANOL	2.662	0.200 min	0.200 min	Ordnr		ISTD1			0.000	0.000	A	0.0000

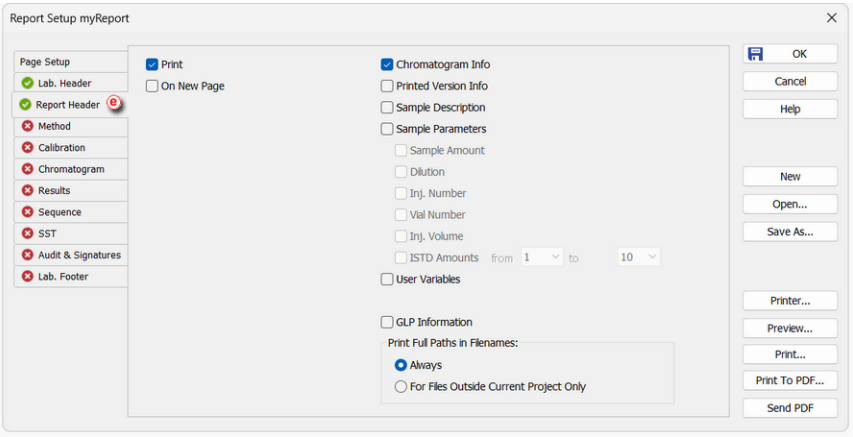
1. Open the chromatograms PERS01 and PERS02 in overlay (located in C:\CLARITY\DATAFILES\DEMO1\DATA).
2. Select the graph area you want to print by clicking and dragging the cursor in the chromatogram graph.
3. Create a new report style.
   - Select the *File - Report Setup*.
   - Click on the *New* button ⓐ to create a new report style.
   - Click on the *Save As...* button ⓑ and save the style under the name (*myReport* in this example).
4. Click and drag the tabs ⓒ to set them in desired order. This will be the order the sections will have in the report.
5. Set the *Margins* as needed.



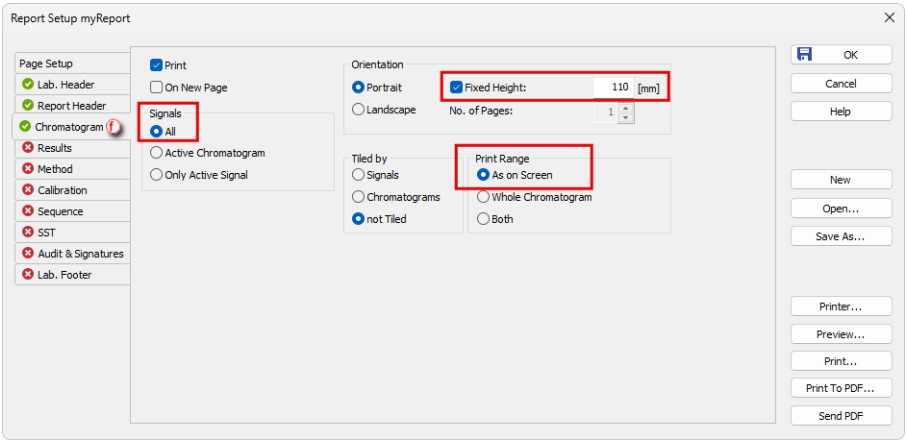
6. Set the *Lab Header*.
    - Click the *Lab Header* tab ⓓ .
    - Check the checkboxes *Print*, *On First Page Only* and *Border*.
    - Check the *Image on the Left* checkbox and click on the *Options...* button to select the logo.
    - Click in each line in the text box and write the you want to have in the header.
    - Click in the first line of text and then on the *Font* icon (icon with "*A*") and select *Bold* as a *Font Style*.



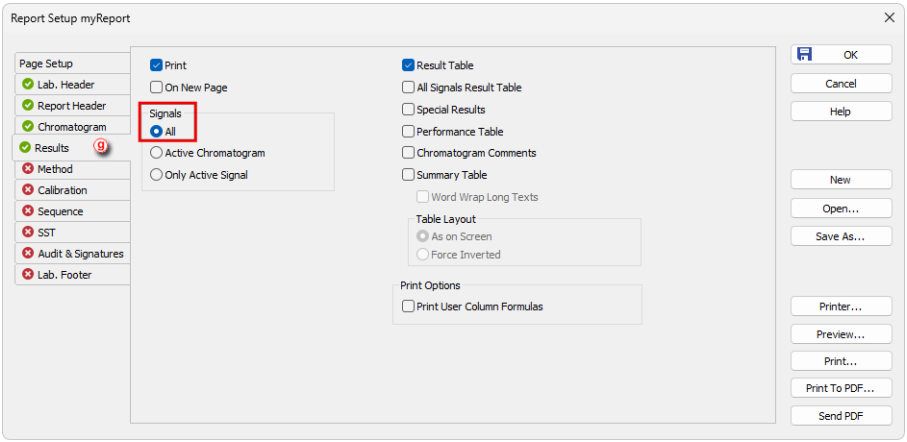
7. Set the *Report Header*.
    - Click the *Report Header* tab ⓔ .
    - Check the options *Print* and *Chromatogram Info*.



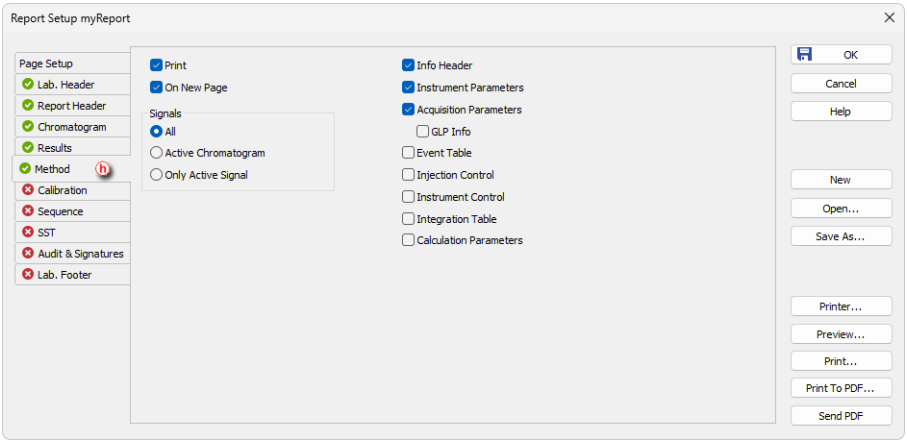
8. Set the *Chromatogram section*. Only the format of printed graphs is set here, result tables are printed based on *Results* tab, see next step.
    - Click the *Chromatogram* tab ⓕ .
    - Check the options *Print* and *Fixed Height* and set the height to 110 mm.
    - Select the options *Signals - All* and *Print range - As On Screen*.



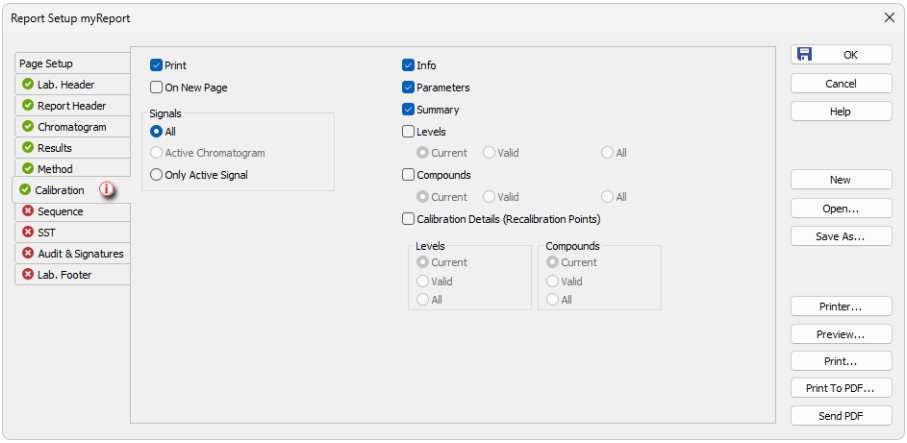
9. Set the *Results* section.
    - Click the *Results* tab ⓖ .
    - Check the options *Print* and *Result Table*.
    - Select the option *Signals - All*.



10. Set the *Method* section.
    - Click the *Results* tab. ⓗ
    - Check the options *Print*, *On New Page*, *Info Header*, *Instrument Parameters* and *Acquisition Parameters*.
    - Select the option *Signals - All*



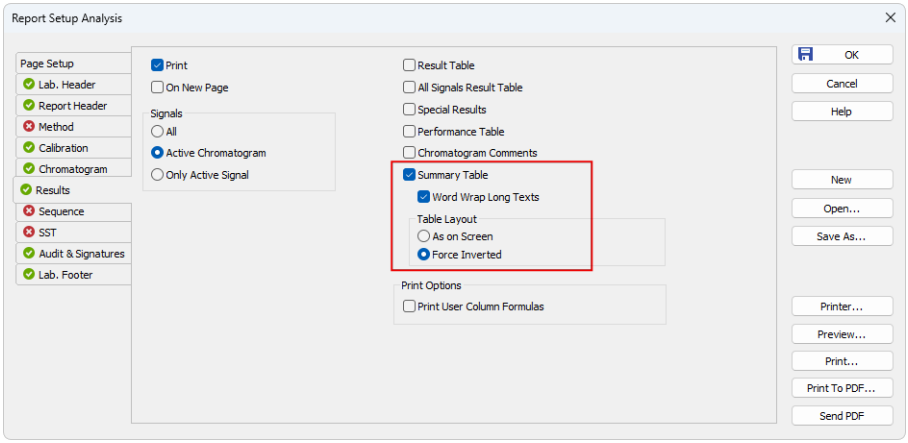
11. Set the *Calibration* section.
    - Click the *Calibration* tab ⓘ .
    - Check the options *Print*, *Info*, *Parameters* and *Summary*.



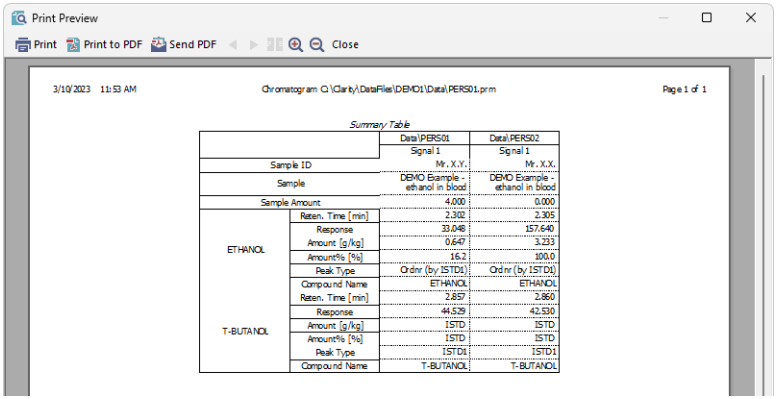
12. You can preview your report by clicking *Preview...*. For more info see ***Printing or previewing a report***.
13. Click the *OK* to save the report style.

14.4 Printing the summary table

1. Setup *Summary* table in *Chromatogram* window. For information on how to create Summary Table, see the chapter **"Comparing the results from several chromatograms"** on pg. **185**.
2. Right-click in the *Summary Table*, if you want to change the visualization of the table, add a custom column, etc.
3. Open the *Report Setup* dialog and check the *Summary Table* checkbox in the *Results* tab.
4. It is also recommended selecting *Word Wrap Long Texts* and *Force Inverted* (table will be printed with inverted layout ignoring the on-screen layout which is more suitable for reports) options. *Print User Column Formulas* can be used when custom columns are included in the table.



5. The results for all opened chromatograms will be printed.



14.5 Printing from sequence

In many workflows, it is useful to have reports printed automatically as part of the sequence — for example, to document each sample, create a summary for the whole sequence, or compare replicate injections. Clarity allows you to set up such automatic printing directly from the *Sequence* window.

Following reports can be printed automatically from the sequence:

- individual reports
- summary reports for the entire sequence
- summary reports for replicates

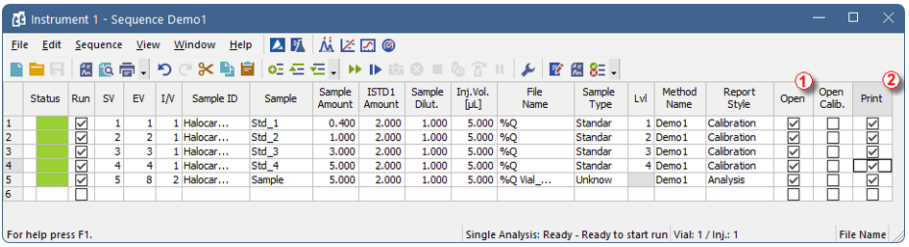
Before printing reports, please notice that printing in Clarity is in most cases WYSIWYG, i.e. when printing chromatograms, they need to be opened in the *Chromatogram* window, graphs and tables are printed as formatted on the screen.

There is common report setup in Clarity, however the data printed may depend on from which window the print is invoked.

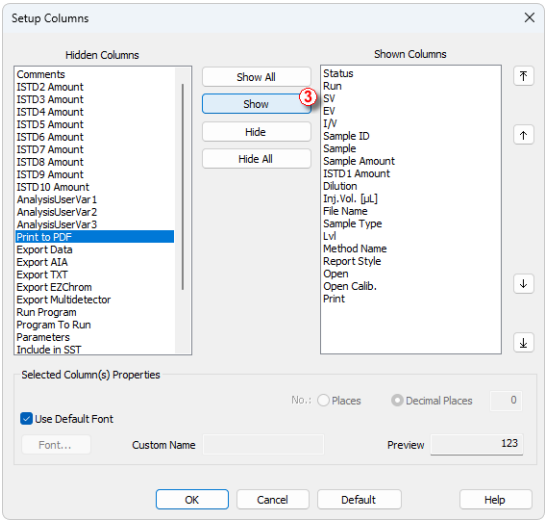
14.5.1 Individual reports

Individual reports can be printed for every analysis in the sequence. In our example, we want to print *Calibration Standards* one at a time, and have a summary report for the *Unknown* samples.

1. In *Chromatogram* window, ensure the *Overlay Mode* is *OFF*.
2. In *Sequence* window, check checkboxes in column *Open* ① and *Print* ② and/or *Print to PDF* for all the rows you want to print from.



3. If required column is not present, invoke local menu and select *Setup Columns* and *Show* ③ the column you want to see.

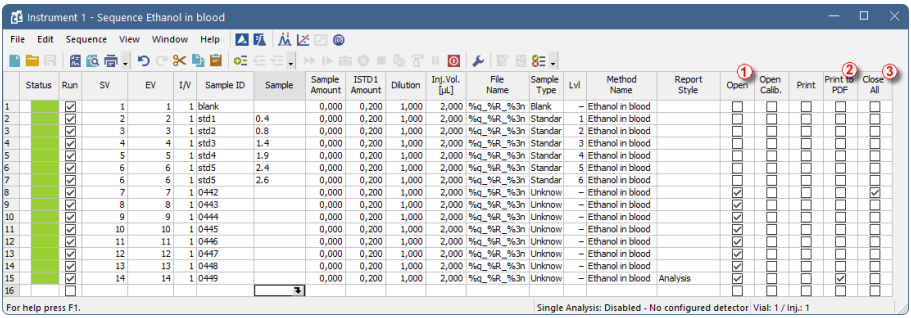


4. Select the *Report Style* you want to use for printing. The chosen *Report Style* determines both the content of the report and its formatting.
5. Run the sequence.

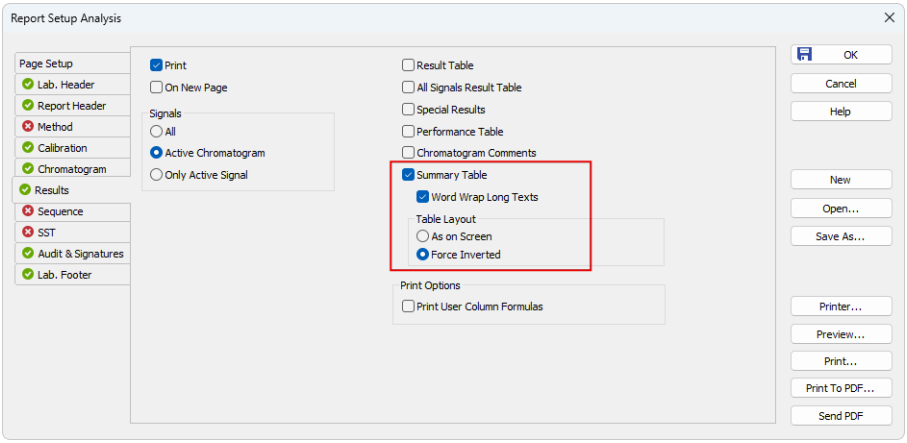
With *Overlay* mode turned *OFF*, only one chromatogram is displayed in the *Chromatogram* window at a time. When an analysis with the *Open* option checked is finished, the resulting chromatogram is opened in the Chromatogram window and printed individually (if *Print* or *Print to PDF* is checked).

14.5.2 Summary reports for the entire sequence

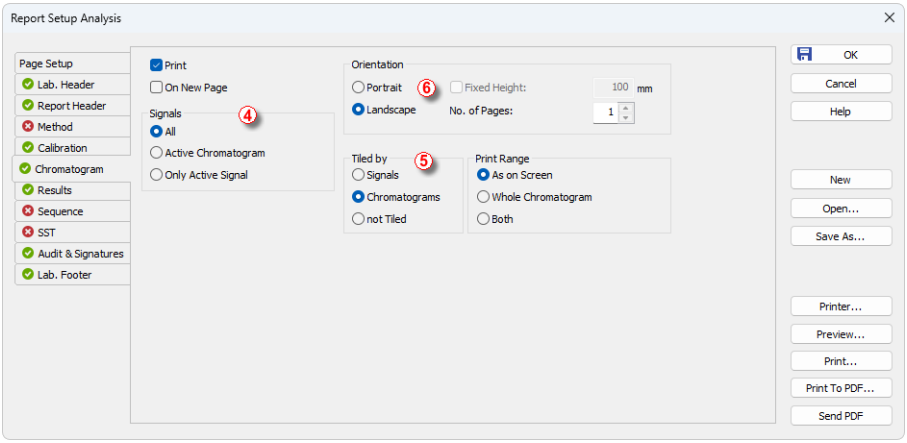
1. In *Chromatogram* window, ensure the *Overlay Mode* is *ON*
2. In *Sequence* window, check checkboxes in column *Open* ① for all the rows you want to include.
3. Print of the sequence will be invoked from the last row where *Print to PDF* ② column is checked.
4. The *Close All* ③ column ensures chromatograms previously opened in overlay will be closed.
5. If required column is not present, invoke local menu and select *Setup Columns* and *Show* the column you want to see.



6. Open the *Report Setup* with *Report Style* you want to use and adjust it accordingly.



7. To print all chromatograms as individual graphs, switch to *Chromatogram* tab and check the *All Signals* ④ and *Tiled by Chromatograms* ⑤



8. To fit the page width, *Landscape orientation* ⑥ may be advantageous. Configure the tables layout in the *Chromatogram* window accordingly. Otherwise the tables will be split across multiple pages but aligned to allow the full table to be reconstructed when the pages are placed side by side.
9. Save the *Report Style* by *OK*.
10. Run the sequence.

The resulting report with setting used in this example will contain: *Calibration Summary table*, *Calibration Level Tables*, each compound calibration and graphs, *Summary table for samples* and *Sequence Audit Trail*.

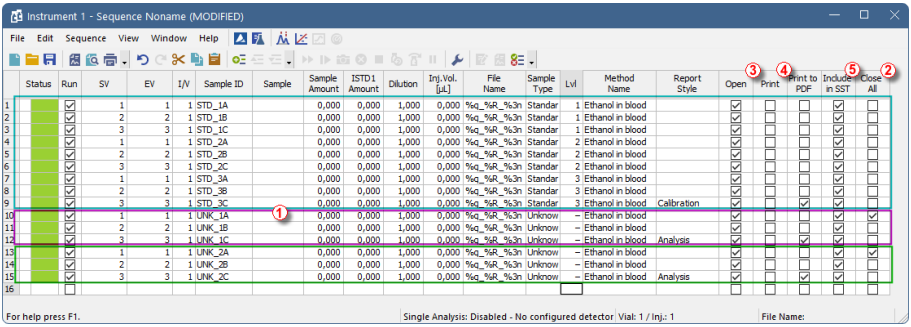
With *Overlay* mode turned *ON*, multiple chromatograms can be opened in the *Chromatogram* window and printed together. On the first row we wanted to include, we

used *Close All* to close any previously opened chromatograms. Each subsequent chromatogram with the *Open* option checked was then automatically opened into the *Chromatogram* window as soon as it was measured, and after the last one was opened, printing was triggered with the *Report Style* correctly adjusted for a summary report.

14.5.3 Summary reports for replicates

The process is similar to printing one summary report for the sequence. The difference is that for each sample there is a block of three rows (3 repetitions) ① . On the first row of the block, the *Close All* ② column should be checked to ensure previously opened chromatograms are closed. In all rows to be printed should be the *Open* ③ column checked. On the last row of the block, the *Print* ④ column should be checked and *Report Style* filled in to trigger printing of the report. If you want the SST results to appear in the report, make sure to check the *Include in SST* ⑤ column for the corresponding chromatograms.

In this example, we want to print calibration report after measuring all standards, and summary report for replicates for each unknown sample.



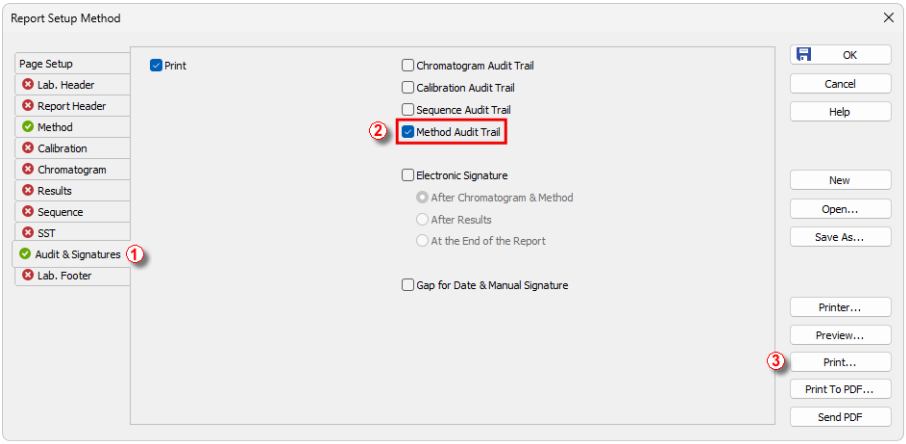
14.6 Printing audit trail of method used for measurement

In Clarity, it is possible to print not only the method itself but also its *Audit Trail*, which documents how the method was created and modified. While the method itself can be printed directly with the chromatogram, its *Audit Trail* can not be printed from other windows than *Method Setup*, even if the option is selected in the *Report Setup* dialog. Therefore, the *Audit Trail* of a method cannot be printed together with the chromatogram to one report.

Method *Audit Trail* can be printed by following these steps:

1. Open the desired method in the *Method Setup* dialog.
2. From there, open *Report Setup* dialog using *CTRL + ALT + P* or the *Report Setup* icon .
3. In the *Report Setup* dialog, on the *Audit & Signatures* tab ① , check the option *Method Audit Trail* ② .

4. Print the report from the *Method Setup* dialog ③ .



15 File Management

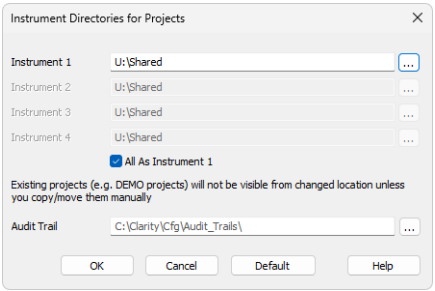
How to set project directories, create new projects, preset file names of measured chromatograms based on variables, store files into subfolders etc.

15.1 Setting up project directories

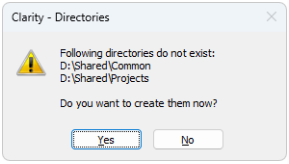
It is possible to set different directories for projects accessible from each instrument and to set the Audit Trail directory. This is useful while working with a shared disk if it is necessary to access measured data from another PC using **Clarity Offline**.

To setup a custom project directories do following:

1. Open Main Clarity window.
2. Open the *Instrument Directories for Projects* dialog using the *System - Directories...* command or the  icon.



3. Set the desired directory e.g., *U:\Shared*.
4. If needed, change the *Audit Trail* directory as well.
5. When saving the changes, the following dialog may appear. Confirming it will create the necessary subfolder structure in your target location. COMMON is filled by default files that are necessary for functioning.



Given that a new COMMON directory has to be created in the custom directory, the report styles and templates for a new method, calibration, and sequence become instrument-specific.

Caution: Be aware that when updating Clarity the COMMON files outside of the installation directory must be updated manually.

15.2 Setting up custom export and import directories

By default, Clarity exports data to the folder where the original chromatograms are stored, and imported files are browsed within the current project directory. If you routinely use specific locations, such as shared folders on a network drive, you can define custom default directories in *Settings - User Options…*, under the *Directories* tab accessible from the *Instrument* window.

Once a custom *Export Directory* is set, all exported files will be saved to that location, regardless of where the chromatograms are stored. Similarly, setting a custom *Import Directory* ensures that the import dialog opens in the predefined location.

Note: These settings are saved in the desktop file (.DSK). If multiple users need to work with the same directories, they must either share the same desktop file or configure their settings individually.

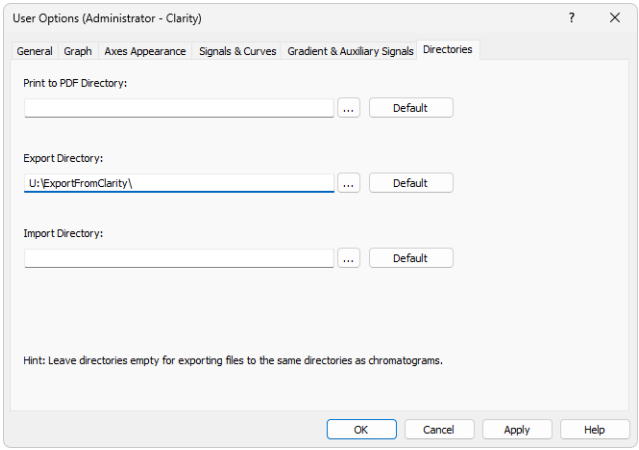


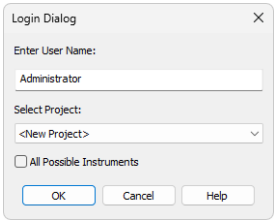
Fig. 15: Setting of the export and import directories

15.3 Creating a new project

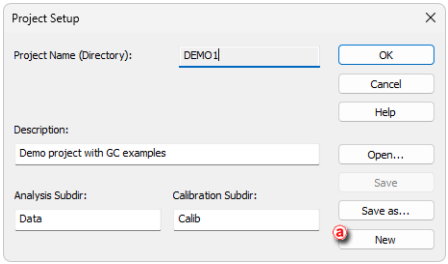
Creating a new project ensures that the measured data will be later easily found. The project itself is a directory in **Clarity's** DATAFILES subfolder or selected directory where all relevant files are saved (methods, calibrations, sequences, chromatograms).

1. To create new project navigate to the *Project Setup* dialog by selecting *Instrument - Project...* in the *Instrument* window.

Note: You can also open a project through the *Login Dialog* opened from the Main Clarity window by selecting the *New Project* option and clicking OK.

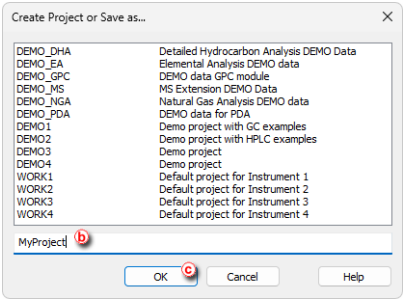


2. In the *Project Setup* dialog click the *New* button ⓐ to create a new project.



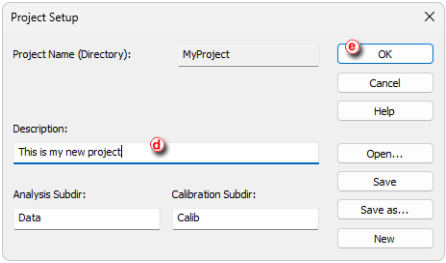
3. Set the name of the new project ⓑ and click *OK* ⓒ .

Note: Entered project name must not contain invalid characters, i. e. \ /:*?"< >|.



4. Fill in the project description in the *Description* field ⓓ and click *OK* ⓔ .

Note: The change of the project will require you to restart the Instrument. If there are any unsaved files opened, you will be prompted to save them. The newly created project does not include any files (for example method, calibration etc.).



15.4 Creating customized file names automatically

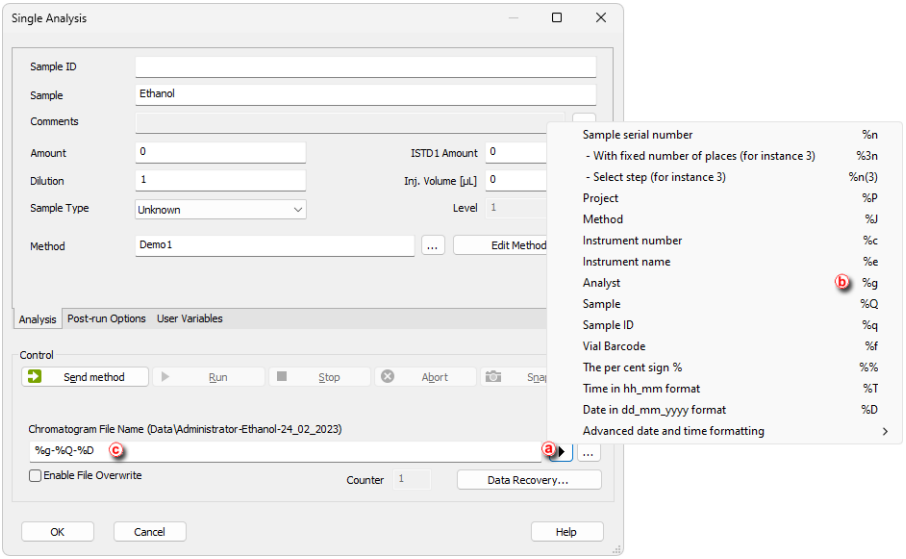
You can create customized file names automatically by appending variables to them.

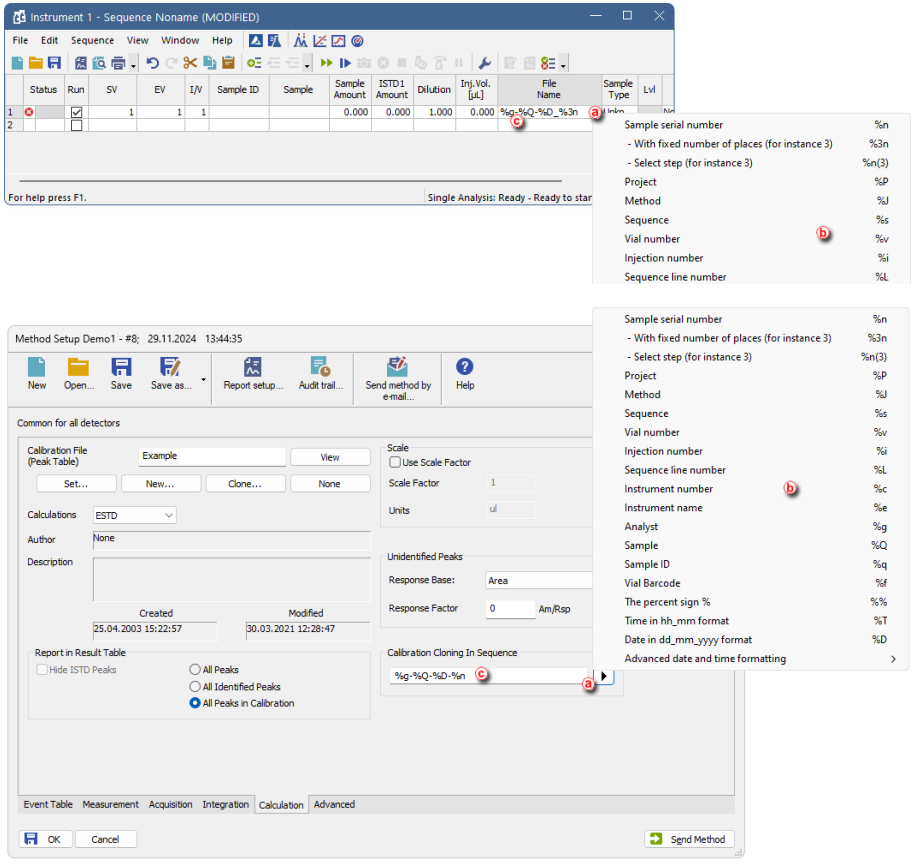
File names can be created in the *Single Analysis* window, in the *Sequence* window and on the *Method Setup - Calculation* tab.

1. Click on the respective icons , , in the *Instrument* window to open the *Single Analysis*, the *Sequence* or the *Method Setup - Calculation* window.
2. Click on to open the variable list. ⓐ
3. Select the variable you want to include in the file name. ⓑ
4. Repeat the previous two steps to add more variables.
5. Insert any allowed characters between the variables to create your file name. ⓒ

More Info:

- Variables are preceded by the "%" character and they are substituted by their value upon file creation. For example "*%g-%Q-%D*" will create a file name with the name of the *Analyst*, the *Sample* and the *date*: "*Administrator-Ethanol-24_02_2023.prm*".
- To prevent an *Unresolved File Name* error you can append the *Sample Serial Number* "%n" or the date and time "%R".


Single Analysis
Sample ID
Sample
Ethanol
Comments
Amount
0
ISTD1 Amount
0
Dilution
1
Inj. Volume [µL]
0
Sample Type
Unknown
Level
1
Method
Demo1
Edit Method
Analysis
Post-run Options
User Variables
Control
Send method
Run
Stop
Abort
Chromatogram File Name (Data\Administrator-Ethanol-24_02_2023)
%g-%Q-%D
Enable File Overwrite
Counter
1
Data Recovery...
OK
Cancel
Help
Sample serial number %n
- With fixed number of places (for instance 3) %3n
- Select step (for instance 3) %n(3)
Project %P
Method %J
Instrument number %c
Instrument name %e
Analyst %g
Sample %Q
Sample ID %q
Vial Barcode %f
The per cent sign % %%
Time in hh_mm format %T
Date in dd_mm_yyyy format %D
Advanced date and time formatting
a
b
c



15.5 Storing chromatograms into subfolders

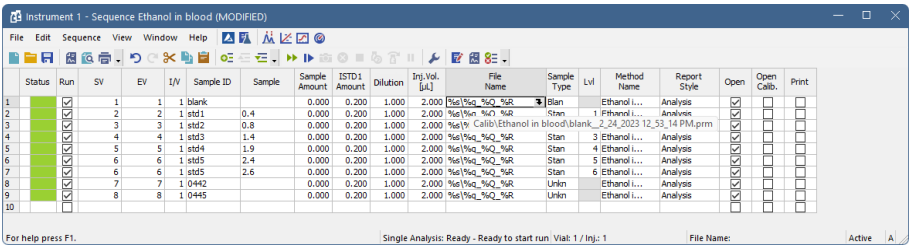
It is possible to include the name of a subfolder in the *File name* to store chromatograms into project's subfolder. If the subfolder doesn't exist, it will be created when the chromatogram is stored. The directory can be set using the **"\"** character. Any string of the variables or characters in front of the **"\"** character is considered as the subfolder name. Any string of variables or characters after the **"\"** character is used as the file name.

Subfolders created this way are present in DATA and CALIB subfolders of used project.

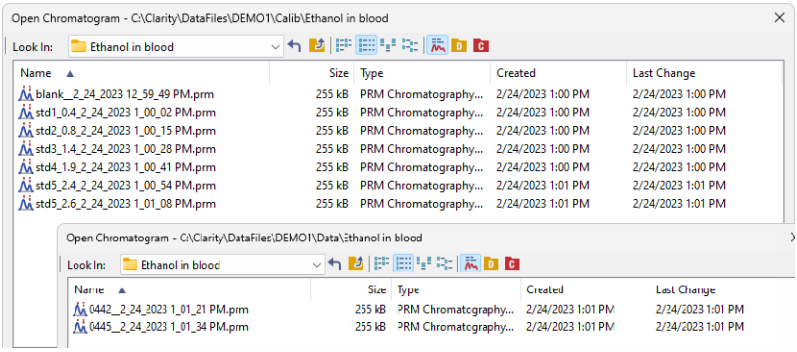
Here we provide an example on how to store chromatograms from one sequence into subfolder named after it.

1. Login to *Instrument* with DEMO1 project.
2. Open the *Sequence* window.
3. Open ETHANOL IN BLOOD.SEQ.

4. Set the File Name of the first row to **%s\%q_%Q_%R**. (To see detailed description on how to create the name using variables see chapter "Creating customized file names automatically" on page 232.)
5. Right click on the *File Name* column and select *Fill down* to apply the name to all rows.



6. The Chromatogram file with a name of SAMPLEID_SAMPLE_DATE-AND-TIME will be stored in *Demo1\Data\Ethanol in blood* folder for unknown samples and in *Demo1\Calib\Ethanol in blood* folder for standards and blank.



- To create subfolder for each month use the %m or %B variables and for each day use the %a or %A variables.
- Same procedure can be also used in *Single Analysis* window.

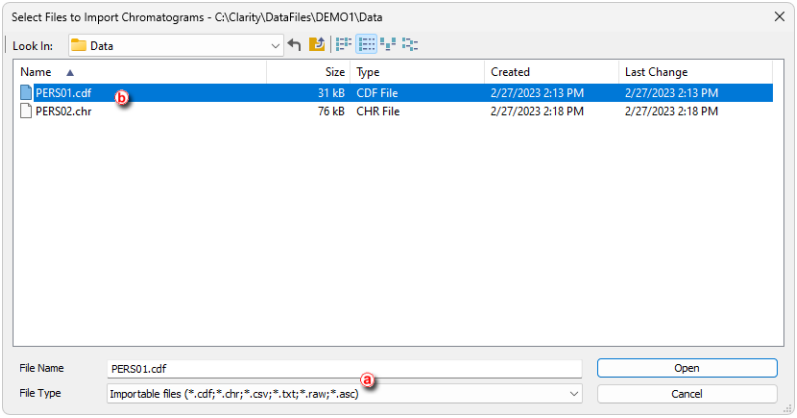
16 Import and Export Data

Clarity allows to import or export chromatograms from/to various formats. Following chapters describe you how to, for example, set exporting chromatograms to a LIMS.

16.1 Importing a chromatogram into Clarity

It is possible to import chromatograms from other chromatography software. Supported formats are : AIA (*.CDF suffix), EZChrom ASCII (*.ASC suffix), Text format (*.TXT), Comma Separated Values format (*.CSV) or Multi-detector format (*.CHR). The particular procedure depends on type of file you want to import.

1. From the *Chromatogram* window open the *Open Files To Import* dialog by selecting *File - Import Chromatogram…*.
2. You can select the *File Type* which you want to import ⓐ . By default you can see all supported formats.
3. Select the file(s) you want to import ⓑ and click on the *Open* button.

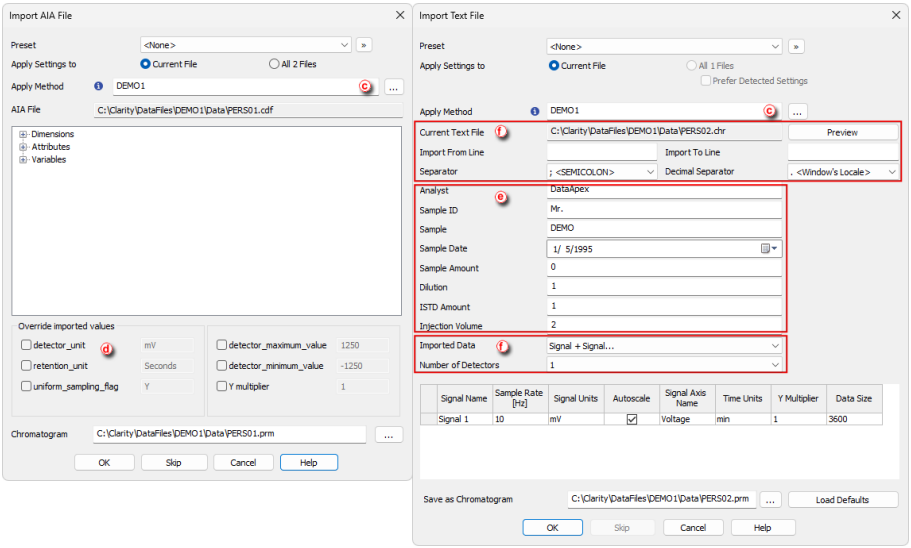


4. Set the parameters as needed in the subsequent dialogs depending on the file format.
5. For all file formats you can select imported file name and which method to apply ⓒ . This will apply integration, calibration etc.

- Import AIA File - when importing AIA file (*.CDF suffix).
  - You have option to inspect data from the source file and override some of them ⓓ e.g, *Detector Unit*.
- Import Text File - when importing Text, Multidetector or EZChrom ASCII file (*.TXT, *.CHR, *.ASC and *.CSV suffixes).
  - You can set information regarding given sample ⓔ like *Dilution* or *Injection Volume* etc. You can also set information regarding source file format ⓕ .

Note: File format related settings is typically detected automatically and there is no need to change it.

- *Save As* - when importing *.RAW file, as there is no need to set other parameters.



16.2 Exporting a chromatogram from Clarity to a different chromatography data station

It is possible to export chromatograms to other formats used by chromatography data stations. The supported formats are : *AIA* (*.CDF suffix), *EZChrom ASCII* (*.ASC suffix), *Text format* (*.TXT), or *Multi-detector format* (*.CHR).

1. Open the *Chromatogram* window by selecting *Window - Chromatogram* on the *Instrument* window or click on  .
2. Open the chromatogram you want to export, then open the *Export Chromatogram* dialog by selecting *File - Export - Export Chromatogram….*
3. Select the export format ⓐ . Notes:

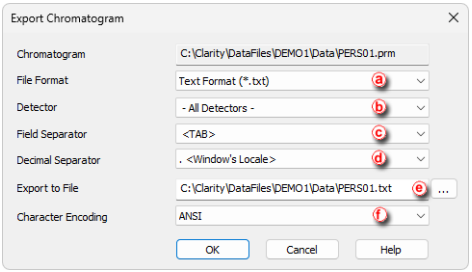
   Note: For PDA export of 3D data only the EZChrom ASCII format is supported.

4. Select the signals to be exported ⓑ .

   Note: You can choose individual signals, *All Detectors*, *3D Data* or *All Detectors + 3D Data* (3D Data variants in EZChrom ASCII only).

5. Select the field separator character ⓒ .
6. Select the decimal separator character ⓓ .

7. Open the *Export Chromatogram As* dialog clicking on ... . Enter the name and location of the file into which you wish to export the chromatogram ⓔ or fill in the file name.
8. Select the character encoding for the exported file (*ANSI* or *Unicode (UTF-8)*) ⓕ .
9. Click *OK* to finish the export.



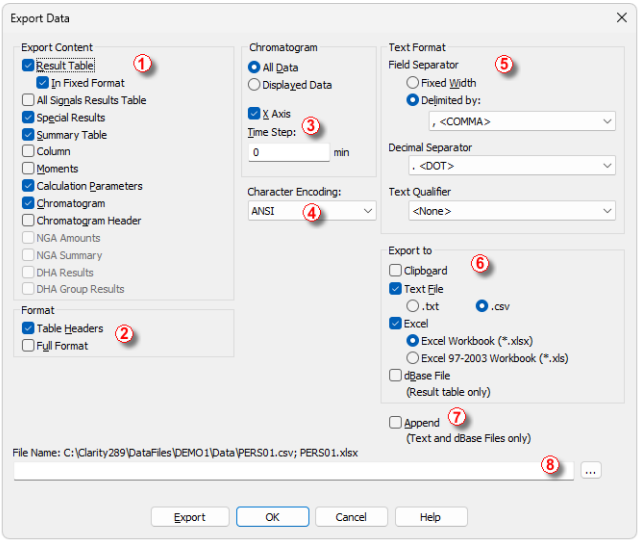
16.3 Exporting data from Clarity

It is possible to export selected parts of the results into external files. All of this can be achieved automatically from *Sequence* or *Single Analysis* window by selecting *Export Data* in *Post-run Options* or manually from the *Chromatogram* window.

1. Open *Export Data* dialog from *Instrument* window by using *Setting - Export Data...*
2. Select which data you want to include in the exported files in the *Export Content* group ① . Detailed description of these fields can be found in the Reference Guide.
3. Select whether you want the tables exported with headers and/or in the full format ② .
4. Select whether the exported chromatogram data will contain time column or not. If you intend to perform bunching for the exported data specify the time period for the bunching ③ .

   Note: The mean value for selected *Time step* period is calculated as a sum of the highest Y_{Max} and lowest Y_{Min} signal curve value found within each *Time Step* period divided by two - $(Y_{Max}+Y_{Min})/2$.

5. Select the character encoding to be used (*ANSI* or *Unicode (UTF-8)*) ④ .
6. Select the appropriate text formatting for the export ⑤ .
7. Select the format or formats to which the data will be exported. You can choose any number of export types at the same time ⑥ .
8. Select whether the exported data should be appended into an existing file ⑦ (in this case file name ⑧ must be filled in) or exported as a new file (leave the file name empty as shown bellow).



- This setting will be used for automated data export from *Sequence* or *Single Analysis*.
- To manually export data you can invoke the same dialog from *Chromatogram* window by using *File - Export - Export Data...* command or icon. In this case dialog also includes *Export* button which can be used the export data from currently opened chromatogram.

16.4 Exporting data for LIMS

For detailed information about **LIMS** integration, configuration, and advanced export settings, refer to the separate *Clarity LIMS Manual* available also at dataapex.com.

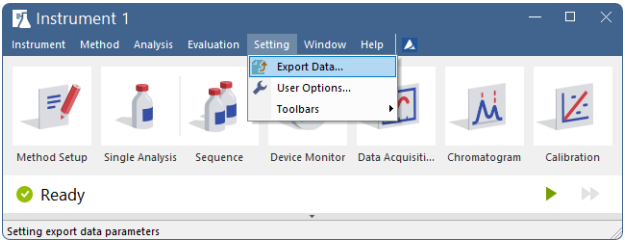
Before exporting data to a **LIMS**, it is recommended to review the chromatograms in Clarity to ensure that all results and calculated values are correct (see chapter Comparing the results from several chromatograms).

Once the results have been verified, Clarity offers several ways to perform the export, depending on the workflow and user preference.

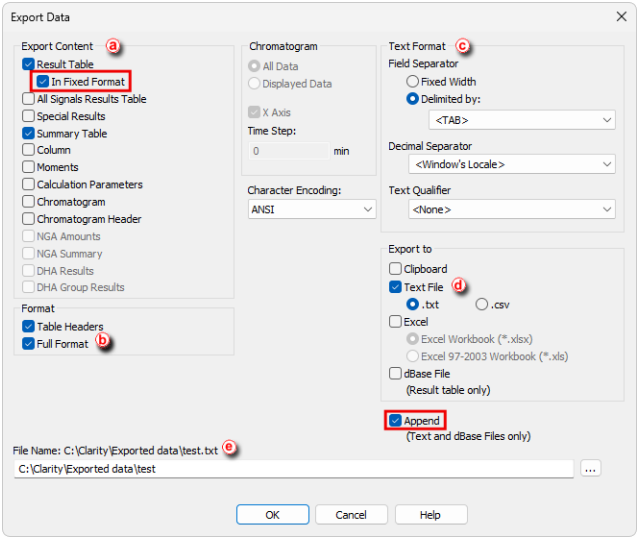
16.4.1 Setting up the Export Format

First, it is necessary to set the format of exported data. To do that, follow these steps:

1. Open *Export Data* dialog by using *Settings - Export Data* from the *Instrument* window.



2. In the *Export Content* section ⓐ , select which data you want to include in the exported files. It is recommended to export the *Result Table* with *In Fixed Format*. This will ensure that the data will be exported always in the same format regardless of the setting on the screen. However, *Fixed Format* can only be used if the predefined set of exported columns meets your needs—if you require custom or user-defined columns, leave this option unchecked.



3. Select *Full Format* ⓑ option. This will add the file name, date and time before each *Result Table* row to allow for easy sorting, which is particularly useful when using the *Append* option.
4. Select the desired file formatting in *Text Format* ⓒ section.
5. Select *Export to - Text File* ⓓ and choose preferred suffix. In the *File Name* ⓔ field, specify the directory where the export files should be created. If the field is left empty, Clarity automatically uses the chromatogram name as the file name and saves the exported file either to the chromatogram directory or to the directory defined in the *User Options – Directories* tab (for more details, see chapter "Setting up custom export and import directories").

6. Check *Append* to export all results to a single file.

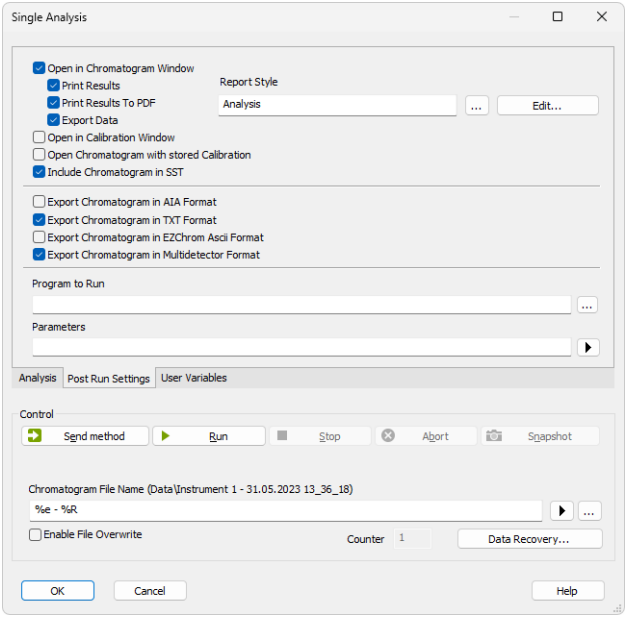
Note: The settings defined in the *Export Data* dialog are stored in the active desktop file (.DSK). If multiple users need to export data in the same format, they must either share the same desktop file or configure their settings individually..

16.4.2 Ways to Export Results

Depending on the workflow and user preference, Clarity provides several ways to execute the export:

Export automatically after each single run

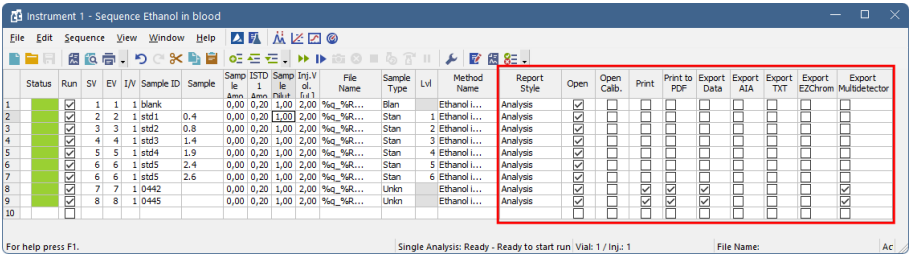
In the *Post-run Options* tab of the *Single Analysis* dialog, select *Export Data*.



Export for individual lines in a sequence

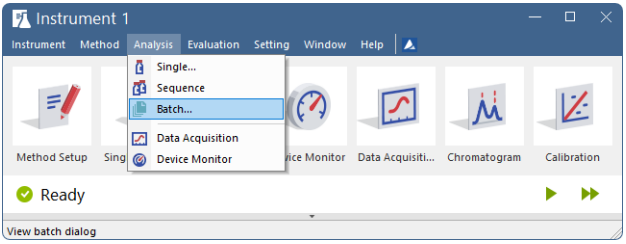
In the *Sequence* window, select checkbox in the *Export Data* column for row(s) to be exported. Note that the export is performed immediately after the run is finished, without any possibility of manual review of the results.

Columns defining export in the *Sequence table* are hidden by default; you can display them using the *Setup Columns...* command and use them to define the export format for each sequence line.

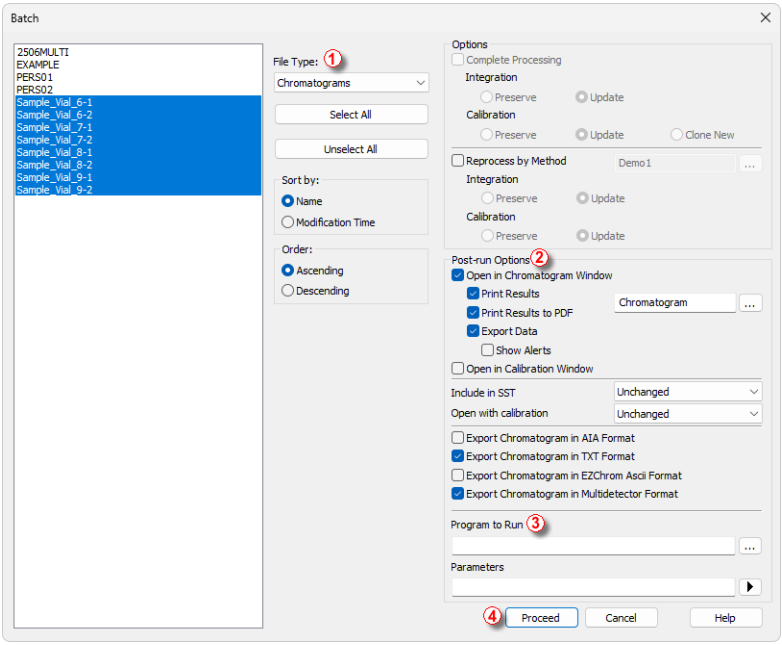


Export on demand for selected chromatograms

This can be done using the *Analysis - Batch* after the results have been reviewed.



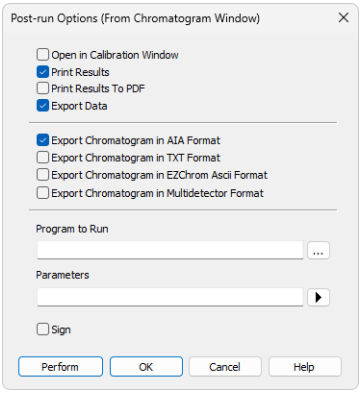
1. Select *File Type* ① and files to be exported from the list on the left.
2. Select what action to perform from *Post Run Options* ② .



3. The *Program to Run* ③ option can start an external application and pass the exported file name to it, allowing the **LIMS** to import the data automatically.
4. Click *Proceed* ④ .

Export directly from the Chromatogram window

This option lets you export data from the chromatogram you are currently reviewing by selecting *File - Perform Post-run Actions...*, which opens the *Post-run Options (From Chromatogram Window)* dialog and performs the export according to the defined settings.



If this action is used on a regular basis, it is convenient to add the command directly to the toolbar. A toolbar button executes the action immediately using the configured settings, without opening the dialog. If you need to modify these settings, you must access the command through the menu (*File - Perform Post-run Actions…*).

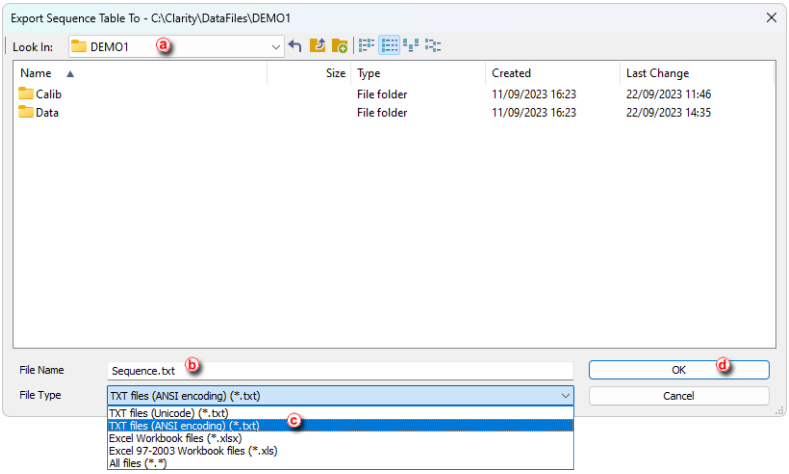
To add the command to a toolbar, right-click any toolbar and select *Customize...*. In the *Commands* tab, find the *Perform Post-run Actions...* command in the *File* category and drag it to the desired position.

The toolbar configuration is stored in the active .DSK file.

16.5 Exporting sequence

It is possible to export sequence to other more common formats. Supported formats are *Excel Table* (*.XLSX and *.XLS suffixes) or *Text format* (*.TXT).

1. Open the sequence you want to export, then use the *File - Export…* command to open the *Export Sequence Table To* dialog.
2. Select the appropriate folder for saving the exported sequence ⓐ .
3. Fill in the name under which the exported sequence will be saved ⓑ .
4. Choose the format in which you want to export ⓒ . For Text format, the *ANSI* or *Unicode* encoding are available.
5. Press the *OK* button to perform the export ⓓ .



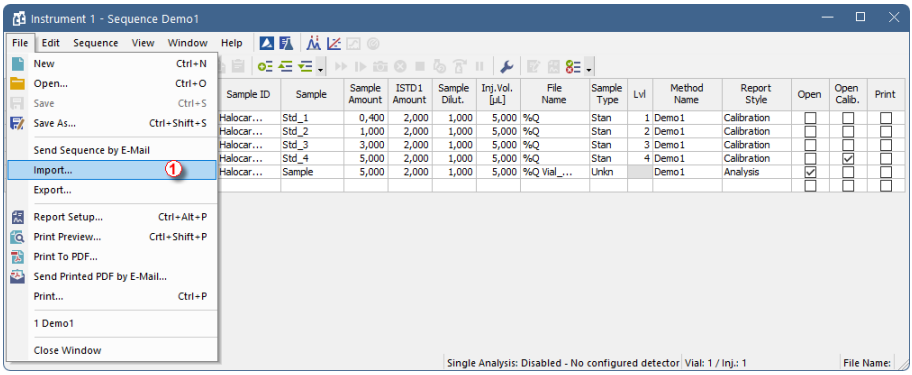
16.6 Importing sequence

It is possible to import sequence that has been stored in a text file. Such a file may be created manually or generated automatically by an external application or script, for example by a **LIMS**. Importing a sequence in this way allows Clarity to prepare the measurement workflow based on data received from other systems.

Clarity supports several file formats for this purpose, including *.txt, *.csv and *.prn. Values have to be in delimited format and separated by an arbitrary delimiter.

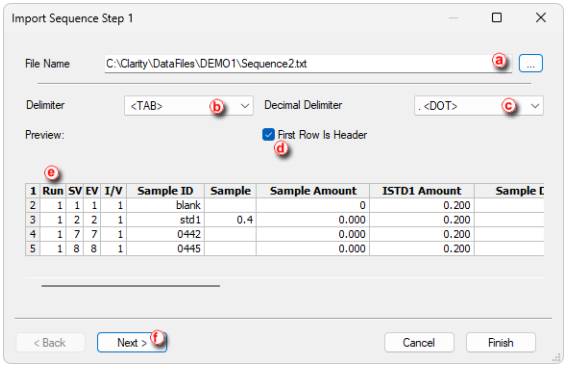
To create a sequence table from an imported file follow the steps below:

1. Open the *Sequence window* and select *File - Import…* ① . This opens the *Import Sequence Step 1* dialog, which opens in the directory defined in chapter "Setting up custom export and import directories".



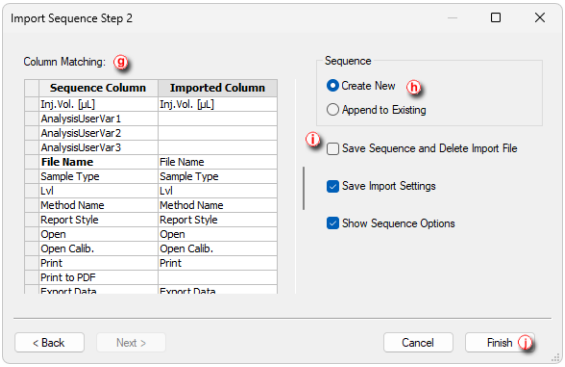
2. Select the file to be imported ⓐ .

3. Select the character used as delimiter ⓑ (possible options are <*TAB*>, <*SPACE*>, <*COMMA*> or <*SEMICOLON*>) and decimal delimiter ⓒ (possible options are <*Windows Locale*>, <*COMMA*>, <*DOT*> or <*SEMICOLON*>).
4. If the text file to be imported contains column headers in the first row, use *First Row Is Header* ⓓ checkbox. This row is used for matching in the *Import Sequence Step 2* dialog.
5. Preview of the first five rows of the imported sequence table is displayed in the bottom part of the dialog ⓔ .
6. Click *Next* to continue ⓕ .



7. Set the *Column Matching* ⓖ to match the imported columns with the ones present in Clarity *Sequence table*. *Start vial number* and *File Name* are required columns and are therefore shown in bold.

   If the imported file contains column headers (the *First Row is Header* option was selected in Step 1), Clarity will try to match the columns automatically based on their names. Any manual changes will overwrite this automatic matching. Clarity will remember the final matching for future imports.
8. Select whether you want to save imported sequence as a new file or just append it to currently opened one ⓗ .
9. You can also use three additional checkboxes ⓘ to adjust the import behaviour:
   - *Save Sequence and Delete Import File* - invokes *Save as* dialog to save the imported sequence and deletes the imported file.
   - *Save Import Settings* - stores current settings so they will be used automatically for future imports.
   - *Show Sequence Options* – opens the Sequence Options dialog immediately after the import finishes, allowing you to adjust additional parameters before the sequence is created.
10. Press the *Finish* button to complete the import and close the dialog Ⓙ .



Clarity also provides command-line parameters that can be used to automate the import process (full list of all available command-line parameters together with their detailed description can be found in *Reference Guide*):

seq_import

Imports the specified *.TXT file as a sequence and replaces the currently opened sequence. The command is ignored when a sequence is already running. The imported sequence is loaded under the default name *Noname*, therefore the *seq_save_as* command must be used to save it before starting a run.

- Example: Clarity.exe i=1 seq_import="C:\CLARITY\DataFiles\<PROJECT>\seq.txt"

seq_save_as

Saves the active sequence under the specified name. The command is ignored when the sequence is running.

- Example: Clarity.exe i=1 seq_save_as="C:\CLARITY\DataFiles\<PROJECT>\results.seq"

seq_import_append

Imports the specified file and appends its content to the currently open sequence. It uses the same settings as when the import is performed manually.

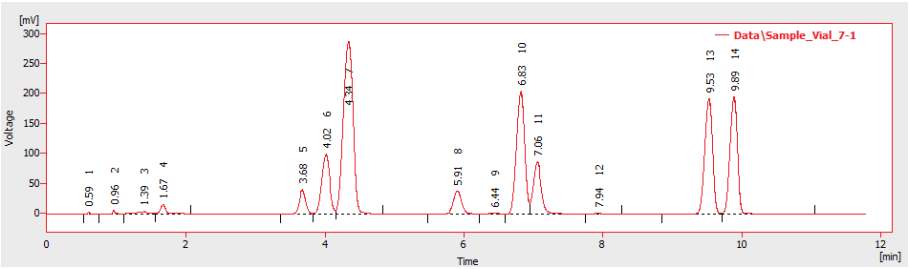
- Example: Clarity.exe i=1 seq_import_append="C:\CLARITY\DataFiles\<PROJECT>\seq.txt"

16.7 Exporting a chromatogram as a picture

You can export a chromatogram as a picture to the clipboard or as a file to a folder of your choice. The picture will include the labels and lines included in the chromatogram.

1. Open the *Chromatogram* window by selecting *Window - Chromatogram* from the *Instrument* window or click on .
2. Open the chromatogram you want to export.

3. Select *File - Export - Export as picture to clipboard* and paste the picture to MS Word, MS Powerpoint, Open Office Writer or any other suitable application of your choice.
   or
4. Select *File - Export - Export as picture to file...* and then select the folder where you would like to save the file in *Enhanced Metafile Format*.



17 Mathematical Operations

This functionality was implemented into Clarity to give users a tool to manipulate already measured data without modifying original raw data. Mathematical operations present a convenient way to perform various actions, such as extraction of a selected signal(s) from multiple signal chromatogram or subtraction of various chromatograms from each other. You can find three examples of *Mathematical Operation* in following chapters. Many other applications may be developed by Clarity users on their own.

For detailed overview of the *Mathematical Operation* dialog, please refer to the *Reference Guide*.

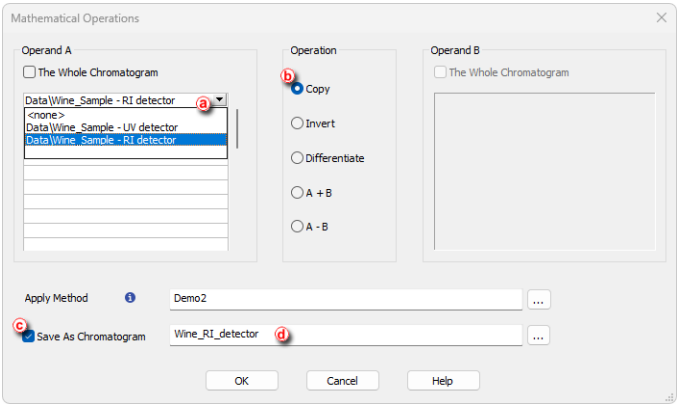
Note that modifications applied in the source chromatogram that change signal processing, such as *Subtraction Chromatogram* (set on *Measurement Conditions* tab) or integration processing options (for example *Spike Removal*, *Detector Delay* or filters), are disregarded by *Mathematical Operations*. *Mathematical Operations* use the chromatographic data processed by the method selected to apply to the resulting chromatogram.

Display adjustments such as *Scale* or *Offset* are taken into account in *Mathematical Operations*.

17.1 Extract chromatogram's signal using Mathematical Operations

You can save a particular signal from a chromatogram that contains several of them. This results in a stand-alone chromatogram file containing only the individual signal of choice, not all of the signals from the original chromatogram which might be confusing when working with a larger number of signals.

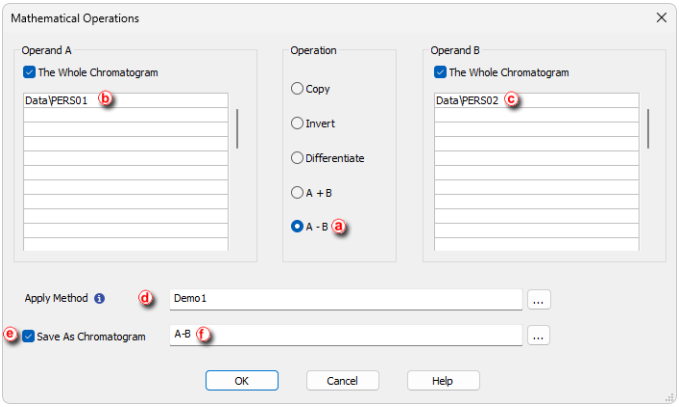
1. Open your a multi-signal chromatogram that you want to work with.
2. In *Chromatogram* window select *Chromatogram - Overlay - Mathematics* to open *Mathematical Operations* dialog.
3. From the drop-down menu ⓐ in the *Operand A* section select the desired signal of chromatogram you want to save separately. Select the *Copy* operation ⓑ , check *Save As Chromatogram* ⓒ , fill a name of the new chromatogram ⓓ and click *OK* to save the signal as standalone chromatogram.



17.2 Subtraction of various chromatograms using Mathematical Operations

If you would like to use one of your chromatograms as a baseline for another chromatogram(s) there is a way to subtract the desired chromatogram from any other chromatogram. It is possible to set *Subtraction Chromatogram* directly in *Chromatogram* window on *Measurement Conditions* tab, however, if you want to have both original and subtracted chromatograms as individual files you can use *Mathematical Operations*.

1. Open your chromatograms that you want to work with in *Overlay*.
2. In *Chromatogram* window select *Chromatogram - Overlay - Mathematics* to open *Mathematical Operations* dialog.
3. Select operation *A - B* ⓐ . From the drop-down menu in the *Operand A* section, select the chromatogram you want to subtract from ⓑ .
4. From the drop-down menu in the *Operand B* section, select the chromatogram you want to subtract ⓒ .
5. Optionally select a method ⓓ to be applied to the newly created chromatogram. If the selected method defines a *Subtraction Chromatogram* or any other *Integration settings*, these **are** applied to the result of the mathematical operation.
6. Check span *Save As Chromatogram* ⓔ , fill a name ⓕ and click *OK* to save the new subtracted chromatogram.



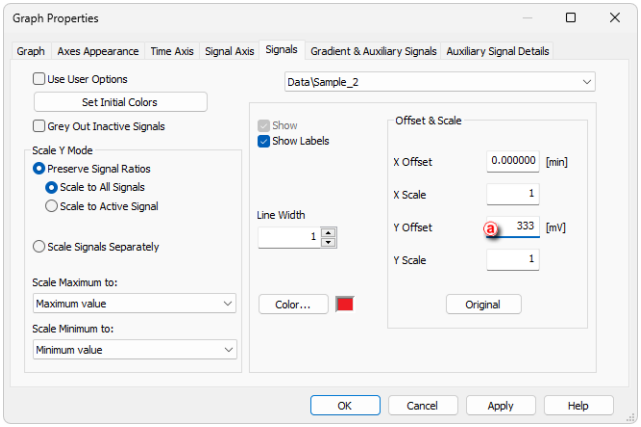
17.3 Saving modified chromatogram using Mathematical Operations

In Clarity, setting an offset in *Graph Properties* only changes how the chromatogram is displayed in the *Chromatogram window*. It does not affect the chromatographic data itself. This display setting is saved in the desktop file (*.dsk), so it can differ for each user.

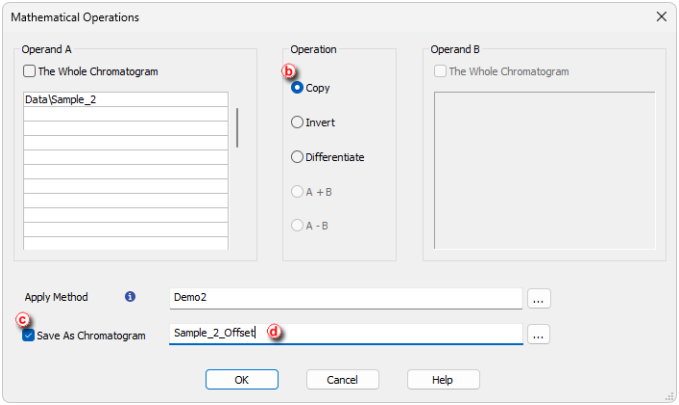
Because of this, a simple *Save As* will not include the offset (or other display settings), since they are not part of the chromatogram itself.

If you want to create a new chromatogram with the offset/scale modification applied to the chromatographic data, you can use *Mathematical Operations – Copy*. This saves the chromatogram with the change included.

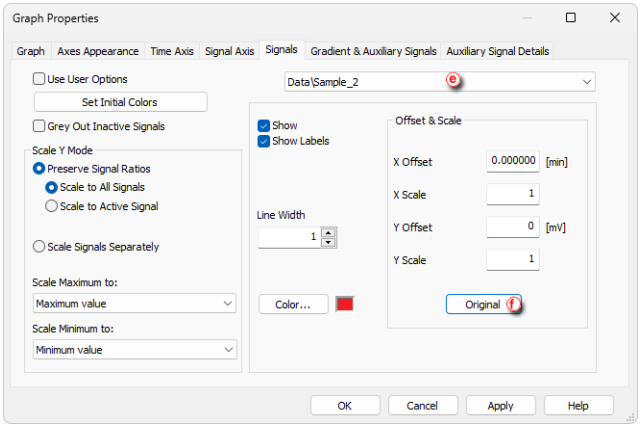
1. Open the chromatogram you want to edit.
2. In *Chromatogram* window, click *Display - Properties* to open *Graph Properties* and go to *Signals* tab.
3. In the *Y Offset* field ⓐ , enter the desired offset in mV (in this example 333 mV), then click *OK* button.



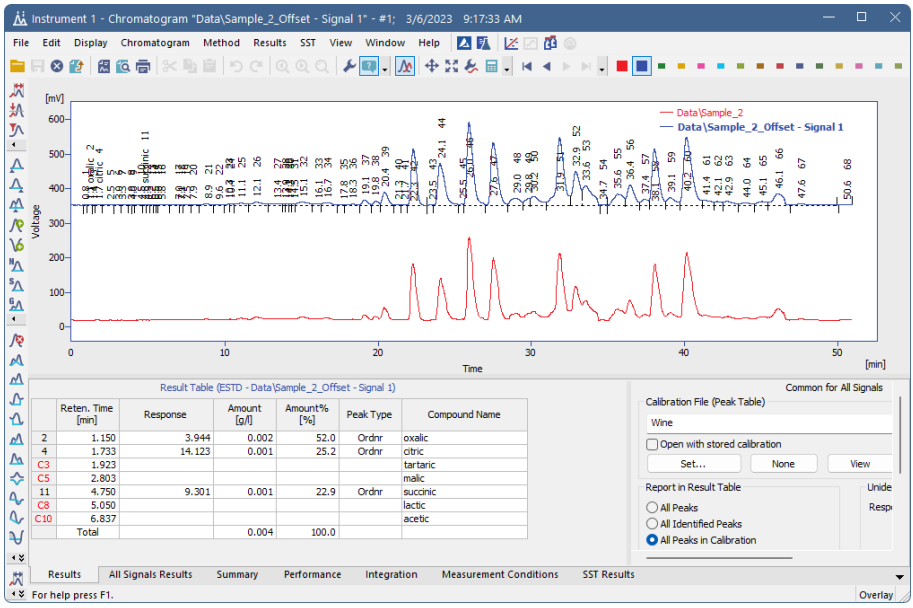
4. Select *Chromatogram - Overlay - Mathematics...* and the *Mathematical Operations* window will open.
5. Select *Copy* option ⓑ. Check *Save as Chromatogram* ⓒ, name the new chromatogram ⓓ and click the *OK* button.



6. Both chromatograms will now be displayed in the overlay mode, overlapping each other.
7. To restore the original chromatogram, open *Graph Properties - Signals* tab as in step 2.
8. Select the original chromatogram ⓔ, click *Original* button ⓕ and close the dialog by clicking *OK*.



9. The original and the modified chromatogram will then be displayed together in overlay mode.



18 Archive and Restore

Clarity allows you to archive your PROJECTS (methods, sequences, measured chromatograms) and also the COMMON folder in which the print styles are stored.

18.1 Archiving a project (Creating an Archive)

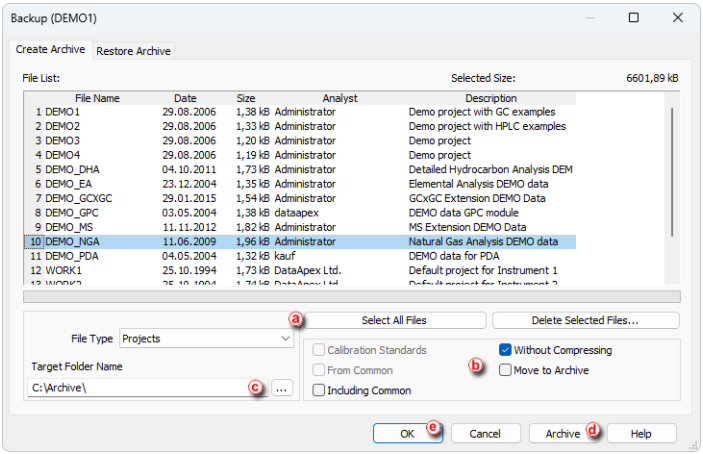
It is strongly recommended to archive the whole project folder after being shelved, but it is also possible to archive specific files only. An archive can be made by simply copying the files or by compressing them into one file (*.DGZ format).

1. Open the *Backup* dialog by selecting *Instrument- Archive...* on the *Instrument* window.
2. Select *Projects* in the *File Type* ⓐ option to archive a complete project directory.
3. Select the project or projects you wish to back up from the list. The *Select All Files* button ⓐ will select all projects.
4. Choose from the following options ⓑ :
   - Uncheck the *Without Compressing* option to archive all files into one compressed file.
   - Check the *Move to Archive* option to have the original files erased after backing them up.
   - Check the *Including Common* option to also back up the COMMON subdirectory.
5. Choose the output directory and name for the archive ⓒ . Compressed files will have the .DGZ extension.

   Caution: If you archive data in compressed format with a previously used name, you can possibly override the former archive and loose all data.

6. Click the *Archive* button ⓓ to back up the project or the *OK* button ⓔ , if you do not need to back up any more files.

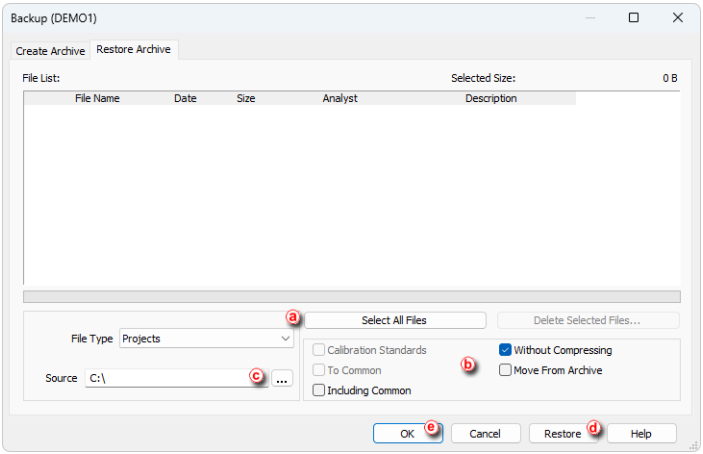
Note: Clicking *OK* will archive current selection.



18.2 Restoring a project from an archive

1. Open the *Backup* dialog by selecting *Instrument - Restore...* in the *Instrument* window.
2. Choose the source directory and select the source file ⓒ . Compressed files will have the .DGZ extension.
3. Select *Projects* in the File Type ⓐ option to restore a complete project directory.
4. Choose from the following options ⓑ :
   - Uncheck the *Without Compressing* option to restore all files from a compressed format.
   - Check the *Move from Archive* option to have the archived files erased after restoring them.
   - Check the *Including Common* option to also restore the COMMON subdirectory.
5. Select the project or projects you wish to restore from the list. The *Select All Files* button ⓐ will select all projects.
6. Click the *Restore button* ⓓ to restore the project or the ***OK*** button ⓔ if you do not need to restore any more files.

Note: Clicking *OK* will restore current selection.

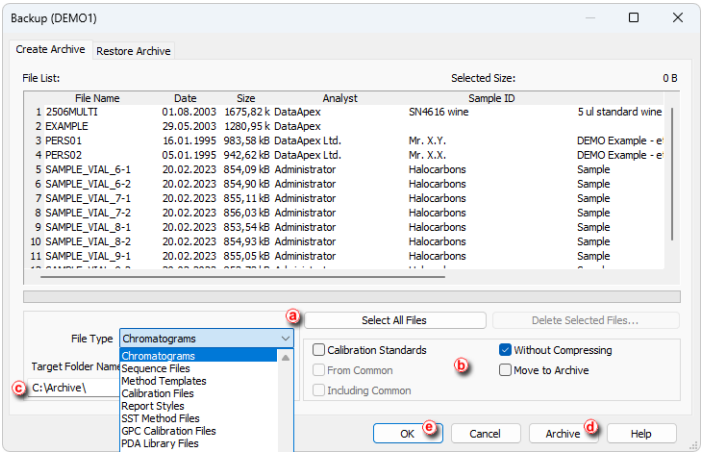


18.3 Archiving specific files (Creating an Archive)

It is strongly recommended to archive the whole project folder after being shelved but it is also possible to archive specific files only. An archive can be made by simply copying the files or by compressing them into one file (*.DGZ format).

1. Open the *Backup* dialog by choosing *Instrument - Archive...* in the *Instrument* window.
2. Select the *File Type* ⓐ option according to the files you wish to archive.
3. Select the files you wish to back up from the list. The *Select All Files* button ⓐ will select them all.
4. Choose from the following options ⓑ :
    - Uncheck the *Without Compressing* option to archive all files into one compressed file.
    - Check the *Move to Archive* option to have the original files erased after backing them up.
    - Check the *Calibration Standards* option when archiving chromatograms. The chromatogram files from the CALIB subdirectory (instead of the DATA subdirectory) should be listed.
    - Check the *From Common* option to display the system files from the COMMON directory.
5. Choose the output directory and name for the archive ⓒ . Compressed files will have the .DGZ extension.
6. Click the *Archive* button ⓓ to back up the file or the *OK* button ⓔ if you do not need to back up any more files.

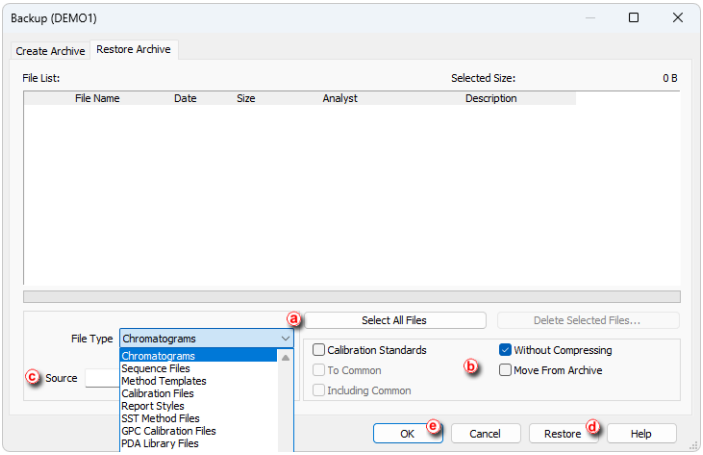
Note: Clicking *OK* will archive current selection.



18.4 Restoring a file from an archive

1. Open the *Backup* dialog by choosing *Instrument - Restore...* on the *Instrument* window.
2. Choose the source directory and select the source file ⓒ .
3. Select the *File Type* ⓐ option according to the files you wish to restore.
4. Choose from the following options ⓑ **:**
   - Uncheck the *Without Compressing* option to restore files from a compressed format.
   - Check the *Move from Archive* option to have the archive files erased after restoring them.
   - Check the *Calibration Standards* option when restoring chromatograms to the CALIB subdirectory (instead of the DATA subdirectory).
5. Select the files you wish to restore from the list. The *Select All Files* button ⓐ will select them all.
6. Click the *Restore* button ⓓ to restore the files or the *OK* button ⓔ if you do not need to restore any more files.

Note: Clicking *OK* will restore current selection.


Backup (DEMO1)
Create Archive
Restore Archive
File List:
Selected Size:
0 B
File Name
Date
Size
Analyst
Description
a
Select All Files
Delete Selected Files...
File Type
Chromatograms
Chromatograms
Sequence Files
Method Templates
Calibration Files
Report Styles
SST Method Files
GPC Calibration Files
PDA Library Files
c
Source
Calibration Standards
To Common
Including Common
b
Without Compressing
Move From Archive
OK
e
Cancel
Restore
d
Help

19 Managing the Chromatography Station

Following chapters contains extended information how to set restrict access to various parts of Clarity to certain users or set up communication with a mobile application.

19.1 Enabling instruments to be used by Clarity2Go application

Clarity enables to send specific parameters over the internet to be monitored via **Clarity2Go** application. In this way you can monitor your analyses while outside the laboratory. Note that both PC with Clarity and smartphone must be connected to internet. For more information regarding Clarity2Go installation refer to www.dataapex.com/product/clarity2go.

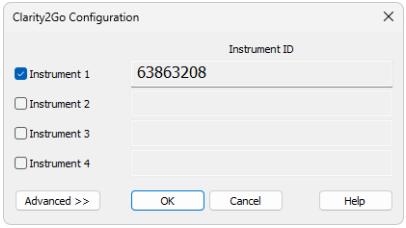
The whole solution consists of three independent parts:

- **Clarity** station (at your side) - sends information about state and running analyses to the server.
- **Server** (at **DataApex's** side) - dispatches the information from **Clarity** stations to **Clarity2Go** clients.
- **Client** (at your side) - device (smartphone or tablet) with installed **Clarity2Go** application processes information from the server.

DataApex is providing a free public server for this use.

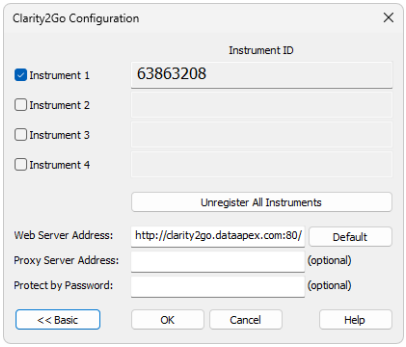
How to set up Clarity:

1. In the *Clarity* main window, go to *System* menu and click on the command *Clarity2Go...*.
2. In the opened *Clarity2Go Configuration* dialog, check the checkbox of *Instrument* 1 to 4, depending on the instruments you want to monitor. Every checked Instrument will get its unique *Instrument ID*.
3. Click the *OK* button to save the configuration and continue with steps described in **How to set up Clarity2Go** section or refer to *Advanced* options bellow.



Options described below are optional and are not obligatory for correct functionality. They are revealed by clicking the *Advanced* button.

- *Unregister All Instruments* - disables the monitoring in the **Clarity2Go** application. Instruments that have been registered will no longer be available for monitoring. If you will later change your mind, you will have to generate new *Instrument ID*.
- *Web Server Address* - do **not** change this field. It defines the address of **Clarity2Go** web server. Address other than default will result in the monitoring to be not functional! Press the *Default* button to set functional web address of the server.
- *Proxy Server Address* - consult with your local administrator if a proxy server is applied in your local network and then provide the proxy server address.
- *Protect by Password* - provided password will be valid for **all** Instruments. The same password needs to be provided in the **Clarity2Go** application to unlock the monitoring.
- Click the *OK* button to save the configuration and continue with steps described in **How to set up Clarity2Go**.



How to set up Clarity2Go:

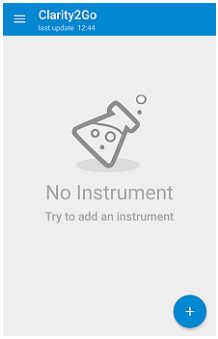
Once you have configured instrument(s) in **Clarity**, it's time to monitor those instruments using **Clarity2Go** application. This part assumes that you have **Clarity2Go** for Android application installed and running.

1. Make sure that you are not in the **Clarity Demo** mode, indicated by a gray stripe at the bottom of the application with the inscription **DEMO mode**. Tap on the *TURN OFF DEMO*.

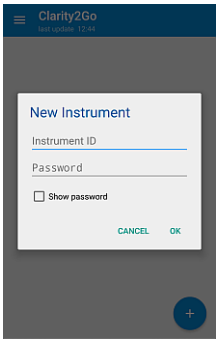
   Note: **Clarity Demo** mode does not allow to add instruments.

2. In the *Settings*, tap on *Demo - Switch to demo mode* which turns the **Clarity Demo** mode *OFF*.
3. Return back. In case you are configuring **Clarity2Go** for the first time, you will see that there is no instrument.



4. Tap on the blue "plus" button at the bottom right corner to add a new instrument.
5. Enter *Instrument ID* that has been generated by **Clarity** and enter password (only if you have set it up in **Clarity**). Tap on the *OK* button to start monitoring this instrument.



6. The newly configured instrument will be added to the list of instruments that are being monitored.

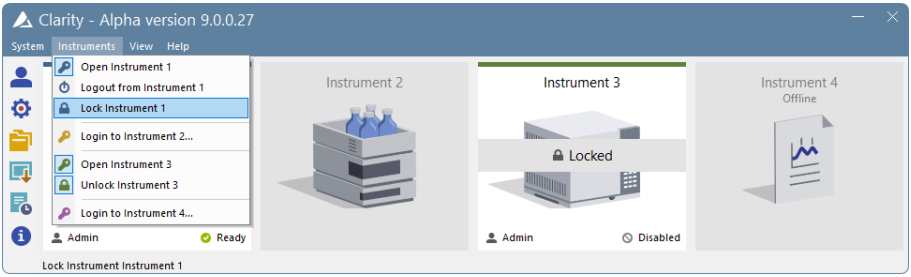
Note: You can invoke the application menu by tapping on the 3 horizontal lines - the menu contains *Settings*, built-in *Help* and *About* options.

19.2 Locking/Auto Locking a Clarity Instrument

You may lock a Clarity Instrument protected by password if you want to prevent unauthorized access to it, for example, when an analysis is running.

Manual Lock

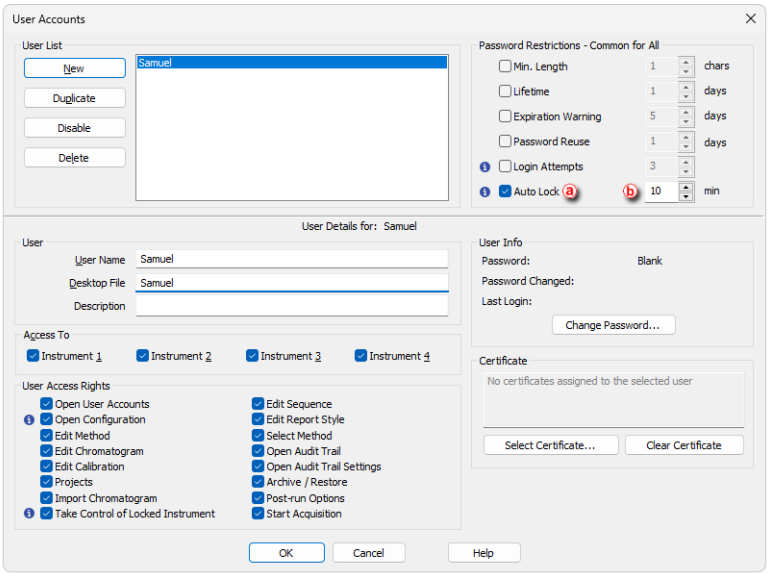
- Instrument can be manually locked either from *Instrument* window by clicking *Instrument - Lock Instrument_Name*.
  or
- From the *Main Station* window by clicking *Instruments - Lock Instrument_Name*.



Auto Lock

It is possible to set the automatic lock function so that all opened instruments will be locked after a period of inactivity.

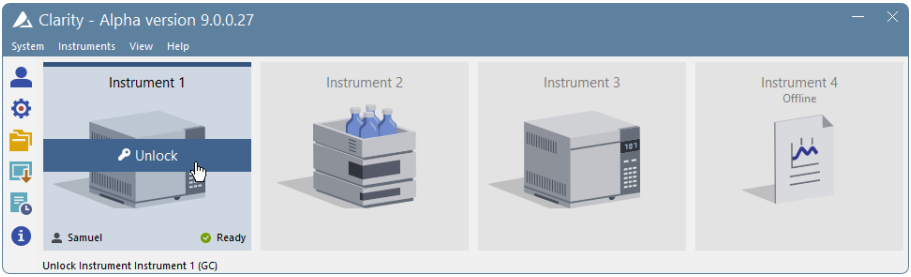
1. Open the *User Accounts* window by clicking on or choose *System - User Accounts*.
2. Check the *Auto Lock* function ⓐ .
3. Set the period of inactivity in minutes after which all opened *Instruments* will be locked ⓑ .



Caution: When an Instrument is Auto Locked, all unsaved changes in modal dialogs (Method Setup, Single Analysis, Report Setup, etc) are discarded and those dialogs are closed.

19.3 Unlocking a Clarity Instrument

1. Select *Instruments - Unlock Instrument 1* from the *Main Clarity* window or click on the *Instrument* image.
2. Enter the password and click OK.

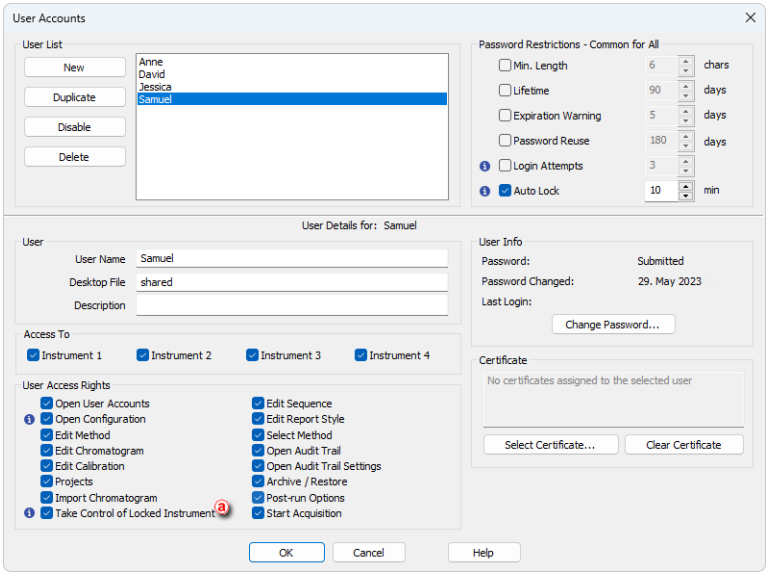


19.4 Taking control of Clarity Instrument

You may take control of an Instrument where a different user is already logged in. To be able to achieve this, the option *Take Control of Locked Instrument* has to be enabled in the *User Accounts* settings for the user who wants to take over.

Setting up the User Right

1. Open the *User Accounts* window by clicking on or choosing *System - User Accounts*.
2. Check the *Take Control of Locked Instrument* in the *User Access Rights* ⓐ part of the dialog for users who should be able to do so.

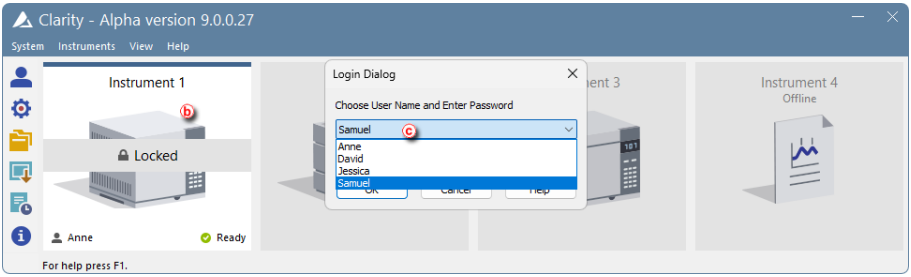


Note: It is recommended to set one common *Desktop File* for all users with this option enabled. Otherwise the desktop of the first logged user will be used for all users that take control over the Instrument, until the Instrument is closed again. It is also recommended to set the same *Edit...* rights for users that plan to take over Instruments (other rights might differ between the users).

Taking Control of Locked Instrument

The steps are similar to the standard logging to instrument.

1. Select *Instruments - Unlock Instrument 1* from the *Main Clarity* window or click on the *Instrument* image ⓑ .
2. Choose your User Name ⓒ .
3. Enter the password and click OK.



Caution: All unsaved changes in files made by the previous user will be discarded.

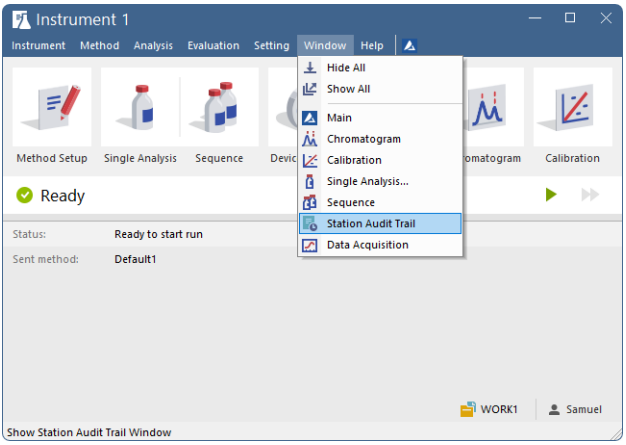
Note: It is possible to take control of a locked Instrument using the Command line parameters. The user *(user=…)* and password *(p=…)* parameters must be included for each command. Althought commands can be run on the locked Instrument this way, the Instrument remains locked.

19.5 Monitoring Events and Operations in Clarity

The ***Audit Trail*** can be used for finding out who did what and when, including file operations, changes to settings, events that take place during data acquisition and system messages. Therefore this is an essential tool for troubleshooting and managing Clarity.

To access the ***Station Audit Trail***:

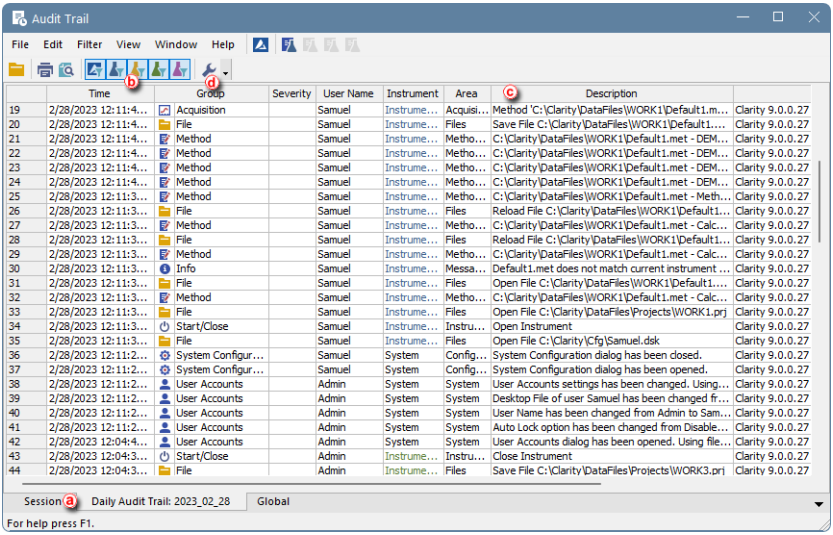
1. Select *Window - Station Audit Trail* from the *Instrument, Chromatogram, Calibration, Sequence* or *Data Acquisition* windows. Alternatively click icon in the *Main Station* window.



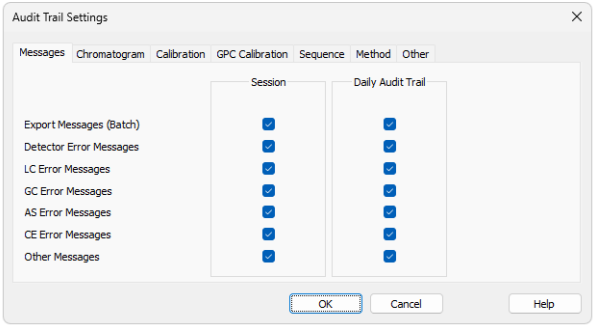
2. Click on the *Session* tab ⓐ if you would like to see the log from the time Clarity was started or on the *Daily Audit Trial* tab for the present day events.

   Note: The *Daily Station Audit Trail* is stored in one separate file every day the station is running. These files can be opened by using the command *File - Open Audit Trail (Append)*.

3. Click on the *Instruments* or *System* icons ⓑ to filter out events and operations based on instrument where they occurred.
4. Inspect the *Description* column to find out about operations and events that have taken place ⓒ .



5. Click on the *Properties* icon ⓓ to set up which events and operations should be recorded in the *Session* or *Daily Audit Trail*.



To access the file-specific *Local Audit Trail* (Chromatogram, Calibration, Sequence and Method):

1. Select *Window - Chromatogram, Calibration or Sequence Audit Trail* from the corresponding window or click on the *Audit Trail* icon in the *Method Setup* window to open corresponding *Audit Trail*.

Note: The *Local Audit Trails* are included in the *Chromatogram, Calibration, Sequence* and *Method* files and contain the whole file history.

19.6 Controlling Clarity from an external application

It is possible to send commands to **Clarity** using Windows command line parameters and also to read its status through Windows Dynamic Data Exchange (DDE).

- For more information on the commands go to our List of commands in the **Clarity Reference Guide**.
- You can also find the list of variables which will give you information on Clarity status on our DDE datasheet.

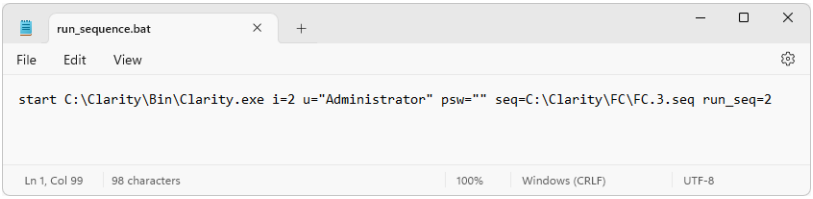
19.7 Starting a sequence from Clarity at a defined time

It is possible to schedule a task that will run **Clarity** with defined parameters to start a sequence measurement automatically. To achieve this, proceed as follows:

1. Prepare a batch script file (e.g., RUN-SEQUENCE.BAT) to perform the required tasks via command line parameters

   The batch file should contain the following line (example):

   start C:\Clarity\Bin\Clarity.exe i=2 u="Administrator" psw="" seq=C:\Clarity\FC\FC.3.seq run_seq=2



   Explanation:

   - *start C:\...\Bin\Clarity.exe* will start Clarity from the specified root directory
   - *i=2* will open the desired instrument (2)
   - *u="Administrator" psw=""* will log in the specified user using the password provided (necessary even if the password is empty)
   - *seq=C:\...\SequenceName.seq* specifies the sequence to be run
   - *run_seq=2* starts the sequence on the desired instrument (2)

2. Prepare the sequence to be run

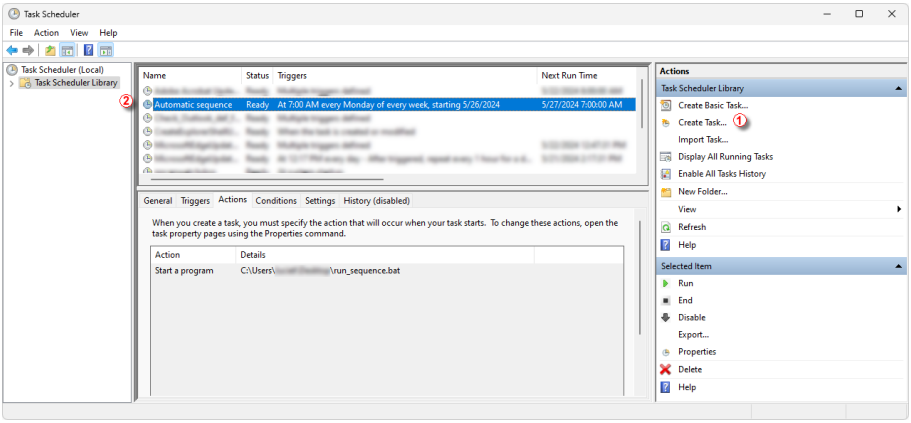
   Set the sequence as necessary for your analysis. The sequence can contain just one row with a start-up method, or additional rows with standards/samples for measurement. The start-up method should prepare the devices for measurements, e.g., switch on the detector lamps, flush the systems as required for equilibration, etc.

3. Use the *Task Scheduler* to schedule starting of the batch script (Windows 11)

   To schedule running the RUN-SEQUENCE.BAT at a specific time and date, use the Windows app *Task Scheduler*. After creating a new task (*Actions* section - *Create Task...* ①), apply the following settings in the *Create Task* dialog:

- tab *General*: set the name of the action (e.g., Automatic sequence), choose the *Run only when user is logged on* option (and do not log yourself off when leaving the PC).
- tab *Triggers* - *New...*: set the date and time of running the script, eventually use further advanced settings to fine-tune the task scheduling (e.g., repeating).
- tab *Actions* - *New...*: choose the *Start a program* option a browse to select the prepared batch script.

The created task is now present in the *Task Scheduler Library* ② . If Windows Updates are available, remember to install them manually (automatic OS updates might log you out due to PC restart - this would prevent the task to be started by the *Task Scheduler*).



20 Clarity in specific scenarios

In this chapter, there are SOPs, that helps you set up Clarity in not-so-usual scenarios, outside of chromatographic laboratory.

20.1 Clarity in the classroom

This section focuses on configuring Clarity to simplify its use in classrooms and students' laboratories, particularly for teaching scientific principles and lab workflows. It explains key settings, like students' account management and evaluating the data on another PC than it was measured on (e.g., in the classroom). In addition there is also tip, how to make your lesson for bigger groups more engaging with some hands-on experience, e.g., to use instrument simulation modes to simulate real measurement.

20.1.1 Creating User Accounts

In *User Accounts* dialog, set up one or more teacher account(s), with complete privileges, and one or more student accounts with limited privileges. Recommended limitation of privileges is access to *User Accounts* and *System Configuration* - so the students can't change privileges of any account, and change configuration of connected devices. Any other limitations depends on what students should perform in your specific use case, e.g., restricting *Edit Method* when student should just use already existing method and not develop new one.

More detailed info on how to set the user accounts can be found in Create New User Account and Restricting Access topics.

20.1.2 Setting the directories

If you want save the files on shared disk to enable access from another computer in the same network, e.g., from the classroom or office. You can set the directories accordingly in the *Instrument Directories for Projects* dialog accessible from main Clarity window.

More detailed info on how to set the directories can be found in Working with Directories topic.

20.1.3 Transferring the projects

It also may be needed to transfer existing project to different disc where you set directories in previous step. To do that, you can simply copy/move whole project (including *.prj file) in File Explorer, or use *Archive/Restore* feature.

More detailed info on how to transfer the project to another disc can be found in *Migrating Projects* topic.

20.1.4 Backing up important files

It is recommended to back up important files, so in the case that any unexpected issue occurs (e.g., someone accidentally power off the computer while Clarity is still

running), and important files are corrupted or deleted, it is simple to get the settings back as it was before.

List of recommended files for back up:

- Clarity.cfg + any other configuration file present in Cfg directory.
- Clarity.dsk + any other desktop file present in Cfg directory.
- Clarity.psw in Cfg directory.
- optional: method(s) validated and used for measurement

20.1.5 Bonus Tip: Simulated Measurement

To showcase Clarity workflow, and simulate laboratory process for larger group of students without need of physical connection to laboratory instruments, you can use Clarity Demo version, accessible from our website www.dataapex.com. In the Demo version, there is simulated connection to any available device you configure on the *Instrument*, so the students can get familiar with Clarity and the work they will do in the laboratories.

20.2 LC Gradient Test – Procedure and Evaluation

The LC gradient test is used to verify correct solvent mixing and proper operation of the LC pump.

It does not generate typical chromatographic peaks or compound separation. However, the acquired signal can be evaluated in Clarity using standard chromatogram processing and comparison tools. This evaluation provides a direct measure of gradient accuracy and overall pump performance.

During the test, the solvent ratios programmed in the method are compared with the actual solvent composition delivered by the system. The actual solvent composition is calculated from the detector response and evaluated against a reference measurement. This reference measurement is performed at the same flow rate using a single solvent containing a low concentration of a marker compound that increases the detector response. This reference enables quantitative assessment of gradient accuracy.

In low-pressure gradient systems, the test mainly checks the correct function of the proportional mixing valve and its ability to combine solvent channels in the specified ratios. In high-pressure gradient systems, the test focuses on the accuracy and synchronization of individual pump channels delivering the mobile phases. In both cases, the results also reflect the performance of the mixing chamber and other components responsible for solvent homogenization.

20.2.1 Integration Events Setup

Integration events and commands are described in detail in the Clarity *Chromatogram* section of the Reference Guide.

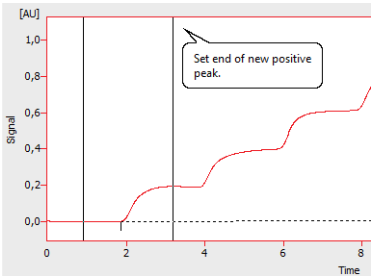
1. Open the measured chromatogram that contains the gradient test record. The signal does not have the shape of a classical chromatogram with peaks; instead it shows step-like changes corresponding to the programmed solvent

composition.

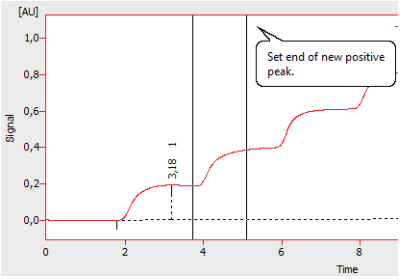
2. Switch to the *Integration* tab in the *Chromatogram* window.
3. Increase the *Global Threshold* value, if necessary, so that the entire gradient test record is integrated as a single peak (see the *Integration Table* example below).

> *Note:* It is recommended to use the *Legacy* integration algorithm in this case, but if you want to use *Wave*, don't forget to also set the *Global baseline slope* to a higher value so that the entire test is treated as a single peak.

4. Use *Chromatogram - Baseline – Together* and use the vertical lines to roughly select the entire measured chromatogram.
5. Use the *Chromatogram - Add Positive* command (or use the corresponding icon in the left-hand panel of the *Chromatogram* window).
6. Click before the start of the gradient test signal, where only the baseline is present, and then click approximately in the middle of the plateau where the signal is constant.



7. Select *Add Positive* again. With the first click, mark the position on the previously selected constant section just before the signal increases to the next solvent ratio. With the second click, mark approximately the middle of the next step (plateau), corresponding to the next gradient ratio.



8. Repeat the previous step (7) for all remaining gradient levels. At the end, the number of *Add Positive* events should match the number of gradient levels in the recorded signal.
9. Mark the second half of the last gradient level as a *Solvent Peak* (the information about its height has already been obtained from the previous peak).

In the left-hand panel of the *Chromatogram* window, select ***Solvent Peak*** and apply it to this section. The Integration Table should match the example shown bellow.

	Chromatogram Operation	Time A [min]	Time B [min]	Value
	Global Peak Width			0,100 min
	Global Threshold			10,0000 mAU
	Global Filter - Bunching			1
	Baseline - Together	0,008	14,868	
	Peak - Add positive	0,930	3,180	
	Peak - Add positive	3,694	5,173	
	Peak - Add positive	5,629	7,252	
	Peak - Add positive	7,632	9,230	
	Peak - Add positive	9,636	11,242	
	Peak - Solvent	11,794	0,141	

Fig. 16: The resulting Integration Table and highlighted Treshhold value

10. Go to the *Results* tab and verify that the *Result Table* contains same number of rows as the number of gradient levels in the chromatogram (mixing ratios defined in the method).

20.2.2 Calibration Setup

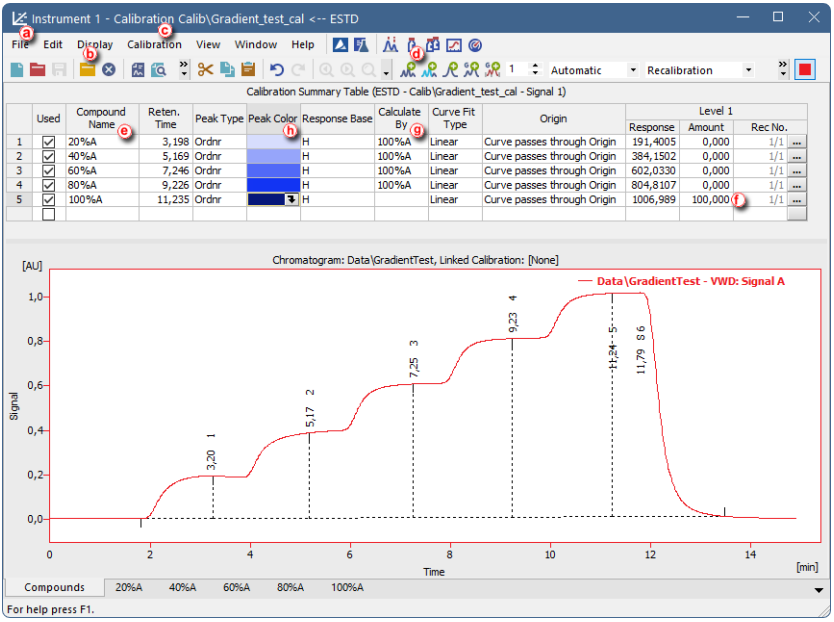


Fig. 17: The figure illustrates the individual steps described in the procedure below.

1. Open the *Calibration* window, select *File – New* ⓐ to create a new calibration.
2. Click *Open Standard…* ⓑ and select the integrated chromatogram from the previous section.

3. Open calibration settings: using the *Calibration - Options...* menu. Compared to the default settings, adjust the following parameters (see the figure below):
    1. Change *Compound Units* from mg to %.
    2. Set *Response Base* to *Height*.

    Note: If you want to use the calibration repeatedly and as a template for future gradient tests, also set *Mode* to *Recalibrate* and *Recalibration* to *Replace*.

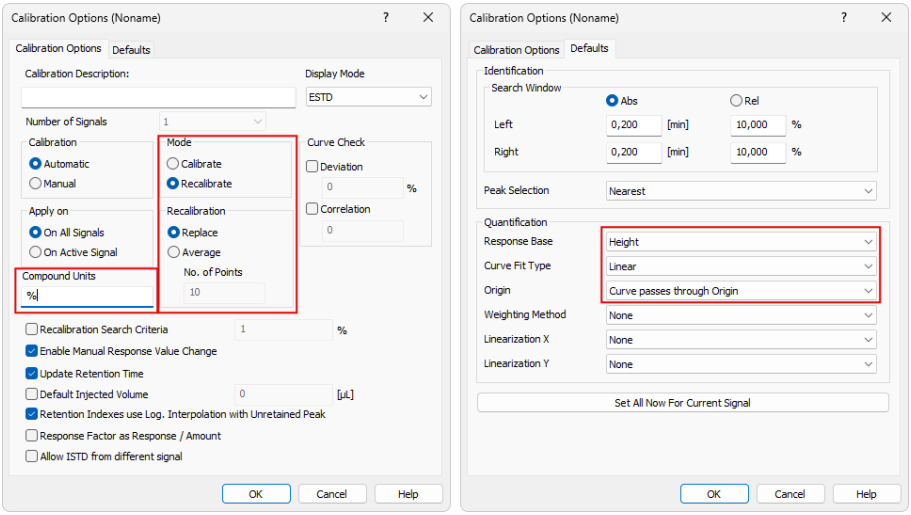


Fig. 18: Correct calibration settings

4. In the upper part of the *Calibration* window, select ***Add All*** ⓓ . The *Calibration* table will be populated with compounds, including the last solvent peak, which is not required. Right-click this compound and select *Delete Compound*. Again, the number of compounds should match the number of gradient levels.
5. Change the compound names so that they describe the defined solvent mixing ratios ⓔ .
6. In the *Amount* column, assign the value 100 ⓕ to the last compound (highest gradient level), which corresponds to 100% of a single solvent without mixing.
7. Display the *Calculate By* column in the *Calibration* table and select the appropriate option for each mixing ratio.
    1. Right-click the table header and select *Setup Columns…*.
    2. In the *Hidden Columns* list, select *Calculate By* and click *Show*.
    3. Close the dialog by clicking *OK*.
    4. In the *Calculate By* column, for all compounds/mixing ratios except the last one (100%), select the last compound/mixing ratio 100% ⓖ .
8. If desired, you can highlight the individual gradient levels using different color shades in the *Peak Color* column ⓗ .

9. Save the calibration. The resulting calibration should match the example shown in the figure above.

20.2.3 Results Evaluation

1. Return to the *Chromatogram* window and assign this calibration to the measured gradient test chromatogram. On the *Results* tab, click *Set...* ① next to *Calibration File - [None]* and select the calibration created in the previous section and click *Open*.
2. Adjust the columns displayed in the *Result Table* so that the relevant information is visible, for example as shown in the following figure. The *Amount* column is the most important for evaluating the gradient test. The resulting chromatogram and *Result Table* should appear as shown below. The *Amount* value for the last gradient level should be exactly 100 % ② .

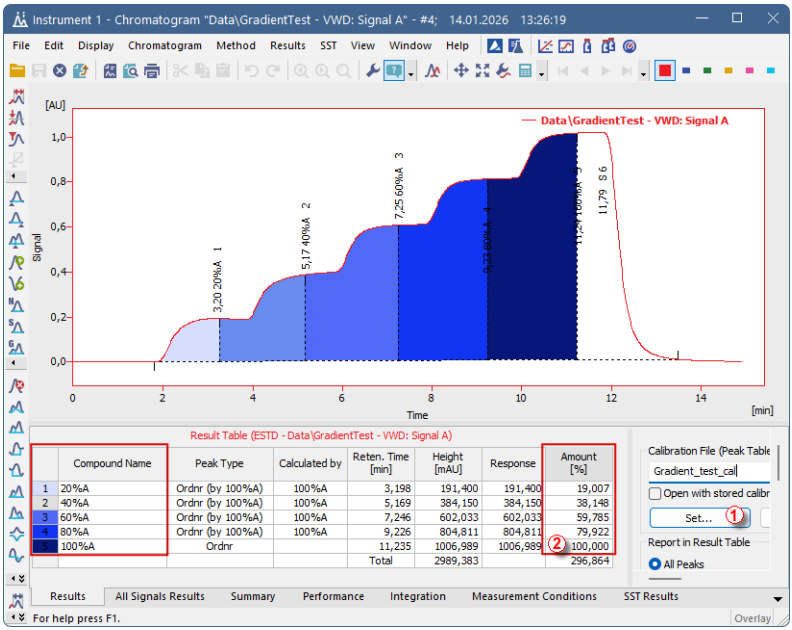


Fig. 19: Resulting evaluated Gradient Test

Note: The result of the gradient test is the difference between the calculated percentages in the *Amount [%]* column and the values defined in the method controlling the gradient pump.

20.2.4 Processing Subsequent Measurements

1. Open the chromatogram with gradient test record you want to finish and use *Method - Copy from Chromatogram* and choose the chromatogram which has already been finished.

2. On the *Results* tab, click *View* to open the calibration.
3. Go to *File* in the menu and select *Save As...*, then save the calibration under a new name and make sure that *Recalibrate* and *Replace* options are set.
4. In the opened *Calibration* window, click *Add Existing* at the top of the window and save the calibration.
5. Return to the *Chromatogram* window and assign this newly created calibration to the chromatogram by clicking *Set* and selecting the calibration. The *Amount* value for the last gradient level should be exactly 100 %.
6. Save the chromatogram.
7. To process and evaluate additional gradient test chromatograms, repeat the procedure starting from step two of this chapter for each chromatogram.

21 Utilities

Clarity installation contains various utilities for validating the installation or predefining various Clarity profiles which helps you in using more configurations of laboratory instruments.

21.1 Checking that the software has been installed correctly (Installation Qualification - IQ)

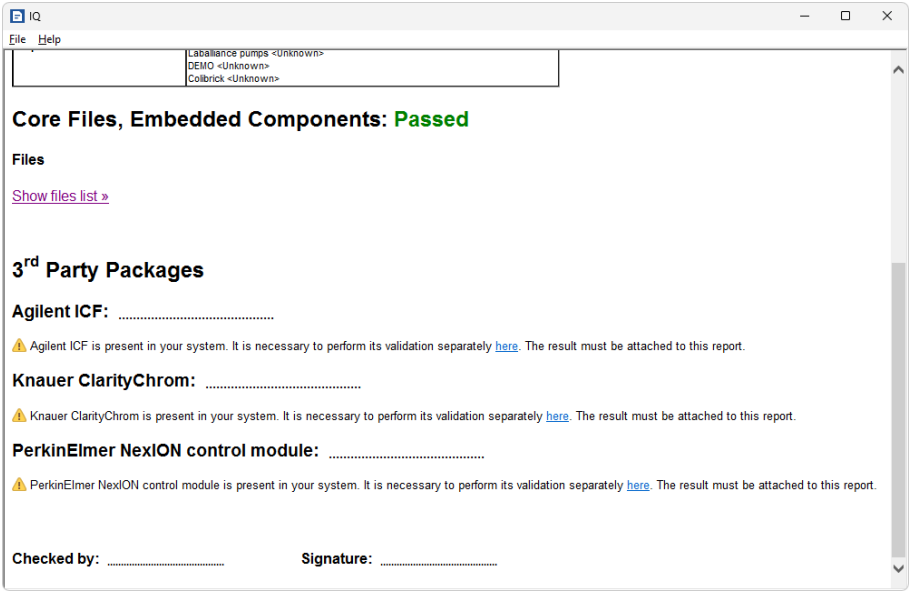
The *Installation Qualification* (**IQ**) is a procedure confirming that the software has been installed successfully and that correct versions of files are present.

1. Install the Clarity station according to the instructions of the *Installation Wizard*.
2. After the installation has been completed, you can open *IQ* by searching for  *IQ Report* in the search field of the Start menu. Alternatively you can start *IQ* by using C:\CLARITY\BIN\IQ.EXE.
3. If the installation has been correctly performed, the status should read: "*Installation Qualification Test: Passed*".
4. If the Installation Qualification fails, it is recommended to uninstall and then re-install Clarity. If it fails again, contact DataApex support.

   Note: You can use *Show files list* to display list of all validated files and search for the ones that are causing issues.

5. The *Installation Qualification* report can then be printed, copied to the Windows Clipboard or sent as an email.

Caution: Some driver packages have standalone IQ that must be performed separately by clicking *here* in given section. Clarity IQ is **NOT** valid unless IQ of all components passed and reports are stored together.

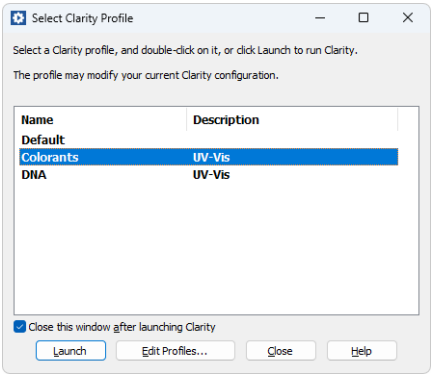


Note: The most common reason for a "Failed" result is the installation of an updated version over an existing installation of Clarity. This itself does not produce any errors but since some of the files are preserved from the original installation, the checksums will not match.

21.2 Editing Clarity profiles for different analyses using the Launch Manager

Launch Manager is a utility that allows you to start the Chromatography Station with specific setting. The collection of these settings is saved as a *Profile* in *Launch Manager*. You can select specific configuration, desktop file containing custom calculations and which instrument and project specifc user will be asked to log in.

1. Start the *Launch Manager* either from the Windows Start menu or using C:\CLARITY\BIN\LAUNCHMANAGER.EXE.
2. Click on the *Edit Profiles* button to create or modify the profiles.



3. Select a profile ⓐ to modify it or click on the *New* button to create a new profile ⓑ .
4. If you created a new profile, fill its name. For easier orientation it is recommended to fill in the *Description* which eases the distinguishing of different profiles.
5. Select the configuration file that will be loaded after the start of Clarity ⓒ .

   Note: The list of configuration files is retrieved from the installation directory (configuration files are located in C:\CLARITY\CFG by default). Clicking on » button opens menu for managing the configuration files, see Creating a duplicate configuration using the Launch Manager for one example of usage.

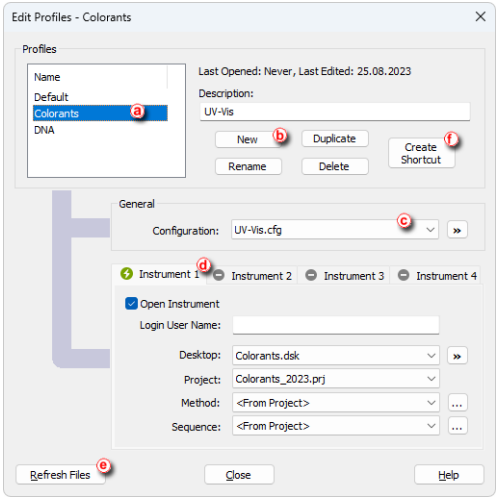
6. If you select the <Last Used> option, Clarity will start with the last configuration it was opened with or if Clarity is running, the present configuration will be preserved.
7. For each Instrument, choose if it should be opened at the Clarity start by *Open Instrument* checkbox. Select the User, Desktop, Project, Method and Sequence files that will be loaded when opening instruments.

   Note: In the desktop file, all layout setting is saved (the width of the table columns, the custom toolbars), but also custom calculations created in *User Columns*.

   Note: If <From Project> is selected, the Method and Sequence that were last opened in selected Project will be used.

8. You can use *Refresh Files* button ⓔ to reload all the files displayed in the *Edit Profiles* dialog.
9. Once the profile is configured, *Close* the *Edit Profiles* dialog and *Launch* the profile either by double clicking on the profile or by selecting a profile and clicking on the *Launch*.

Note: You can use *Create Shortcut* ⓕ to place shortcut on the desktop which can be directly used to launch given profile.

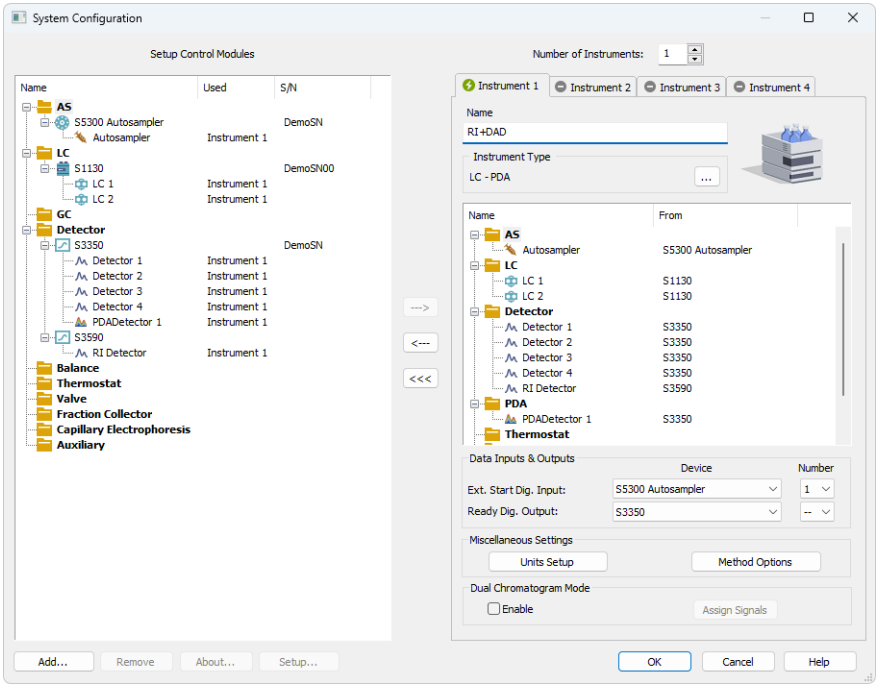


21.3 Creating a duplicate configuration using the Launch Manager

This topic describes how to create a duplicate configuration using the *Launch Manager*. This becomes especially handy when you have system with two detectors (e.g., RI + DAD) but you don't need to run them together every time.

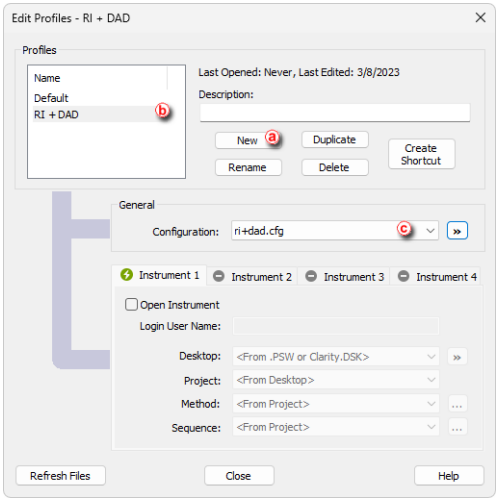
1. If you don't have any configuration yet, start Clarity and configure your device(s) according to the chapter "Adding a new device" and close Clarity. Otherwise start with the next step.

   Note: In this example we start with LC system with both DAD and RI detectors configured.

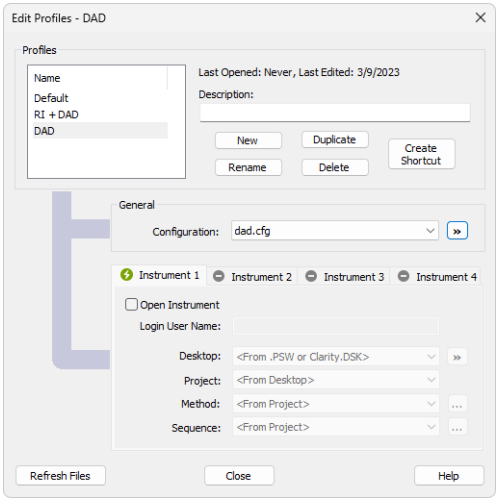


2. Open *Launch Manager* either from the Windows Start menu or by using C:\CLARITY\BIN\LAUNCHMANAGER.EXE.
3. In the *Select Clarity Profile* dialog click *Edit Profiles...*.
4. In the *Edit Profiles* dialog, click the *New* button ⓐ to create a new profile and name your profile (e.g. *RI + DAD*). Click *OK* to save the profile. Newly created profile is displayed in the small table on left ⓑ .
5. From the drop-down list ⓒ , select CLARITY.CFG, click the » button, from the selection choose *Duplicate* and in the following dialog name your configuration (e.g. ri+dad.cfg).

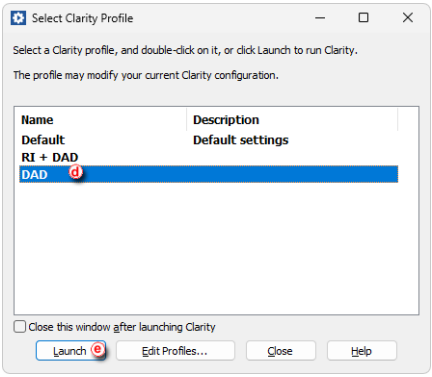
Note: This step will create a duplicate configuration (.cfg file) based on the current Clarity setup (as described in step 1.).



6. Create a new profile (DAD) with a different configuration (duplicated ri+dad.cfg named as dad.cfg), similarly to steps 4.-5. Once done, your profile should look similar to the image below.

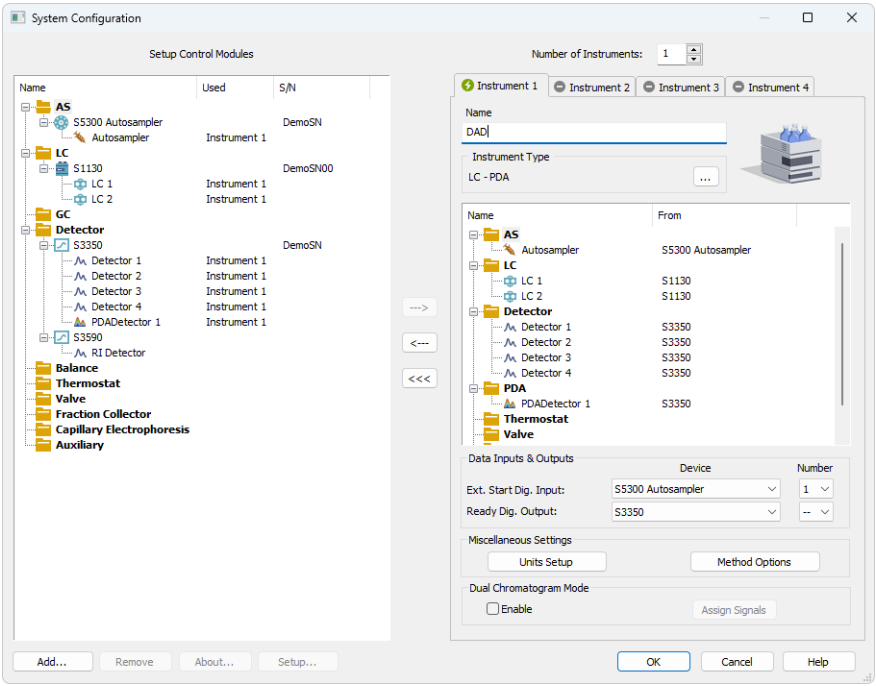


7. Close this dialog to return to the main *Launch Manager* window.
8. In the *Launch Manager* window select the *DAD* profile ⓓ which has not been configured but simply duplicated and click on the *Launch* ⓔ button.



9. Clarity has launched with the selected profile, open *System Configuration*. Since the configuration has been duplicated from the initial configuration, both detectors are present. Remove the RI detector from instrument and save the configuration by click *OK* in the *System Configuration* window.

   Note: This step may differ based on used control modules. In our case simply drag the RI module from right side to the left one. In other modules e.g., when using ICF you have to invoked the control module setup and change it there.



10. Launch each profile using the *Launch Manager* to make sure that correct configuration is loaded.

22 Best Practices for Using Clarity Effectively

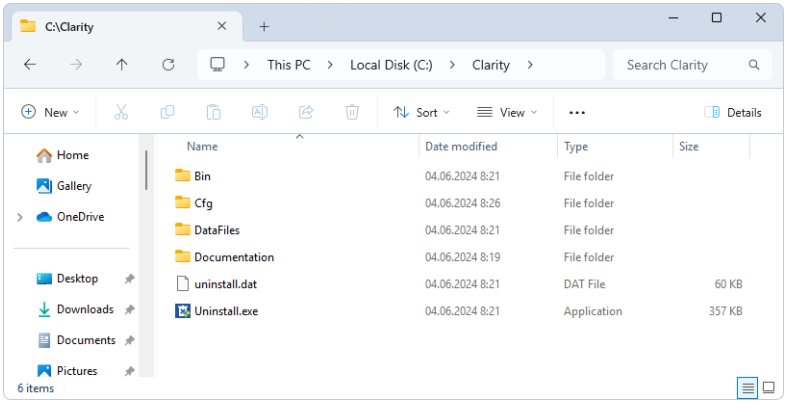
To ensure Clarity operates smoothly and delivers accurate results, it is important to follow certain practices when working with the software and your computer.

These principles cover topics like maintaining Clarity's file structure, proper data management, and adhering to recommended workflows. This section introduces these foundational guidelines, which help avoid errors, prevent data loss, and ensure a seamless experience.

22.1 Respect Clarity's file structure

Maintaining Clarity's file structure is crucial for ensuring smooth operation and reliable data acquisition. The Clarity folder includes four subfolders:

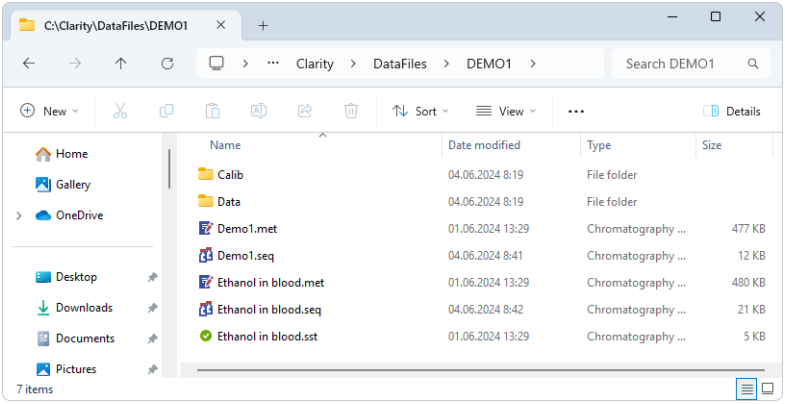
- *Bin Folder* contains executable files for the software and tools like Launch Manager.
- *Cfg Folder* stores software configurations, audit trails, and diagnostic data. Important files like .cfg, .dsk, and Clarity.psw should be backed up regularly.
- *Data Files Folder* organizes chromatographic data using a project- based structure. Each project has its own folder with subfolders for calibrations and sample data.
- *Documentation Folder* provides datasheets and manuals specific to your version.



The Data Files folder stores chromatographic data using a project-based approach:

- *Projects Folder* contains **.prj* file for each project.
- *Common Folder* stores shared files, such as report styles **.sty*, and templates, accessible to all projects.
- *Individual Project Folders* contains all the files belonging to each project in this structure:

- *Calib Folder* holds calibration **.cal* files and standard or blank chromatograms.
- *Data Folder* contains chromatograms of unknown samples.
- The root project directory contains method **.met*, sequence **.seq*, and SST **.sst* files.



Subfolders can be created in Data and Calib folders for organization of chromatograms, for more details see Storing chromatograms into subfolders topic. However, avoid adding folders directly to the project folder or storing files outside of this structure, as this may disrupt file linking and cause errors, if you want to change the location of Data Files directory it can be done in the Directories dialog, for more details see Setting up project directories topic.

22.2 Avoid switching Windows OS users and entering Sleep mode

Switching Windows user profiles or entering sleep mode while Clarity is running can disrupt communication with the hardware key or connected instruments. Active Clarity station (with an Instrument window open) prevents entering the sleep mode to ensure reliable data acquisition. However, in some BIOS configurations, this safeguard may fail.

To avoid issues, do not switch users while Clarity is active, and disable Power Saving features in both Windows OS (for all users) and the BIOS settings.

22.3 Protect Clarity from unexpected shutdowns

Unexpected computer shutdowns, such as those caused by Windows updates, power outages, or forced restarts, can interrupt ongoing measurements and potentially corrupt critical files that store station settings.

To minimize the risk of loss of settings or its corruption:

- Regularly back up important files stated below.
- Schedule Windows updates during off-hours when Clarity is not running to prevent forced restart.
- Ensure reliable power through a UPS (Uninterruptible Power Supply).

List of recommended files for back up:

- Clarity.cfg + any other configuration file present in Cfg directory.
- Clarity.dsk + any other desktop file present in Cfg directory.
- Clarity.psw in Cfg directory.
- optional: method(s) validated and used for measurement

22.4 Version Compatibility Across Clarity Stations

To ensure proper functionality of all Clarity stations, it is essential that the same version of the Clarity software is installed on every PC. If the PC used for instrument control is running a different version than the Clarity Offline used for processing results or preparing methods, this may lead to incompatibility when attempting to use files created in a higher version. This applies not only to combinations of Clarity and Clarity Offline, but also to setups with multiple Clarity installations.

Clarity is designed to maintain backward compatibility, allowing data and methods created in older versions to be opened and processed in newer versions of the software without issues. This ensures continuity when upgrading systems or working across multiple stations. However, files created or modified in a newer version may not be usable in an older version of Clarity, and attempting to do so can result in errors or limited functionality.

To prevent these issues, all Clarity installations within the same environment should always run the identical software version.

23 Troubleshooting

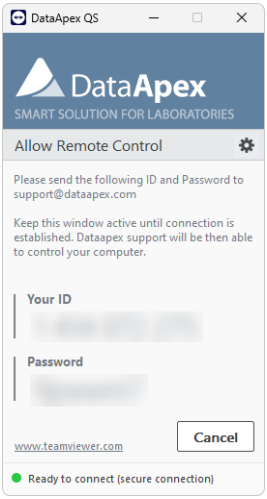
This chapter contains a set of Standard Operating Procedures (SOPs) designed to assist you in resolving any issues you may encounter while working with Clarity. The SOPs include instructions on which information and data to collect and sent to our Support team, enabling them to offer effective solutions to your problems.

Note: Video tutorials and How To videos regarding Troubleshooting can be found in the Troubleshooting playlist on our YouTube channel.

If you do not find your answers here, use the www.dataapex.com website where the *Support* menu will navigate you to video tutorials, frequently asked questions (FAQ), and the *Support request form*. Alternatively, you can contact your distributor or the **DataApex** helpdesk via e-mail. Please note that we can request the collection of some configuration files. In case you have an e-mail client installed, you can collect these files using the *Help - Send Report by E-mail* menu in the main **Clarity** window.

Solutions to problems connected to particular **hardware** can be found in the corresponding manuals.

As the last option when troubleshooting complicated issues, **DataApex** may provide remote support via **TeamViewer QuickSupport** to registered customers (paid sevice). To use this option, the user must first contact **DataApex Technical Support** (support@dataapex.com). The **TeamViewer QuickSupport** application can be downloaded by clicking *Help - TeamViewer QS* in the main *Clarity* window. The application is ready to be used directly after downloading.



23.1 Missing hardware key

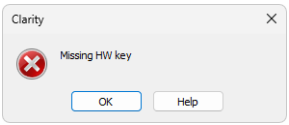


Fig. 20: Missing HW key error dialog

If you try to start **Clarity** without a properly recognized hardware key connected to the PC, an error message saying "Missing hardware key" is displayed and the application will not start. The hardware key must be plugged into a USB port and correctly detected by Windows. This error may occur if the key is not plugged to the PC, or if the key is malfunctioning and is not recognized by the operating system, or if the required USB driver is not installed correctly.

Reason: Your hardware key is not detected by Windows

Solution: Check if the hardware key is properly inserted in the USB port. Check whether the USB port is working (e.g., try to connect a different device, etc.), check if the hardware key diode is lighting steadily, if blinking or is dimmed try another USB port.

Under normal circumstances, the driver for the currently supplied hardware key is installed automatically when the key is inserted into a USB port; however, if you are using an older type of hardware key, a dedicated driver may be required. Older hardware keys are easily identified by their blue casing (current key is supplied in a transparent grey casing).

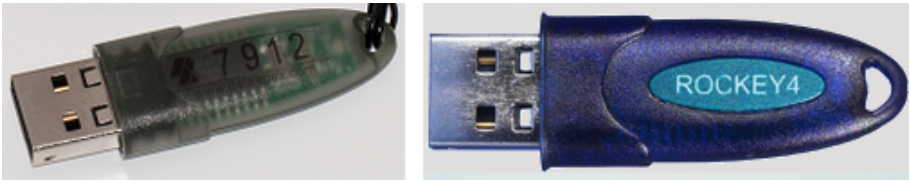


Fig. 21: Current (left) and older (right) hardware key

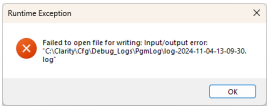
Troubleshooting the older hardware key

If none of the steps described in the previous section resolve the issue, the reason may be that you are using an older type of hardware key that requires a dedicated driver.

For this older hardware key in blue casing, a specific driver must be installed for the key to function correctly. This driver is normally installed automatically during the Clarity installation. Plugging in the older hardware key before installing Clarity may lead to problems with installing the drivers.

If problems persist, try reinstalling the driver. For the complete installation procedure and common issue resolutions, refer to Installing a USB hardware key – Older hardware key with blue casing.

23.2 Failed to open file for writing



For Clarity to operate correctly, the logged-in Windows User must have *Read* and *Write* access privileges to the entire Clarity folder. Without these permissions, Clarity cannot be started.

Reason: You probably have insufficient access rights to the C:\CLARITY directory.

Note that this solution requires a user with administrator rights.

- Right-click on the C:\CLARITY directory and choose *Properties*.
- In the *Clarity Properties* on the *Security* tab, locate the User/Group of Users and click *Edit*.
- Provide the administrator password when prompted.
- In the next dialog, grant the User/Group of User the necessary permissions by checking the *Allow* option for: *Read & Write*, *List folder contents*, and *Read*.

In case insufficient privileges are applied only to a part of the Clarity folder, Clarity still may not work properly, causing similar error messages to pop up.

23.3 The User Code Errors

In some cases, the entered User Code may not be accepted and as a result, **Clarity** cannot be started. This situation can occur for several different reasons and may trigger various error messages. Below are the most common messages related to User Code rejection, along with their possible causes and suggested solutions.

Note: The ***User Code*** dialog does not distinguish between upper case and lower case letters. However, be careful not to confuse the letter "l" with the number "1".

In the case that the User Code is intended for unlocking additional extensions/add-ons for the station, the previously accepted one is still saved.

If necessary, contact the manufacturer or your distributor to request the correct User Code. In this case, be prepared to provide the serial number (S/N) of the workstation.

23.3.1 The User Code is not valid for version x.y

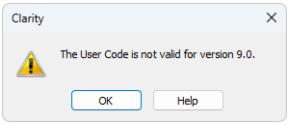


Fig. 22: The User Code not valid for version error dialog

Reason: You have probably entered a User Code for a different version.

Solution: You have to enter the User Code corresponding to your current version. For example, when you purchase additional extensions/control licenses, a new User Code is generated for your station. The new User Code is valid only for the most recent **Clarity** major version, so you will probably need to install the latest version of the software.

23.3.2 Wrong User Code

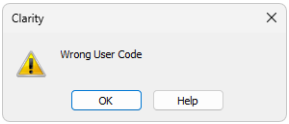


Fig. 23: Wrong User Code error dialog

The User Code of the workstation does not match the code in the HW key.

Reason: You have entered a User Code that does not match the serial number of the HW key plugged into the PC.

Solution: Submit a correct User Code. The User Code can be found on the back of the plastic card provided with the installation USB.

23.3.3 Wrong Software Version

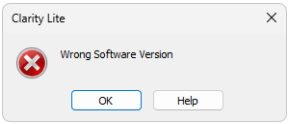


Fig. 24: Wrong Software Version error dialog

Reason: You have probably installed a different application than you had purchased. For example, you installed Clarity Lite instead of Clarity.

Solution: Install the correct application you had purchased. If you are not able to locate the correct installer, contact the manufacturer or your distributor.

23.4 Trial Expired

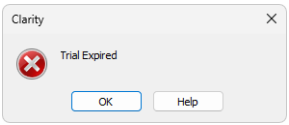


Fig. 25: Trial Expired error dialog

The Trial period (time period when **Clarity** works without a User Code filled in) expired. You are prompted to enter a User Code or a Trial Prolongation Code.

Reason: Your Clarity station just ended its trial period.

Solution: a) Enter the correct User Code, which switches **Clarity** from the Trial mode into the full mode ① .

b) Or switch to section ② and enter a Trial Prolongation Code to extend the trial mode period. Trial Prolongation Codes must be requested from your distributor or DataApex.

Once a correct User Code or Trial Prolongation Code has been provided, click the *OK* button to start **Clarity**.

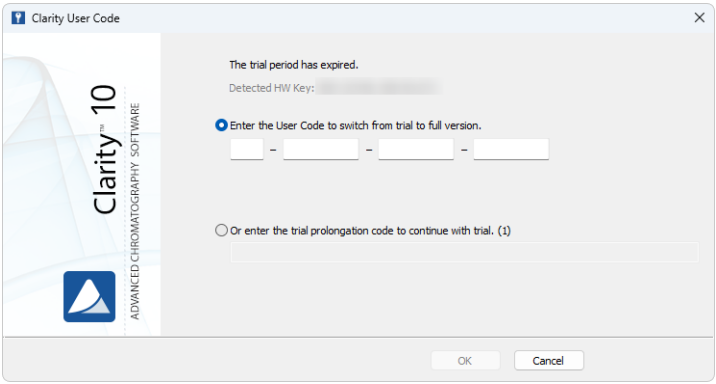


Fig. 26: Clarity User Code dialog

In the case you need to enable trial on the station where the User Code was previously entered check the *D037 Clarity Trial-Full mode switching* datasheet.

23.5 IQ Report failed

The IQ Report (Installation Qualification) may occasionally fail, especially when upgrading from significantly older versions of Clarity. The IQ program verifies all registered files, and if some are no longer used in the new version, the check may not pass.

Despite the failure, Clarity will typically function correctly.

Reason: In Bin folder, unexpected files are present.

Solution:

1. Uninstall Clarity (e.g. from the Windows Start menu or by running uninstall.exe from the Clarity folder). This process does not remove your chromatographic data and system settings (these files are not included in the IQ).
2. If there are any remaining *.dll files in the C:\Clarity\Bin folder, delete them manually.
3. Install Clarity again. Make sure that the "Keep the configuration files" option remains selected (this is the default setting) to preserve your data.

23.6 The XX file is corrupted or missing

In most cases, corruption happens when Clarity is unexpectedly closed, e.g., due to power outage or Windows updates forcing the system to restart, or when some important file is moved outside of the expected location. The type of the file indicates the severity of the situation. In majority of cases, Clarity is restarted and a backup file is used instead.

To prevent the problems caused by the corrupted files, we recommend following of the tips in the Best Practices for using Clarity effectively chapter, especially backing up of important files regularly.

23.6.1 Clarity.psw file

The Clarity. psw file holds the information about user accounts. If it is corrupted, Clarity cannot be started.

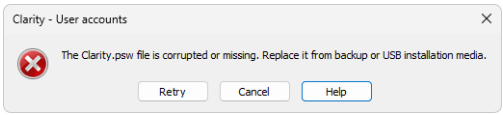


Fig. 27: The Clarity.psw file is corrupted or missing.

- In the case you have backed up the file previously, replace the corrupted .psw file in the *Cfg* folder of your Clarity station, and the *User Accounts* saved in the backup will be ready to use.
- If you have not backed up the .psw file, you have to use the default backup from the CFG\BACK folder or from the USB installation media. In this case, you will have to set up the *User Accounts* again.

23.6.2 Configuration *.cfg file

The configuration *.cfg files holds the information about the setting of the directories, the devices configured on Instruments, and some additional settings that is done in the *System Configuration* dialog.

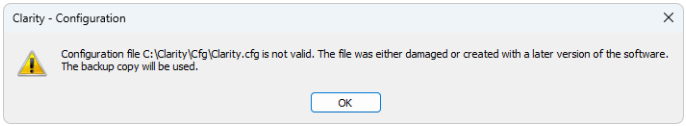


Fig. 28: Configuration file x.cfg is not valid. The file was either damaged or created with a later version of the software.

To repair the damage, follow this process:

1. Open the *System Configuration* dialog and configure your system manually (eg. add detectors, LCs, GCs, valves and so on to the configuration), fill in their settings and distribute them to particular instruments.
2. Close the *System Configuration* dialog by clicking OK.
3. If you had the *Directories* dialog set before, set it once more. Then, close the dialog.
4. Open the Instrument and select the Project that was used before.
5. Check the used methods. If you did not saved the methods in the time the loaded backup configuration was empty, they should have the correct settings as before the problem.

23.6.3 Project *.prj file

The project file contains only information about the last opened documents that are "prepared" for you when you log in next time, so no damage to your data has been done upon corruption. The easiest way to fix this is to delete the corrupted project file and create a new one with the same name.

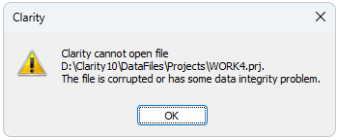


Fig. 29: Clarity cannot open file x.prj.

1. Close Clarity.
2. Find the corrupted file using the File Explorer and delete it - by default it is located in the DATAFILES\PROJECTS subfolder.
3. Go back to Clarity.
4. When logging in to an *Instrument*, select *New Project*.
5. Fill in the same name as the corrupted project had.
6. Confirm that the directories exist and you want to create the project file.

23.7 Data Acquisition - Disabled

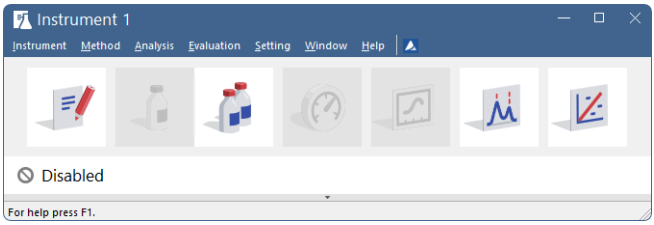


Fig. 30: Data Acquisition disabled

The "**Disabled**" label appears, and the *Single Analysis* dialog and *Data Acquisition* windows are not available. Other manifestations of this error are also: ***Method Setup - Acquisition*** tab missing, *Run*, *Stop*, and *Abort* commands non-functional in the ***Sequence*** window.

Reason 1: No detector is allocated to the Clarity Instrument.

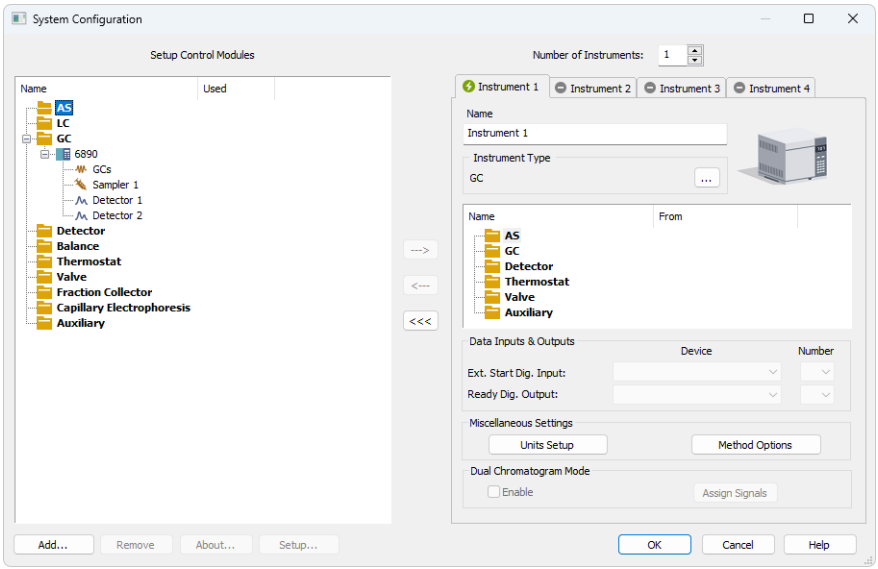


Fig. 31: Detector not allocated to the Instrument

Solution: Open the ***System Configuration*** dialog from the ***Clarity*** window using the *System - Configuration...* command and check the tab of the corresponding Instrument - **Instrument X**. If it has no allocated detectors, add them.

In the list on the left side of *Setup Control Modules*, select the correct detector, and drag it to the corresponding instrument section on the right.

If the appropriate detector is not in the list, add it using the *Add* button and repeat the previous step.

Reason 2: You purchased a license for data collection on fewer Instruments.

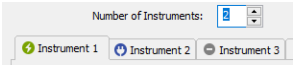


Fig. 32: Small number of Instruments purchased

Solution: Open the *System Configuration* dialog from the *Clarity* window using the *System - Configuration...* command and check the tab of the corresponding Instrument - **Instrument X**. The icon indicates that the Instrument is not available for data acquisition. If you want to use this Instrument for data acquisition, contact your distributor and order an Add-On Instrument.

Reason 3: You are using the Clarity Offline version, which is not intended for data acquisition.

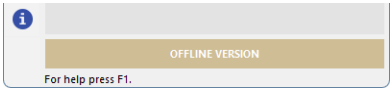


Fig. 33: Clarity Offline

Solution: Check whether there is a brown band with the text **OFFLINE VERSION** on the main *Clarity* window under the instrument icons. If it is, remove the HW key with the **Offline** license and insert a key with the **Clarity** full license.

23.8 Data Acquisition - Simulated

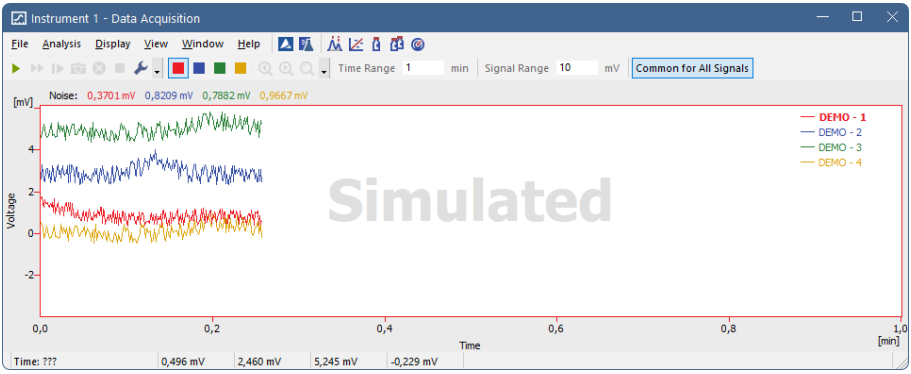


Fig. 34: Data Acquisition Simulated

The title "**Simulated**" is displayed. The corresponding Instrument only displays a simulated curve in the *Data Acquisition* window.

Reason 1: You are using Clarity Demo version.

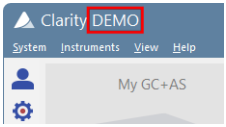


Fig. 35: Clarity DEMO

Solution: Check whether the title **DEMO**is in Clarity window header. If so, uninstall the demo version and install the full version of Clarity.

Reason 2: A DEMO detector is allocated to the Instrument.

Solution: Open the *System Configuration* dialog from the *Clarity* window using the *System - Configuration...* command and check the tab of the corresponding Instrument - **Instrument X**. If it obtains detector signals only from the **DataApex DEMO** detector, it is necessary to reconfigure it. You can find more information on how to add a detector in the chapter "Configuration"

23.9 Clarity is unable to find HW key

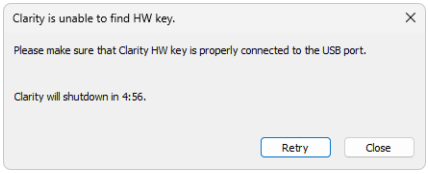


Fig. 36: Clarity is unable to find HW key

When **Clarity** has lost communication with the HW key, the "Clarity is unable to find HW key" error message is displayed. The user has 5 minutes to try to reestablish the communication between Clarity and the key. Once this time elapses, Clarity will automatically shut down.

Retry

Check for the HW key again and resume running **Clarity** in case it was detected.

Close

Close **Clarity** Chromatography Station.

There are two possible explanations for this error message:

Reason 1: The key was removed while *Clarity* was running.

Solution: Plug the key in again. Click the *Retry* button to reestablish the communication.

Reason 2: The USB port which the key is plugged in entered the sleep mode.

Solution: Go to *Start - Control Panel - Hardware and Sound - Device Manager* , locate **Universal Serial Bus Controller**. Right-click each **USB Root Hub** item and choose *Properties*. Click the *Power Management* tab and uncheck the box for "Allow the computer to turn off this device to save power".

Caution: Another way to forbid USB ports from entering the sleep mode is in **BIOS**. This option is however recommended only for **advanced** users and is usually performed by the local System Administrator.

23.10 Clarity sequence does not progress when started or running

There may be multiple different reasons. Please check the detailed status in the *Instrument* window and *Device Monitor*.

Status: Waiting for Injection

Description: Indicates parameters for injection were sent to the sampler, but the start signal has not yet been received. Suppose the sampler is not working on the injection. In that case, it may indicate wrong synchronization settings in the System Configuration or that the start signal was not received or ignored for some reason.

Status: Waiting for Hardware to be Ready to Run

Description: Indicates some of the devices configured on the instrument do not report Ready state. Check the status reported by individual devices in the Device Monitor.

Status: Sequence Paused

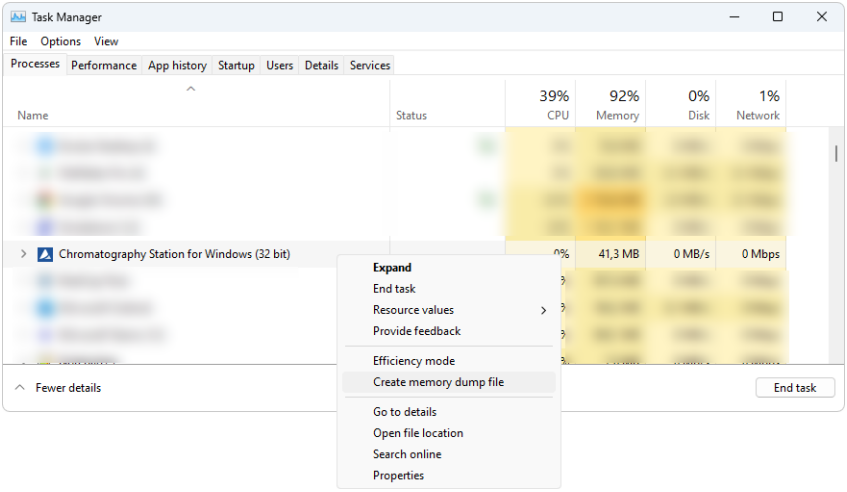
Description: Indicates the sequence was paused. An automatic pause may happen if an invalid value is entered during the editing of the running sequence to prevent locking a line with an invalid value. After correcting the value, the sequence must be manually resumed.

23.11 How to create a dump (*.dmp) file from running Clarity

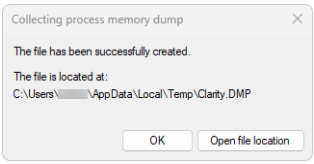
Sometimes if you encounter problems while working with Clarity, you may be asked by our Support team to provide a dump (*.dmp) file created from the problematic Clarity process. Specifically, this is useful when you are encountering freezes during Clarity operations.

Here is a simple guide on how to create such dump file:

1. Run the 32-bit Task manager with the option Run as administrator (Clarity is a 32-bit process thus the 32-bit Task Manager must be used), it is located here: C:\WINDOWS\SYSWOW64\TASKMGR.EXE.



2. Locate the Clarity process, right click on it, and in context menu select *Create memory dump file*.
3. Wait a moment.



4. A dialog informing that the dump has being successfully created will pop up, including information on where it is located.
5. Send this file to our support team either via email support@dataapex.com, or the Support Request form on our website.

23.12 Recovering data after crash or freeze

If Clarity crashes or freezes during data acquisition, it is possible to recover the data up to that moment.

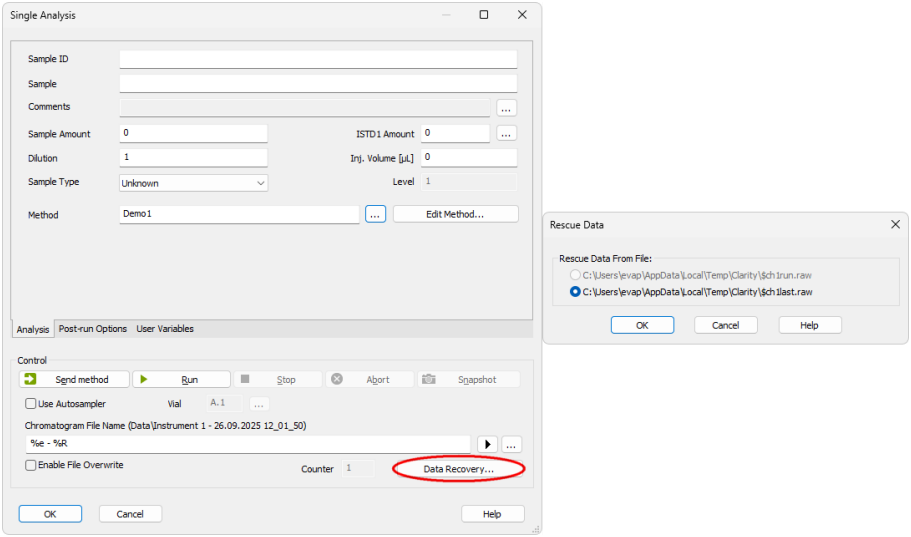
During acquisition, data are stored in the temporary directory (by default C:\USERS\<USER NAME>\APPDATA\LOCAL\TEMP\CLARITY\$CH1RUN.RAW file). The data are stored from memory to disk approximately every 10-90 seconds intervals (the exact interval depends on the detector frequency).

Here is a simple guide on how to restore the data:

1. Open *Single Analysis* dialog.
2. Select the *Data Recovery* command to reconstruct the chromatogram. There can be two files to choose from:

- *RUN.RAW file will be created only when Clarity station has been unexpectedly terminated while measuring data (e.g. after a power failure)
- *LAST.RAW file always contains the last measured chromatogram

Note that the recovered chromatogram will be processed using the method and parameters defined in the *Single Analysis* dialog. Only the processing part of the method (e.g., integration settings, calculations) is applied. Instrument control parameters (such as pump flow) are not taken into account.



After a freeze, recovery depends on whether the background thread writing data was still running. After a crash, data can usually be recovered up to the last minute before the failure. If freezes happen repeatedly, we advise to investigate the cause - please do not hesitate to contact us via the Support Request form on our website and send us the respective a diagnostic files (including a memory dump file).

23.13 Resolving “Out of Memory” error

Clarity operates as a 32-bit process, which limits the available memory to 2 GB of RAM. When multiple demanding instruments are used simultaneously, overall system performance can be affected. Although Clarity itself cannot use more than 2 GB, it is still recommended to equip the computer with at least 8 GB of physical RAM to ensure sufficient resources for the operating system and other applications.

The *Out of Memory* error may appear, for example, when opening measured chromatograms while a sequence is running, or when working with a method file that has been saved repeatedly after multiple modifications. Each time a method is saved, Clarity creates a new version of the file, shown in the *Method Setup* dialog title as *#number*. A large number of versions significantly increases the file size, and when a

method becomes too large, memory resources may be depleted, leading to instability or malfunction.

Recommended solutions in Clarity

- Save the method under a new name. Use *File → Save As* to save the current method under a new name. This creates a fresh method file without previous versions, which reduces the file size.
- Avoid overlaying chromatograms during sequences. When opening chromatograms, do not use *Open in Overlay* while a sequence is running, since overlay display increases memory consumption during data acquisition.
- Do not open resulting chromatograms automatically. In the *Sequence Table*, disable the check box in the *Open* column. This prevents Clarity from opening each chromatogram as it is acquired.
- Limit the number of chromatograms in summary reports. When generating a *Summary Report*, include only the necessary chromatograms. Excessive data in reports may consume additional memory resources.

Additional recommendations

- Restart your PC or Clarity once in a while to release memory resources.
- Check which programs consume most memory in the *Task Manager*. Try to uninstall or disable unnecessary programs with the highest RAM (memory) consumption.
- Limit the number of programs that start automatically when you turn on your PC and run in the background. Open *Task Manager → Startup apps* tab and disable unnecessary startup entries.
- If the issue persists, verify that the PC meets or exceeds the recommended hardware requirements or consider buying a new PC with better hardware (mainly increase RAM capacity).