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:

Instrument (blue text) marks the name of the window to which the text refers.

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 (when you already are in the topic describing the window).

WORK1 (capitals) indicates the name of the file and/or directory.

ACTIVE (capital italics) marks the state of the station or its part.

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

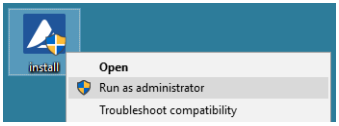
These are the basic steps you have to follow for the First installation of Clarity.

First installation of the software (since version 7.0)

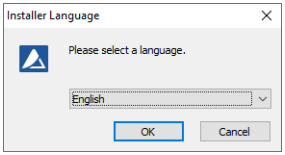
1. **Install the software** BEFORE connecting any hardware.

   More Info:

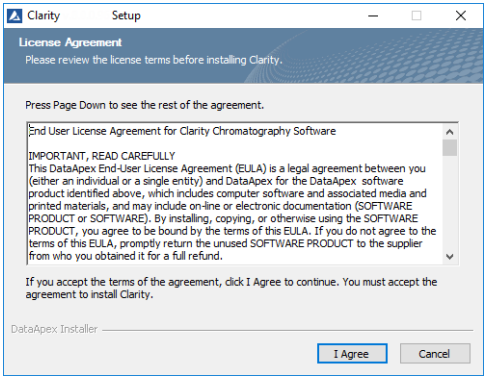
   - The software can be installed by inserting the installation USB and running install.exe or by downloading the installation from the download center at our website.
   - On administered systems use „*Run as Administrator*“ from intended User account. Administered systems are managed by an administrator 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.
   - On Windows 7, 8.1 and 10 User Account Control may have to be disabled in order to install some control modules (PAL, Shimadzu and ICF) correctly.

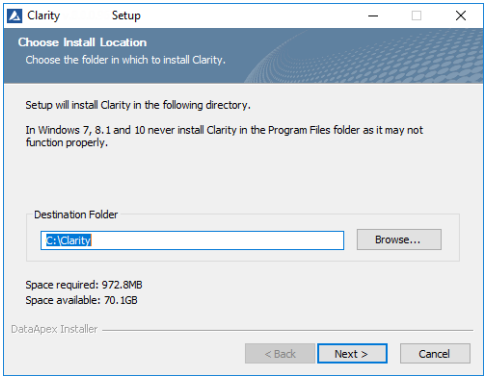
2. **Select the language.**

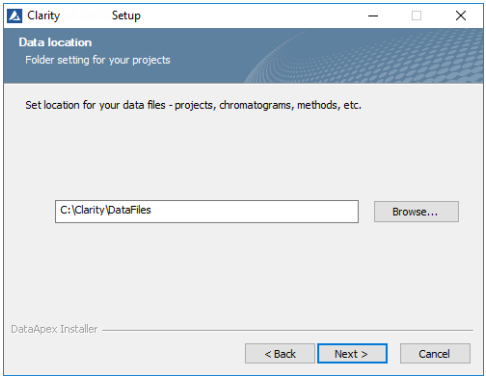
3. **Confirm the License Agreement.** It is possible to continue only in case you agree with the statement.



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



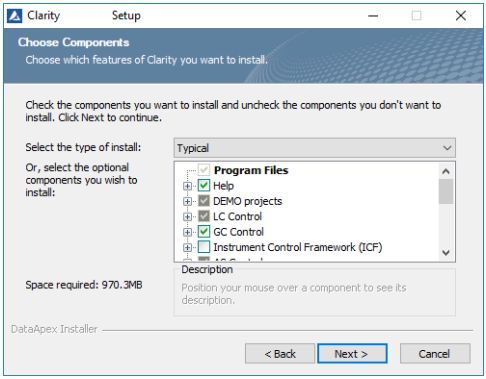
5. **Set location for your data files.** C:\CLARITY\DataFiles is set by default. Notice that Data location folder name cannot contain following characters / : * ? " < > | and also cannot start or end with a space and cannot end with a dot.



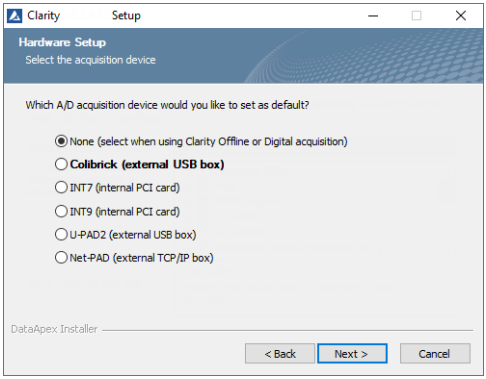
6. **Select the type of installation.**

More Info:

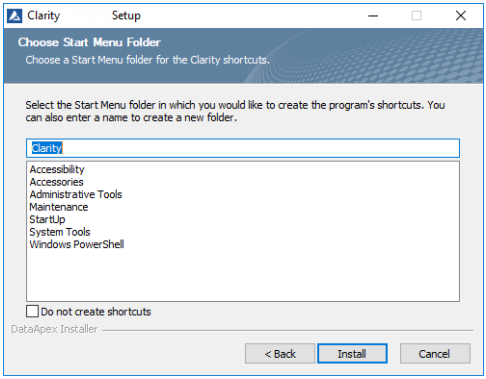
In most cases "Typical" should be selected. A "Custom" installation is necessary for Agilent HPLC control via ICF, CTC PAL, Shimadzu LC-10/20 system, Master GC, ESA Coulochem III and possibly some others.



7. In case you will use an **A/D converter**, select the one you have. It will be preconfigured in the **System Configuration**. Select **None** in case you want later configure will later configure detectors with digital acquisition.



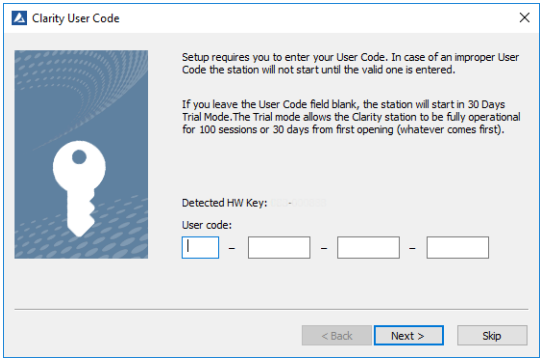
8. **Select the Start Menu folder or create a new one.** After clicking on Install you will get a screen showing the installation in progress.



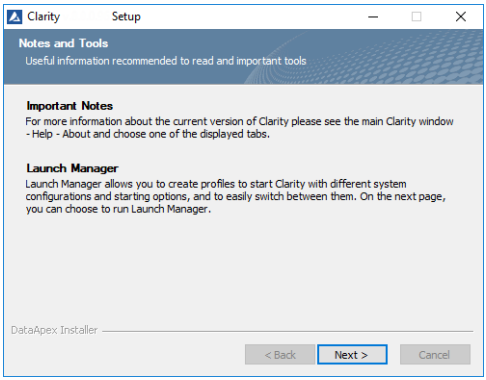
9. **Enter the User code** corresponding to your hardware key **or leave blank** for a 30 day trial mode.

More Info:

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



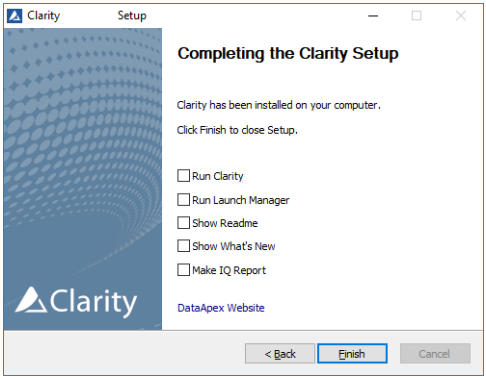
10. When installation is finished Notes and Tools window will be opened.



11. Finally the last window will offer you several actions which may be executed after the installation is completed.

More Info:

- The Launch Manager allows you to start Clarity using different profiles that correspond to different configurations and combinations of instruments, projects, methods, etc. For example, different users or groups of users can have the chromatography station configured on the same computer.
- The Installation Qualification - IQ (Make IQ report option) is a procedure that confirms that the software has been installed successfully and that the files are in the correct version.



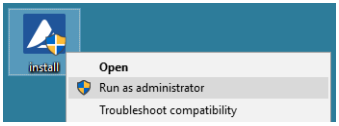
1.2 Updating Clarity Software

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

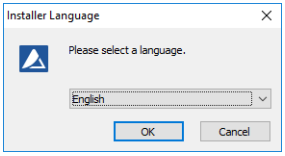
1. **Check for the updates:** click *Help - Check for Updates...* or download new version of software from the download center at our website.
2. **Run the installer.**

   More Info:

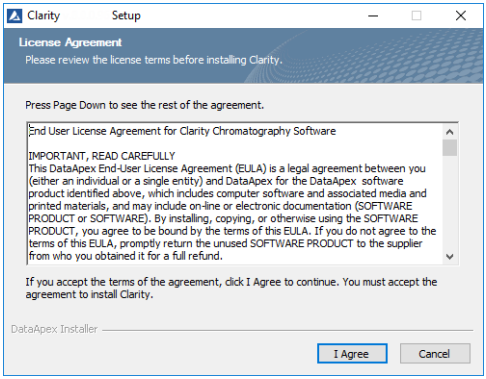
   - On administered systems use „*Run as Administrator*“ from intended User account. Administered systems are managed by an administrator and users using the PC may not have administrator privileges. Insufficient privileges may result in:
     - Clarity not being installed.
     - When installed from Administrator account, the installation directory may be read only for users with limited privileges and the station will be inoperable.
   - On Windows 7, 8.1 and 10 User Account Control may have to be disabled in order to install some control modules (PAL, Shimadzu and ICF) correctly.

3. **Select the language.**

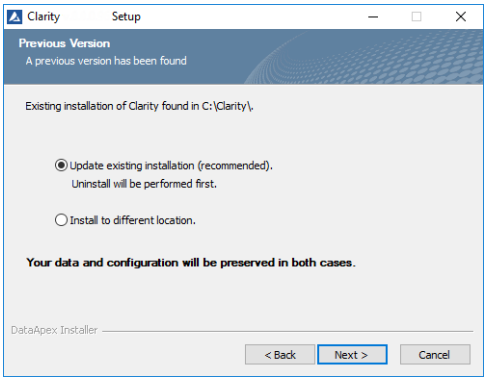
4. **Confirm the License Agreement.** It is possible to continue only in case you agree with the statement.



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

More Info:

In both cases your data and configuration will be preserved.

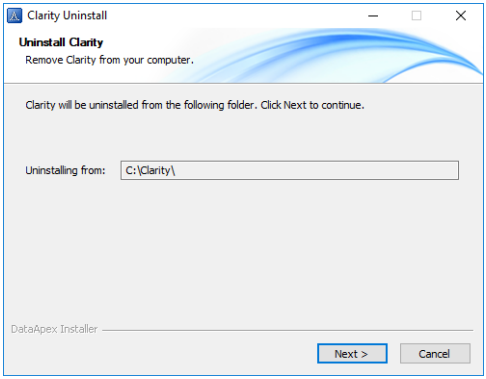


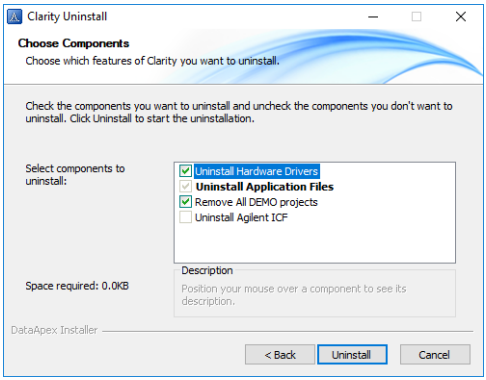
6. If you select to **Install to different location**, continue from step 8.

More Info:

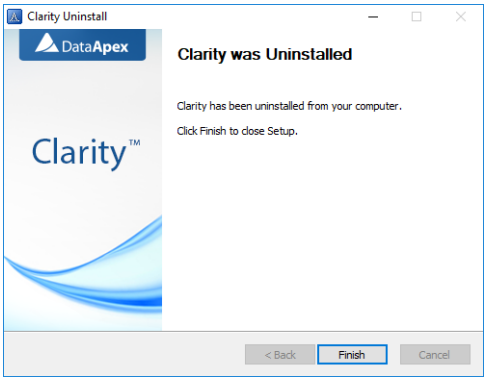
Note that update cannot be installed to the current destination folder because it already contains an installed program. Select another location or uninstall the program manually.

7. If you select to **Update existing installation**, Clarity will be uninstalled first and following window appear.





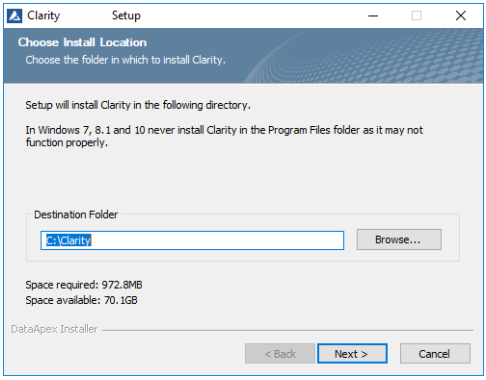
8. **Finish Clarity uninstall.**

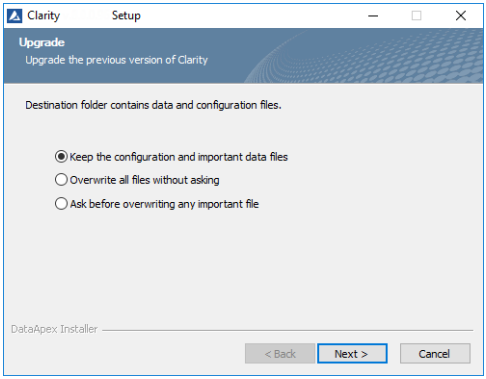


9. **Choose the destination folder for new installation.**

More Info:

- Note that now update can be installed to the current destination folder. In that case following window will appear, you can decide whether keep old data and configuration or overwrite them.
- DEMO projects are always overwrite by default.
- Notice that Destination Folder name cannot contain following characters / : * ? " < > | and also cannot start or end with a space and cannot end with a dot.

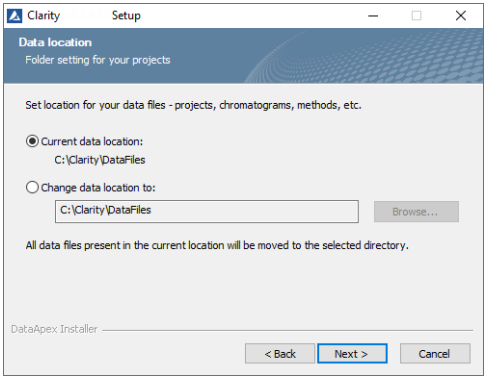




10. **Set destination folder for your data files.**

More Info:

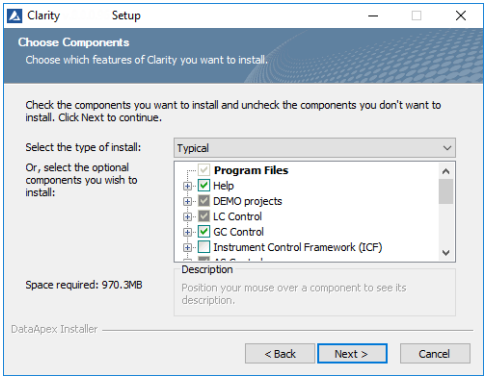
- Since Clarity 7.0 recommended default data location is *C:\CLARITY\DataFiles*. All your data will thus be stored in one place.
- If you change data location, all data files present in the current location will be moved to the selected directory.
- Notice that data location folder name cannot contain following characters / : * ? " < > | and also cannot start or end with a space and cannot end with a dot.



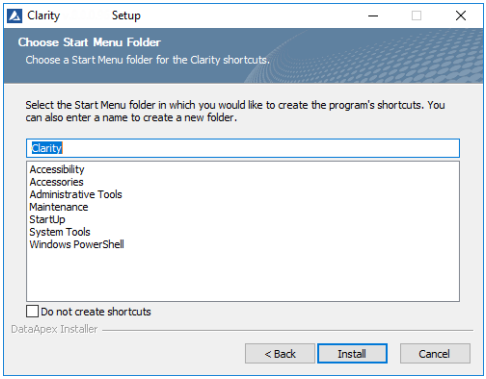
11. **Select type of installation.**

More Info:

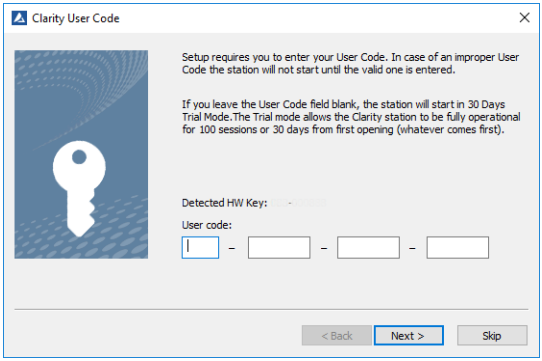
In most cases "Typical" should be selected. A "Custom" installation is necessary for Agilent HPLC control via ICF, CTC PAL, Shimadzu LC-10/20 system, Master GC, ESA Coulochem III and possibly some others.



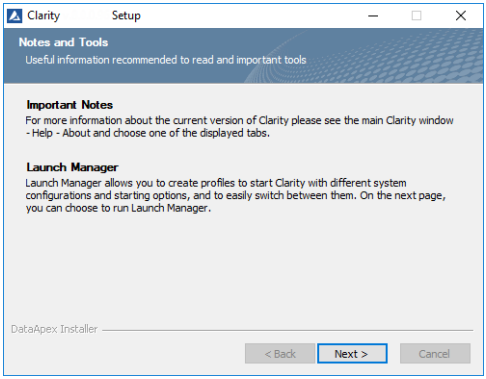
12. **Select the Start Menu folder or create a new one.** After clicking on Install you will get a screen showing the installation in progress.



13. **Confirm the User code.**



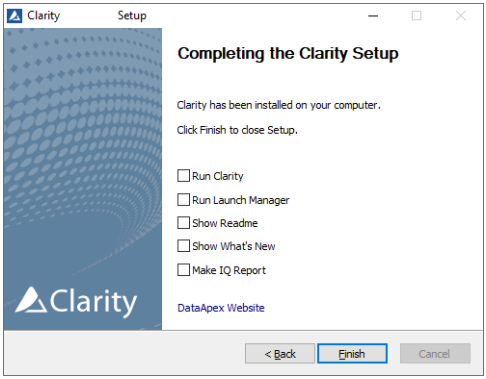
14. When installation is finished Notes and Tools window will be opened.



15. Finally the last window will offer you several actions which may be executed after the installation is completed.

More Info:

- The Launch Manager allows you to start Clarity using different profiles that correspond to different configurations and combinations of instruments, projects, methods, etc. For example, different users or groups of users can have the chromatography station configured on the same computer.
- The Installation Qualification - IQ (Make IQ report option) is a procedure that confirms that the software has been installed successfully and that the files are in the correct version.



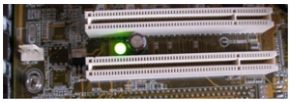
Caution: When upgrading from Clarity 6.2 or older to Clarity 7.0 or newer be aware that there is change in the installation structure - the content of the original installation folder is separated to three new subfolders BIN, CFG and DataFiles. The respective files are moved automatically during update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

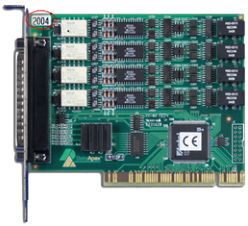
Caution: During eventual downgrade between those versions the files need to be moved manually to the original locations.

1.3 Installing an internal card

Please install the software BEFORE connecting any hardware. To install an internal card on your PC follow these steps:

1. **Switch off the computer.**
2. **Insert the INT7 or INT9 A/D board** to a free PCI slot.





3. **Switch on the computer.**
4. In Windows 7, 8.1 and 10 **the drivers will be installed in the background**.

1.4 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.

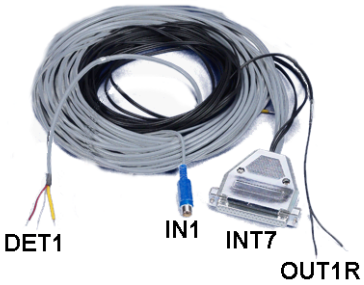
1. **Install *Clarity* first.**

   More Info:

   - The drivers will be installed automatically during the installation of Clarity. Ensure that you have Administrator access rights in your Windows OS before you proceed with the installation.
   - 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 Starting, Digital output and Analog Signal cables 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.

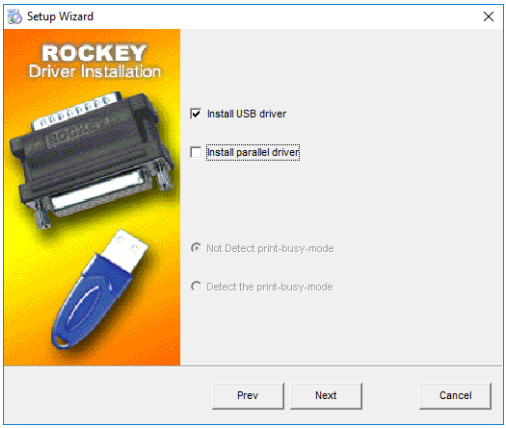
More Info:

- 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.

1.5 Installing a Rockey USB dongle

Currently supplied RkNDUSB HW keys use the HID (Human interface device) technology and do not require any drivers.
For old RkUSB keys the drivers will be installed automatically during the installation of Clarity. If the installation did not proceed as expected or you have an old version of Windows, follow the procedure below.

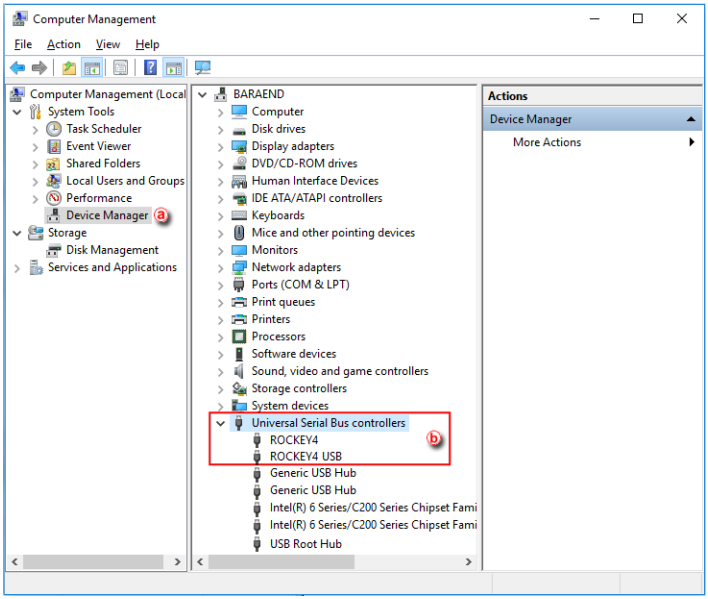
1. **Install Clarity first.**
2. **Connect the USB dongle to a USB port on the computer.**
3. **Install the Rockey drivers** by running INSTDRV.EXE in C:\CLARITY\BIN\HW_DRIVERS\ROCKEY\. The following window will appear.
4. **Select the Install USB driver option and click on Next** to finish the installation.



5. **Verify that the driver has been installed correctly**

More Info:

- Go to the Windows *Start* menu in the lower left corner of the screen and select *Control Panel*.
- Click on the *System* icon.
- Verify 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 dongle, **Windows** will detect a new **Plug and Play** device and the Found New Hardware Wizard will appear.

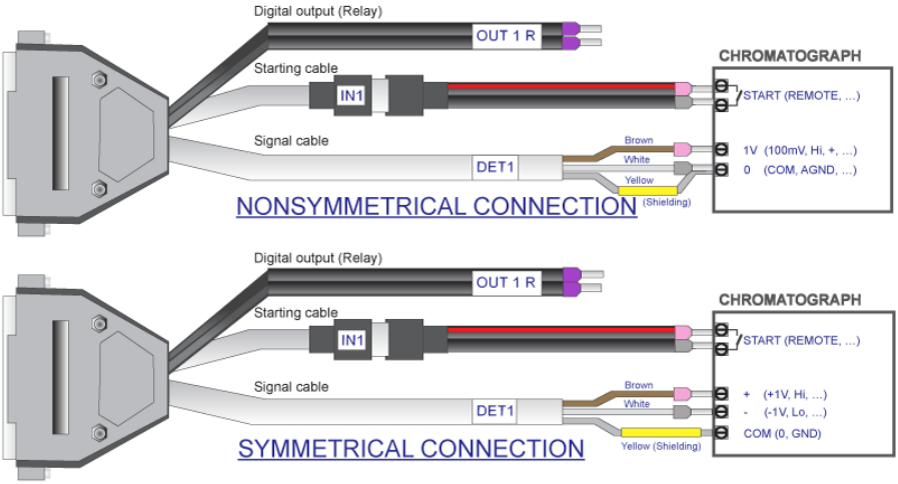
1. **Select "*Search for a suitable driver for my device.*"**
2. **Select "*Specify a location*" and then select the C:\CLARITY\BIN\HW_DRIVERS\ROCKEY\folder**. The rest of the installation will be carried out automatically.
3. **Verify that the driver has been installed correctly**

More Info:

- Go to the Windows *Start* menu in the lower left corner of the screen and select *Control Panel*.
- Click on the *System* icon.
- Verify that the Device Manager ⓐ has the item "*Universal Serial Bus Controllers*" - "*Rockey4 USB*" ⓑ.

1.6 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 A/D converter** card as explained in Installing an internal card **or an external A/D converter** like *Colibrick*, Installing Colibrick.
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 board.**
5. **Switch on your computer and your chromatograph.**

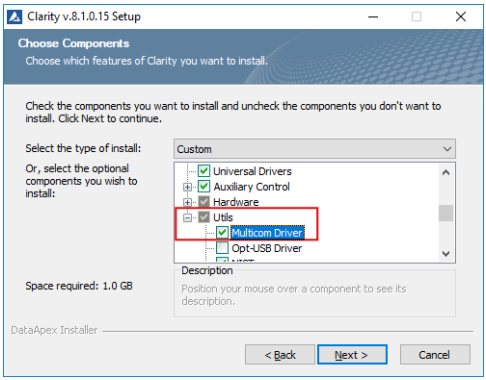
1.7 Installing Multicom

MultiCOM is a USB to RS232 converter developed for controlling LC and GC systems 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. **Install *Clarity* first selecting the *Multicom* driver under *Utils* at the end of the components list.**

More Info:

Ensure that you have Administrator access rights in your Windows OS before you proceed with the installation.

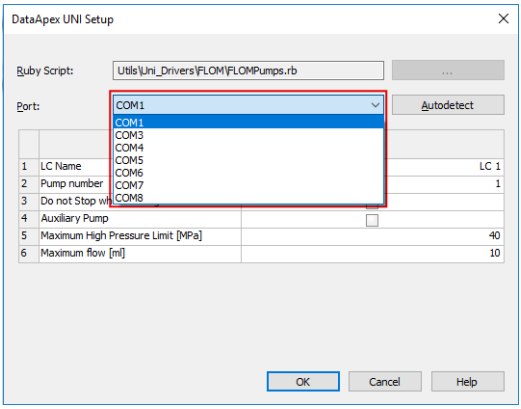


2. **Connect *Multicom* to a USB port in your computer.** It will be detected automatically.

More Info:

The “Found New Hardware” message will appear on the Windows taskbar and the LED diodes on the *MultiCOM* will be turned on one by one. Finally the message “New hardware is installed and ready to use” will appear.

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.**



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 Solid – 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.

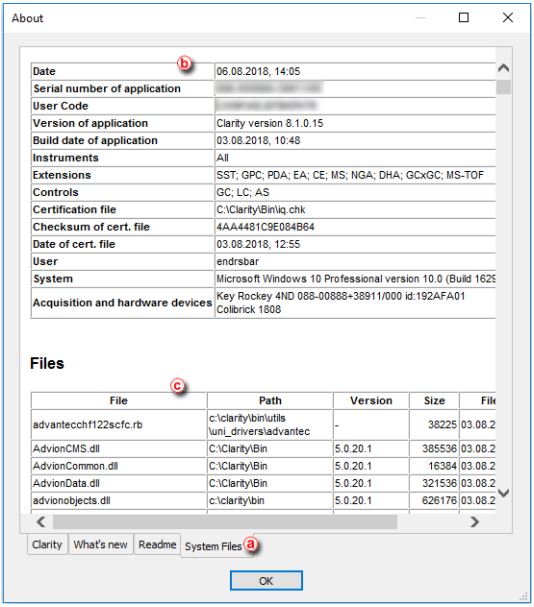
2.1 Obtaining information about Clarity configuration

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* window:** 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. **Go to the first table** ⓑ to find 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.

More Info:

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.



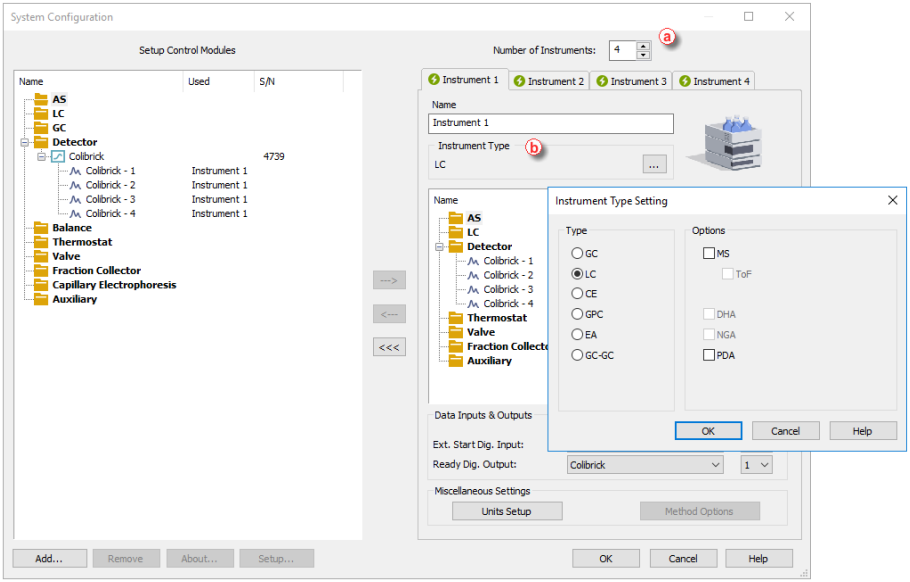
2.2 Setting the number and type of instruments

- **Enter the System Configuration dialog:** select *System - Configuration…* on the *Main* window.
- **In the Number of Instruments field** ⓐ a number of instruments can be set, based on licenses you bought.

  Note: The remaining instruments (up to four) can be used as offline instruments, e.g. if you bought 2 instruments, remaining 2 can be used as offline instruments. These instruments can be used in the same way as your standard ones except for data acquisition.

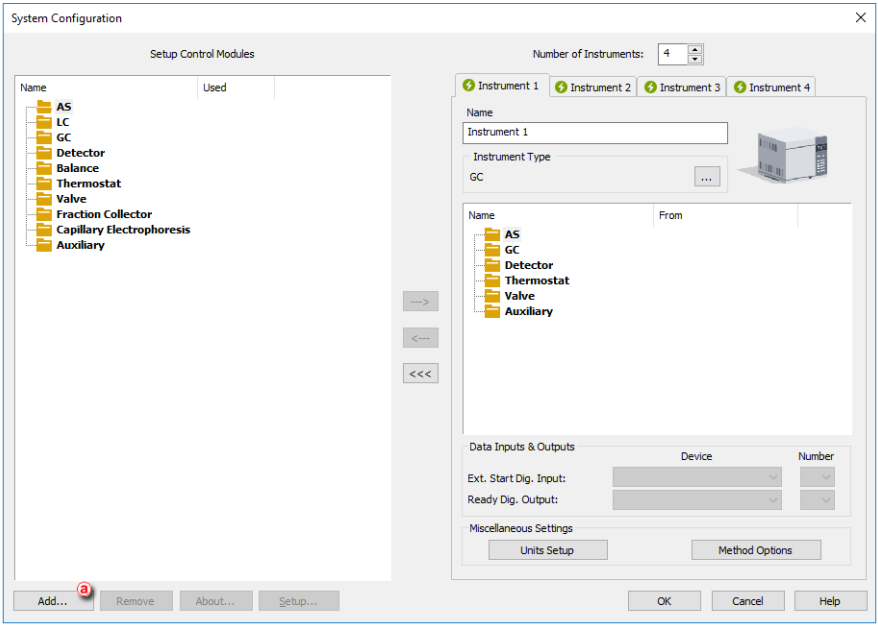
- **Set the Instrument Type** field ⓑ depending on the type of the device, GC or LC.

  For the rest of the instrument types GPC, PDA, EA, NGA, etc., you should purchase the license for the appropriate Extension.



2.3 Adding a new device

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

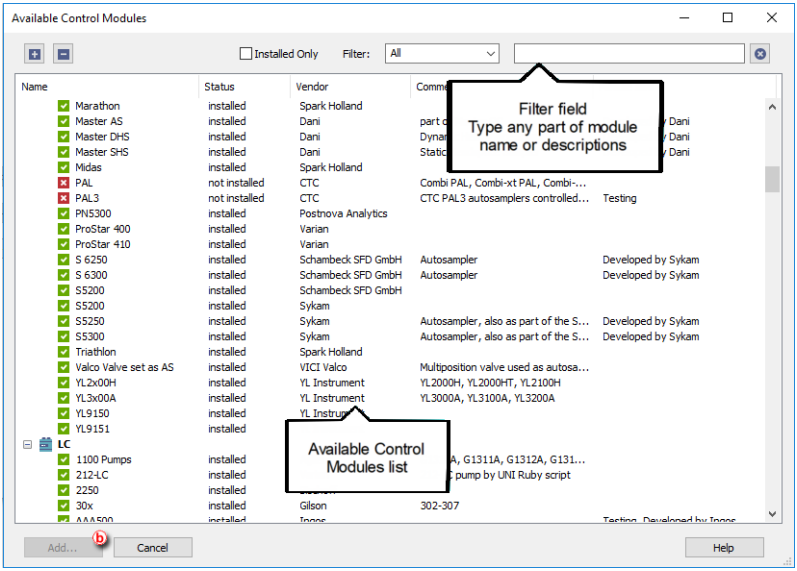


2. If the device you want to add is not in the list, **click on *Add*** ⓐ and the following window will open. Here you can filter the list by typing some text in the filter field or filter by Name, Vendor, etc.

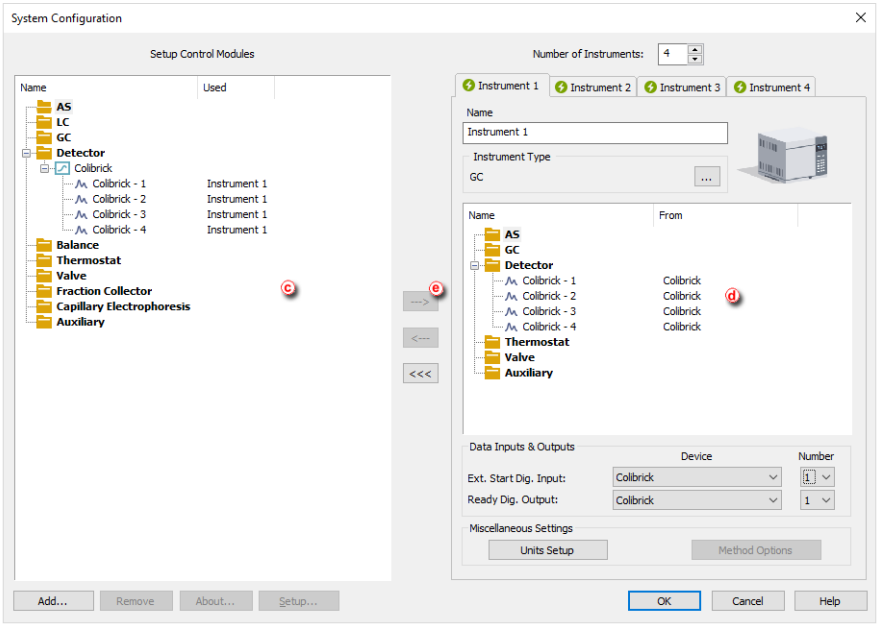
   More Info:

   If on the status column, says the module is not installed, you could install it by re-installing Clarity, clicking on *Custom Install* and selecting the module you wish to install.

3. **Select the device and click on *Add*.** ⓑ



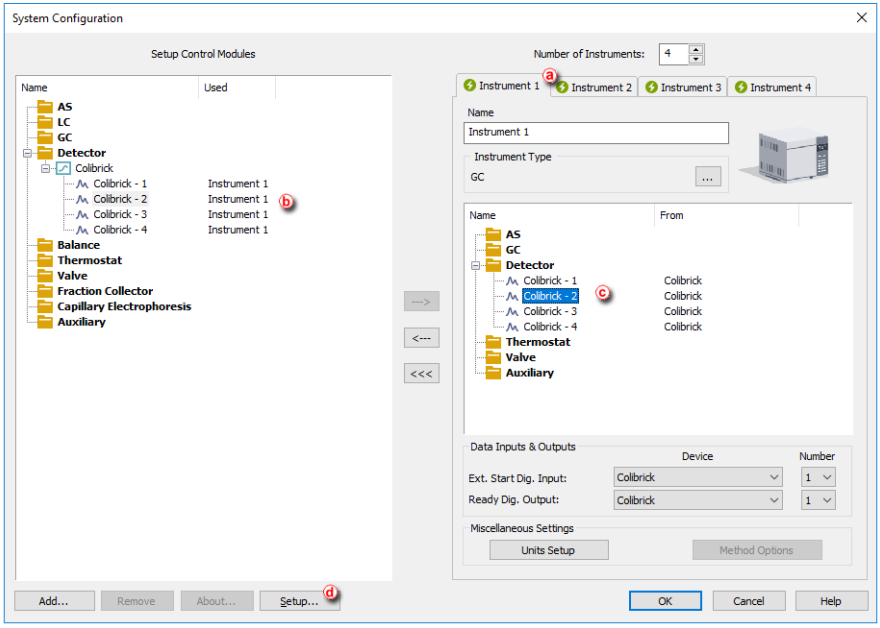
4. **Add new devices** to the appropriate instrument: drag and drop the instrument from the left pane ⓒ to the *Instrument* pane on the right ⓓ or select the device and click on ---> ⓔ.



5. If you need to configure a device, **go to the topic** Configuring a device.

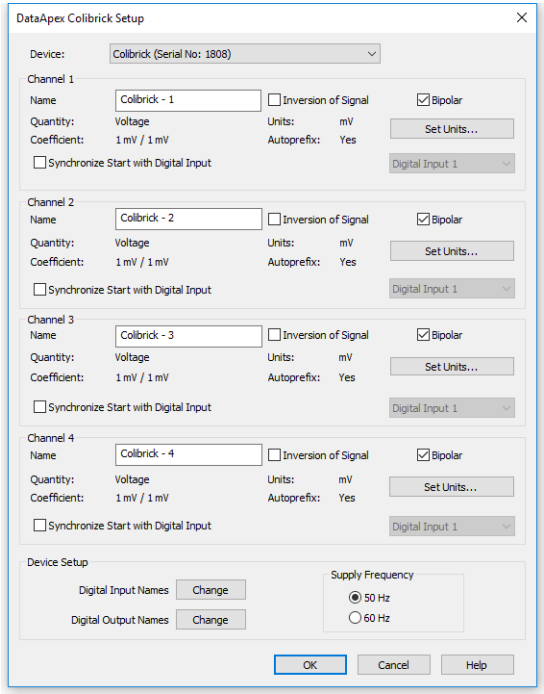
2.4 Configuring a device

1. **Enter the System Configuration dialog:** select *System - Configuration…* on the *Main* window.
2. **Select the Instrument 1..4:** click on the corresponding tab ⓐ.



3. **To configure a device, double click on it** ⓑ / ⓒ or click on *Setup...* ⓓ after selecting it. A device setup dialog will appear.

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

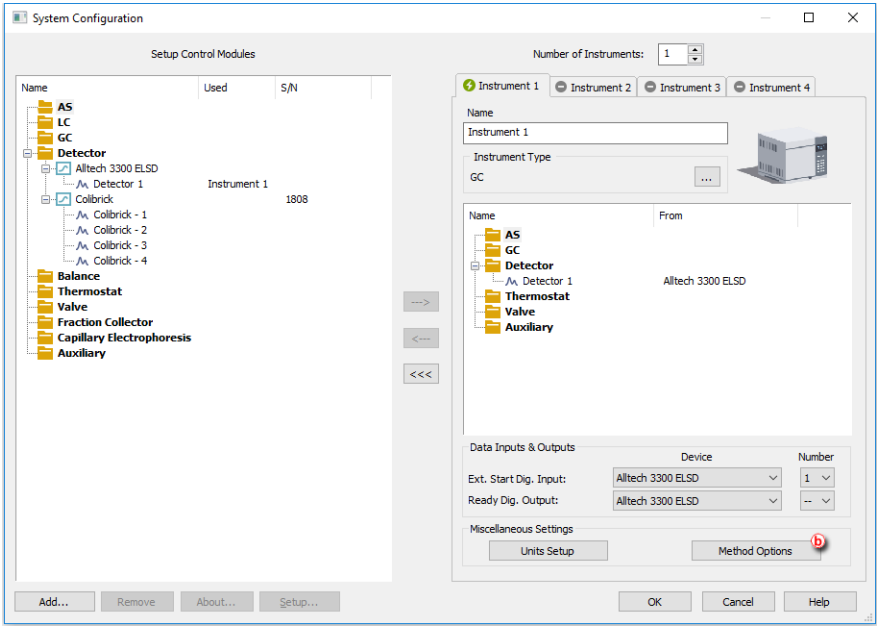


2.5 Automatic sending of a method to an instrument after each change

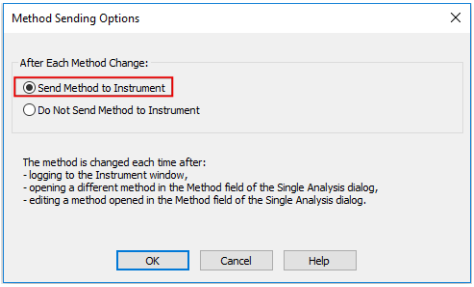
In a default Clarity installation, each time you change the method on Instrument, you need to send it manually to configured devices. Let's describe how to change that behavior that the method will be automatically sent to devices after each time you change the method.

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. **Set up the options** for sending the method to the instrument: in the group *Miscellaneous Settings* click on *Method Options* button. ⓐ



3. **Configure when to send the method to the instrument**.



If you select the *Send Method to Instrument* option, every time the instrument is opened or the method selected in Single Analysis window is modified, the method will be automatically sent. The method will be also sent when the sequence is finished.

2.6 Assigning digital input and output to start acquisition

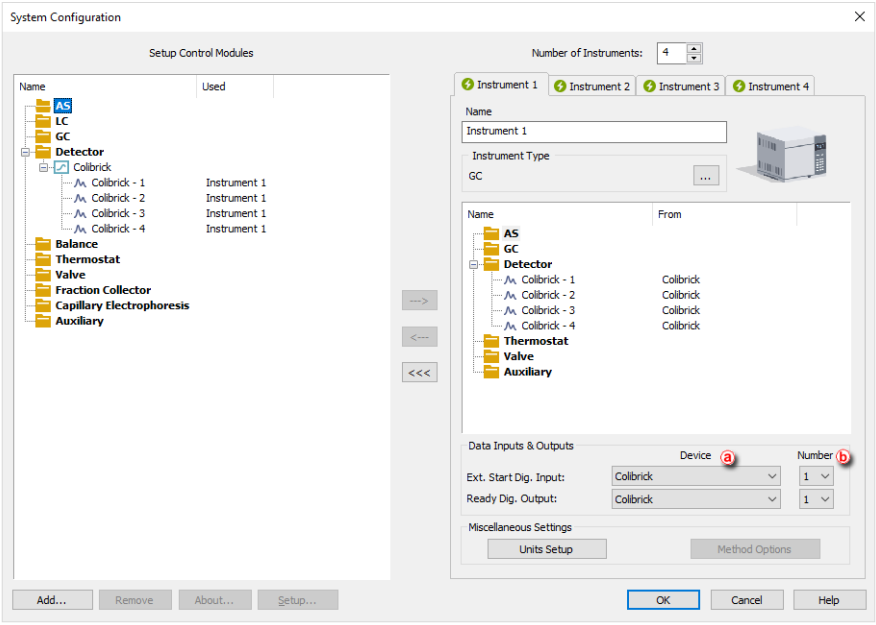
This chapter describes the most common wiring of autosamplers and start synchronization configuration through *Ext. Start Dig. Input* and *Ready Dig. Output* functions.

For more detailed information about connecting autosamplers and active or passive sequence see **Getting Started Manual.**

AS + GC set - ACTIVE sequence

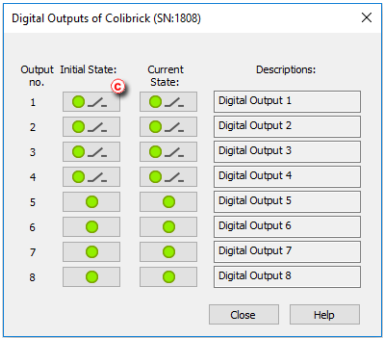
Variant A - Autosamplers started by **closing** the contacts.

1. Enter **System Configuration** dialog: Click *System - Configuration...* or on  icon.



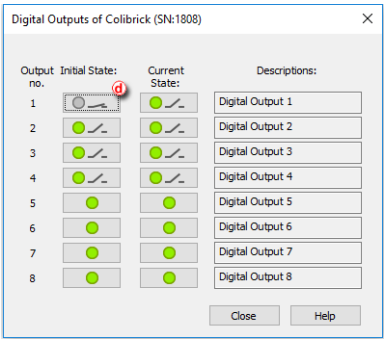
2. Add the required autosampler and assign it to the instrument according to "Add new device" and "Configuring a device".
3. In *Ext. Start Dig. Input* and *Ready Dig. Output* line set **Device** ⓐ to *Colibrick* and **Number** ⓑ to *1*.
4. Close **System Configuration** dialog.
5. Enter **Digital Outputs** dialog: Click *System - Digital Outputs...* or on  icon.

6. Set the **Output Initial State** to *HIGH* ⓒ.



Variant B - Autosamplers started by **opening** the contacts.

1. Perform steps 1-5 as in **Variant A**.
2. Set the **Output Initial State** to *LOW* ⓓ.

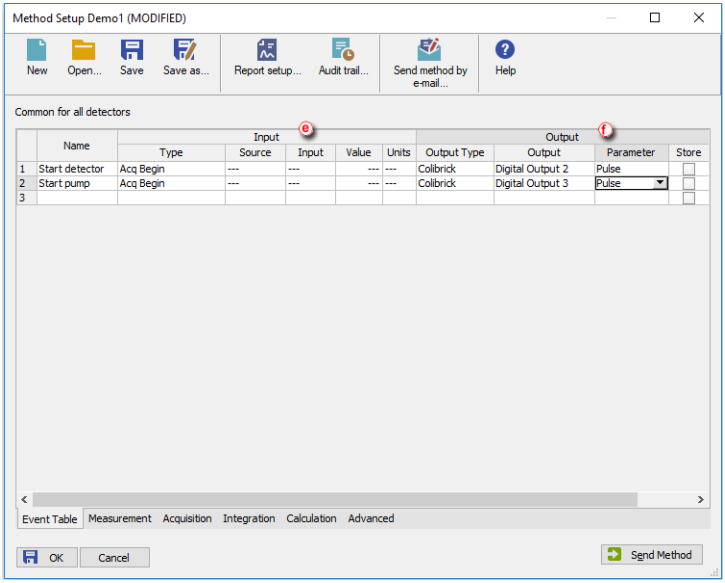


AS + LC set - ACTIVE sequence

Variant A - Autosampler sends the command to start acquisition directly back to **Clarity**. Event to start additional detectors and pumps from **Clarity** must be set in the Event Table.

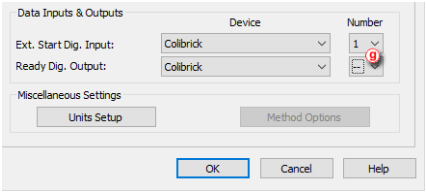
1. Enter **System Configuration**dialog: Click *System - Configuration...* or on icon.
2. Add the required autosampler and assign it to the instrument according to "Adding a new device" and "Configuring a device".
3. In *Ext. Start Dig. Input* and *Ready Dig. Output* line set **Device** to *Colibrick* and **Number** to *1*.
4. Close **System Configuration** dialog.

5. Enter **Event Table** dialog: Login to the Instrument and click *Method -Event Table...*
6. Set Events for Detector and Pump Inputs ⓔ and Outputs ⓕ.



Variant B - Autosampler sends the command to other device which sends the command to **Clarity** (in case when AS cannot be connected directly to **Clarity**).

1. Enter **System Configuration** dialog: Click *System - Configuration...* or on icon.
2. Add the required autosampler and assign it to the instrument according to "Add new device" and "Configuring a device".
3. In *Ext. Start Dig. Input* line set **Device** to *Colibrick* and **Number** to *1*.
4. In *Ready Dig. Output* line set **Device** to *Colibrick* and **Number** to -- ⓖ.



AS + GC set - PASSIVE sequence

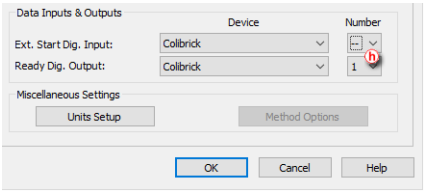
Autosampler initiates the injection after manual start on the device, GC then sends the command to start acquisition to **Clarity**.

1. Enter **System Configuration** dialog: Click *System - Configuration...* or on icon.
2. Add the required autosampler and assign it to the instrument according to "Add new device" and "Configuring a device".
3. In *Ext. Start Dig. Input* line set **Device** to *Colibrick* and **Number** to *1*.
4. In *Ready Dig. Output* line set **Device** to *Colibrick* and **Number** to -- .

AS + LC set - PASSIVE sequence

Variant A - Autosampler initiates the injection after manual start on the device and sends the command to start acquisition directly back to **Clarity**. Event to start additional detectors and pumps from **Clarity** must be set in the Event Table.

1. Enter **System Configuration** dialog: Click *System - Configuration...* or on icon.
2. Add the required autosampler and assign it to the instrument according to "Add new device" and "Configuring a device".
3. In *Ext. Start Dig. Input* line set **Device** to *Colibrick* and **Number** to --.
4. In *Ready Dig. Output* line set **Device** to *Colibrick* and **Number** to *1* ⓗ.
5. Close **System Configuration** dialog.
6. Enter **Event Table** dialog: Login to the Instrument and click *Method - Event Table...*
7. Set Events for Detector and Pump refer to **AS + LC set - ACTIVE sequence Variant A**



Variant B - Autosampler initiates the injection after manual start on the device and sends the command to other device which sends the command to **Clarity**.

1. Enter **System Configuration** dialog: Click *System - Configuration...* or on icon.
2. Add the required autosampler and assign it to the instrument according to "Adding a new device" and "Configuring a device".
3. In *Ext. Start Dig. Input* line set **Device** to *Colibrick* and **Number** to --.
4. In *Ready Dig. Output* line set **Device** to *Colibrick* and **Number** to *1* ⓗ.

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

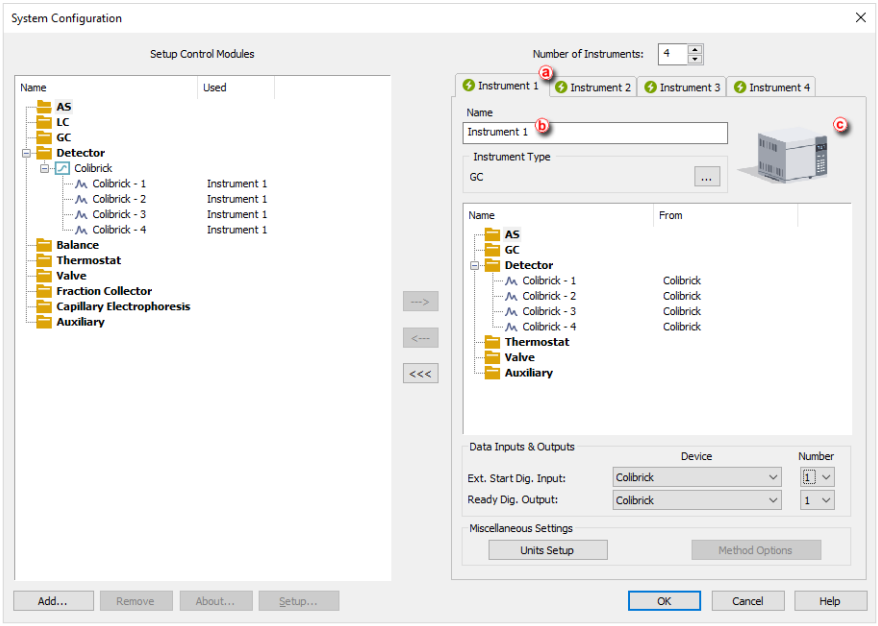
Refer to **AS + LC set - ACTIVE sequence Variant B**.

AS with Clarity control module - Active Sequence + digital acquisition

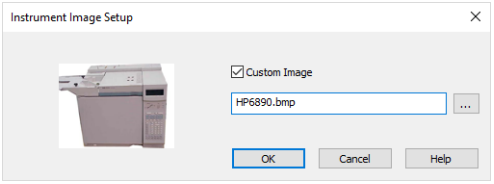
Refer to the corresponding **Clarity Control** manual.

2.7 Setting a custom image and a name for an instrument

1. **Enter the System Configuration dialog:** select *System - Configuration…*on 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 labeled *Image for Opened Instrument*** ⓒ to change the image.



5. **Click the *Custom Image* check box and then on ... to select your image. Click *OK* to save your changes.**
6. **Repeat steps 3 - 5** if you wish to change the names or the pictures on the other instruments.

3 Configuring the 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.

3.1 Configuring the User Accounts

The User Accounts can be configured from the System Configuration window. It allows you to configure the settings for each user (Name, Password, Access Rights and Digital Certificates).

1. **Open the *User Accounts* window:** click on  or choose *System - User Accounts*.

   More Info:

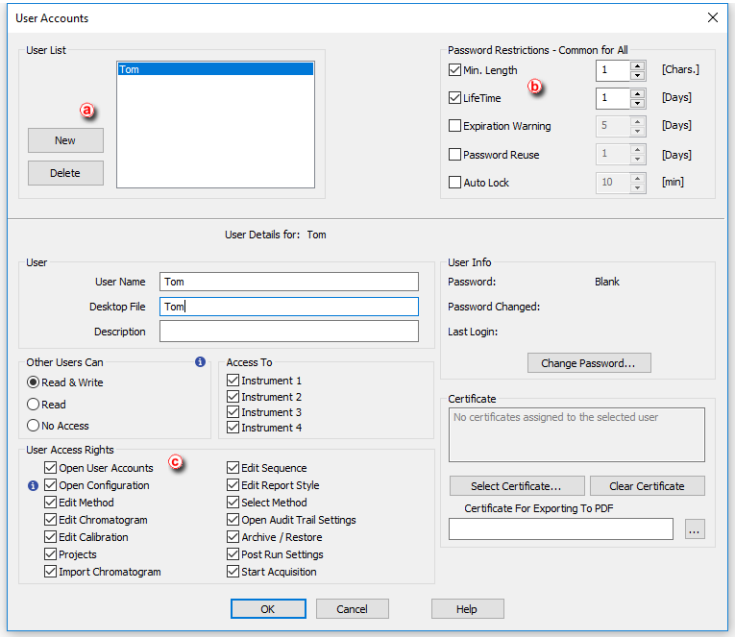
   The User Accounts window allows you to configure the settings for each user (Name, Password, Access Rights and Digital Certificates).

2. To create a new user**, click on the *New* button**ⓐ and then choose the preferred options from the ones offered.

   More Info:

   - Leave blank for unprotected mode - all users will share a common desktop file.
   - The desktop file (user profile) stores information about the last used project, table and graph settings, the files opened last, etc.

3. **Set the minimum password length and life time** ⓑ .
4. **Fill in the User Access Rights section**ⓒ in accordance to your company rules for GLP (Good Laboratory Practice) and CFR PART 11 compliance.



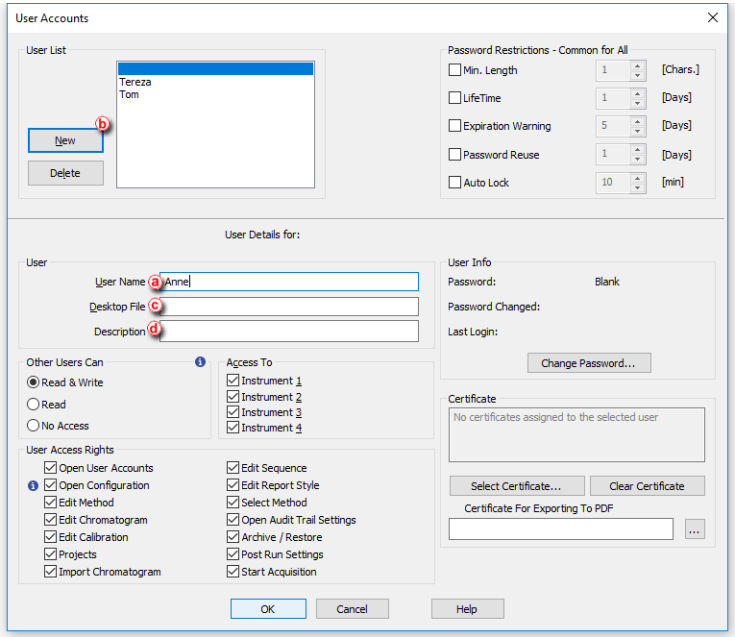
3.2 Creating a new user account

1. **Open the *User Accounts* window:** click on or choose *System - User Accounts*.
2. **To create a new user, fill in the New User Name ⓐ and click on the New button ⓑ.**

   The User's name will be placed on the headers of the files created while working in the station.
3. **Enter the desktop file name.** ⓒ

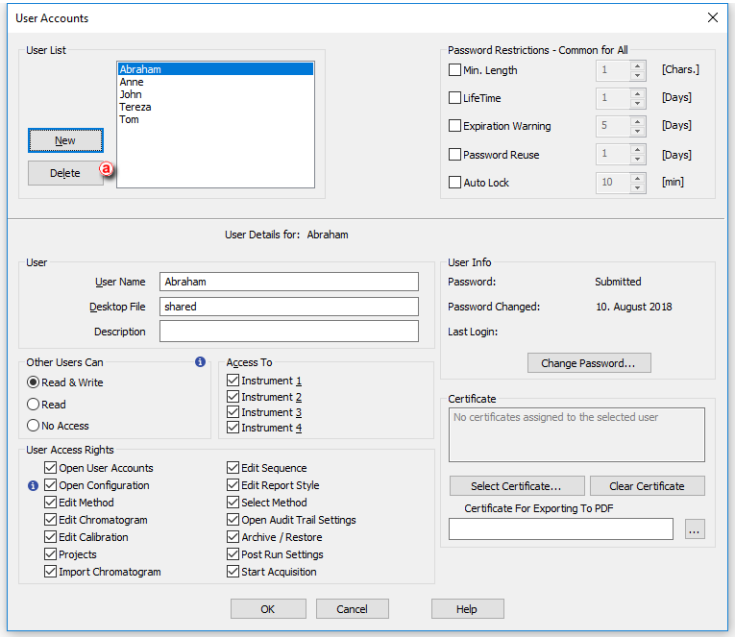
   More Info:

   This file contains settings about the size, location and visibility of the Instrument windows as well as all the amendable Instrument parameters which are not part of system files.
4. **Write here a user detailed description.** ⓓ
5. **Click *OK*** to accept the changes.



3.3 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 on the User List and then click on the Delete button ⓐ.**
3. **Click on the OK button to accept the changes.**



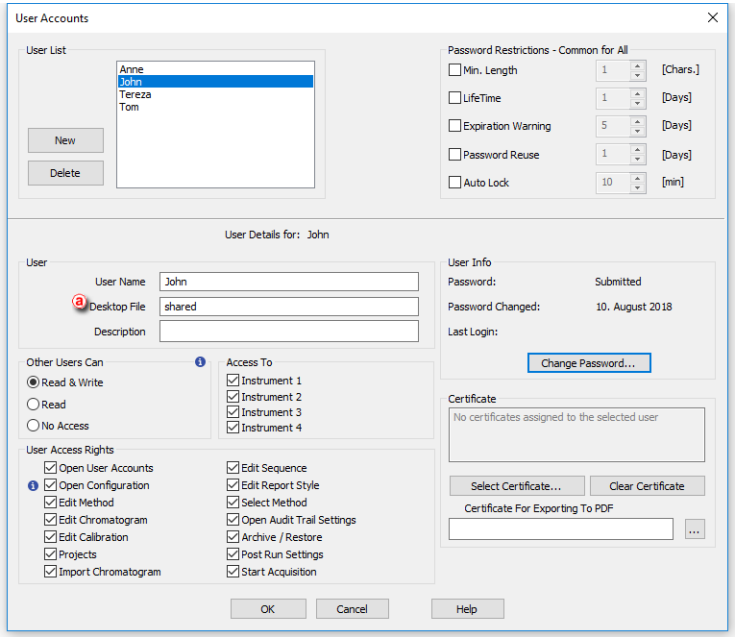
3.4 Sharing settings among users

1. **Open the *User Accounts* window:** click on or choose *System - User Accounts*.
2. **Select the user** with whom you want to share the settings from the users list.
3. **Then type the name of the desktop file** (user profile) to be shared by different users ⓐ.

   More Info:

   This file contains settings about the size, location and visibility of the Instrument windows as well as all the amendable *Instrument* parameters which are not part of system files.

4. **Click *OK* to accept the changes.**

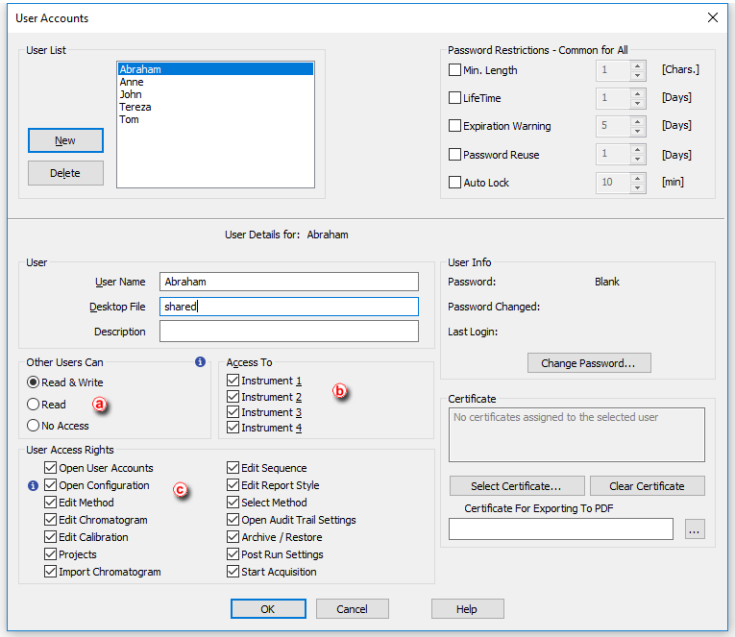


3.5 Restricting access

In Clarity it is possible to:

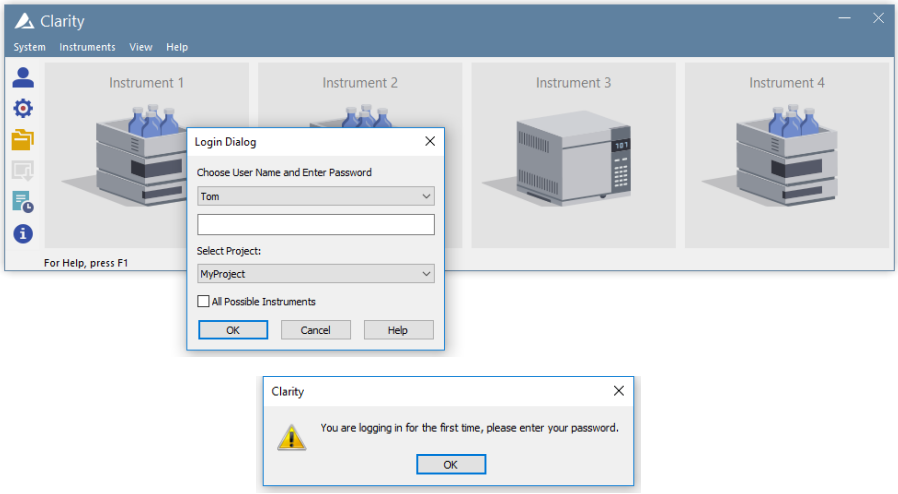
- Restrict other users' access to your files
- Restrict user's access to instruments
- Restrict user's access to Clarity procedures

1. **Open the *User Accounts* window:** click on or choose *System - User Accounts*.
2. **Configure the file access rights** for other users ⓐ.
3. **Tick the instruments** the user will have access to ⓑ.
4. **Tick the Clarity procedures** the user will have access to ⓒ.
5. **Click OK** to accept the changes.

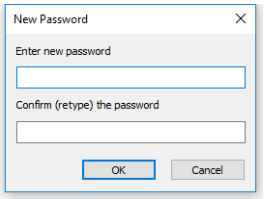


3.6 Setting a password for the first time

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 on the *Instrument* window, after selecting the user and clicking OK on the *Login Dialog*, you will be asked to enter a new password.



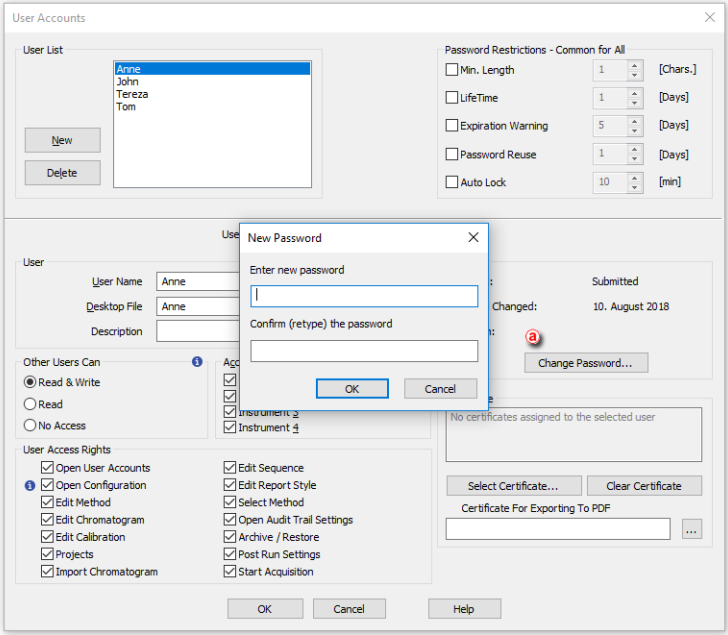
2. **Type in and confirm the new password and then click *OK*.**



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.**

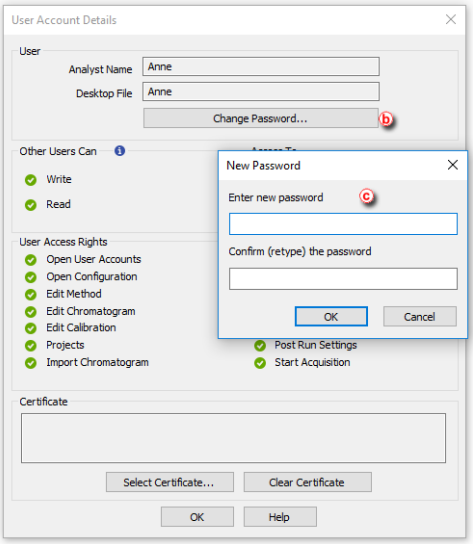
3.7 Changing a user password

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



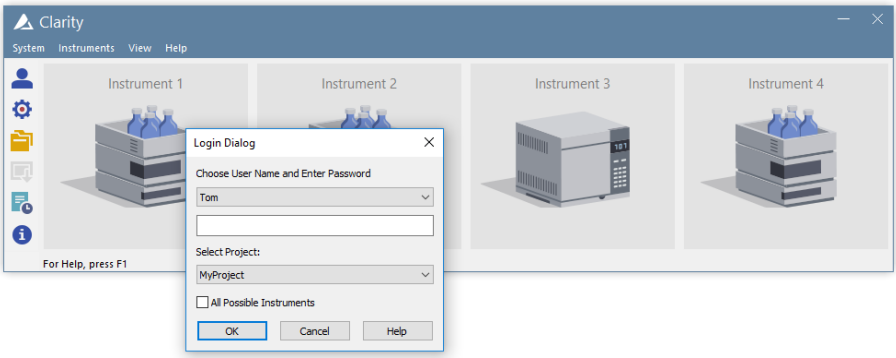
Alternatively you can change a new password by following these steps:

1. **Open the User Accounts Details window** by choosing *System - User Details*, selecting the user and entering the present password.
2. **Click on *Change Password* ⓑ and enter and confirm the new password.** ⓒ



3.8 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 set, in an previously created account as explained in Changing a user password.
2. **Click on the *Instrument*** you wish to open in the *Instrument* window.
3. **Select the user name and click OK** while leaving a blank password.



4 Method Setup

How to set up a method and set it as a template.

4.1 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 new sequence measurement each row has to be set manually.

Template Method vs. Chromatogram Method

- The sent method is used as a template for new chromatograms and its contents are copied onto the chromatogram file after acquisition or batch file reprocessing. You can open the different sections of the sent method setup from the icons in the Instrument window or with the command *Method - .....* on the toolbar.
- The changes to the chromatogram method do not affect the template method and they are performed in the lower pane of the Chromatogram window.
- The calibration file is linked to the template method and to the chromatogram method by its name.

Method Setup window

- The title of the Method Setup dialog displays a method that is currently opened. 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 it will be automatically saved and Method Setup dialog will close.

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 - just as before.
    - 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.

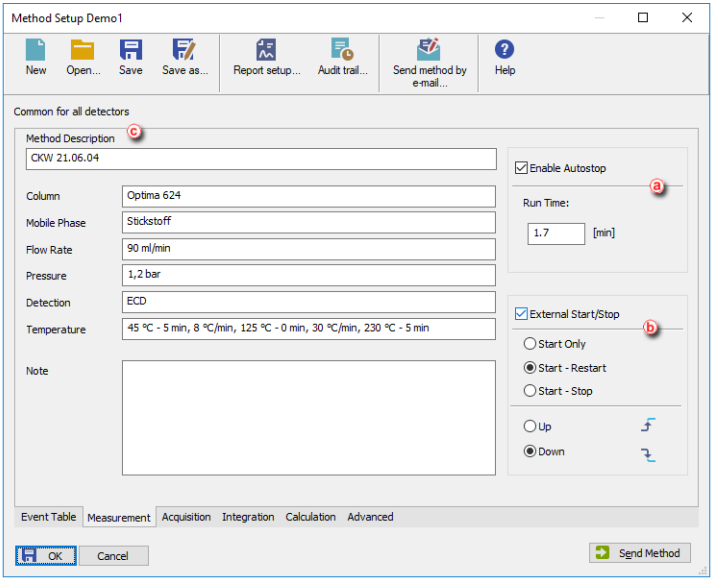
Method Development

You can edit or develop any method without changing the current method until you send the new on by pressing *Send Method*
When developing a method, you can configure the following settings among others:

1. **Set the measurement conditions.**

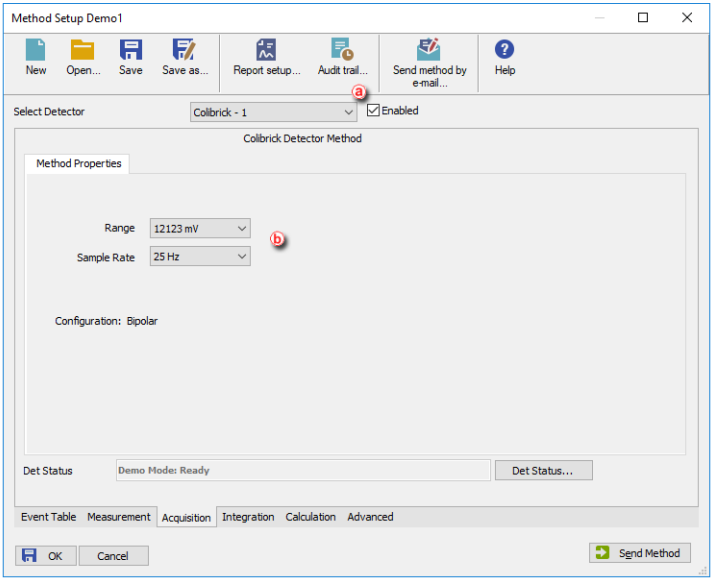
More Info:

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 ⓑ. Also you can describe some options of the method and add a note ⓒ.



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

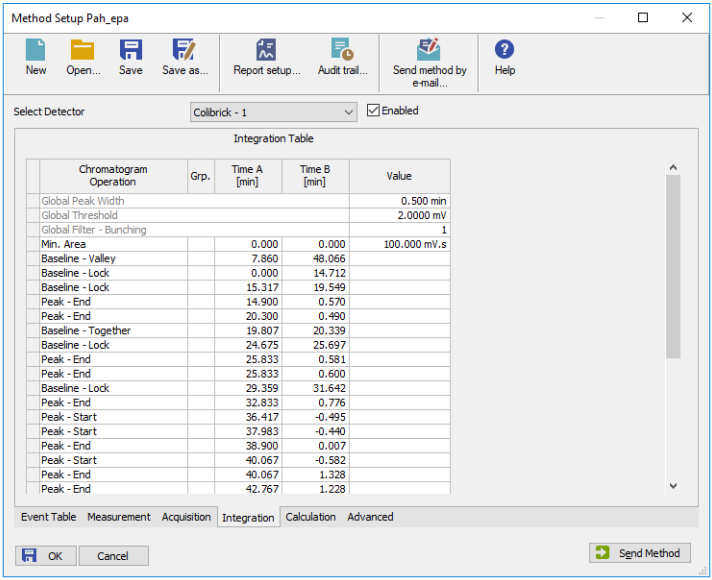
   It allows you to select and enable the detector ⓐ and to set the signal range and sample rate ⓑ. At any time at least one detector has to be *Enabled*.



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

More Info:

When using a multi-detector configuration, there is a specific integration table for each detector.
All operations are editable and programmable in time. If you aren't able to edit tab parameters the current detector probably isn't *Enabled*.
The integration parameters are optimized for a sample rate of 10 Hz and a 10000 mV range.

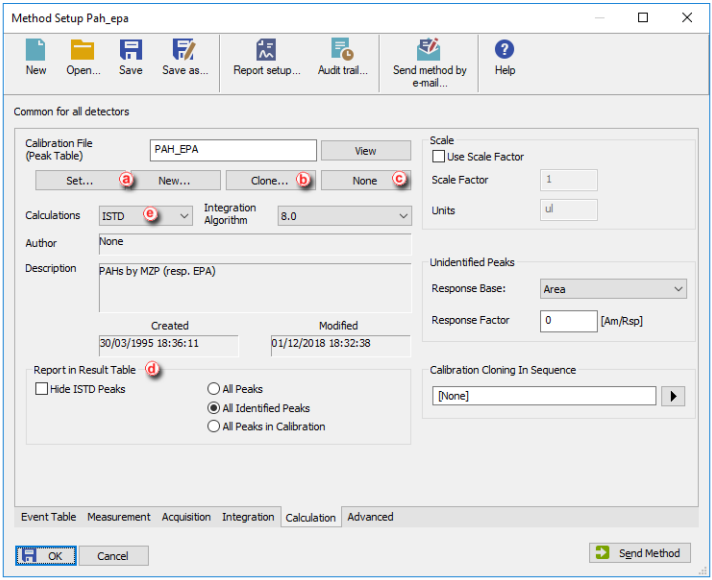


Note: Although Integration parameters are editable on the method setup window they are usually modified manually after data acquisition on the chromatogram window itself. Then you can manually rewrite them into any method in the Method Setup dialog or you can use the *Method - Save as Template* menu command in the Chromatogram window. For more details see the chapter **Saving the chromatogram method as a template method** on pg **73**..

4. **Set the calculation options.**

More Info:

- In this tab you can create *New...* calibration file or *Set...* the one created previously ⓐ and configure the different settings related to it.
- After data acquisition, chromatograms from unknown samples will be calibrated and chromatograms from calibration standards may be used to automatically re-calibrate the attached calibration file.
- *Clone...* ⓑ button will create a copy of a current calibration file. By using the *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 reports ⓓ and set Calculation Type ⓔ to see detail about each type invoke help (F1).



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

More Info:

The table also has an Event Table tab, used for configuring what events will be triggered and when. It may also have some extra tabs corresponding to the control modules (LC, GPC, EA, etc.). For more information on this or any of the settings above, press F1 in Clarity and go to the corresponding section or go to the **Clarity Reference Guide**.

4.2 Saving the chromatogram method as a template method

The method saved in the chromatogram file may be needed as a template method for further use - for example because the integration table is fully customized to that type of analysis, the chromatogram has a linked calibration file that will be later linked to new chromatograms or simply because the original template method was lost.

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Select the *Method - Save as Template...* to save the method** (including the integration parameters) from the current chromatogram as a new method.

More Info:

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

4.3 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 option is only available for some pumps controlled by Zebrick, CB20 D/A converters or UNI Ruby scripts.

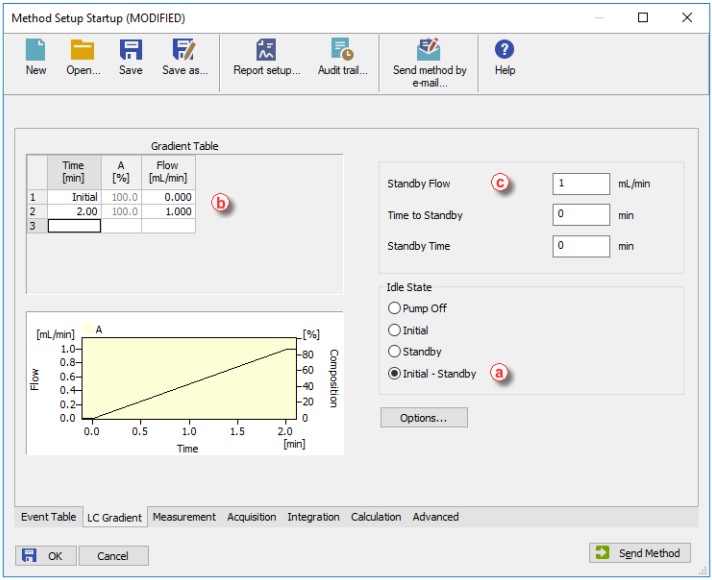
1. **Set the *Instrument Method Sending* options to *"Do not send Method to Instrument"*** as explained in Setting the options for sending the method to the instrument.

Startup Method

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

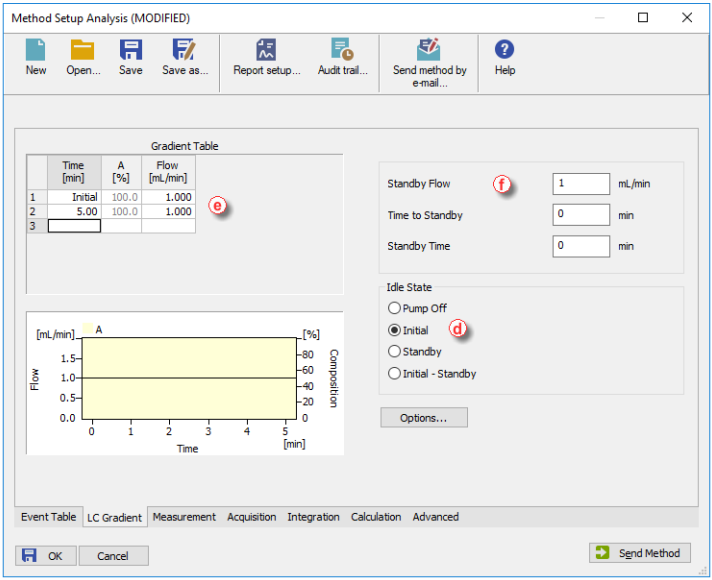
More Info:

In our example, the *Standby Flow* rate is 1 ml/m and the time 2 min.



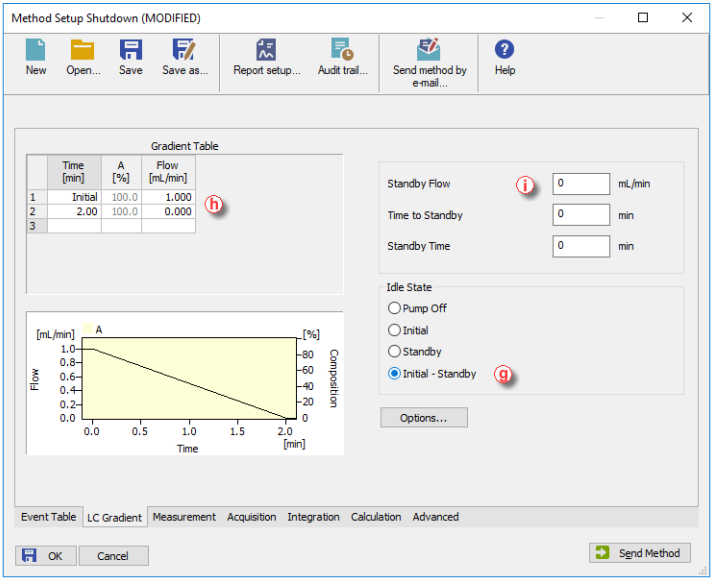
Analysis Method

8. **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* and the *Flow* on the second row ⓔ to the previous *Standby* value. ⓕ
   - Set the *Time* to the total duration of your analysis. ⓔ



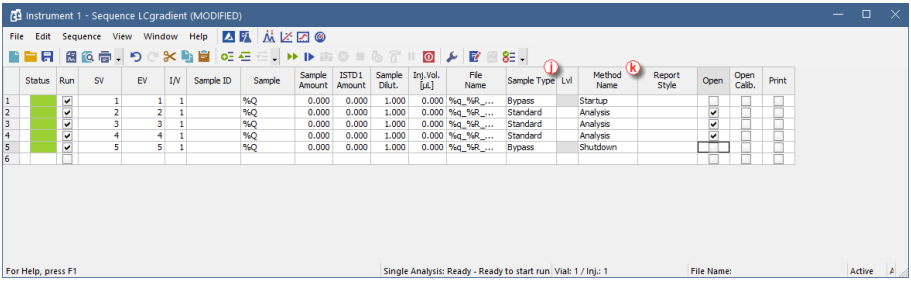
Shutdown Method

9. **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

10. **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*.

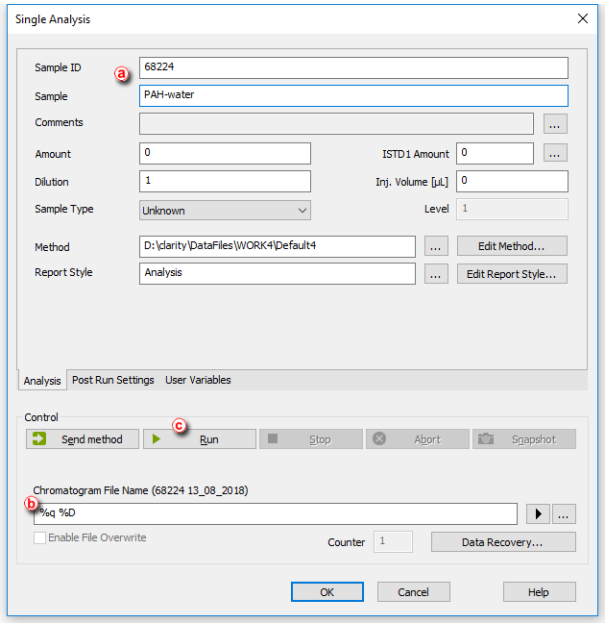


5 Data Acquisition

Chapters describing how to perform a measurement using *Single Analysis* or *Sequence* and how to evaluate chromatograms during run.

5.1 Running a single analysis

1. **Open the *Single Analysis* dialog:** select *Analysis - Single* from the *Instrument* window or click on  .



2. **Fill in the information on the sample** into the *Sample ID* and/or *Sample* fields ⓐ.
3. **Fill in the *Chromatogram File Name*** ⓑ.

More Info:

If you use variables (for example, *%q* will use the *Sample ID* as a part of the file name), the resulting file name will be shown in brackets just above the *Chromatogram File Name* field. For more info on variables go to "Chromatogram File Name" in the **Clarity Reference Guide**.

4. **Run the analysis:** click on the *Run* button ⓒ or click  on the *Data Acquisition* window.

More Info:

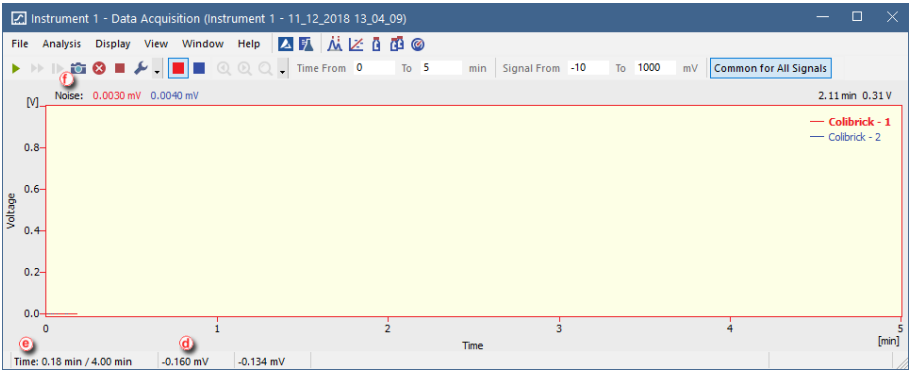
Also it can be triggered by *External Start* from the Chromatograph. The Instrument will get to the *RUNNING* state and the *Single Analysis* dialog will close. The state is visible in the status line on the *Instrument* window.

5. **Open the *Data Acquisition* window** to monitor the analysis: select *Analysis - Data Acquisition* or click on the Instrument window.

6. **Watch the signal both in the graph and in the status bar** ⓓ.

More Info:

The analysis time is shown in the leftmost part of the status bar ⓔ. You can also take a snapshot of the acquired signal ⓕ. More info in Pre-evaluating a chromatogram during acquisition.



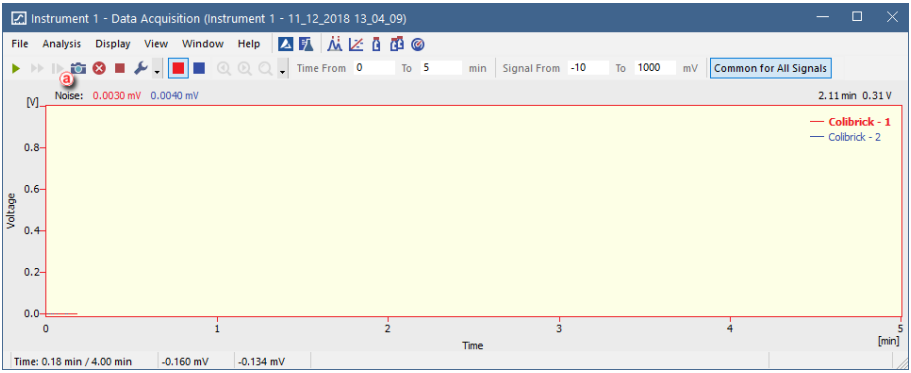
5.2 Pre-evaluating a chromatogram during acquisition

1. **Open the *Data Acquisition* window:** select *Monitor - Data Acquisition* or click on on the *Instrument window*.

2. **To create a temporary chromatogram**, select *Analysis - Snapshot* or click on ⓐ.

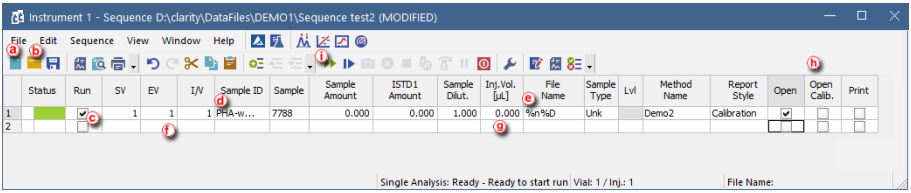
More Info:

- Every time you take a snapshot, the data will be evaluated again from the beginning up to the point where you clicked.
- If you would like to preserve the snapshot, save it. Otherwise it may be overwritten, for example if you selected the Autostop option on the Method.



5.3 Creating and running a sequence

1. **Open the *Sequence* window:** select *Analysis - Sequence* or click on .
2. **Create a new sequence file:** click on ⓐ. or open an already created sequence ⓑ.
3. **Give it a name** (*MySequence* in this case) and **save it** selecting *File - Save As*….



4. **Check the checkbox in the first (empty) row** in the *Run* column ⓒ.
   The first row will be pre-filled with default basic information on the analysis (such as the method file used).
5. **Fill in the *Sample ID* and/or *Sample* columns**. ⓓ
6. **Fill in the *File Name* .** ⓔ

   More Info:

   You can use variables, for example, *%q* (*Sample ID*) as a part of the file name. Hold the mouse pointer over the file name field to see resulting name. For more info on variables go to "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.
8. **Fill in volume of the injection in the *Inj. Vol.* column ⓖ.**

9. Tick any of the **Open, Open Calib. or Print options** ⓗ in case you wish to open measured chromatogram, open measured standard or print the results after each measurement of a sample.
10. **Repeat the steps 4-8**for any rows you need to add to the Sequence Table.
11. **Check the validity of the sequence:** select *Sequence - Check Sequence* or click on .

More Info:

In valid sequences, all rows will show the symbol in the *Sts.* column. Invalid sequences will issue a warning message with the cause of the problem.

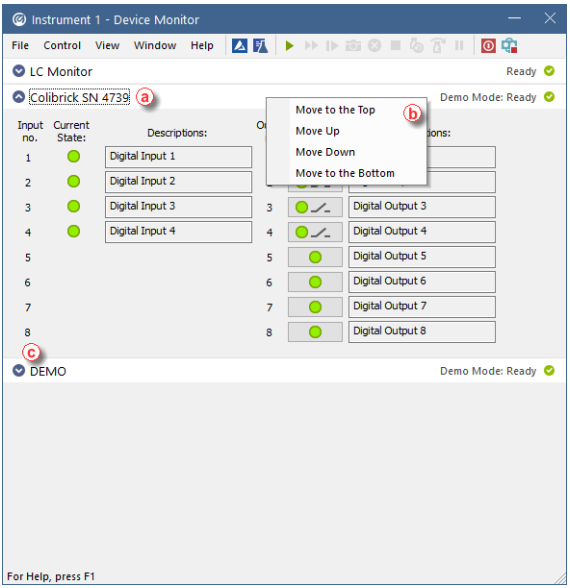
12. **Save the sequence:** select *File - Save* or click on .
13. **Run the prepared sequence:** select *Sequence - Run* or click on ⓘ.

More Info:

The sequence state will change to *WAITING FOR INJECTION*, if no controlled autosampler is connected, or to *INJECTING*, if a controlled autosampler is connected and correctly configured, and all other controlled modules are on *READY* state. The state is visible at the bottom of the Sequence window.

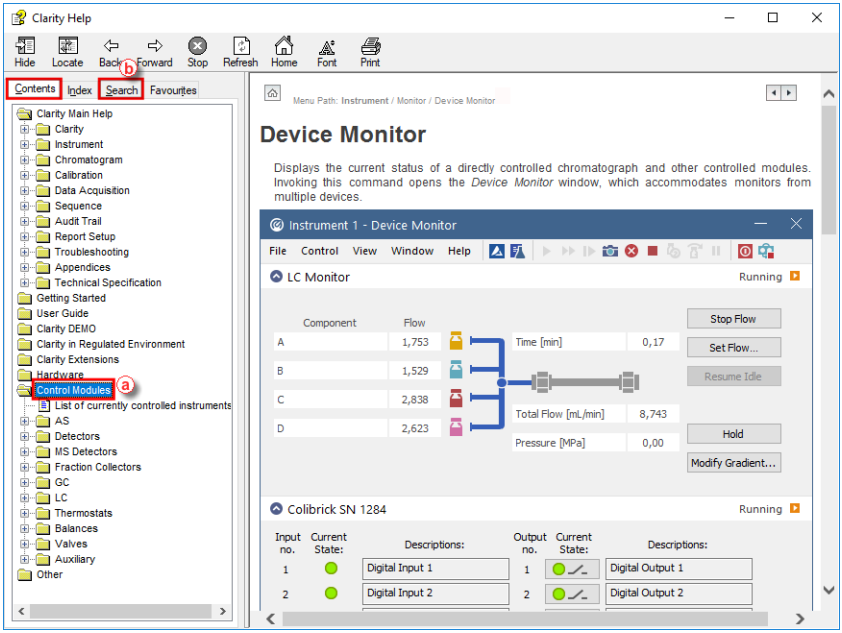
6 Device Monitor

The Device Monitor window serves firstly to show the current status of each control module and secondly for direct control of the device.
The 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 icon ⓒ in the header of the panel.



6.1 How to set parameters during run

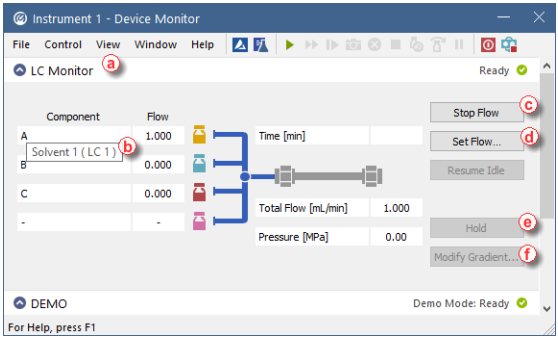
Besides performing some service commands outside run, in some cases it is possible to perform some actions also during run. This is individual for specific control modules and could be found in the Help filer or espective control module manual using the *Contents tab*(the *Control Modules* folder ⓐ) or using the *Search tab*ⓑ or go to www.dataapex.com/downloads.
Common for the pumps configured to the LC Gradient is the LC Gradient pane described in next chapter.



6.2 How to directly control LC gradient pumps during run

For gradient pumps, the monitor consists of the LC Monitor ⓐ section common to all pumps present in the gradient. Maximum number of solvents configured to LC Gradient is 4 - it could be any combination of isocratic and gradient pumps. If another pump needed, it has to be add as auxiliary pump.

Note: Tooltip ⓑ over each component shows name of the current pump.



It is possible to change parameters in the Device Monitor - LC Monitor window such as stopping the pumps ⓒ without stopping the acquisition. The *Flow* for each solvent, *Total Flow* and *Max Pressure* can be also

changed using the Set flow ⓓ window. When using the *Stop Flow* or *Set Flow* button, gradient cannot be restored and the set flow will be used for the rest of acquisition.
For selected pump models (typically those controlled by Clarity in real time) are available further commands to amend the gradient conditions during run.

How to keep current gradient conditions for longer than set in the Method Setup - LC-Gradient

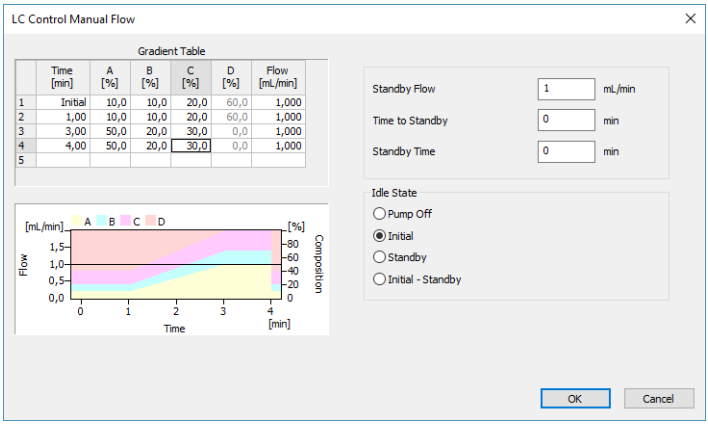
When the desired gradient is current, press *Hold* ⓔ button. To continue with the gradient use the same button, which changed to *Resume*.

How to change gradient

Invoke the LC Control Manual Flow window via *Modify Gradient...* ⓕ button. This window resembles the Method Setup- LC Gradient functionality and once the OK button is pressed the original LC - Gradient method data are replaced for this measurement. All such operations are recorded into the current chromatogram Audit Trail and the amended gradient will be stored within the chromatogram.

Note:

- The LC Control Manual Flow dialog is only available during the analysis run.
- The template method is not affected.



7 Chromatogram Editing

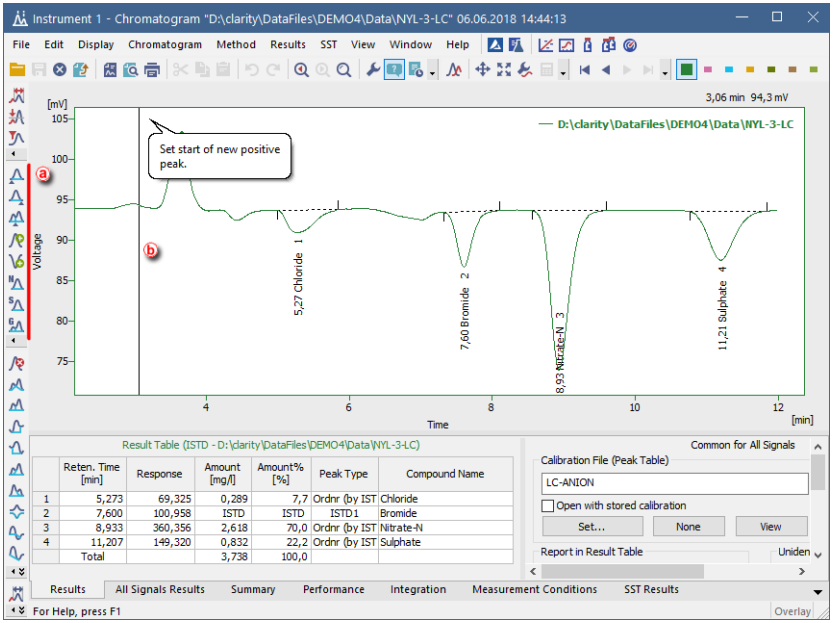
Following topics help you how to navigate in the chromatogram window, adjust integration table or preset basic parameters.

7.1 Modifying a peak not integrated correctly

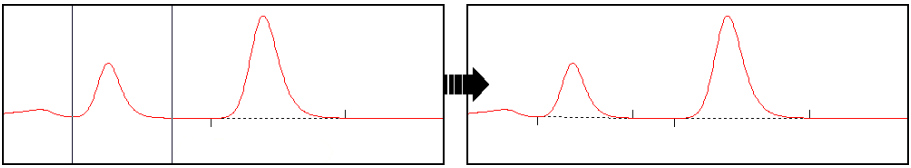
1. If you want to re-calculate a peak integrated incorrectly, follow the steps in section Remove a peak from integration.Then add the peak as explained on section Add a new peak.
2. If you need to change the position of beginning and / or end of the peak, go to section Modifying the beginning and the end of a peak.
3. You can also modify the **Global Peak Width and / or Threshold** (minimum width or height of the peak for it to be integrated) for the whole Chromatogram or the **Local Peak With and / or Threshold** if a group of peaks needs to be corrected at once as explained in section Modifying Minimum Width and Threshold.

7.2 Adding a new peak manually

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Select *Chromatogram - Peak - Add Positive/Negative*** in the main menu or in the context menu (right mouse-click in the graph) or click on  and  in the *Peak* toolbar ⓐ.
3. **Click in the chromatogram and set the beginning ⓑ and the end of a new peak**.

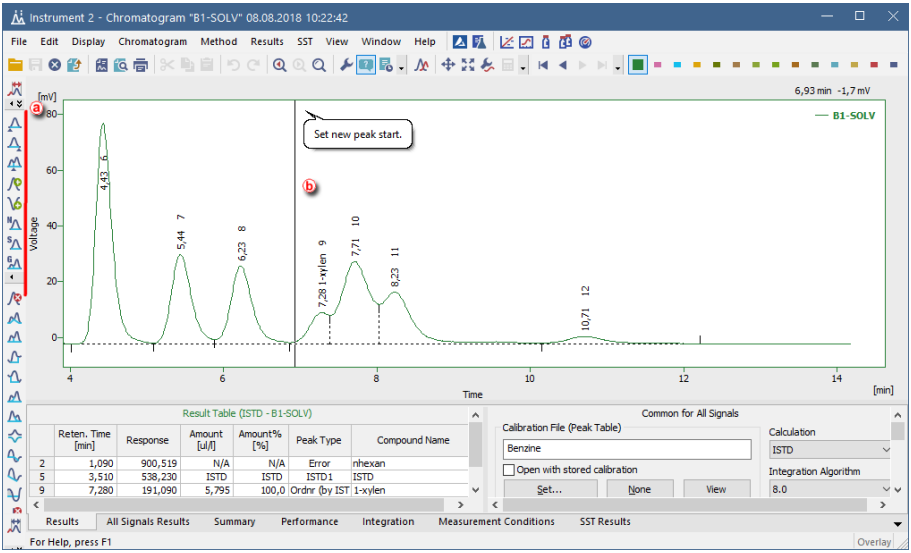


Note the two vertical guidelines marking the beginning and end of the peak.



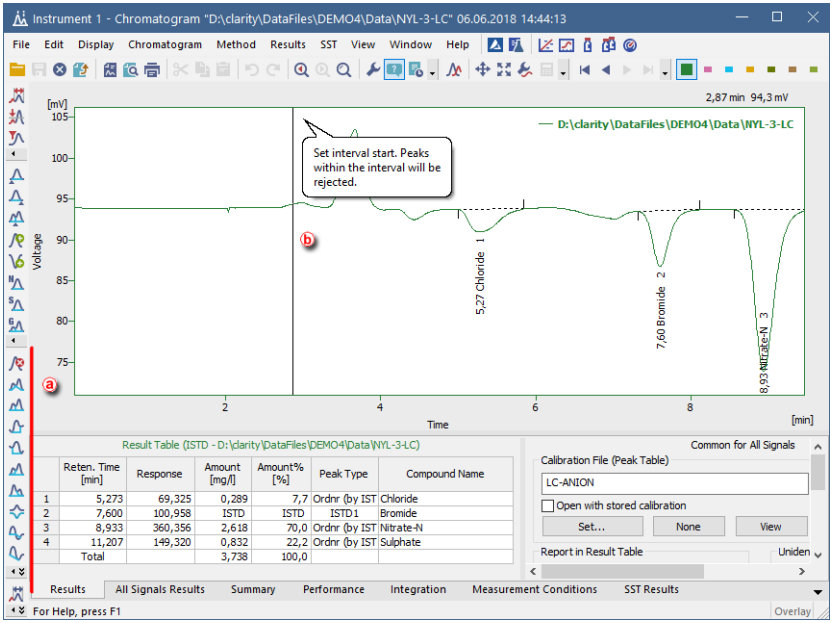
7.3 Modifying the beginning and the end of a peak

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Change the position of beginning and/or end of the peak:** select *Peak-Start* or *Peak-End* or click on or in the *Peak* toolbar ⓐ.
3. **Set the new beginning ⓑ and/or end by clicking on the new position**

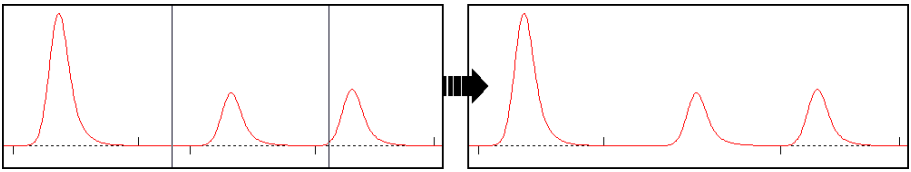


7.4 Removing a peak from integration manually

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Launch the *Lock* command:** select *Chromatogram - Baseline - Lock* on the main menu or in the context menu (right mouse-click in the chromatogram curve area) or click on in the *Baseline* toolbar ⓐ.
3. **Click once before and after ⓑ the apex of particular peak.**

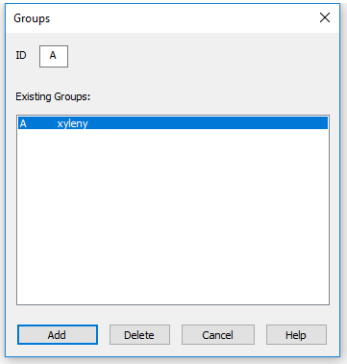


Note the two vertical guidelines marking the beginning and end of the peak. More than one peak can be removed from integration at once.

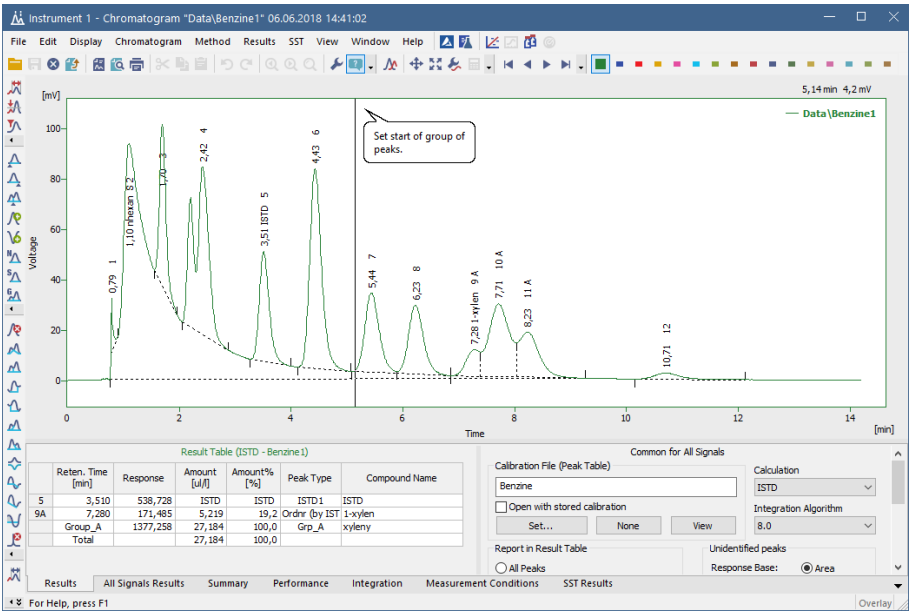


7.5 Adding a peak to a group

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Click on the *Chromatogram - Peak - Groups…*** menu to display the dialog.

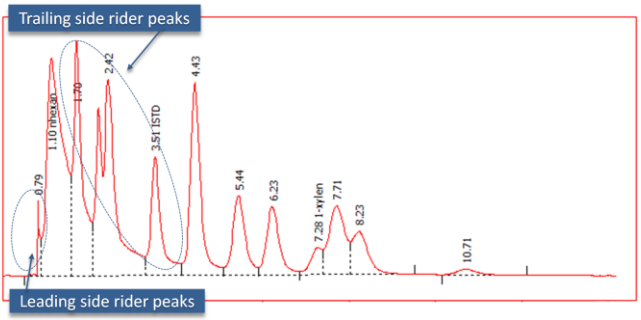


3. **Select an existing group from the list and click the *Add* button.**
4. **Click on the chromatogram for the first time to select the start point and second time for selecting the end point of the interval.** Peaks with apexes found in the interval will be added to the new group.

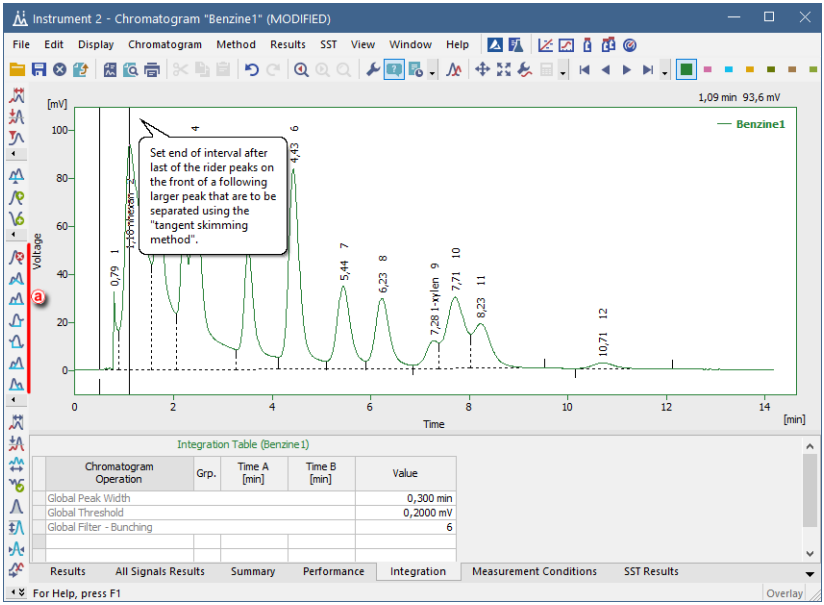


7.6 Separating rider peaks by tangent

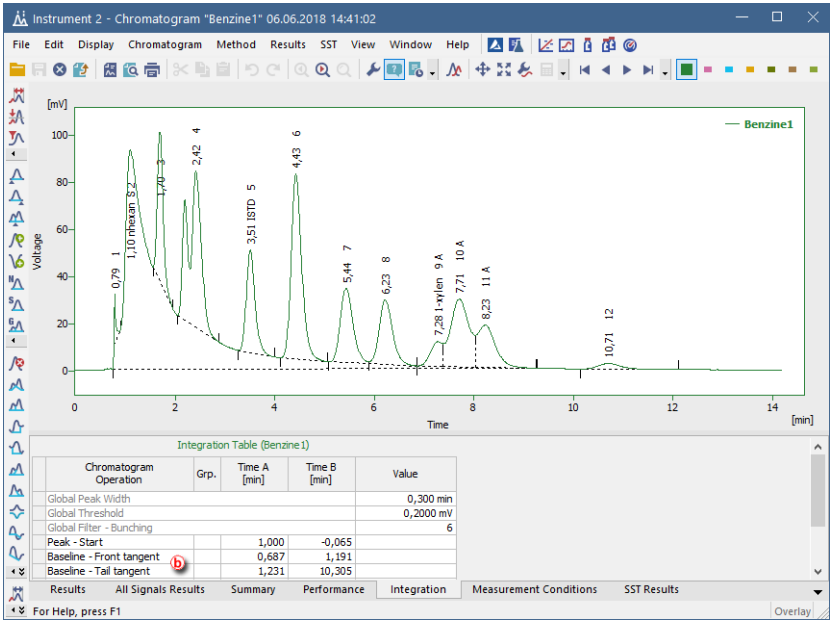
Rider peaks are small peaks which are not well resolved from a large and asymmetrical neighbor but sit on its leading or trailing side.



1. **Open the *Chromatogram* window and then the chromatogram**.



2. **Select the rider peaks you want to separate on the leading side of the mother peak:** choose *Chromatogram - Integration - Front Tangent* or click on the toolbar ⓐ.
3. **Select the rider peaks you want to separate on the trailing side of the mother peak:** choose *Chromatogram - Integration - Tail Tangent* or click on the toolbar ⓐ.
4. **You can check, modify the range or delete this operations** in the Integration tab (Baseline - Front tangent and *Baseline - Tail tangent*) ⓑ.

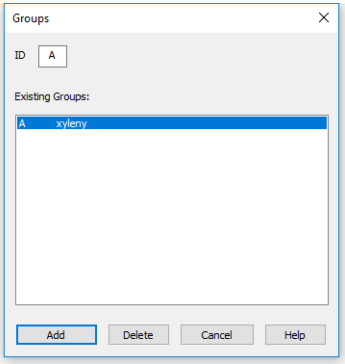


More Info:

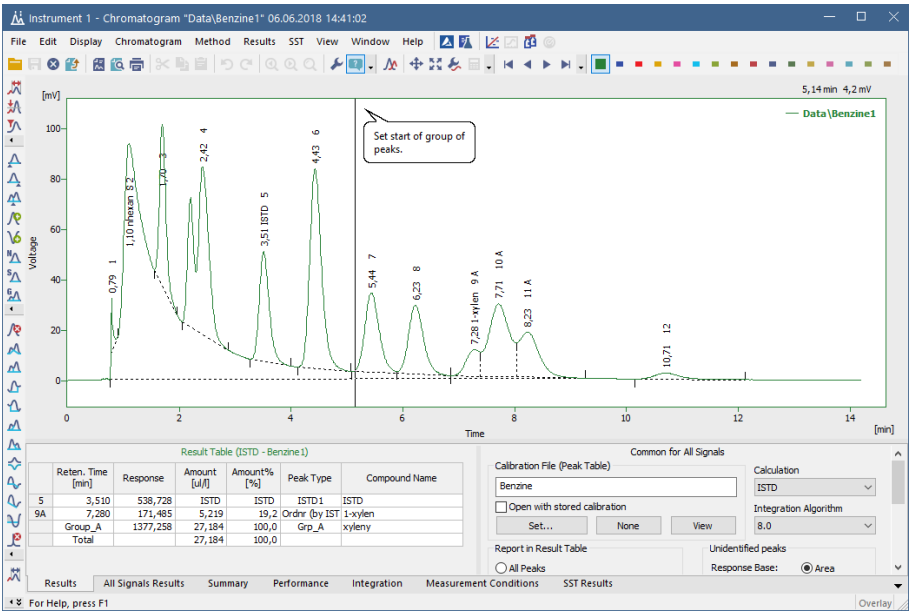
You can also use the Tangent Slope Ratio and Tangent Area Ratio under *Chromatogram - Separation* to establish a threshold for the separation of rider peaks based in those two parameters.

7.7 Removing a peak from a group

1. **Open the *Chromatogram* window and select *Chromatogram - Peak - Groups…***



2. **Select an existing group from the list and click *Delete.*** The *Chromatogram* window will show a cursor for removing peaks from the selected group.
3. **Click on the chromatogram to select the start and again to select the end of the interval** to be removed from the group.

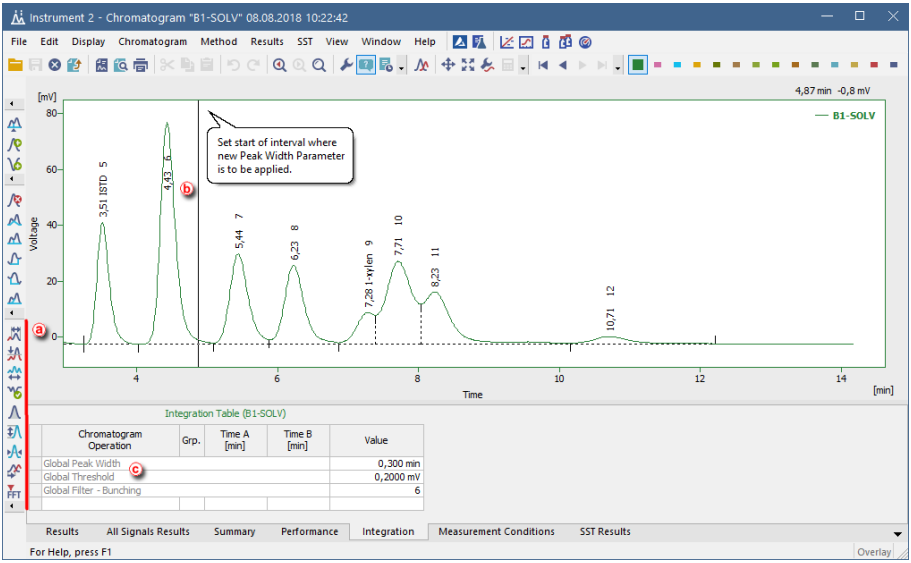


7.8 Modifying Minimum Width and Threshold

Peaks are only integrated if they exceed a minimum width and height. If you wish to exclude peaks from the integration according to this criteria, it can be achieved both globally or locally in a specified interval.

For setting the Local Peak Width or Threshold:

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Set the interval you want to modify:** ⓑ select *Local Peak Width or Threshold* on the menu item *Chromatogram - Integration* (or click on and on the toolbar ⓐ.

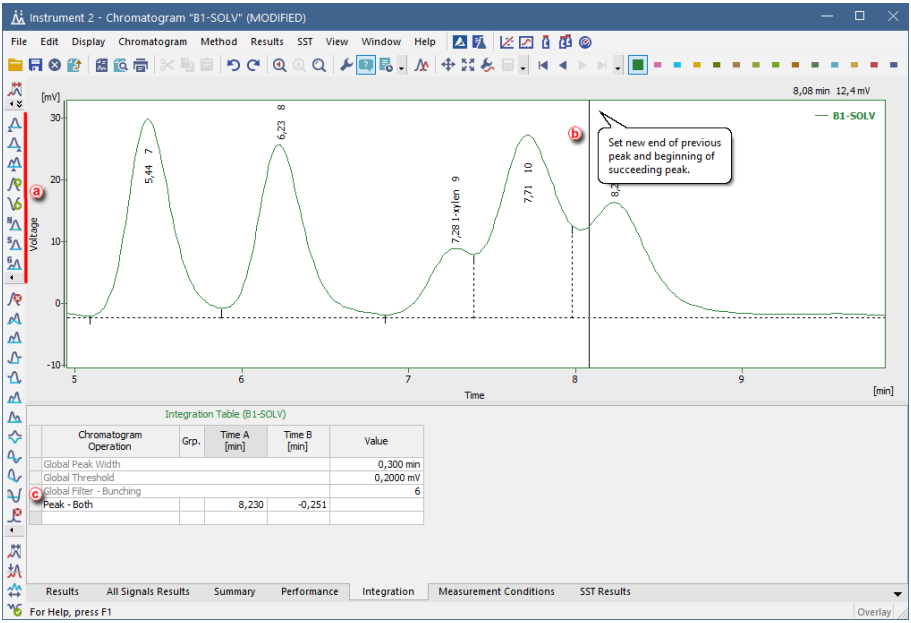


For setting the Global Peak Width or Threshold:

Set the interval you want to modify: select *Global Peak Width or Threshold* from the *Chromatogram* menu or edit their value on the integration table ⓒ on the *Integration* tab.
The new values will be applied to the whole chromatogram.

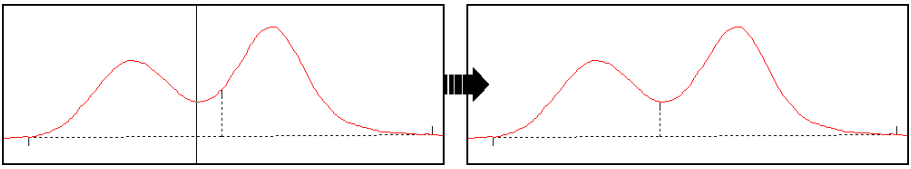
7.9 Changing the position of a peak separating line

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Select *Chromatogram - Peak - Both*** from the main menu or from the context menu (right mouse-click in the chromatogram curve area) **or click on** in the *Peak* toolbar ⓐ.



3. **Set the new position of peak- separating line** by clicking in the chromatogram area ⓑ.

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



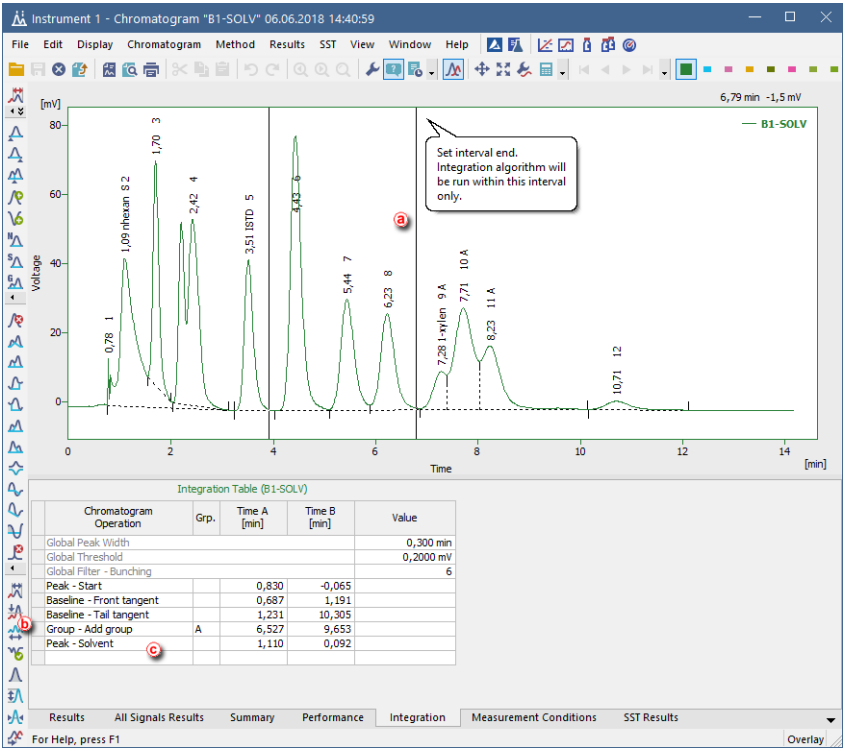
4. You can check, modify the position or delete this operation in the Integration tab ⓒ.

7.10 Setting the integration interval

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Set the interval on which to apply the integration** ⓐ: select *Chromatogram - Integration - Integration Interval* or click on the toolbar ⓑ.

More Info:

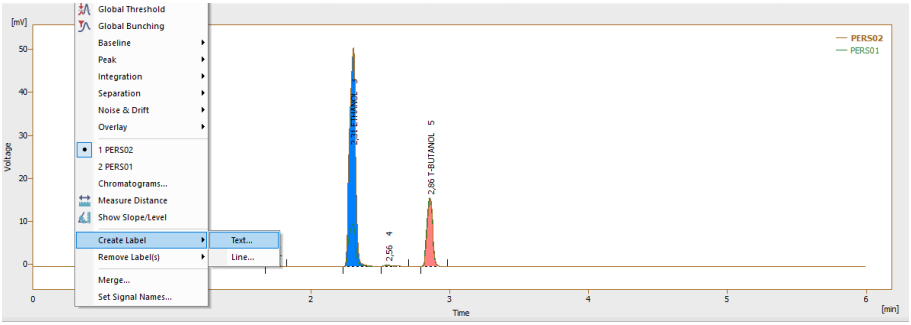
Subsequent uses of the same command will add further integration intervals to the previously selected.



3. If you want **to exclude some specific interval from the integration,** click on the icon on the toolbar as explained in Remove peak from integration (or use *Chromatogram - Baseline - Lock*).
4. **You can check, modify the range or delete this operations** in the Integration tab (*Integration Interval* and *Baseline - Lock* items) ⓒ.

7.11 Adding text and lines to a chromatogram

1. **Right click on the chromatogram in the *Chromatogram* or the *Calibration* window.**



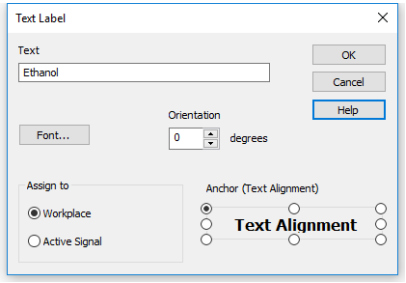
2. **Select the option *Create Label - Text* to add text.**

More Info:

- Write the text in the text box.
- Select the font by clicking on the *Font* button.
- Enter the *Orientation* of the text.
- Select the *Anchor point* for the text.
- *Assign to the workplace*, if you want the text to stay in the same location regardless of the chromatogram opened and its position (labels stored in the desktop file).

Assign to the active chromatogram, if you want the text to shift as the chromatogram moves, zooms in and out (labels stored in the chromatogram file). The text will be displayed only when the respective chromatogram is active.

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



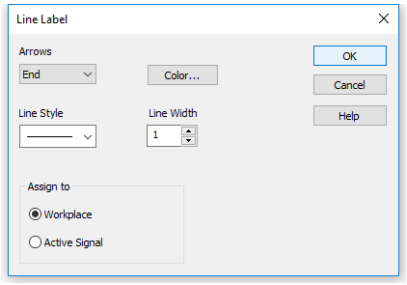
3. **Click and drag the text if you wish to move it to a different location.**
4. **Select the option *Create Label - Line* to add a line.**

More Info:

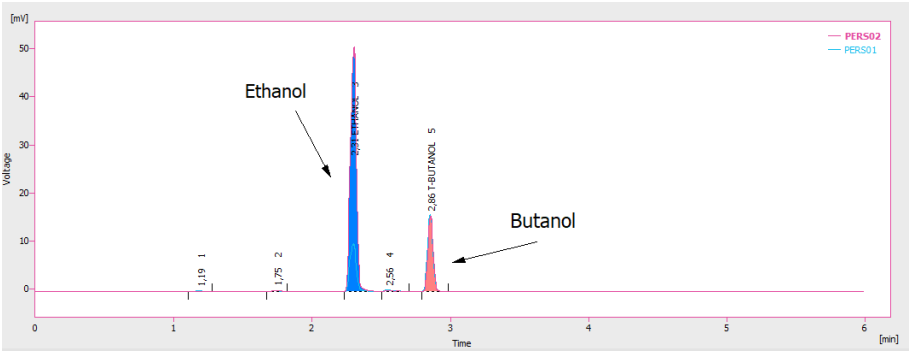
- Select whether you want to add an arrow tip at the beginning, end or at both ends of the line.
- Select the color by clicking on the *Color* button.
- Enter the *Line Width*.
- Select the *Line Style*.
- *Assign to the workplace*, if you want the line to stay in the same location regardless of the chromatogram opened and its position (labels stored in the desktop file).

Assign to the active chromatogram, if you want the line to shift as the chromatogram moves, zooms in and out (labels stored in the chromatogram file). The text will be displayed only when the respective chromatogram is active.

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



5. **Click and drag the line, if you wish to move it to a different location or click and drag the ends to lengthen or shorten it.**



7.12 Saving the chromatogram method as a template method

The method saved in the chromatogram file may be needed as a template method for further use - for example because the integration table is fully customized to that type of analysis, the chromatogram has a linked calibration file that will be later linked to new chromatograms or simply because the original template method was lost.

1. **Open the *Chromatogram* window and then the chromatogram**.
2. **Select the *Method - Save as Template…* to save the method** (including the integration parameters) from the current chromatogram as a new method.

More Info:

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

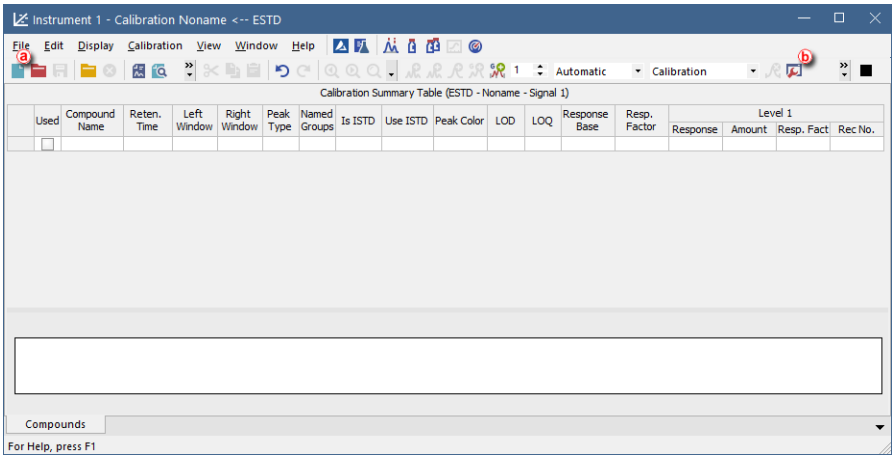
8 Calibration

Following chapters contains multiple topics which will guide you through the basic principles of calibrating in **Clarity** and also introduces you to advanced solution, for example using the *Bracketing*.

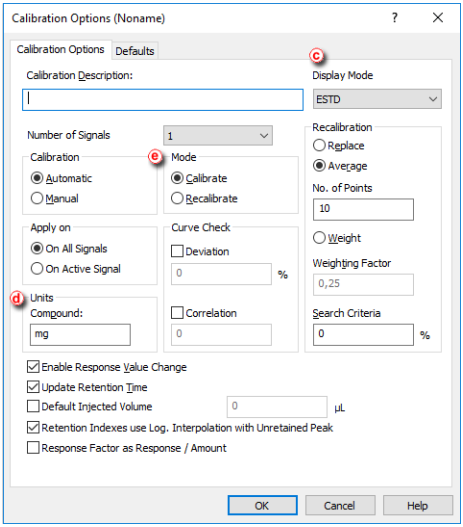
8.1 Creating a new calibration

This chapter concerns 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* on the *Instrument* window or click on .



2. **Create a new calibration file:** select *File - New* or click on ⓐ .
3. **Fill in the calibration name** in the *New File* dialog and click *OK*.
4. **Open the Calibration Options dialog:** choose *Calibration - Options…* or click on ⓑ.



5. **Set the *Display Mode*** ⓒ to the option that will be used in the calibration.
6. **Fill in the units *in the Units* section** ⓓ to suit your analysis conditions.
7. **Set the *Mode* to *Calibrate*** ⓔ.
8. ***Set the Calibration* option to *Automatic*** to add the peaks without modification **or *Manual*** to modify them one by one ⓔ.
9. **Press the *OK* button** to exit the dialog.
10. **Open integrated chromatogram of a standard:** choose *File - Open Standard…* or click on ⓕ on the *Calibration* window.

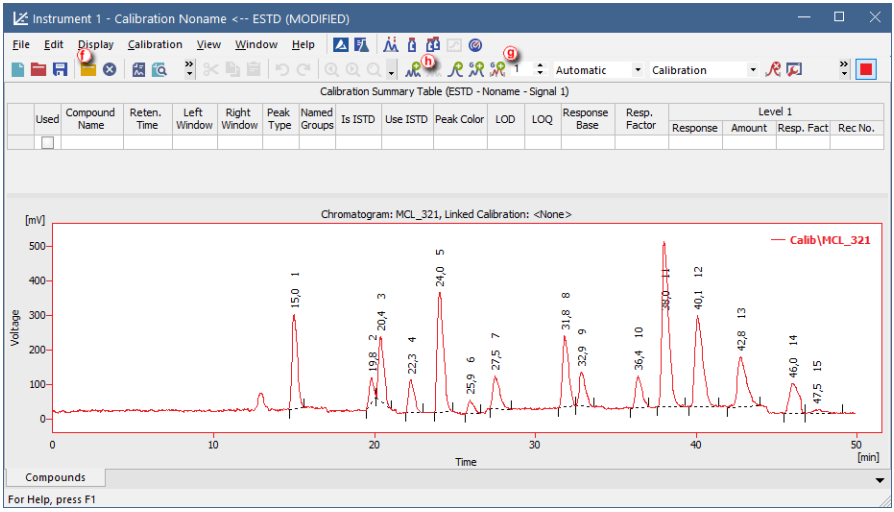
More Info:

The standard should contain peaks of compounds of interest with a known concentration.

11. **Add peaks in the chromatogram of the calibration standard to the calibration file**

More Info:

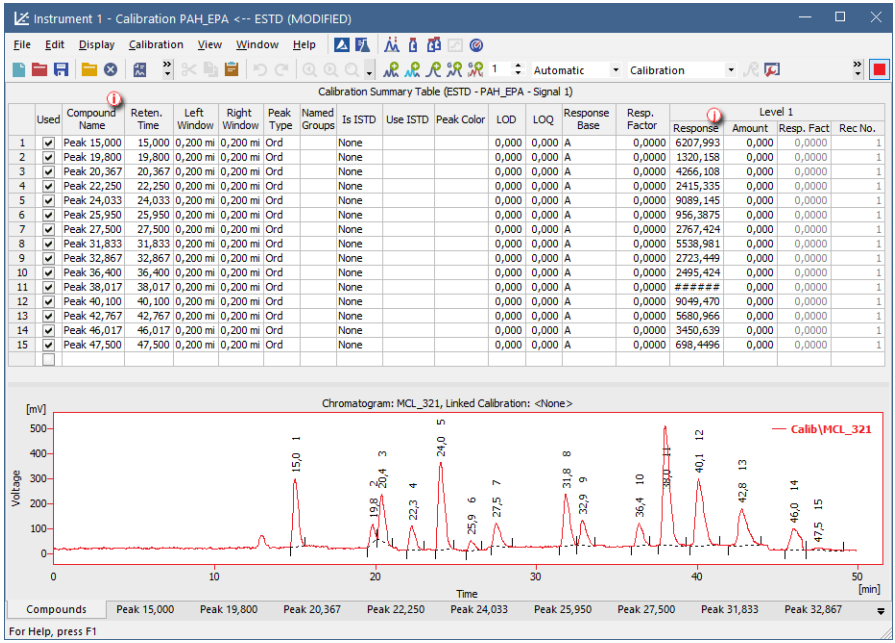
Select *Calibration - Add All* or click on to add all peaks or the Add Peak / Add Group icons to add specific peaks ⓗ. Regardless of the set Current Level ⓖ the peaks will be added to the first free level.



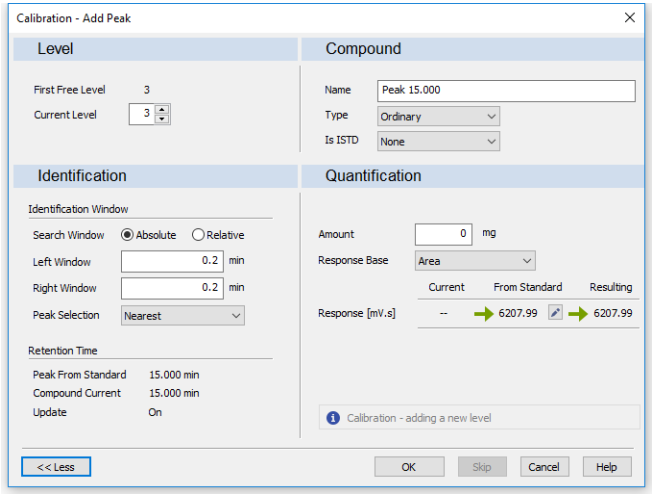
12. If you selected ***Automatic*** calibration:
    - **Name the peaks identified** in the *Calibration Summary Table* ⓘ by their retention times by typing the *Compound Name* for each peak. No peak name may be used more than once.
    - **Fill in the *Amount*** ⓙ for each compound into the *Calibration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

    More Info:

    Make sure you enter the units ⓓ in the *Calibration Options* dialog.



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

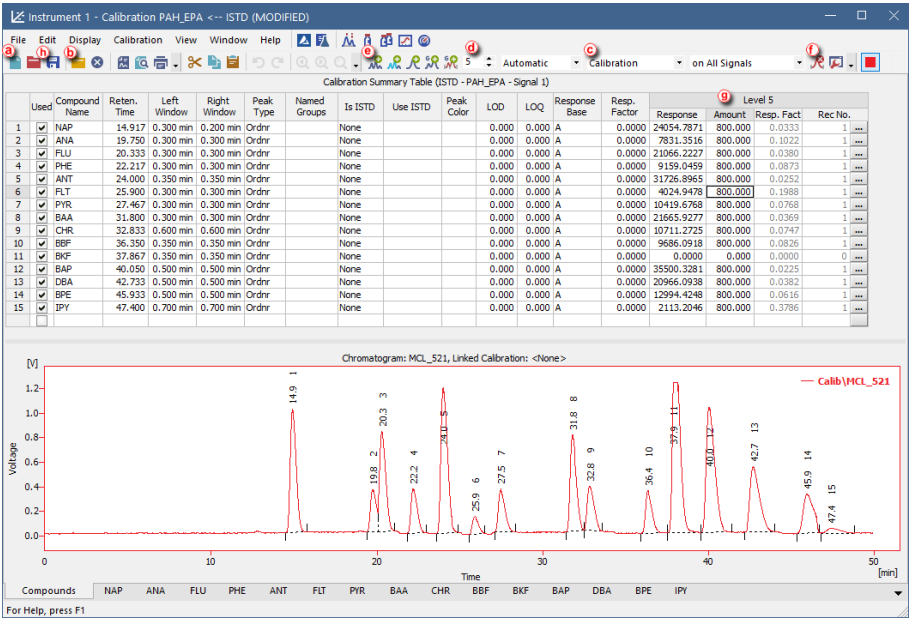


14. **Save the calibration file** from *File - Save* or click on .

8.2 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 on



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

   More Info:

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

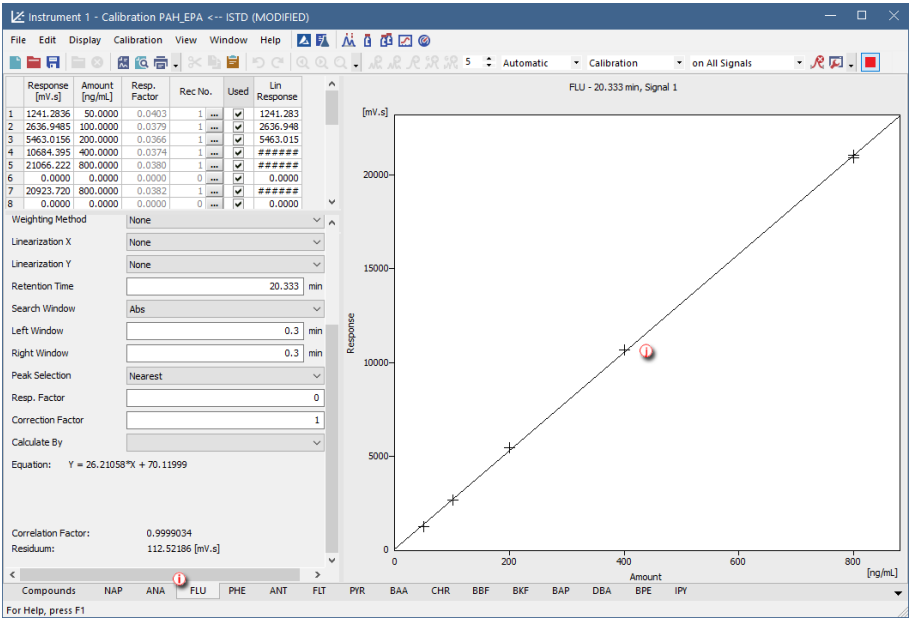
4. **Check that the *Automatic* option is selected in the first field** and the *Calibrate* option in the second field of the calibration mode settings ⓒ.
5. **The calibration level number is in the *Current Level* field** ⓓ set automatically to the first free level.
6. **Add all peaks in the chromatogram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

   More Info:

   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 from *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 on ⓗ

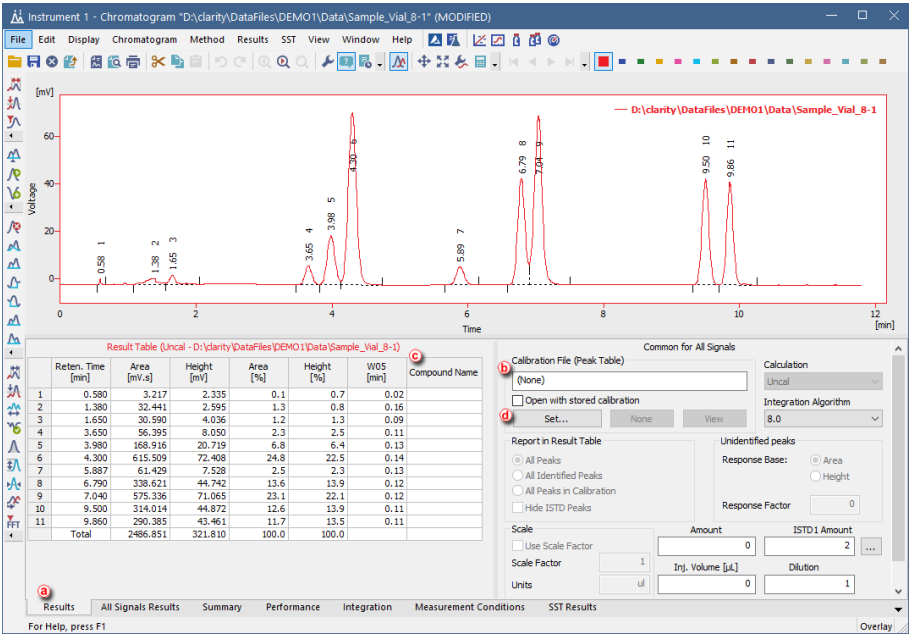
9. **Click on any of the tabs below** ⓘ and you will be able to see the calibration curve with all the levels added for one specific compound ⓙ.



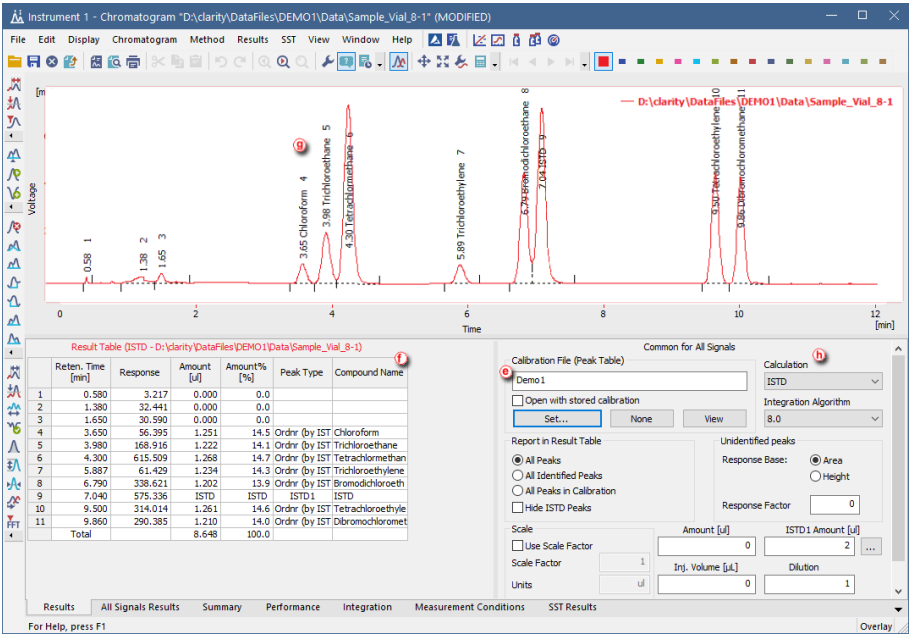
8.3 Applying a calibration to a chromatogram

If the calibration file was not assigned in the template 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.
   - **Select the correct calibration file from the list and click *OK***.
     The content of the Chromatogram window will change.

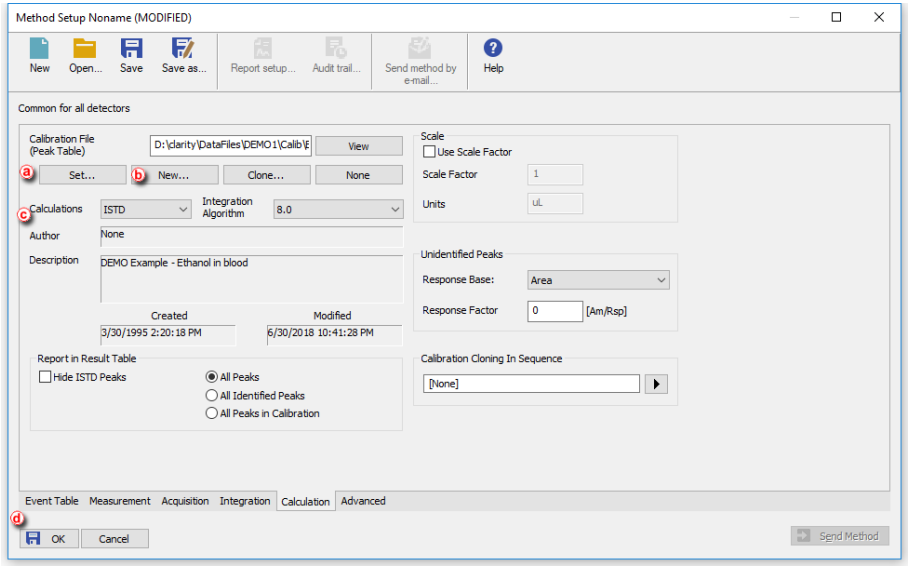


6. **Check that the *Calibration File (Peak Table)* field contains the name of the calibration file.** ⓔ
7. The *Compound Name* column ⓕ in the *Result Table*, as well as the identified peaks in the graph ⓖ, will now have the names of the identified peaks from the calibration file.
8. **Check the *Calculation*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

8.4 Setting the calibration in the template 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 template method** from the Instrument window by using the *File - Open Method…* command.
2. **Open the Method Setup - Calculation dialog:** select *Method - Calculation* on the *Instrument* window.

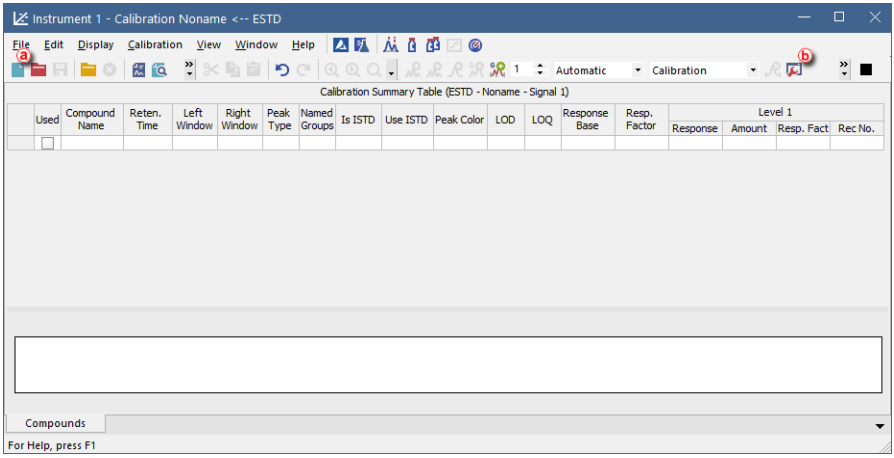


3. **Click the *Set…* button** ⓐ **to select a calibration file for the template method, or create a new calibration file** by clicking the *New…* button ⓑ.
4. **Change the default calibration type** in the *Calculations* field ⓒ.
5. **Click *OK*** ⓓ **to apply the changes** to the template method and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

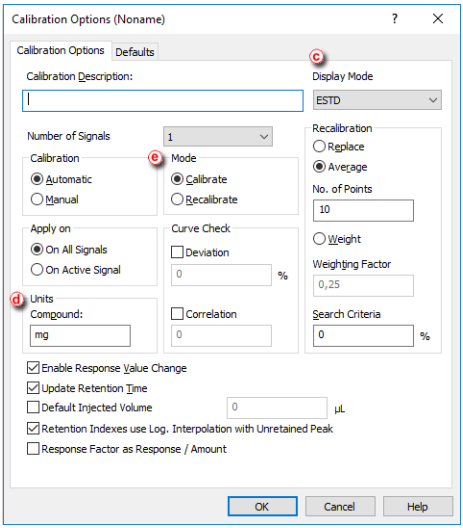
8.5 Calibrating with manually entered Response Factors

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

1. **Open the Calibration window:** choose *Window - Calibration* on the *Instrument* window or click on  .
2. **Create a new calibration file:** select *File - New* or click on  ⓐ.

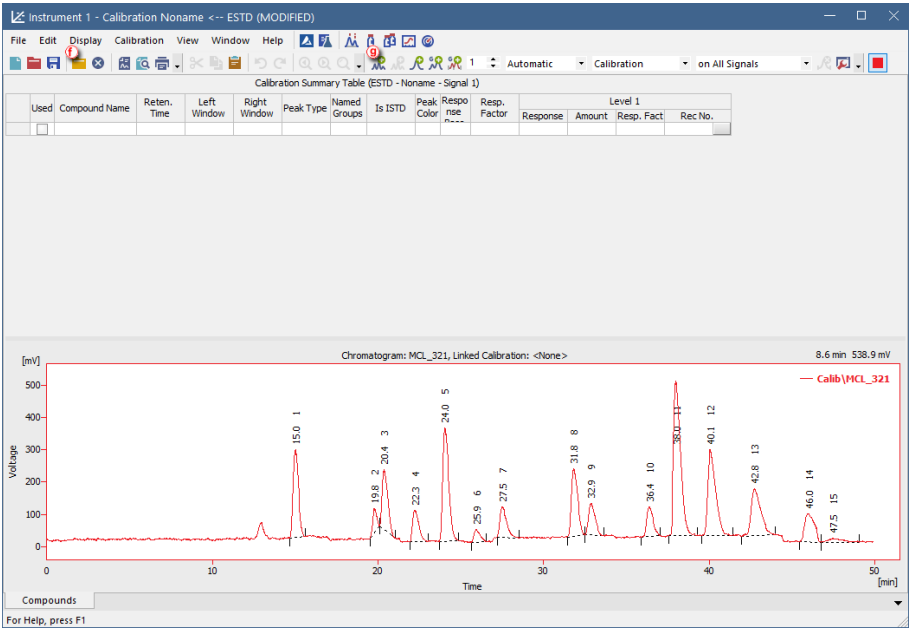


3. **Fill in the calibration name** in the following dialog and press the *OK* button.
4. **Open the Calibration Options dialog:** choose *Calibration - Options…* or click on . ⓑ



5. **Set the *Display Mode*** ⓒ to the option that will be used in the calibration.
6. **Fill in the units *in the Units* section** ⓓ to suit your analysis conditions.
7. **Check that *Calibration* option is set to *Automatic* and *Mode* to *Calibrate.*** ⓔ
8. **Press the *OK* button** to exit the dialog.

9. **Open an integrated chromatogram of a standard** (containing peaks of compounds of interest with a known concentration): select *File - Open Standard…* or click on ⓕ on the Calibration window.
10. **Add all peaks in the chromatogram of the calibration standard to the calibration file:**choose *Calibration - Add All* or click on ⓖ.

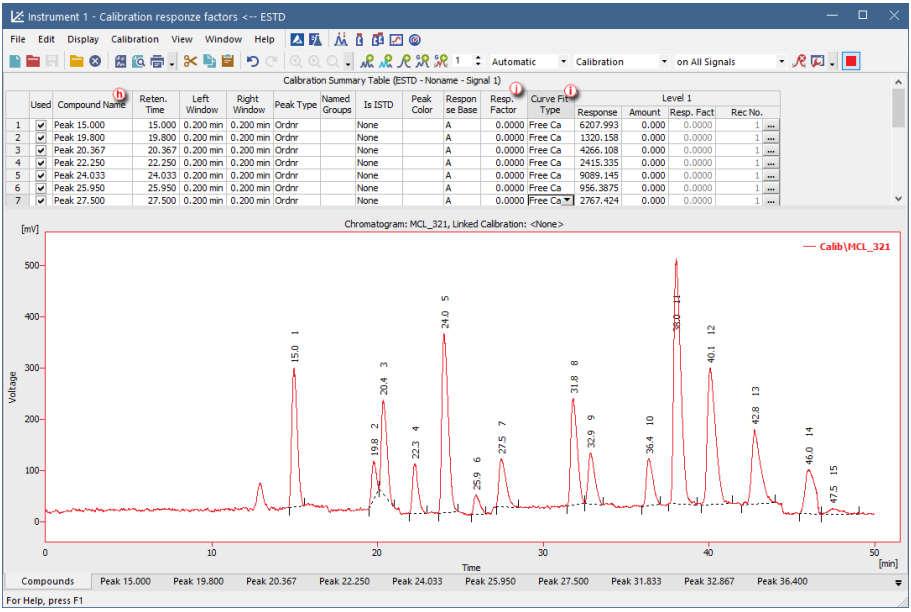


11. **Name the peaks identified in the Calibration Summary Table** ⓗ by their retention times by typing the *Compound Name* for each peak. No peak name may be used more than once.
12. **Set the *Calibration Fit Type* to *Free Calibration*** ⓘ for each one of the compounds in the *Calibration Summary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

13. **Type in the *Response Factor* for each one of the compounds.** ⓙ
14. **Save the calibration file:** choose *File - Save* or click on .

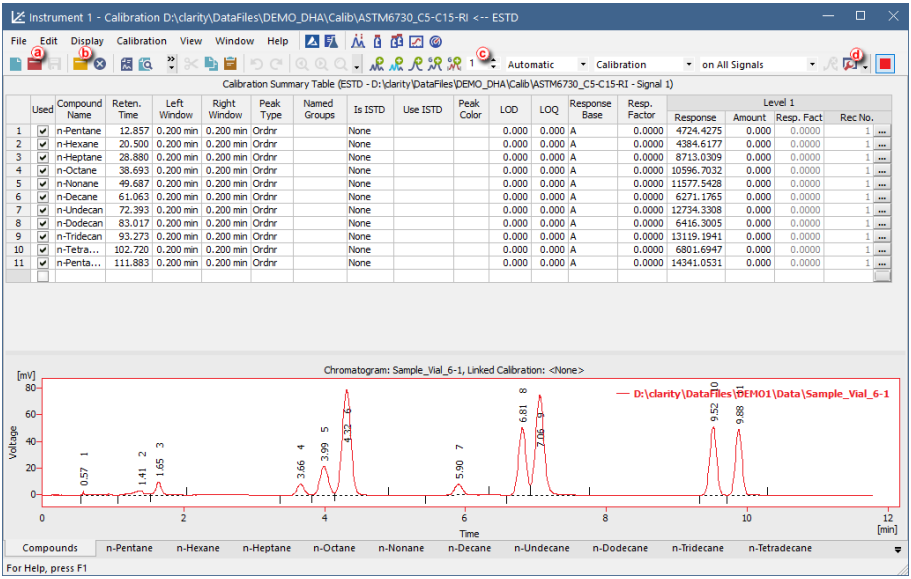


Since **Clarity** 8.0 when constructing calibration curve there is check that calibration curve could be constructed, that means all amounts have nonzero value. In case calibration curve could not be constructed for any compound, no results are calculated (as the total amount could be wrong]. If you do not want to calculate amounts for all identified compounds, you could use free calibration with zero response factor.

8.6 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 on .

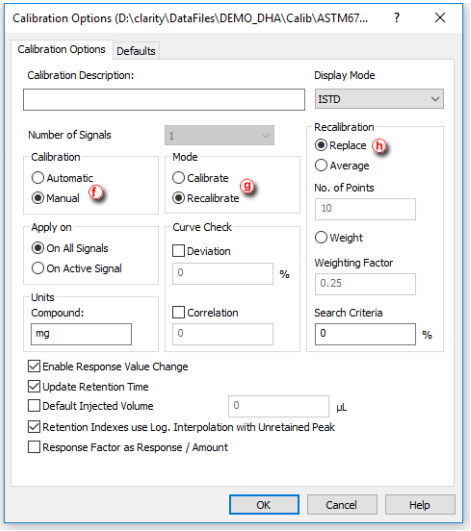


2. **Open the calibration file:** choose *File - Open…* or click on ⓐ.
3. **Open calibration standard:** select *File - Open Standard…* or click on ⓑ .

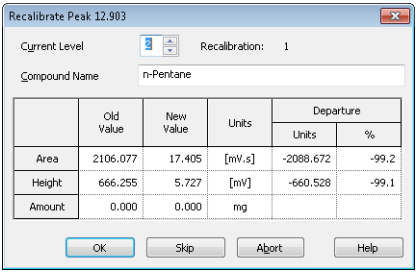
   More Info:

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

4. **Select the *Level* you wish to recalibrate.** ⓒ
5. **Open the Calibration Options dialog:** choose *Calibration - Options…* or click on ⓓ.



6. ***Set the Calibration* option to *Automatic* to add the peaks without modification or to *Manual* to modify them one by one ⓕ.**
7. **Set the *Mode* to *Recalibrate*** ⓖ.
8. **Select how and whether the new values will be added** (Replace, Average, Weighting Factor and Search Criteria) on the *Calibration Options* dialog ⓗ.
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 *Calibrate Peak* window. This window will open once for each one of the peaks processed.

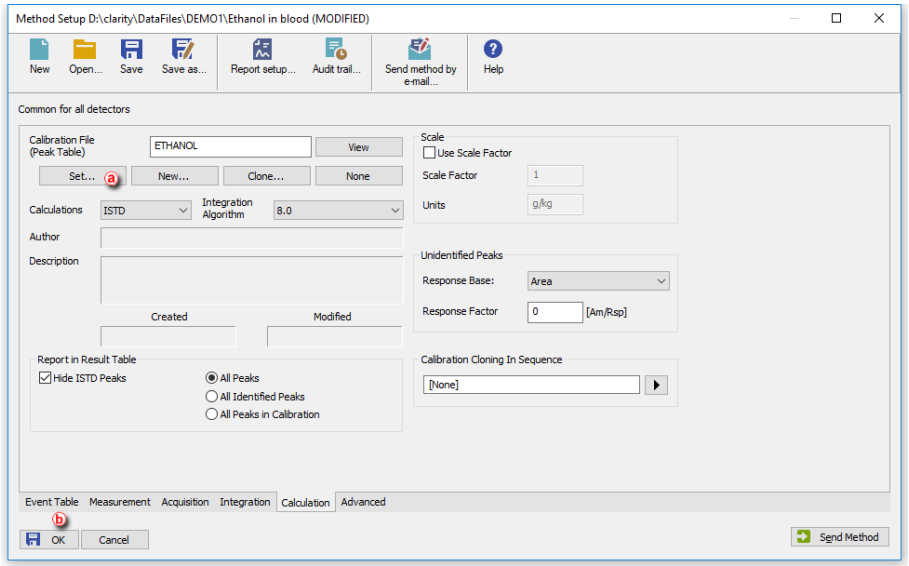


11. **Save the calibration file:** choose *File - Save* or click on .

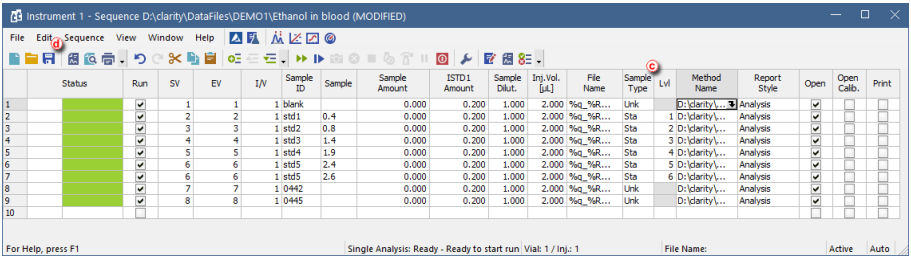
8.7 Recalibrating a calibration automatically using a sequence

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 on .
2. **Open the Method Setup - Calculation dialog:**select *Method - Calculation* on the Instrument window.



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



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

More Info:

The *Std* 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 calibration standards). For a blank sample, select *Blank* in the *Std* column.

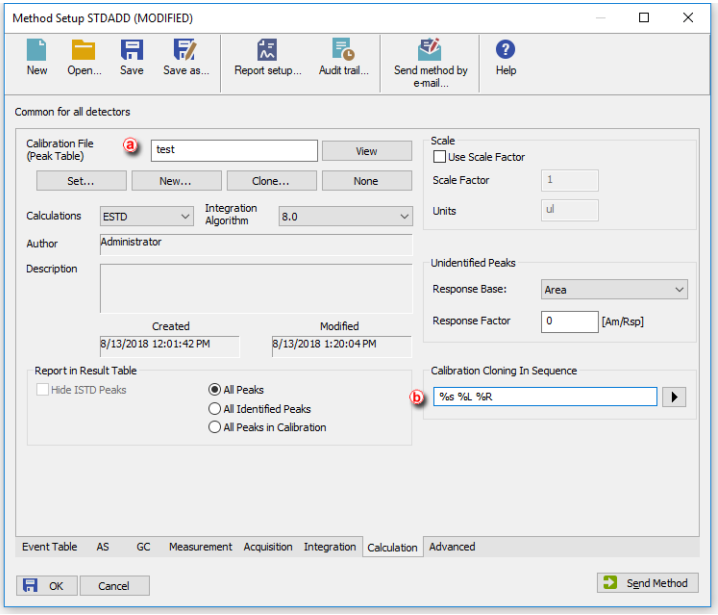
8. **Save the sequence file:** select *File - Save* or click on . ⓓ

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

8.8 Calibrating using clone at first recalibration

Option *Clone at 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.

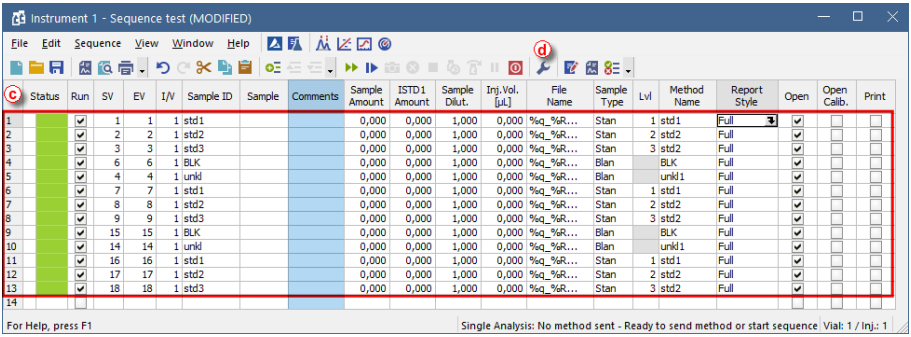
1. **Open the template method** from the *Instrument* window by selecting *File - Open Method…*
2. **Open the Method Setup - Calculation dialog:** select *Method - Calculation* tab on the *Instrument* window.



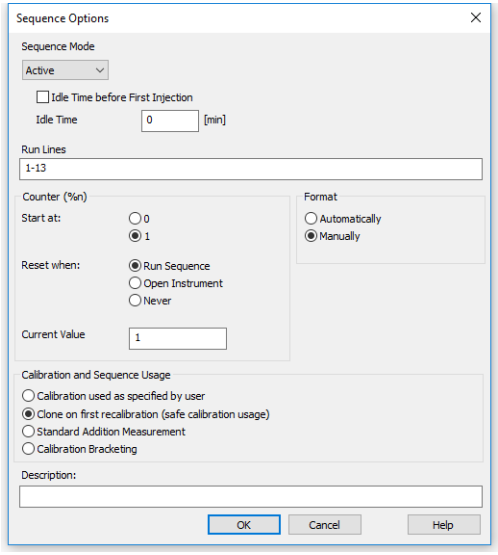
3. **Click on *Set...* button and select a calibration file** ⓐ**.** to be used during cloning at first recalibration. Note that this calibration will remain unchanged as newly created clone of the calibration will be used with new responses.
4. **Create a custom name for the calibration files in *Calibration Cloning in Sequence*** ⓑ as explained in Creating customized file names automatically. The name of the final calibration file will match just the contents of this field - if you wish to include the name of the model calibration, include the name in this field again (e.g. "test - %s %L %R"). Note that when using %R parameter, the name of the calibration will reflect the time of Sequence start, not the time of creating the clone.
   - **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. ⓒ
     - 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 after the unknown sample/s.
     - Repeat the previous three steps for every unknown sample you wish to add.
     - Before running the sequence, go to the following step.



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



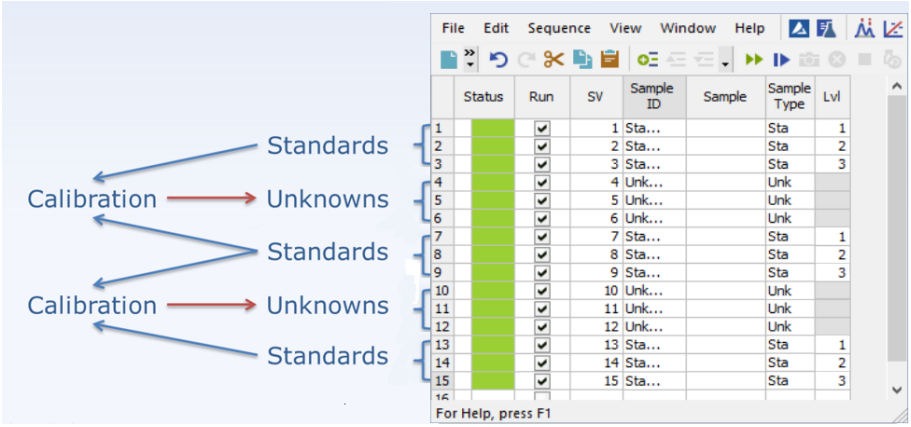
8. **Run the sequence as explained in Creating and running a sequence .**

8.9 Compensating for response drift using bracketing

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

In bracketing sequence contains 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 on average of both calibrations after both calibrations are measured. As every unknown sample series is demarcated by calibration standards and as such uses a single calibration file, calibration will be cloned from the previous calibration clone whenever an unknown sample or blank follows the calibration standard. Newly cloned calibration file has all responses cleared - apart from the responses from the last series (immediately preceding the current unknown samples) of calibration standards.

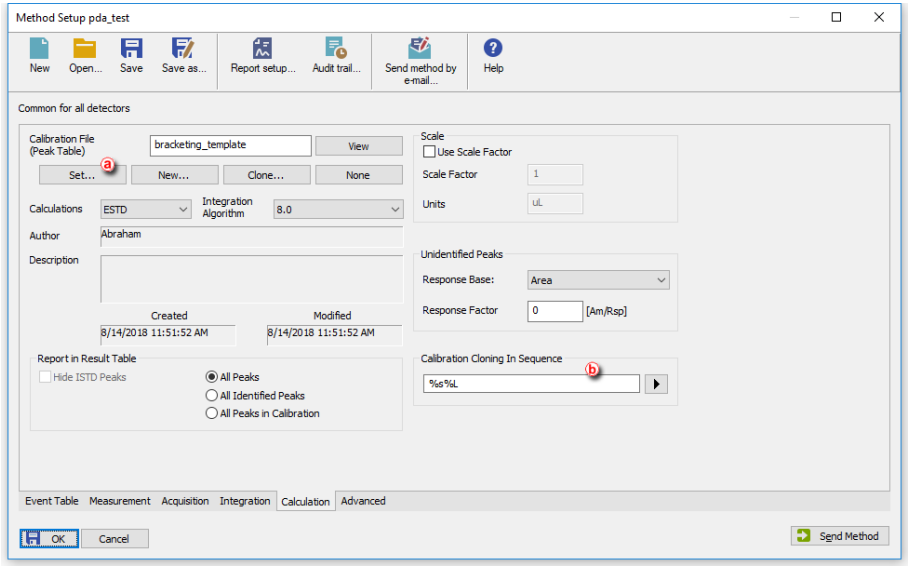
Bracketing in Clarity



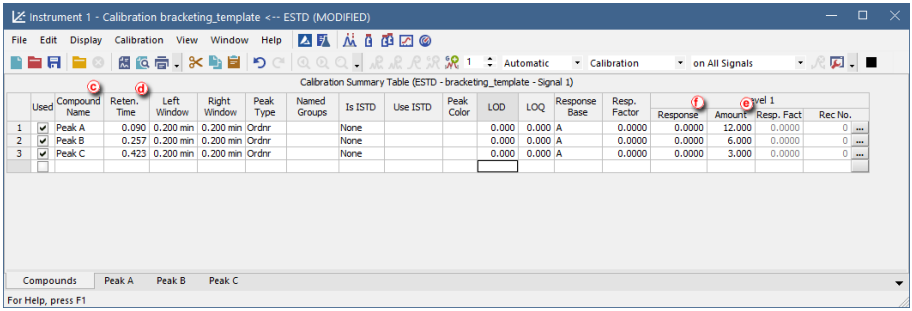
1. **Open the method that will be used in the sequence**: click *File - Open Method…* from the *Instrument* window.
2. **Open the Method Setup - Calculation dialog:** click *Method - Calculation* or from *Instrument* Window click on *Method - Calculation*
3. **Set the template calibration as Calibration File:** click *Set...* ⓐ and select the calibration.

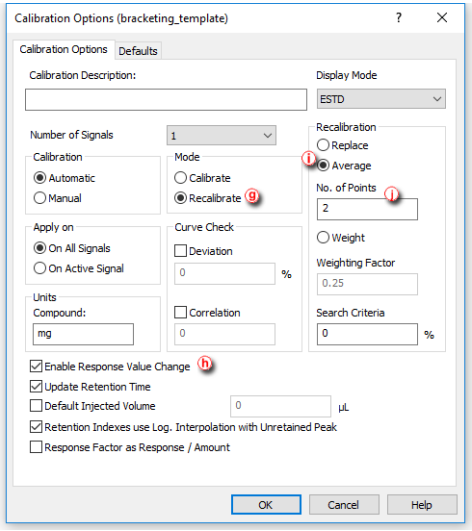
   Note that this calibration will remain unchanged, newly created clone of the calibration will be used with new responses.
4. **Set the name of the cloned calibration** ⓑ **:** you can use predefined parameters (refer to Creating customized file names automatically).

Note that when using %R parameter, the name of the calibration will reflect the time of Sequence start, not the time of creating the clone.

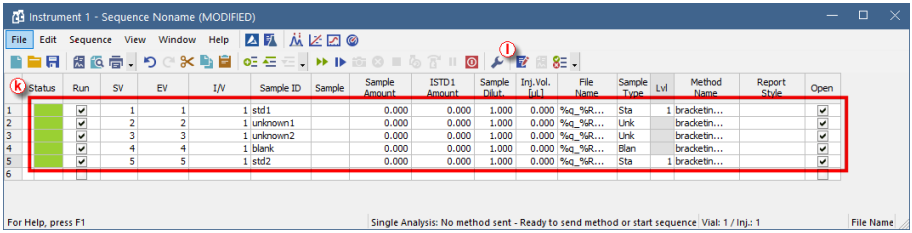


5. **Click OK and Save the modified method.**
6. **Open Calibration window and the template calibration:** click *Window - Calibration* from the *Instrument* window and *File - Open...* in the *Calibration* window, select the template calibration (in this case bracketing_template.cal).
   - Set *Compound Names* ⓒ, *Retention Time* ⓓ, *Amounts* ⓔ, etc., but no *Responses* ⓕ.
   - Click *Calibration - Options* and select *Recalibrate* ⓖ, *Enable Response Value Change* ⓗ item is optional.
   - Set *Recalibration* to *Average* ⓘ and *No. of Points* to *2* ⓙ (no more points needed as they would not be applied anyway)
   - Save changes and close the calibration.

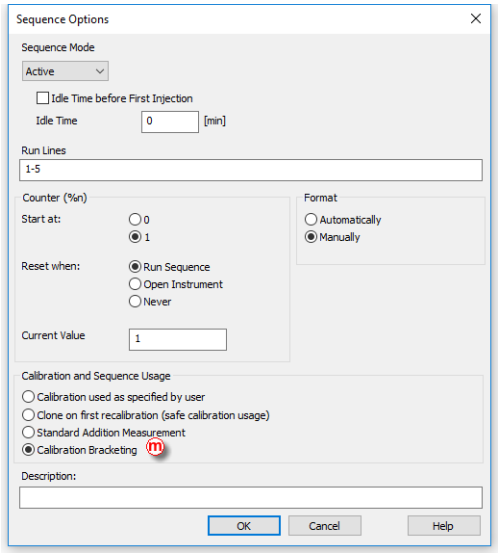




7. **Open Sequence window and create a new sequence:** click *Analysis - Sequence* and then on icon.
8. **Set the sequence according to the following steps** (for more details about creating the sequence refer to **Creating and running a sequence**):
   - Set the row/s for the standard/s. (k)
   - Add 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 that the sequence must start and end with a row containing calibration.
   - Repeat the previous four steps for every "bracket" of unknown samples you wish to add.



9. **Set the sequence to operate in the calibration bracketing mode:**
   - Click on icon to open the Sequence Options dialog. ⓛ
   - Check Calibration Bracketing. ⓜ
   - Click OK.
     Note that 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.



10. **Run the sequence** (for more details about running the sequence refer to **Creating and running a sequence)** .

More Info:

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.

8.10 Creating a Multisignal Calibration

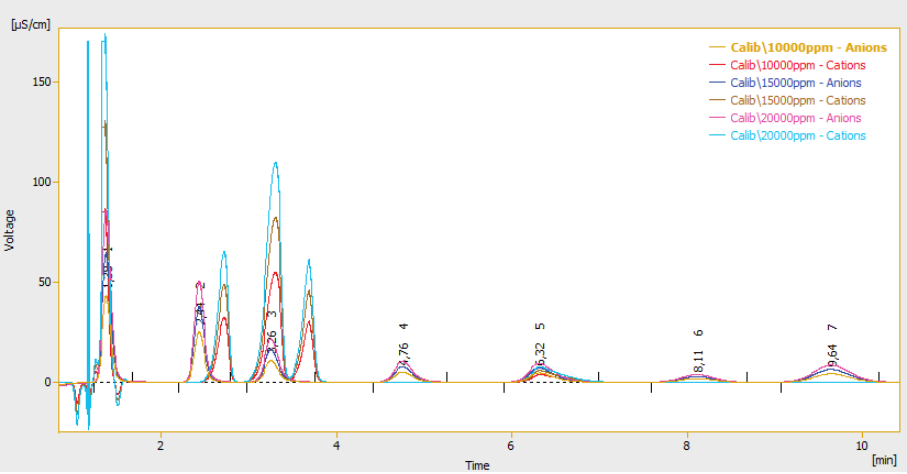
This topic describes how to construct a multisignal calibration in Clarity. Below is an example of creating and constructing a three (concentration) level calibration which provides calculation parameters for calculating results in two-signal chromatograms.

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.

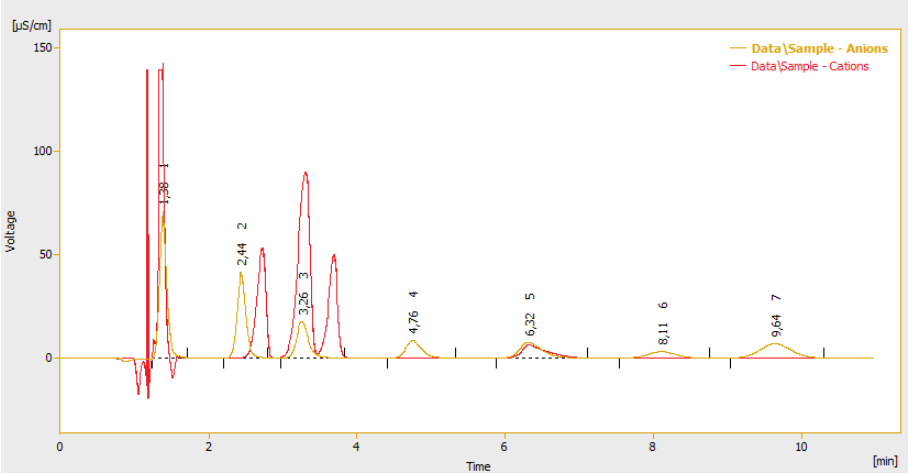
This guidance is based on two-signal chromatograms of standards of cations and anions on three concentration levels (10 000 ppm, 15 000 ppm and 20 000 ppm) and one chromatogram of sample from ion chromatography. All chromatograms used in this guidance have been integrated in manner to fit the demonstration purpose.

Prerequisites:

- Integrated chromatograms of standards.

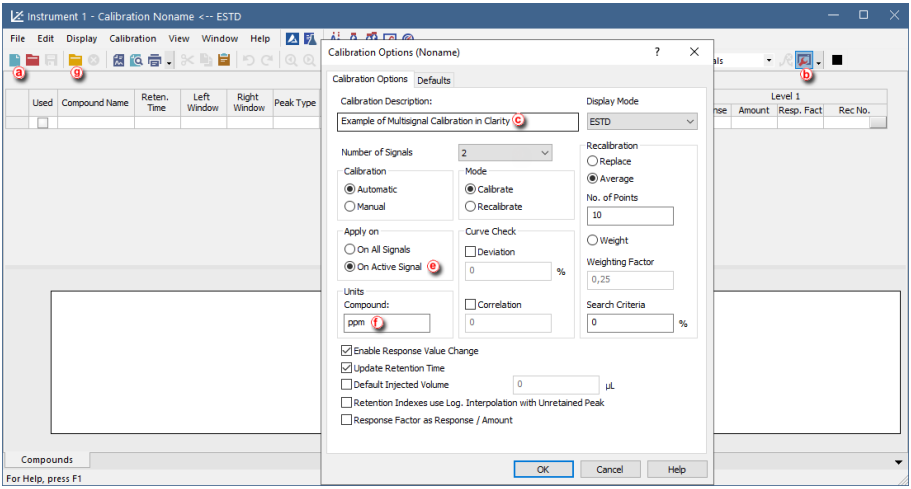


- Integrated chromatogram of sample.

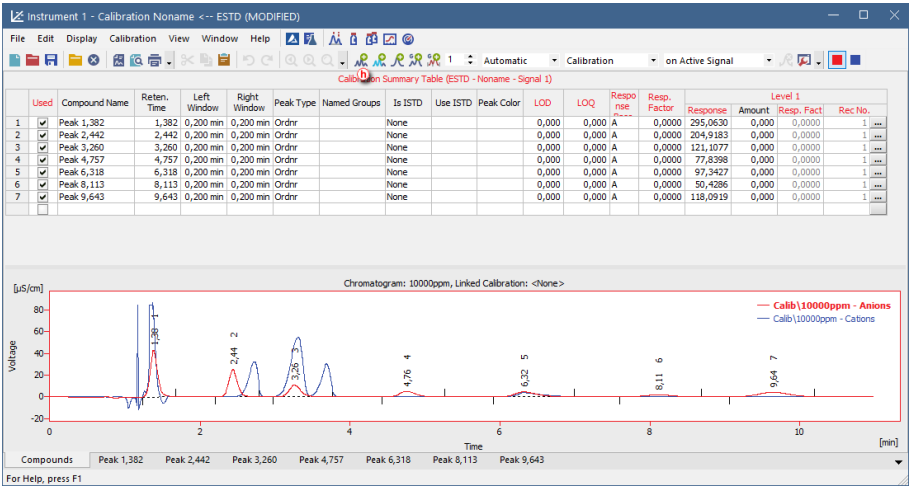


1. **Open the Calibration window:** select *Window - Calibration* in the *Instrument* window or click on .
2. **Create a new calibration file:** select *File - New* or click on ⓐ.
3. **Open the Calibration Options dialog:** select *Calibration - Options…* or click on ⓑ.
4. Enter *Calibration Description*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

   If all peaks in the standard chromatogram are unique across all signals it is viable to change the option to *on All Signals*.
7. Set section *Units* to *ppm* field ⓕ and click *OK* button then.



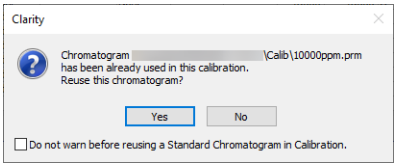
8. **Open calibration standard:** select *File - Open Standard…* or click on  to open measured and integrated chromatogram with the lowest concentration level where all peaks are available.
9. Make sure the upper toolbar displays *on Active Signal*. It is also recommended to make sure you are currently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



12. **Switch** to the second signal in chromatogram to make it active.

13. Fill the *Calibration Summary Table* with peaks from the currently selected (second) signal in chromatogram using *Add All* icon. After clicking *Add All* icon there will be invoked dialog with question if reuse an already used chromatogram for this calibration. It is necessary to confirm the reuse by clicking *Yes* button.

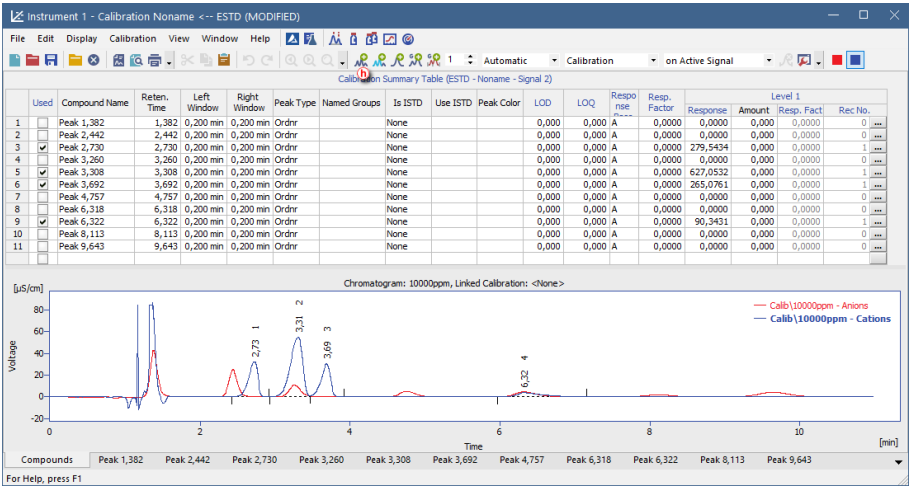
Note: In case of constructing more signal calibration these last two steps have to repeated as many times as necessary in order to fill in peaks from all signals to *Calibration Summary Table*.



Note: For more signal calibration this dialog will be invoked respectively times based on required number of signals in calibration. It is possible to switch off invoking of the dialog using the checkbox in the bottom of the dialog.

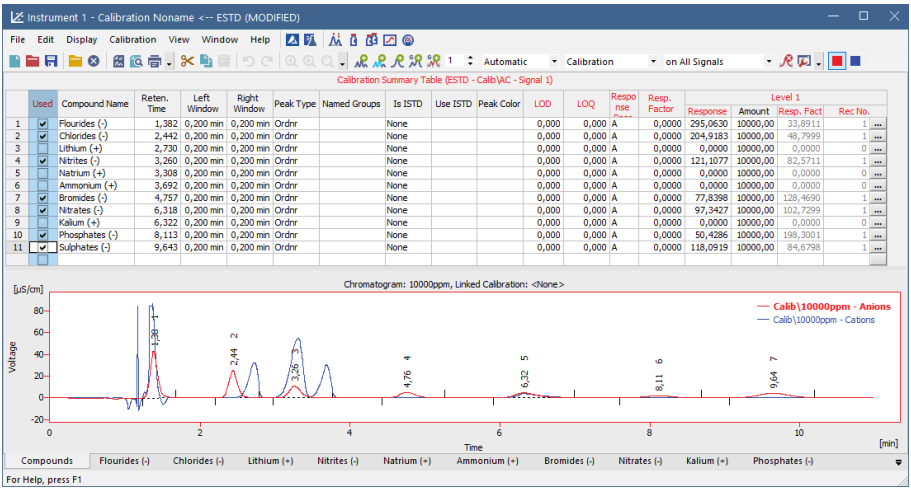
More Info:

Be noticed the that for resolution what 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.

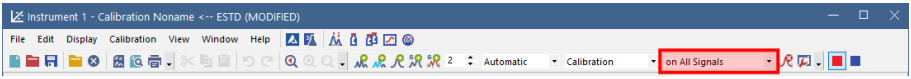


14. Rename the automatically pre-filled names in the *Calibration Summary Table* column.
15. Enter value into *Amount* column. As in this guidance this chromatogram refers to concentration 10 000 ppm of each ion there will be filled in all rows with this value. The first concentration level is finished now. It is possible to proceed building up to next levels of calibration.

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



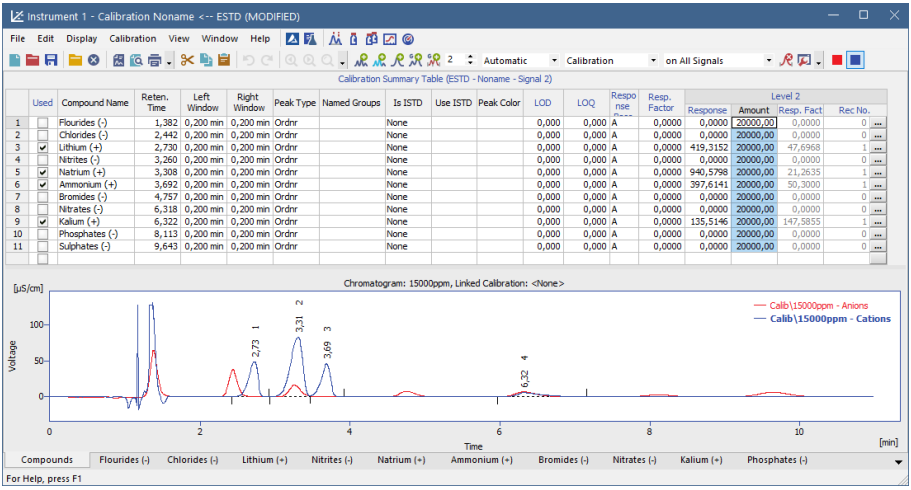
16. Open chromatogram of standard of the next (second) concentration level.
17. Change the setting of the calibration to *on All Signals*.



18. Fill the *Calibration Summary Table* with Responses from both signals of currently chromatogram using *Add All* icon.

Note: There will be transferred all responses of all peaks for both signals into calibration by this single click.

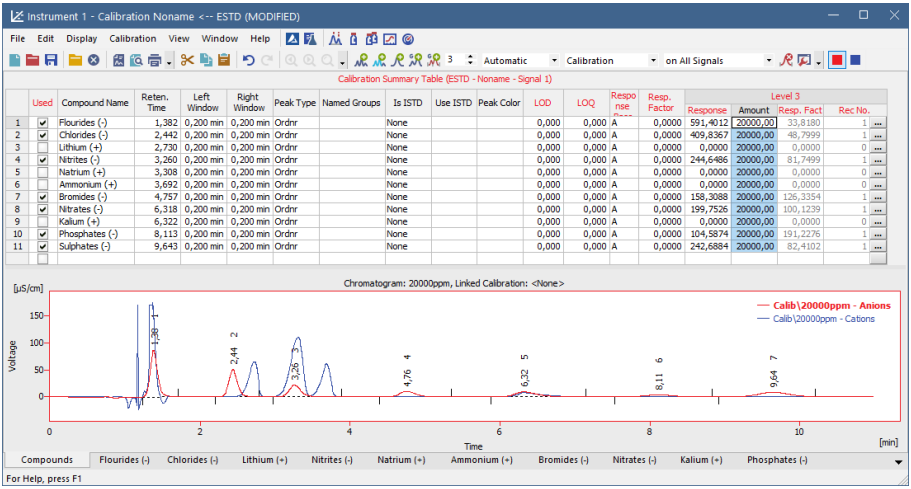
19. Enter value into *Amount* column. As in this guidance this chromatogram to concentration 15 000 ppm of each ion there will be filled in all rows with this value.



20. Open chromatogram of standard of the next (third) concentration level. Make sure there is still set *on All Signals* as given in point *16* of this guide.
21. Fill the *Calibration Summary Table* with Responses from both signals of currently chromatogram using *Add All* icon.

Note: There will be transferred all responses of all peaks for both signals into calibration by this single click.

22. Enter value into *Amount* column. As in this guidance this chromatogram to concentration 20 000 ppm of each ion there will be filled in all rows with this value. The last concentration level is finished now.

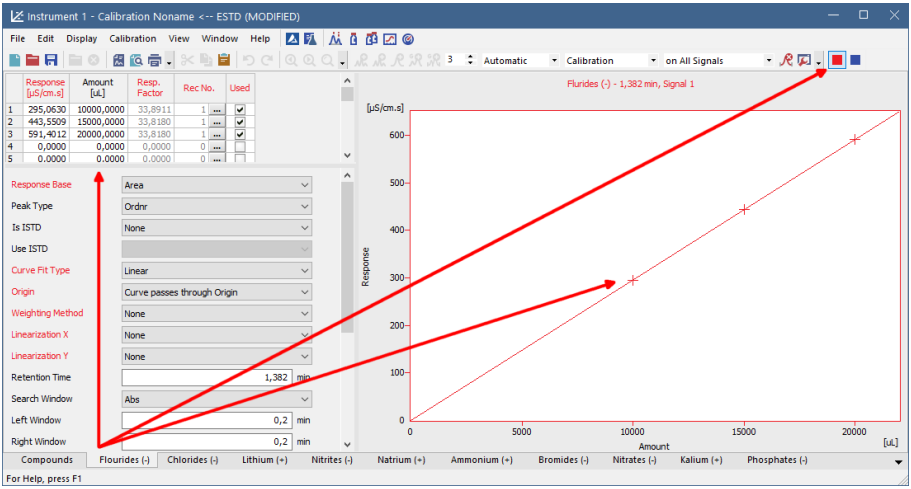


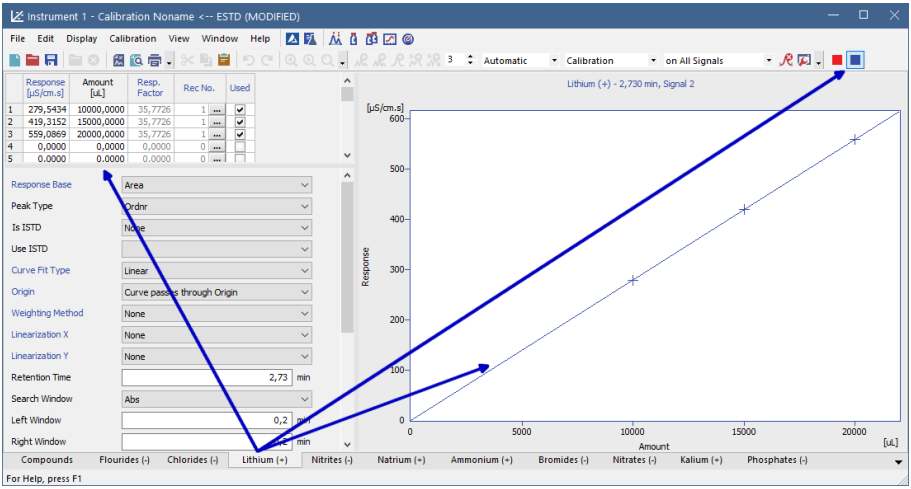
	Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Named Groups	Is ISTD	Use ISTD	Peak Color	LOD	LOQ	Response	Resp. Factor	Level 3 Response	Level 3 Amount	Level 3 Resp. Fact	Level 3 Rec No.
1	☑	Flourides (-)	1,382	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	591,4012	20000,00	33,8180	1
2	☑	Chlorides (-)	2,442	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	409,8367	20000,00	48,7999	1
3	☐	Lithium (+)	2,730	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
4	☑	Nitrites (-)	3,260	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	244,6486	20000,00	81,7499	1
5	☐	Natrium (+)	3,308	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
6	☐	Ammonium (+)	3,692	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
7	☑	Bromides (-)	4,757	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	158,3088	20000,00	126,3354	1
8	☑	Nitrates (-)	6,318	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	199,7526	20000,00	100,1239	1
9	☐	Kalium (+)	6,322	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	0,0000	20000,00	0,0000	0
10	☑	Phosphates (-)	8,113	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	104,5874	20000,00	191,2276	1
11	☑	Sulphates (-)	9,643	0,200 min	0,200 min	Ordnr		None			0,000	0,000	A	0,0000	242,6884	20000,00	82,4102	1

More Info:

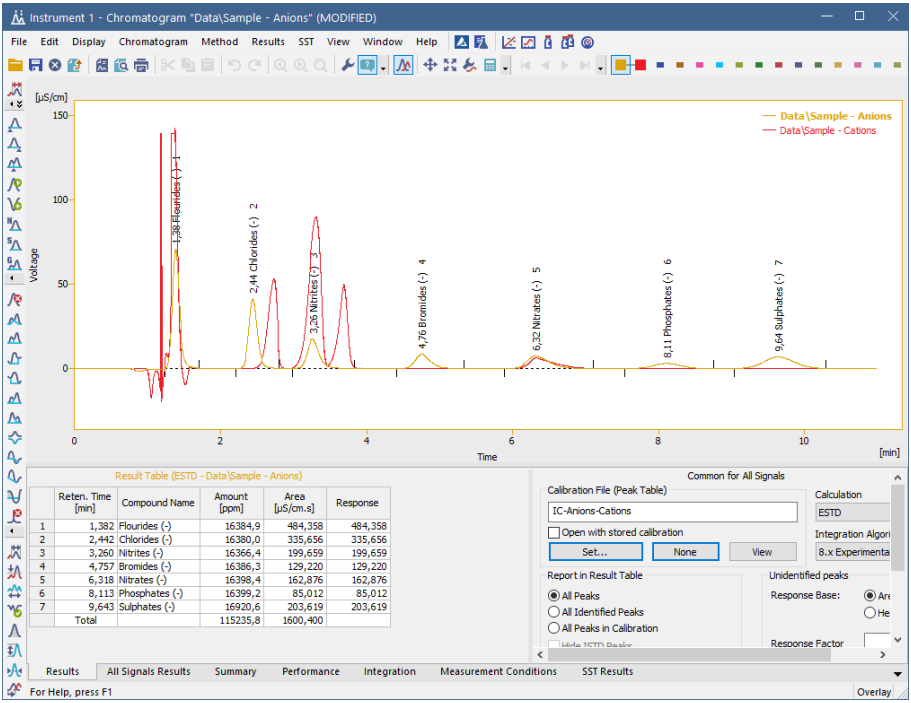
It is possible to review calibration curves for each ion on the respective tabs of individual ions. Be noticed that calibration curve are displayed only for valid signal.

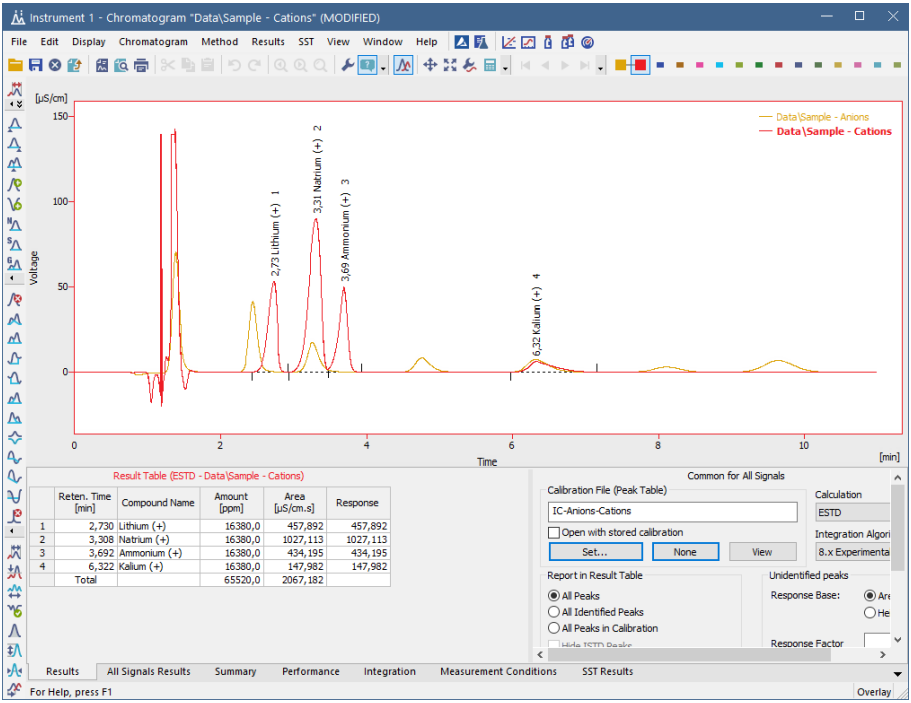
Note: If you want to review calibration curve of ion which is calibrated on second signal you need to select second signal within the tab. Signal selection is still located in right upper corner of the *Calibration Window*.

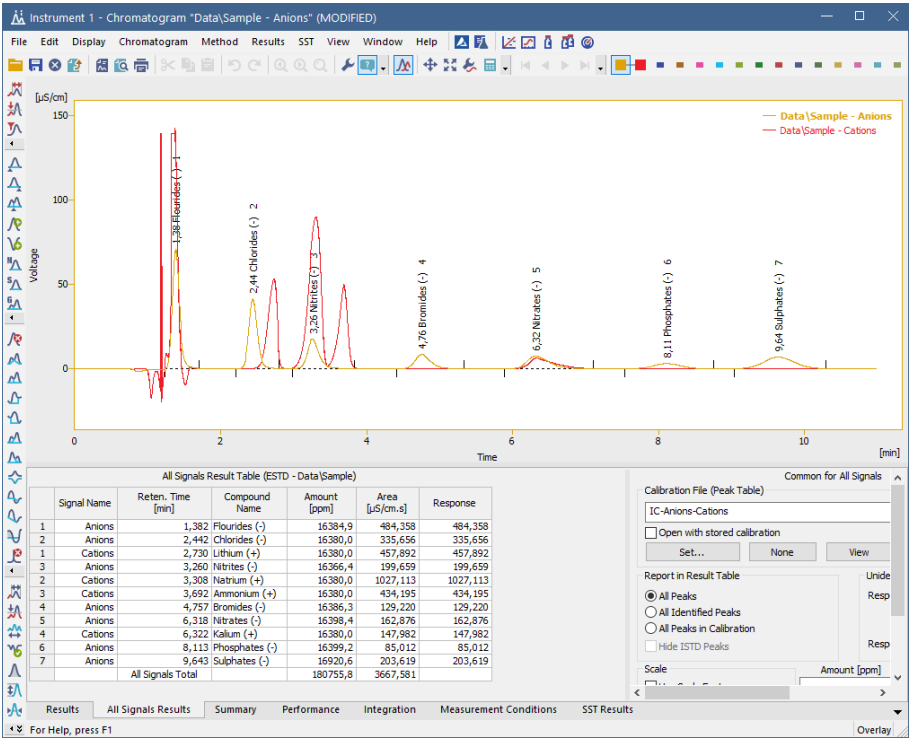




23. If calibration is finished do not forget to save it using select *File - Save* or click on .
24. For calculating result in sample open the **Chromatogram window** select *Window - Chromatogram* on the *Instrument* window or click on and open chromatogram of sample and link the calibration to chromatogram.
25. Review results on *Results Table* of each individual signal or review results for all signals on *All Signals Results* Table.


Instrument 1 - Chromatogram "Data\Sample - Anions" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[µS/cm]
Voltage
Time
[min]
Data\Sample - Anions
Data\Sample - Cations
1,38 Flourides (-) 1
2,44 Chlorides (-) 2
3,26 Nitrites (-) 3
4,76 Bromides (-) 4
6,32 Nitrates (-) 5
8,11 Phosphates (-) 6
9,64 Sulphates (-) 7
Result Table (ESTD - Data\Sample - Anions)
Reten. Time [min] | Compound Name | Amount [ppm] | Area [µS/cm.s] | Response
1 | 1,382 | Flourides (-) | 16384,9 | 484,358 | 484,358
2 | 2,442 | Chlorides (-) | 16380,0 | 335,656 | 335,656
3 | 3,260 | Nitrites (-) | 16366,4 | 199,659 | 199,659
4 | 4,757 | Bromides (-) | 16386,3 | 129,220 | 129,220
5 | 6,318 | Nitrates (-) | 16398,4 | 162,876 | 162,876
6 | 8,113 | Phosphates (-) | 16399,2 | 85,012 | 85,012
7 | 9,643 | Sulphates (-) | 16920,6 | 203,619 | 203,619
Total | | 115235,8 | 1600,400
Common for All Signals
Calibration File (Peak Table)
IC-Anions-Cations
Open with stored calibration
Set... None View
Calculation
ESTD
Integration Algori
8.x Experimenta
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Unidentified peaks
Response Base:
Response Factor
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
For Help, press F1
Overlay

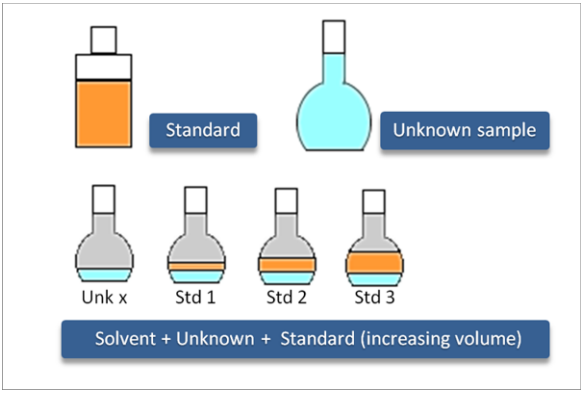

Instrument 1 - Chromatogram "Data\Sample - Cations" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[µS/cm]
Voltage
Time
[min]
Data\Sample - Anions
Data\Sample - Cations
2,73 Lithium (+) 1
3,31 Natrium (+) 2
3,69 Ammonium (+) 3
6,32 Kalium (+) 4
Result Table (ESTD - Data\Sample - Cations)
Reten. Time [min] | Compound Name | Amount [ppm] | Area [µS/cm.s] | Response
1 | 2,730 | Lithium (+) | 16380,0 | 457,892 | 457,892
2 | 3,308 | Natrium (+) | 16380,0 | 1027,113 | 1027,113
3 | 3,692 | Ammonium (+) | 16380,0 | 434,195 | 434,195
4 | 6,322 | Kalium (+) | 16380,0 | 147,982 | 147,982
Total | | 65520,0 | 2067,182 |
Common for All Signals
Calibration File (Peak Table)
IC-Anions-Cations
Open with stored calibration
Set... None View
Calculation
ESTD
Integration Algori
8.x Experimenta
Report in Result Table
All Peaks
All Identified Peaks
All Peaks in Calibration
Unidentified peaks
Response Base:
Response Factor
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
For Help, press F1
Overlay



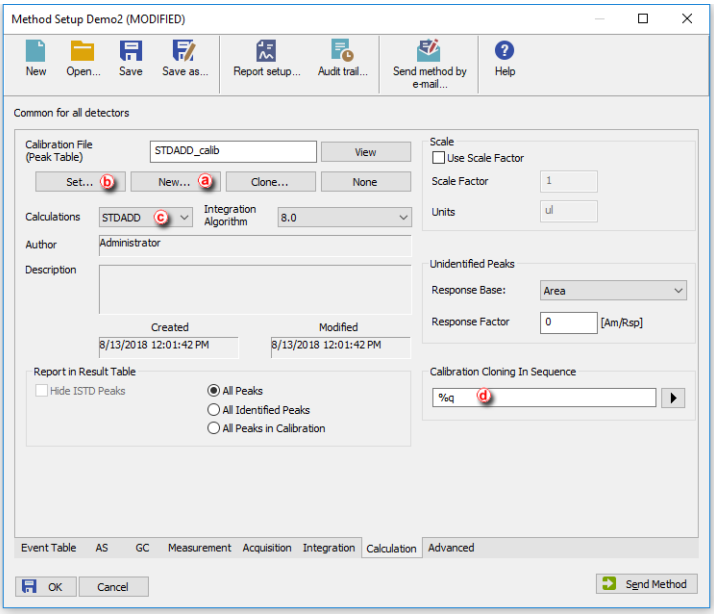
	Signal Name	Reten. Time [min]	Compound Name	Amount [ppm]	Area [µS/cm.s]	Response
1	Anions	1,382	Flourides (-)	16384,9	484,358	484,358
2	Anions	2,442	Chlorides (-)	16380,0	335,656	335,656
1	Cations	2,730	Lithium (+)	16380,0	457,892	457,892
3	Anions	3,260	Nitrites (-)	16366,4	199,659	199,659
2	Cations	3,308	Natrium (+)	16380,0	1027,113	1027,113
3	Cations	3,692	Ammonium (+)	16380,0	434,195	434,195
4	Anions	4,757	Bromides (-)	16386,3	129,220	129,220
5	Anions	6,318	Nitrates (-)	16398,4	162,876	162,876
4	Cations	6,322	Kalium (+)	16380,0	147,982	147,982
6	Anions	8,113	Phosphates (-)	16399,2	85,012	85,012
7	Anions	9,643	Sulphates (-)	16920,6	203,619	203,619
		All Signals Total		180755,8	3667,581	

8.11 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.



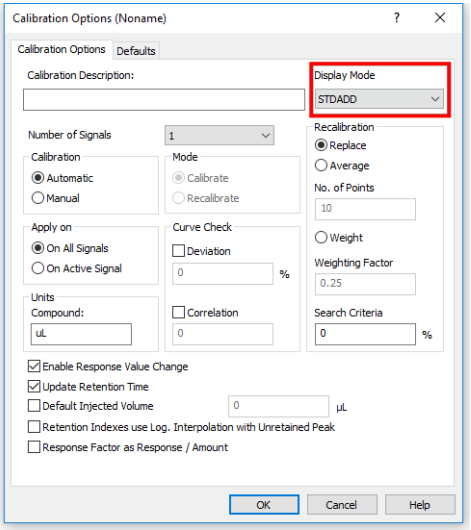
1. **Create a new method** from the *Instrument* window by selecting *File - New Method…* or open your already prepared method.
2. **Navigate to Method Setup - Calculation pane**.
3. **Create new Calibration file** ⓐ or Set already created your Calibration file ⓑ.



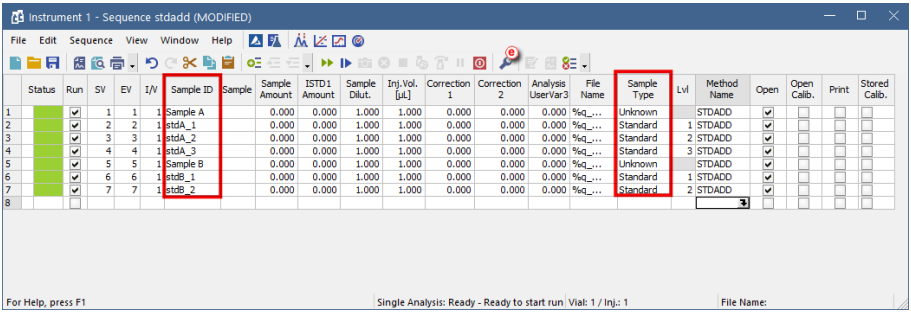
4. **Select STDADD in the *Calculations* combobox** ⓒ.
5. **Create a custom name for the cloned calibration files in** *Calibration Cloning in Sequence* ⓓ and click *OK*.

Note: Make sure that each of the samples measured will have a unique calibration name; good example might be using unique sample ID for each sample (duplicating it over the standard addition files) and using it as a name of new calibration by inputting the parameter %q.

6. **Open the Calibration window** by selecting *Window - Calibration* in the *Instrument* window.
7. **Open the Calibration Options dialog:**choose *Calibration - Options…* or click on . Select the *STDADD* in the Display Mode combobox and click *OK*.

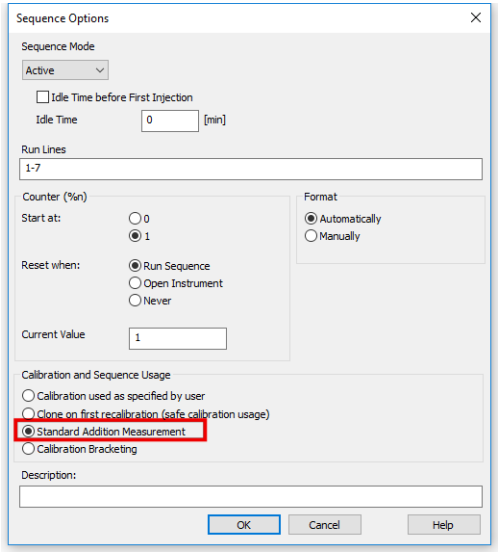


8. **Create a new sequence** with the given order of the lines:
   - Sample A
   - Sample A with Standard level 1
   - Sample A with Standard level 2
   - Sample A with Standard level X
   - Sample B
   - Sample B with Standard level 1
   - Sample B with Standard level X
   - *continue with the given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

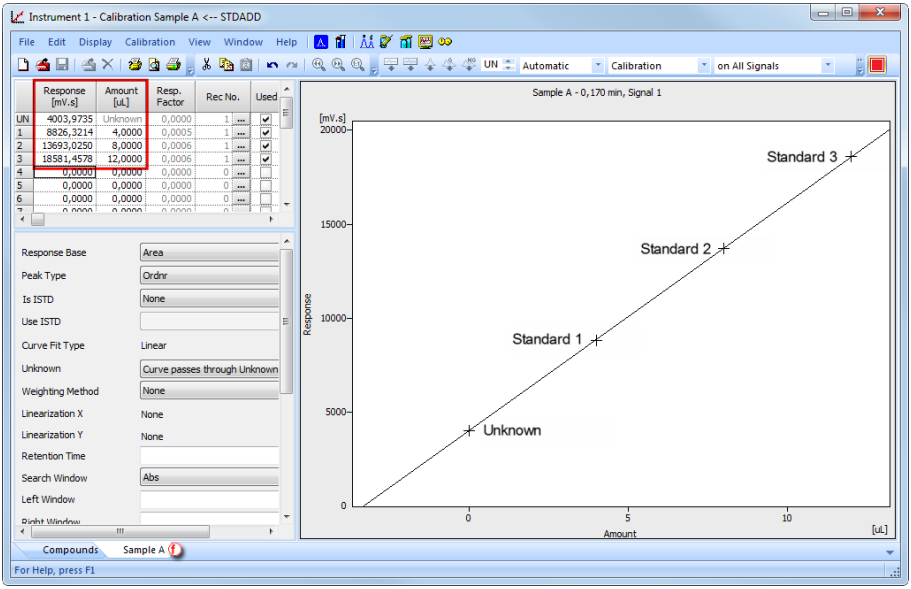


Note: In case you want to use a blank sample too, such sample shall be always put in the sequence before the unknown sample.

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



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

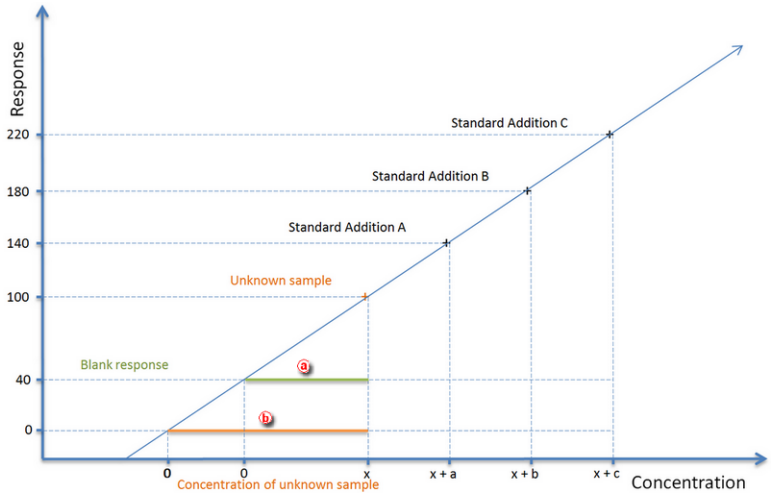


15. **Open chromatogram of the desired unknown sample.** The Result Table now contains amount of the unknown sample, calculated using Standard Addition.

How the concentration is calculated

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

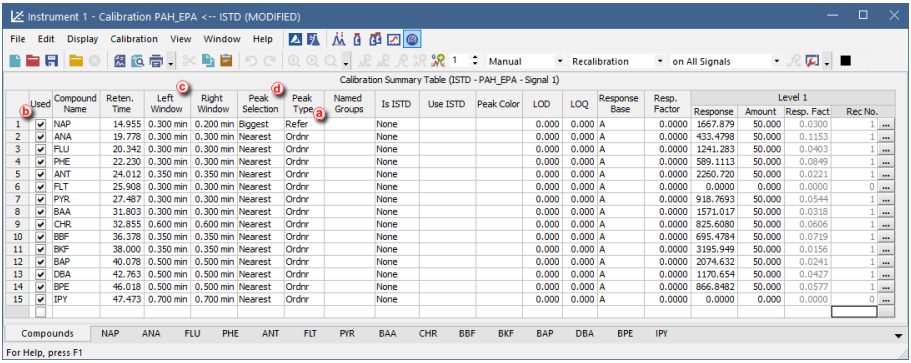
As shown in the picture below, the concentration when using Blank samples equals the green line ⓐ, whereas the concentration of an unknown sample equals the orange line ⓑ when using no Blank samples at all.



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



2. **Open the calibration file:** choose *File - Open…* or click on .
3. **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 ⓑ. If not checked, ordinary peaks would not be recalculated.
4. **Edit the Left and Right window values to define the range within which the peak should appear**. ⓒ

   More Info:

   This window may include other peaks if the selected reference peak meets the *Peak Selection* criteria.

5. **Select the Peak Selection criteria**: biggest, nearest, first or last peak ⓓ.

   More Info:

   Ordinary peaks are identified by the nearest option. 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*.

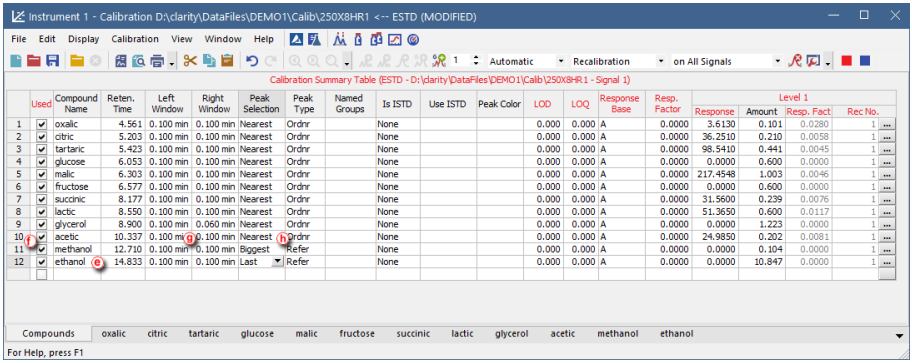
6. **Repeat steps 3 to 5 to add more reference peaks.**

7. **Set reference peak on other signals.**

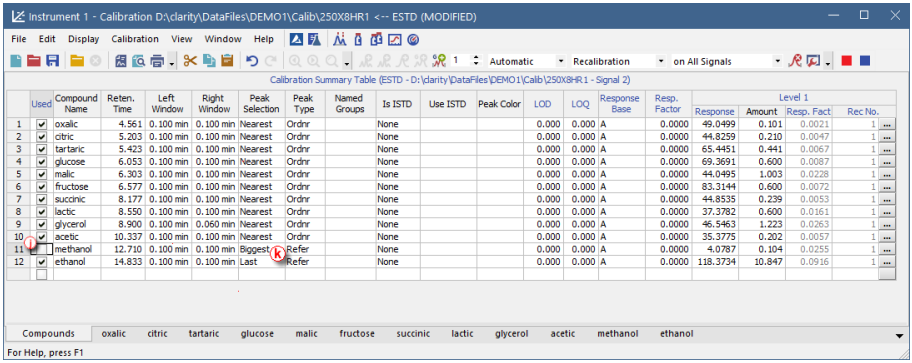
More Info:

When using reference peak with multisignal chromatogram, check that the reference peak fulfills the given Reference peak's *Peak Selection* criteria on all signals. If not, follow these steps:

- Duplicate the reference peak row in the calibration ⓔ (as many times as the number of different Peak Selection criteria will be used).
- Uncheck *Used* check-box for all newly added rows ⓕ.
- Duplicate **Retention time** to all reference peaks' rows ⓖ.
- Select *Refer* on the *Peak Type column* for all reference peaks' rows.
- For each reference peaks' row select the *Peak Selection* criteria according to current signal ⓗ. Note that the same reference peak can be the biggest in Signal 1, but not in Signal 2, where the same reference peak is the first.
- Switch to Calibration Summary Table of another signal ⓘ.

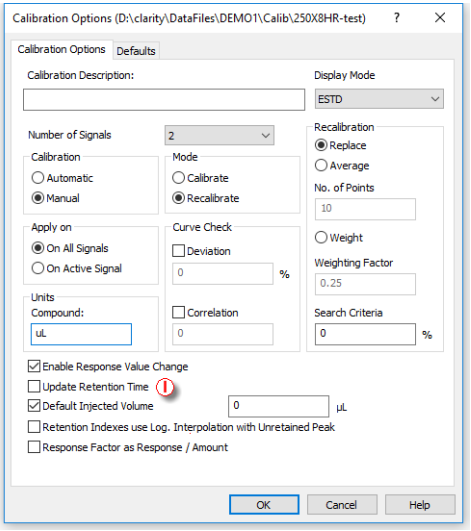


- Check *Used* check-box ⓙ for reference peak with *Peak Selection* criteria corresponding to displayed signal ⓚ.



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

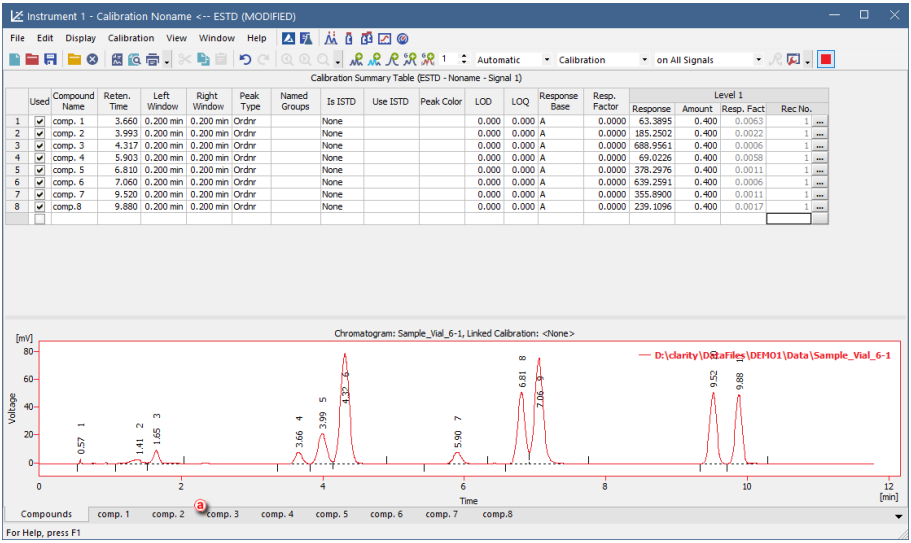
9. **Link the calibration to your chromatogram** as explained in Applying a calibration to a chromatogram.
10. **It is advisable to disable the update of retention times when recalibrating in Calibration options**ⓛ.



8.13 Calibration adjustments

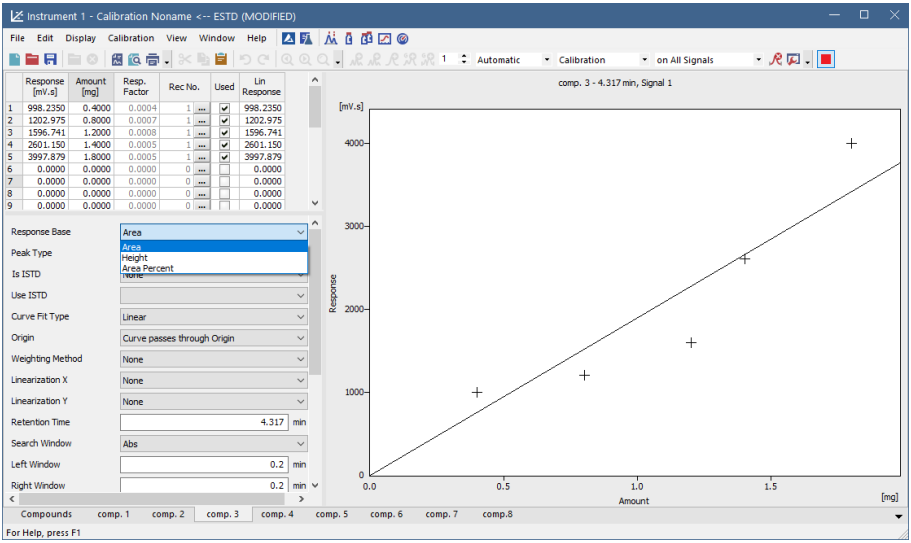
Following articles will describe how to perform some of the most common calibration modifications that can improve your calibration. Using this guide you manage to fit your calibration closer to your analytical application.

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.



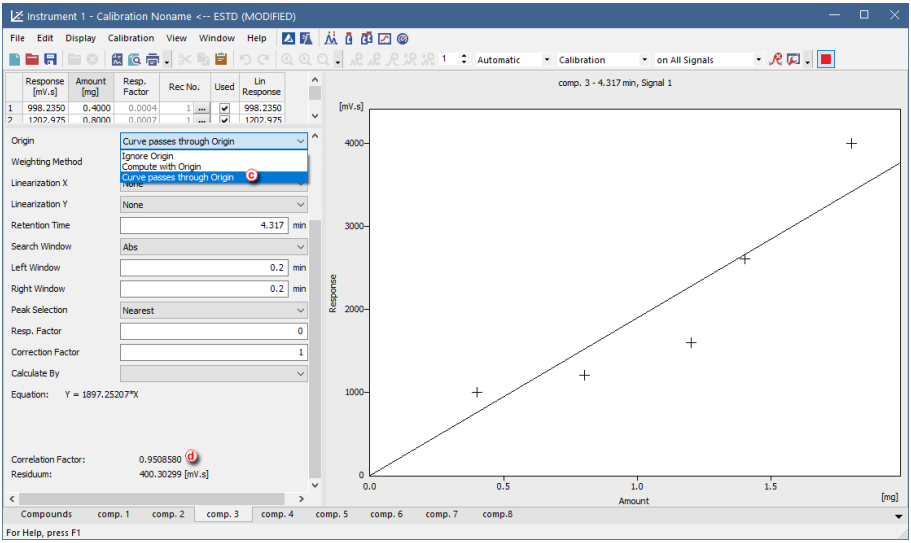
Modifying Response Base

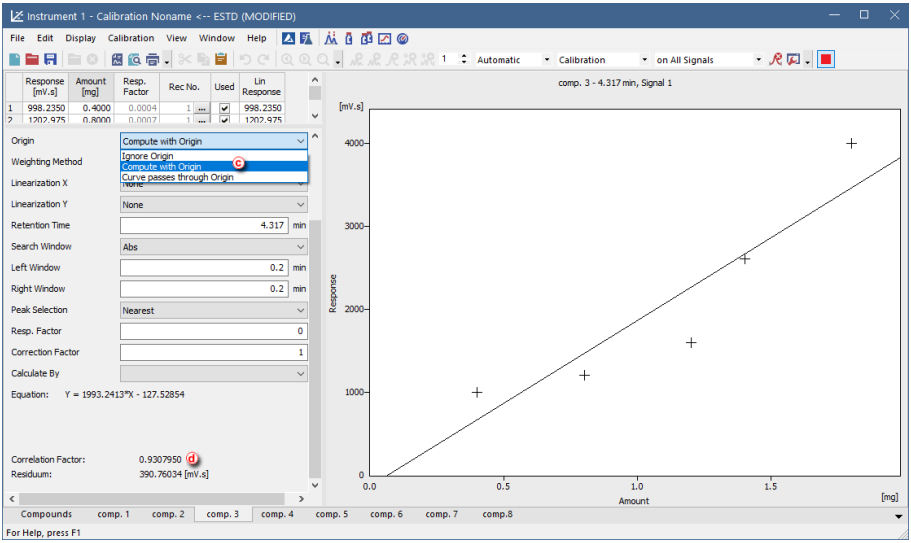
Set the *Response Base* ⓑ to modify whether the calibration curve will be calculated using *Area* or *Height* of the corresponding peak belonging to the specific compound. Changing the *Response Base* can help to create better fitting of the calibration to not well resolved peaks.

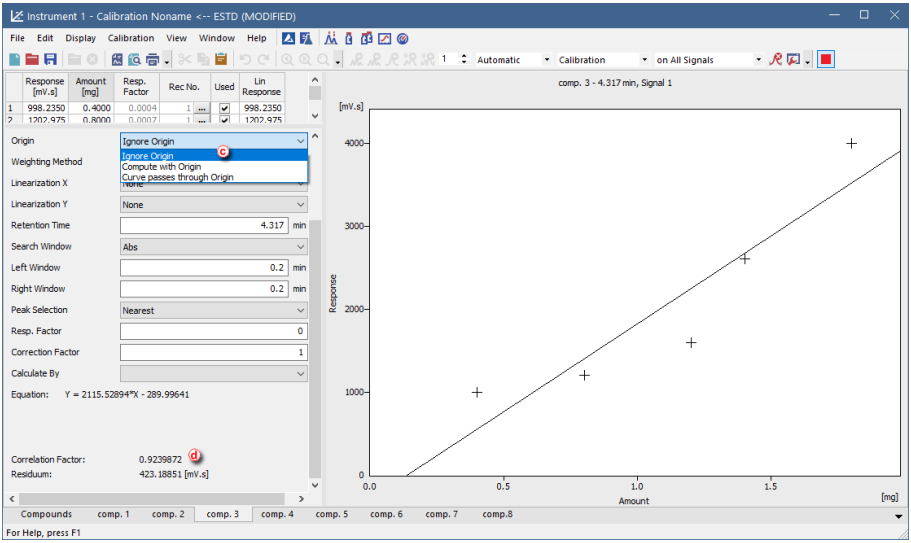


Modifying Origin

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 Noname <-- ESTD (MODIFIED)
File Edit Display Calibration View Window Help
Automatic
Calibration
on All Signals
Response [mV.s]
Amount [mg]
Resp. Factor
Rec No.
Used
Lin Response
1 998.2350 0.4000 0.0004 1 998.2350
2 1202.975 0.8000 0.0007 1 1202.975
Origin
Curve passes through Origin
Ignore Origin
Compute with Origin
Curve passes through Origin
Weighting Method
Linearization X
Linearization Y
None
Retention Time
4.317
min
Search Window
Abs
Left Window
0.2
min
Right Window
0.2
min
Peak Selection
Nearest
Resp. Factor
0
Correction Factor
1
Calculate By
Equation: Y = 1897.25207*X
Correlation Factor: 0.9508580
Residuum: 400.30299 [mV.s]
comp. 3 - 4.317 min, Signal 1
[mV.s]
Response
4000
3000
2000
1000
0
0.0
0.5
1.0
1.5
Amount
[mg]
Compounds
comp. 1
comp. 2
comp. 3
comp. 4
comp. 5
comp. 6
comp. 7
comp.8
For Help, press F1





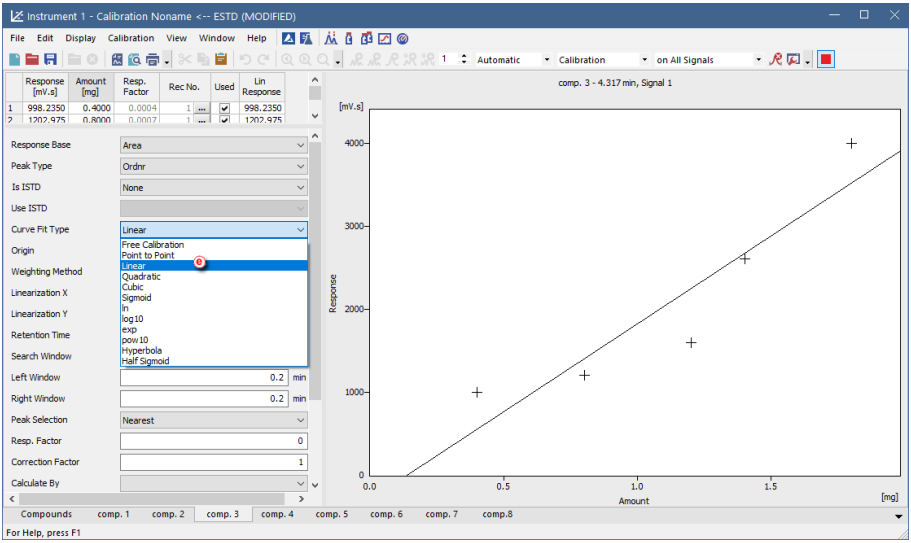
As you can see from the *Correlation factor* ⓓ values, changing the *Origin* setting from the *Curve Passes through Origin* to *Compute with Origin* improved the curve fit. However, the option *Ignore Origin* has proved to be the best match for the used detector.

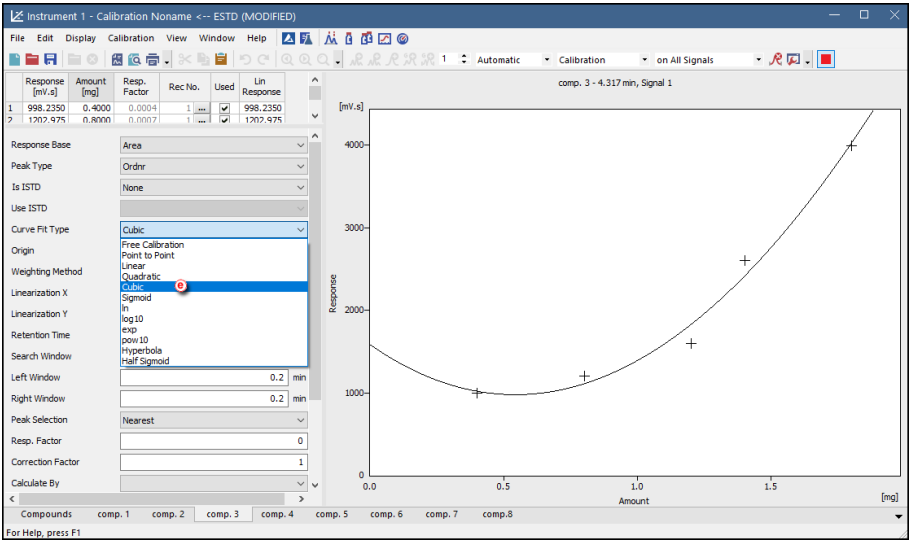
Modifying Curve Fit Type

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.



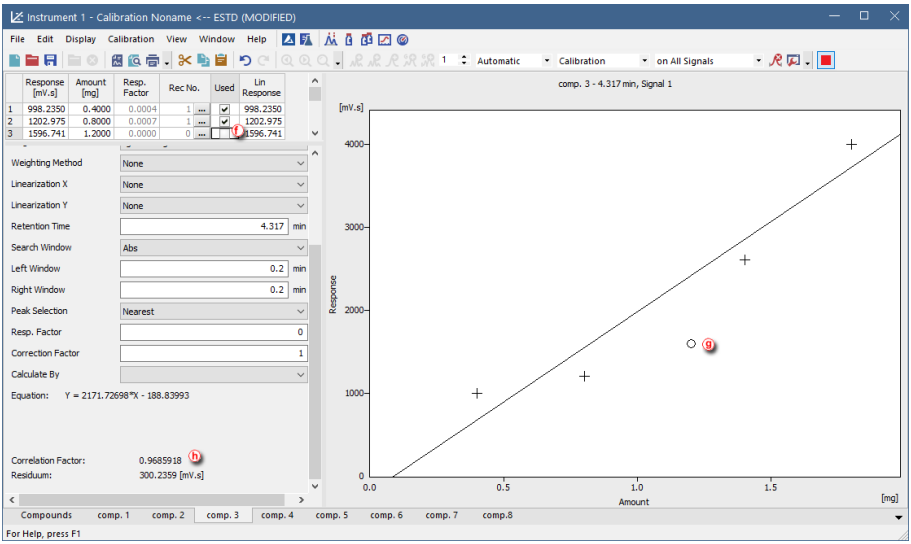


As you can see, changing the *Curve Fit Type* from *Linear* to *Cubic* increased the *Correlation Factor* from 0.951 to 0.999.

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.

8.14 Normalized Area % Calculation

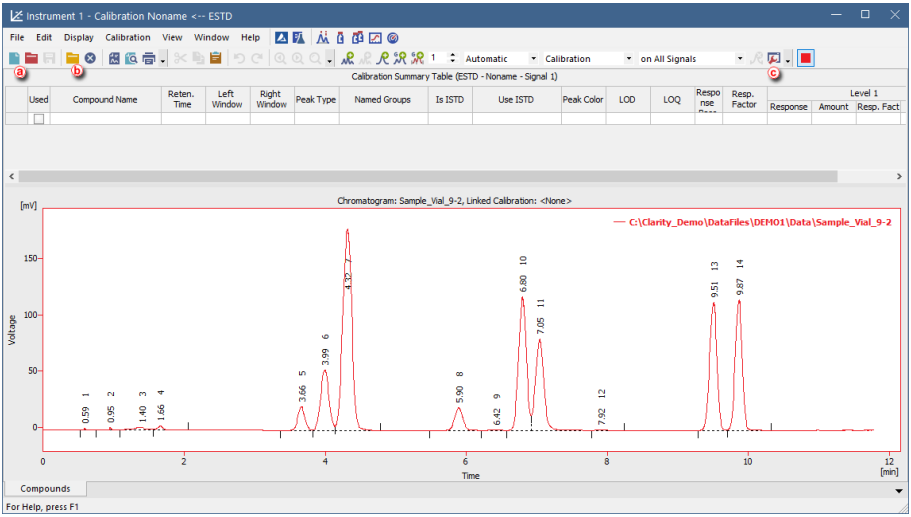
For Normalized Area% calculation no specific settings are necessary, the calculation results are always present in the *Area%* column in the Result table.

8.15 Normalized Amount % Calculation

This topic describes how to set all necessary settings in Clarity, in order to obtain correct results calculated according to normalization calibration method. The normalization can be achieved by two means. First option is application of 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.

A) Application of specific Response Factors

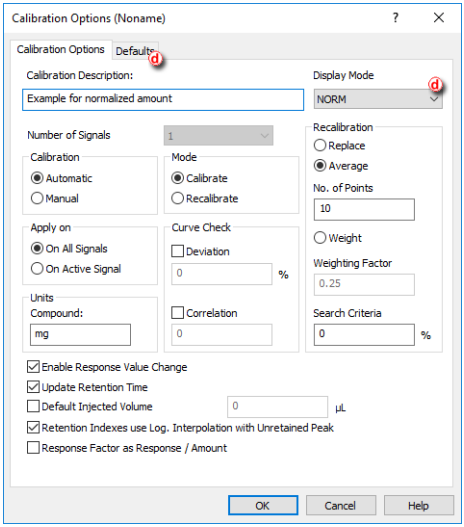
1. **Open the Calibration window:** select *Window - Calibration* on the *Instrument* window or click on .



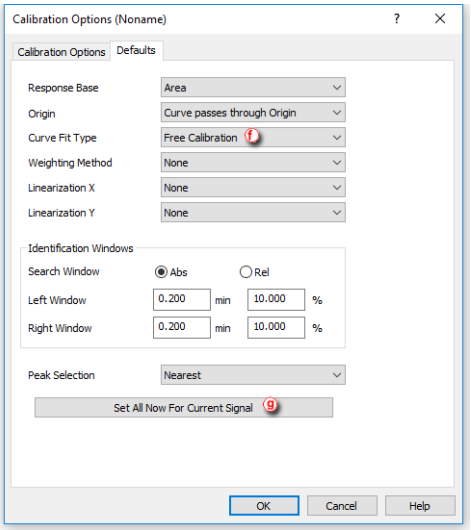
2. **Create a new calibration file:** select *File - New* or click on ⓐ and insert name for this calibration.
3. **Open calibration standard:** select *File - Open Standard…* or click on ⓑ.

   More Info:
   Select a measured and qualitatively evaluated chromatogram where all peaks are available.

4. **Open the Calibration Options dialog:** select *Calibration - Options…* or click on ⓒ.



5. Set ***Display Mode*** to ***NORM*** ⓓ.
6. Switch to ***Defaults*** tab ⓔ to set other necessary options.

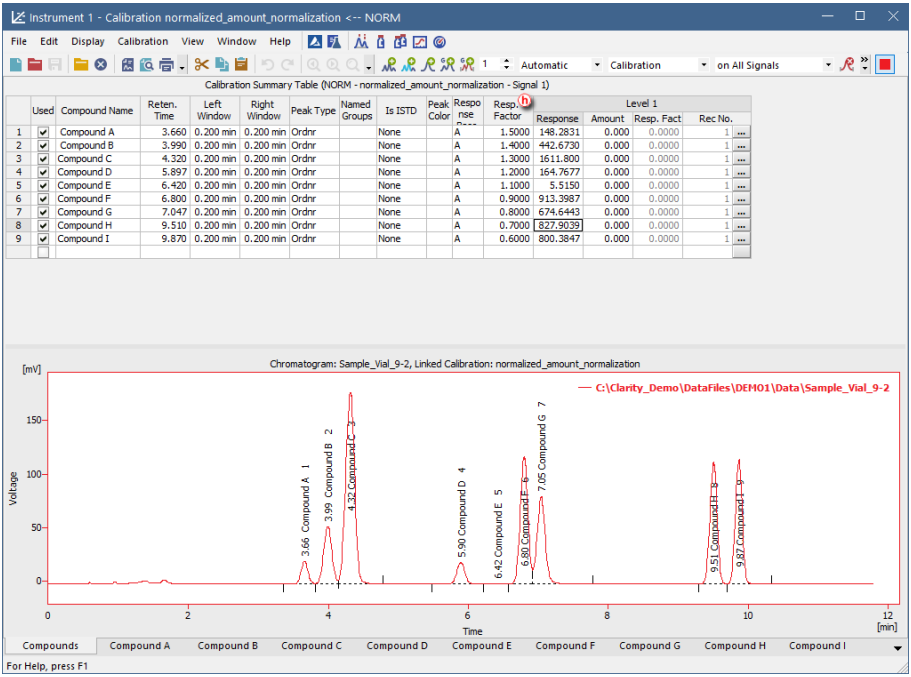


7. Set ***Curve Fit Type*** to ***Free Calibration*** ⓕ and then click ***Set All Now For Current Signal*** ⓖ.
8. Click **OK**.
9. Add peaks in the chromatogram of the calibration standard to the calibration file.

More Info:

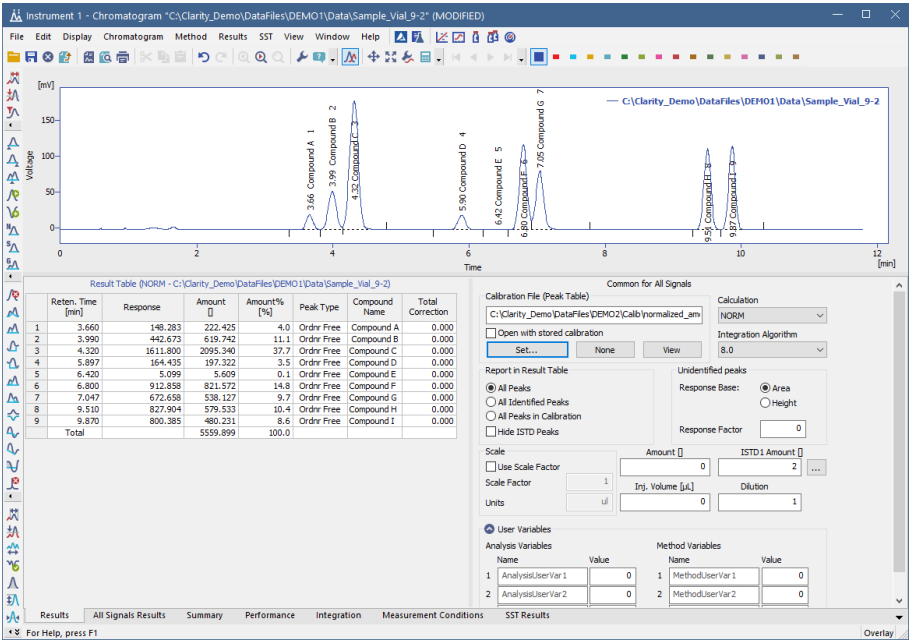
Select *Calibration - Add All* or click on to add all peaks or the Add Peak / Add Group icons to add specific peaks.

10. Set ***Response Factors*** ⓗ to corresponding values.



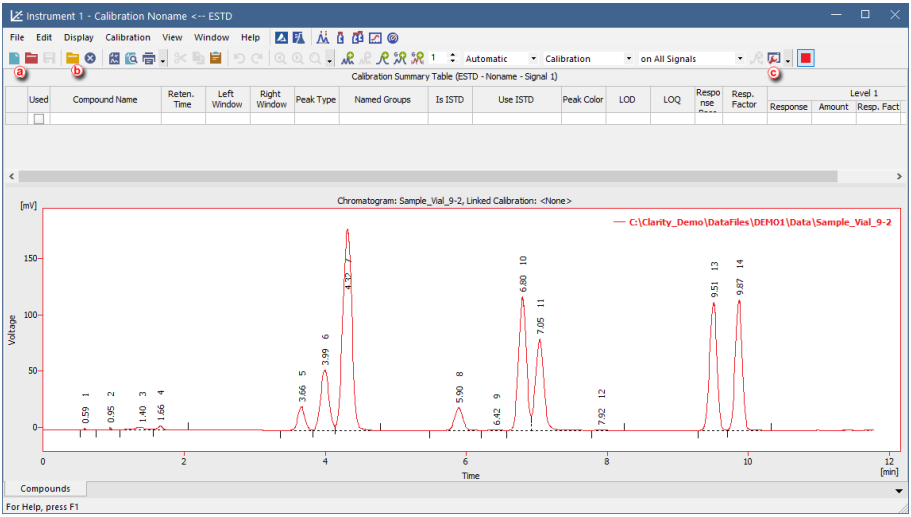
11. **Save the calibration file:** select *File - Save* or click on .

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



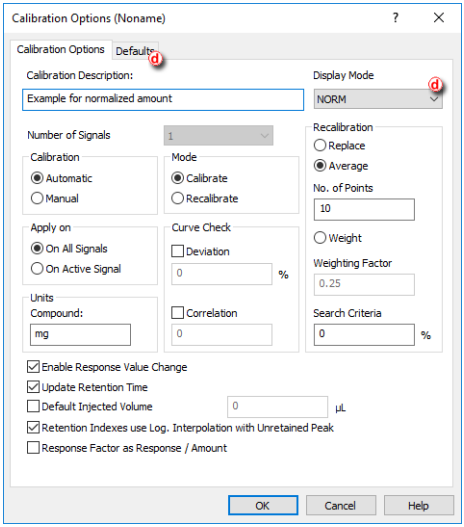
B) Application of automatically calculated Response Factors based on calibration with standard sample with known composition

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

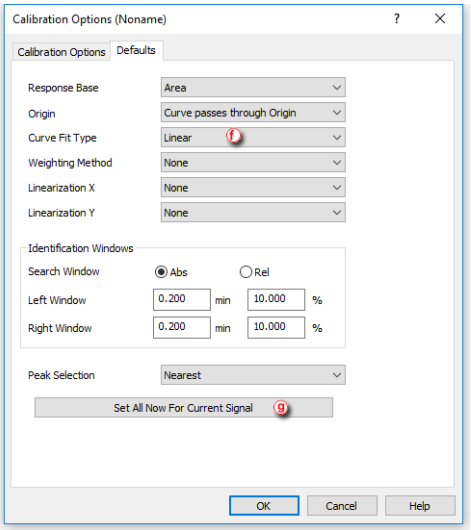


2. **Create a new calibration file:** select *File - New* or click on ⓐ and insert name for this calibration.
3. **Open calibration standard:** select *File - Open Standard…* or click on ⓑ.

   More Info:
   Select a measured and qualitatively evaluated chromatogram where all peaks are available.
4. **Open the Calibration Options dialog:** select *Calibration - Options…* or click on ⓒ.



5. Set ***Display Mode*** to ***NORM*** ⓓ.
6. Switch to ***Defaults*** tab ⓔ to set other necessary options.

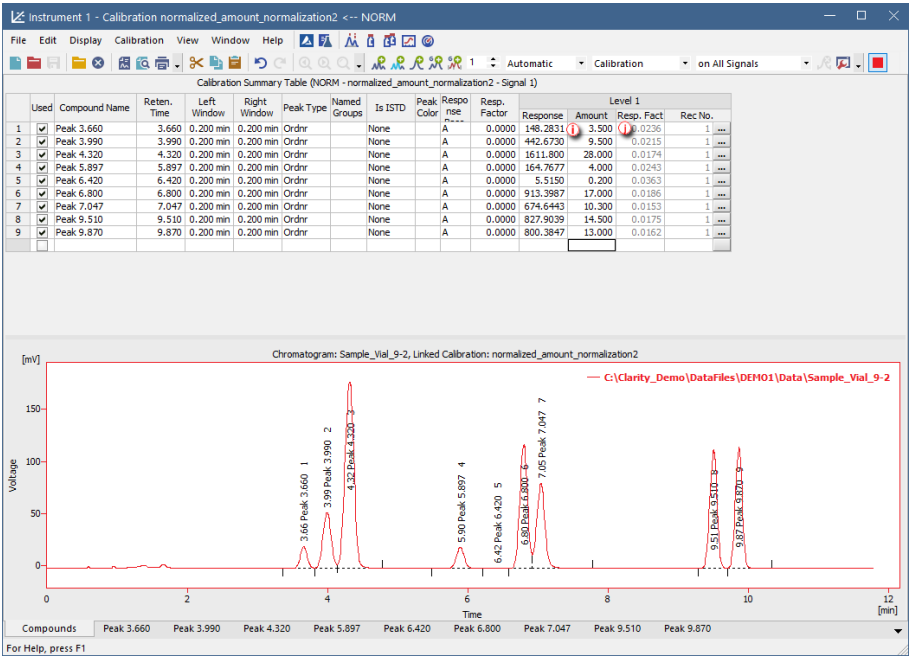


7. Set ***Curve Fit Type*** to ***Linear*** ⓕ and then click ***Set All Now For Current Signal*** ⓖ.
8. Click **OK**.
9. Add peaks in the chromatogram of the calibration standard to the calibration file.

More Info:

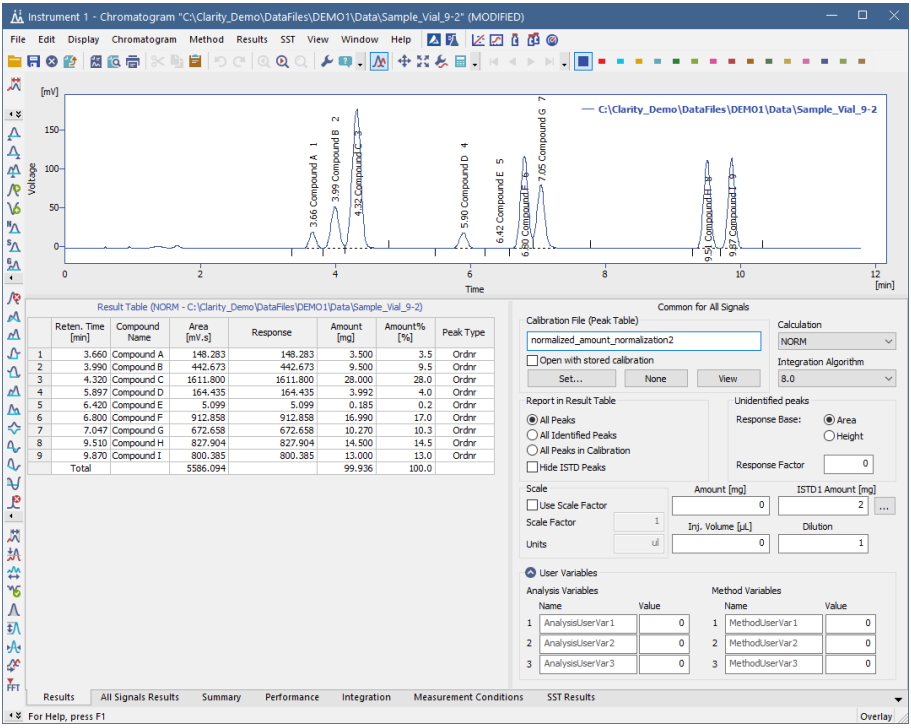
Select *Calibration - Add All* or click on to add all peaks or the Add Peak / Add Group icons to add specific peaks.

10. Insert values in ***Amount*** column ⓘ. These values represent actual fraction composition of the standard sample. Note that ***Response Factor*** ⓙ values are calculated immediately.



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

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


Instrument 1 - Chromatogram "C:\Clarity_Demo\DataFiles\DEMO1\Data\Sample_Vial_9-2" (MODIFIED)
File Edit Display Chromatogram Method Results SST View Window Help
[mV]
Voltage
C:\Clarity_Demo\DataFiles\DEMO1\Data\Sample_Vial_9-2
3.66 Compound A 1
3.99 Compound B 2
4.32 Compound C 3
5.90 Compound D 4
6.42 Compound E 5
6.80 Compound F 6
7.05 Compound G 7
9.51 Compound H 8
9.87 Compound I 9
Time
[min]
Result Table (NORM - C:\Clarity_Demo\DataFiles\DEMO1\Data\Sample_Vial_9-2)
Reten. Time [min] | Compound Name | Area [mV.s] | Response | Amount [mg] | Amount% [%] | Peak Type
1 3.660 Compound A 148.283 148.283 3.500 3.5 Ordnr
2 3.990 Compound B 442.673 442.673 9.500 9.5 Ordnr
3 4.320 Compound C 1611.800 1611.800 28.000 28.0 Ordnr
4 5.897 Compound D 164.435 164.435 3.992 4.0 Ordnr
5 6.420 Compound E 5.099 5.099 0.185 0.2 Ordnr
6 6.800 Compound F 912.858 912.858 16.990 17.0 Ordnr
7 7.047 Compound G 672.658 672.658 10.270 10.3 Ordnr
8 9.510 Compound H 827.904 827.904 14.500 14.5 Ordnr
9 9.870 Compound I 800.385 800.385 13.000 13.0 Ordnr
Total 5586.094 99.936 100.0
Common for All Signals
Calibration File (Peak Table)
normalized_amount_normalization2
Open with stored calibration
Set... None View
Calculation
NORM
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
Amount [mg] 0
ISTD 1 Amount [mg] 2
Inj. Volume [µL] 0
Dilution 1
User Variables
Analysis Variables
Name Value
1 AnalysisUserVar1 0
2 AnalysisUserVar2 0
3 AnalysisUserVar3 0
Method Variables
Name Value
1 MethodUserVar1 0
2 MethodUserVar2 0
3 MethodUserVar3 0
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results
For Help, press F1
Overlay

9 Results and Calculations

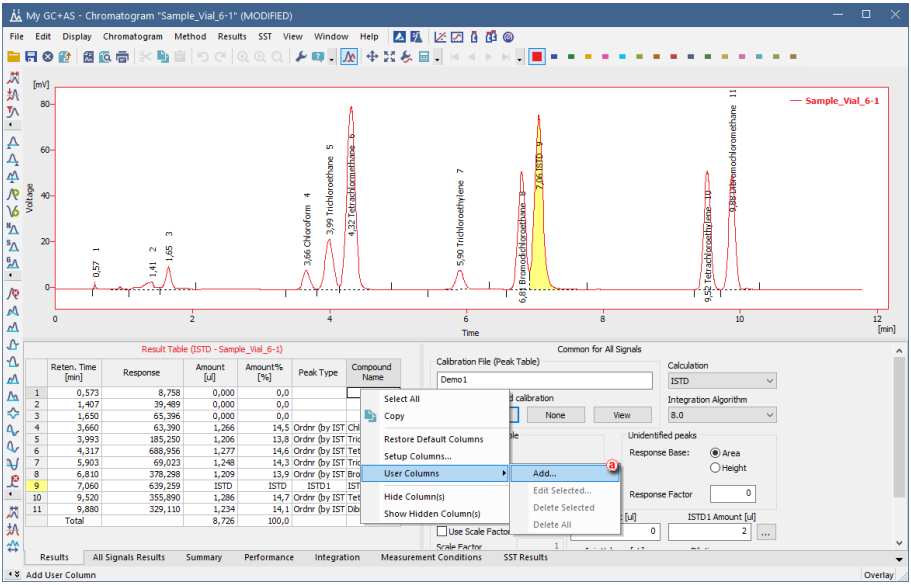
Advanced topics describing how to use *User Columns* displaying custom results, etc.

9.1 User Columns

This article describes how to append a new column with user-defined calculation to the *Chromatogram - Result Table*. For more details about User Columns refer **Reference Guide Manual**.

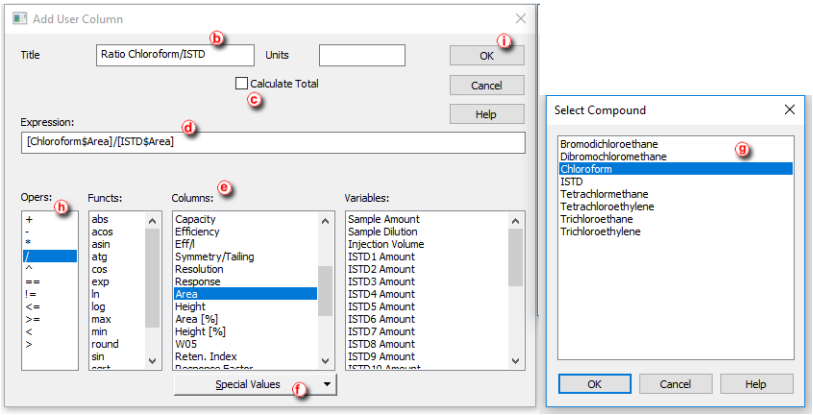
Note that to perform defined calculation it is mandatory to have chromatograms with calibration. Only for first or last peaks in the chromatogram calibration is not mandatory.

1. Open **Chromatogram window**: select *Window - Chromatogram* from the *Instrument* window or click on  icon.
2. Open chromatogram you want to edit: click *File - Open Chromatogram...* or click on  icon.
3. Switch to ***Results*** tab and right-click on it.
4. Select ***User Columns - Add...*** ⓐ, the **Add User Column dialog** will be opened.

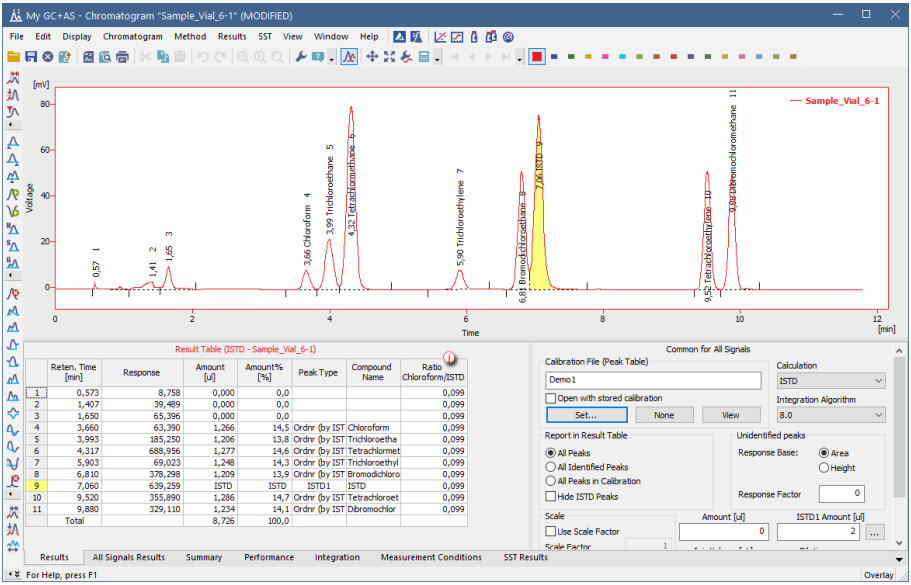


5. Fill in the **Title** ⓑ on a new column. In our case *Ratio Chloroform/ISTD*.
6. Check/Uncheck *Calculate Total* ⓒ (depends on column Expression result).

7. Fill in **Expression** ⓓ line , which presents the user's defined calculation. In our case:
    - In **Columns:** ⓔ list select *Area*, then click on **Special Values - Compound** ⓕ and choose *Chloroform* ⓖ. Click OK.
    - In **Opers:** ⓗ list select / and double-click.
    - In **Columns:** list select *Area*, then click on **Special Values - Compound** and choose *ISTD*. Click OK.



8. Click **OK** ⓘ in **Add User Column dialog**.
9. New User Column is added in the end of Result Table ⓙ.



9.2 User Variables

This article describes how to set *Analysis* and *Method User Variables* subsequently used in *User Columns* calculations. *Analysis User Variables* can be defined in Single Analysis or Sequence window. *Method User Variables* can be defined in Method Setup window.

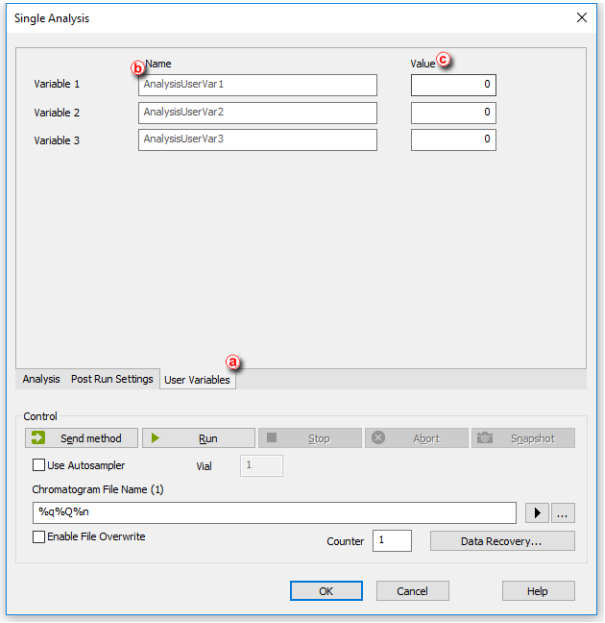
A) Setting of Analysis User Variables in Single Analysis window

1. Open **Single Analysis window**: select *Analysis - Single...* from the *Instrument* window or click on  icon.
2. Unroll the *Analysis User Variables* section, click on the chevron button ⓐ.
3. Define **Name** of the variable ⓑ.

   More Info:

   Note If the field is left empty, default name *AnalysisUserVar1-AnalysisUserVar3* would remain filled in.

4. Define numerical **Value** of the variable ⓒ.



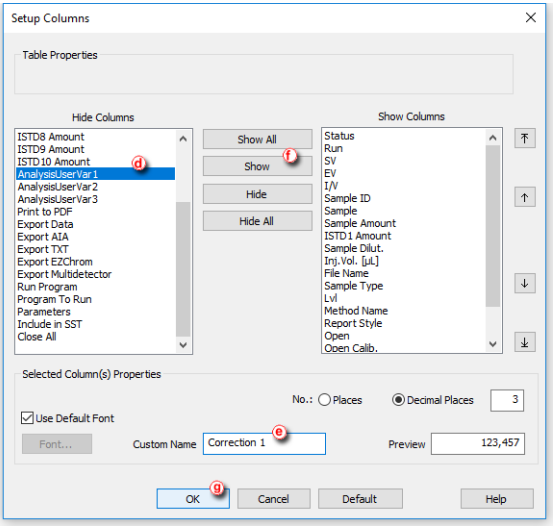
B) Setting of Analysis User Variables in Sequence window

1. Open **Sequence window**: select *Analysis - Sequence* from the *Instrument* window or click on icon.
2. Show the User Variable columns: Click *Edit - Setup Columns...*

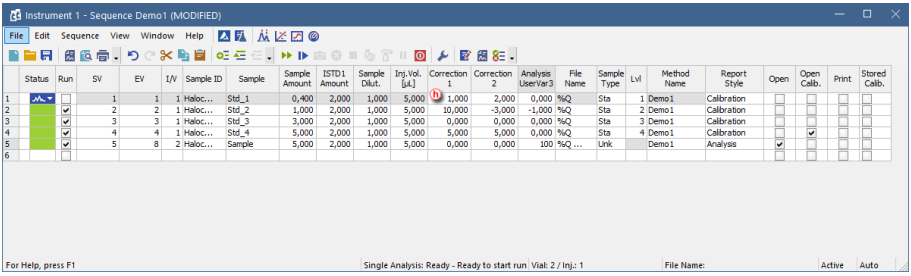
   More Info:

   AnalysisUserVar1 - AnalysisUserVar3 columns are hidden and set to value *0* by default.

3. Define **Name** of the variable: select the variable ⓓ and fill in the name in *Custom Name* field ⓔ.
4. Click Show ⓕ.
5. Click OK ⓖ.



6. Define **Name** of the variable: type the value directly in the appropriate row ⓗ.



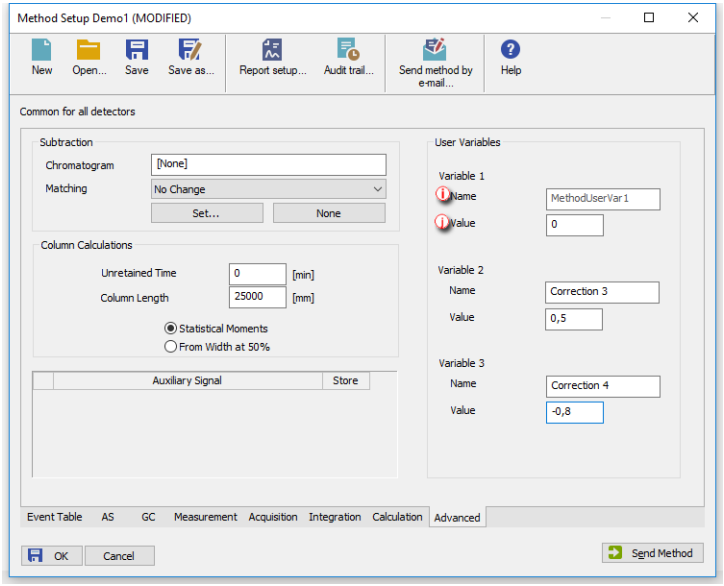
C) Setting of Method User Variables in Method Setup window

1. Open **Method Setup window**: select *Method - Advanced...* from the *Instrument* window.
2. Define **Name** of the variable ⓘ.

   More Info:

   Note If the field is left empty, default name *MethodUserVar1-MethodUserVar3* would remain filled in.

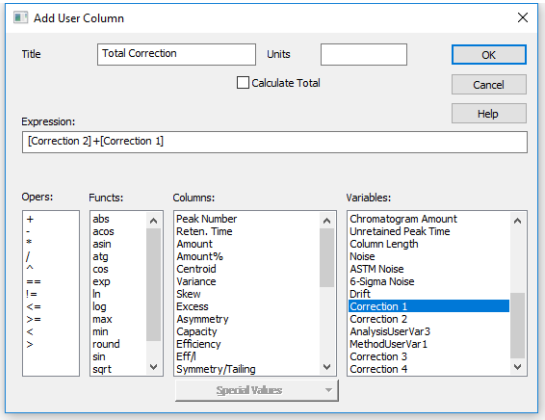
3. Define numerical **Value** of the variable ⓙ.

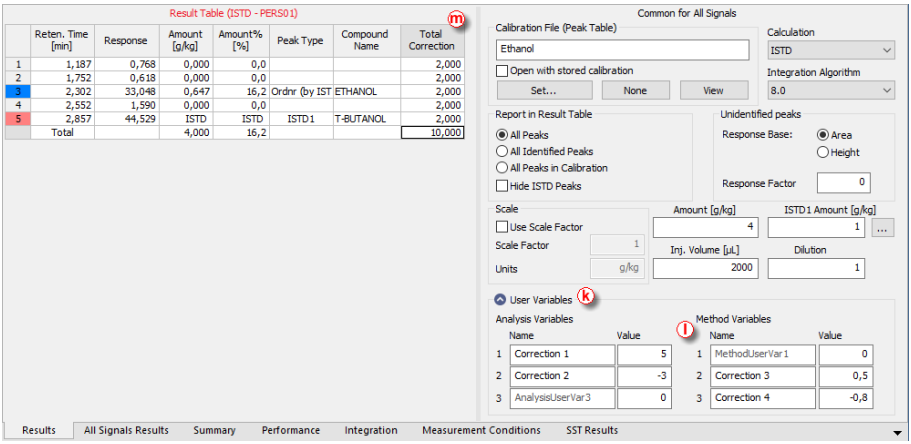


D) Setting of User Columns with User Variables

Analysis and *Method User Variables* are editable also directly from *Chromatogram - Result Table*.

1. Open **Chromatogram window**: select *Window - Chromatogram* from the *Instrument* window or click on  icon.
2. Unroll the *User Variables* section in the right side of the window, click on the chevron button ⓚ.
3. Define / re-type the Name or Value ⓛ of the variable.
4. Add User Column ⓜ as described in User Columns using User Variables.





9.3 Signal to Noise Ratio Calculation

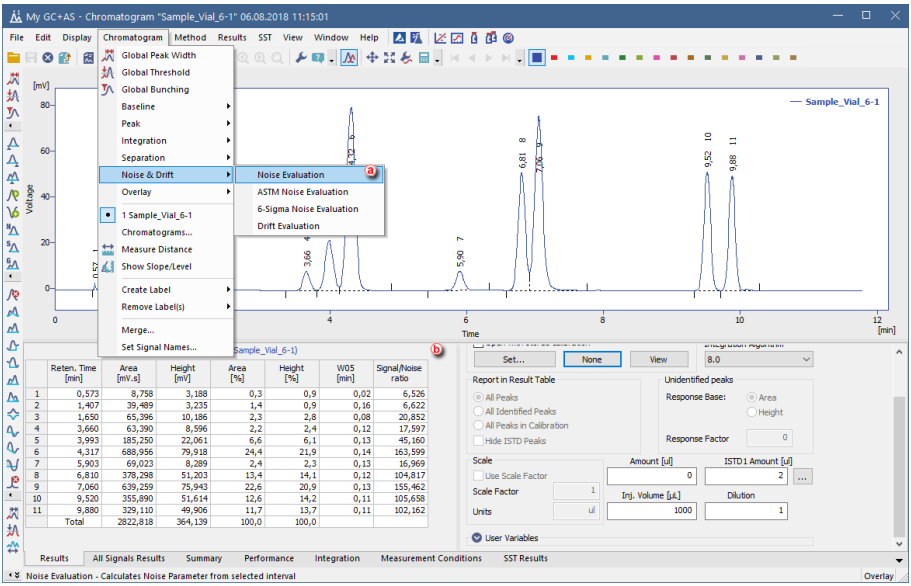
This article describes how to calculate Signal to Noise Ratio using User Columns calculations with Variables.

9.3.1 Noise Parameter Evaluation

At first the 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. After selecting *Chromatogram - Noise & Drift - Noise Evaluation* ⓐ the interval for Noise calculation can be selected. 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* ⓔ.



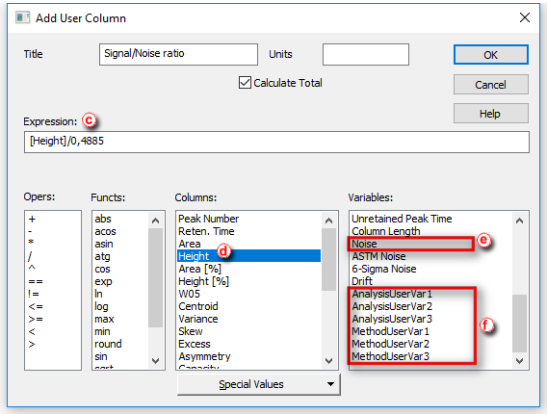
9.3.2 Calculating Signal to Noise Ratio

Once the Noise Parameter value is evaluated, such value can be used to calculate Signal to Noise Ratio either as a numerical value or as a defined User Variable.

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 [Height]/[Noise].
- 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. [Height]/0,4885, where the number 0,4885 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]/0,4885 or 2*[Height]/([Noise] + 3,141).

Note: Setting the *Analysis User Variable* or the *Method User Variable* is described in the section **User Variables on pg 134**.

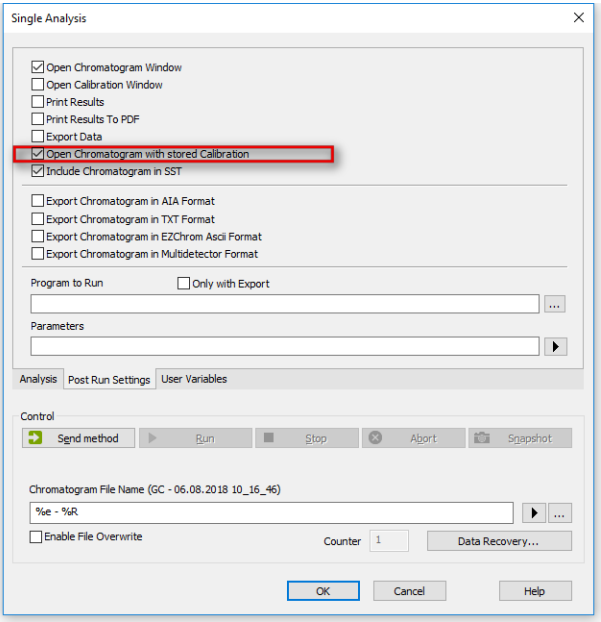
9.4 How to Display Older Results when Linked Calibration is Modified

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:

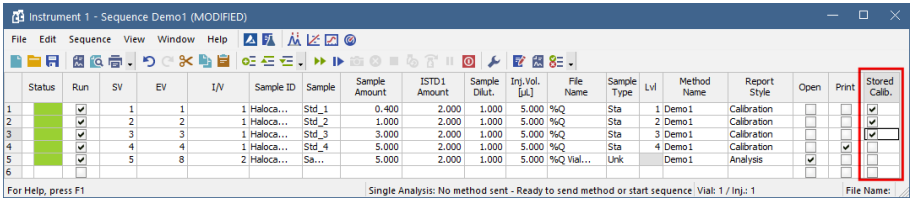
1. Make a copy of the calibration file so each series of measured chromatograms will be linked to a separate calibration file. This has advantage in case some amendments to the calibration will be necessary later, as the amendments will affect only the related chromatograms. Such

procedure could be automated from sequence. For more information on this procedure, see the chapter **"Calibrating using clone at first recalibration"** on pg **91**..

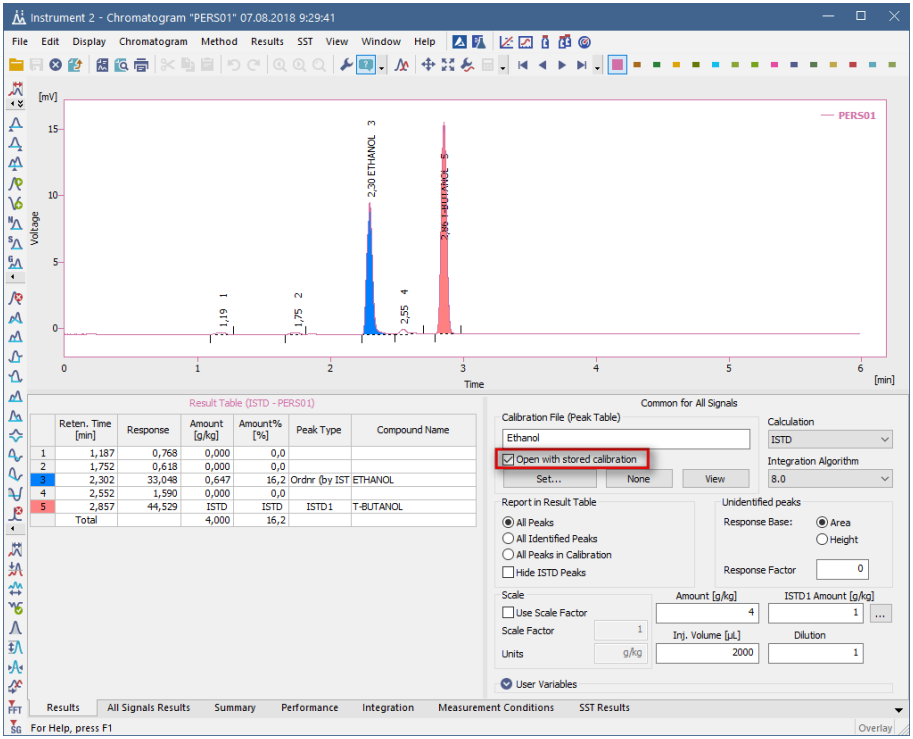
2. Using the *Open with stored calibration* option. Such option is accessible from multiple dialogs, depending on whether Single Analysis or Sequence is measured (automated approach) or this option can be selected upon opening the chromatogram.
    - In the Single Analysis dialog - Post Run Settings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



9.5 Calculating percentage content of a compound in a solid sample

It 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 Calibration** window with your calibration.
2. **Click the**  to open Calibration Options window ①.
3. **Specify correct units** for the calibrated amount ②. Confirm changes by clicking **OK** button.

   More Info:

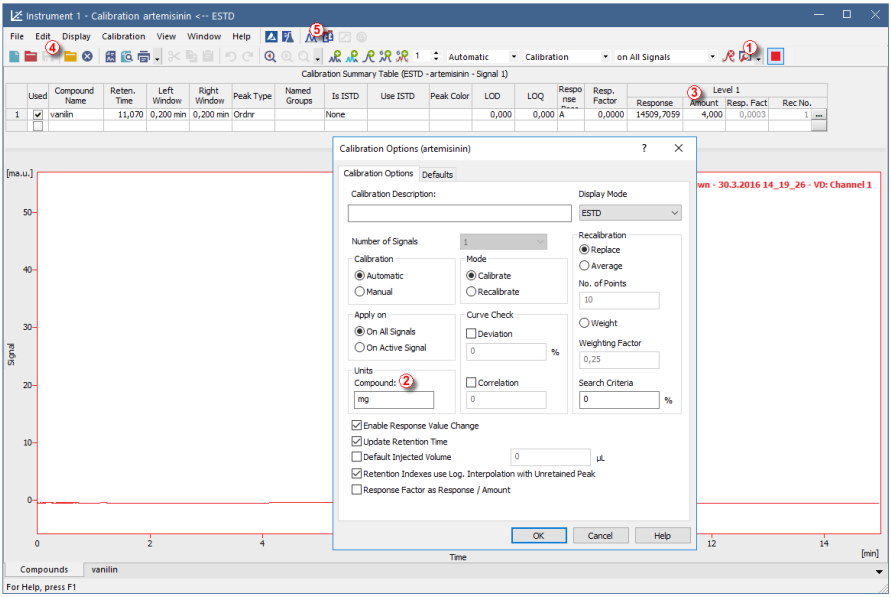
   Fill the units specified in the **Compound** field according to the used amount units. In our specific case *mg* are used. Set units are used in the Chromatogram window for further calculations.

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

   More Info:

   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 ④ and open Chromatogram window ⑤.



6. **Open chromatogram(s)** using the yellow folder ⑥.
7. **Assign each chromatogram a calibration** using the *Set...* button ⑦.
8. **Fill the amount** of the sample that had been used ⑧.

   More Info:

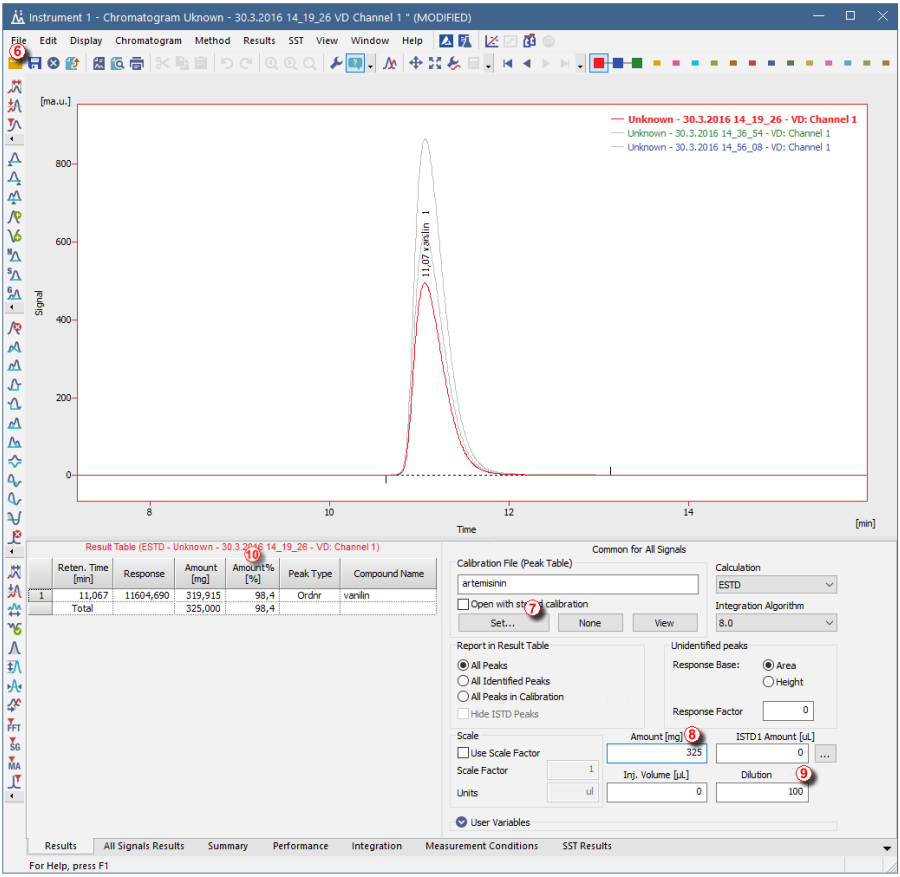
   Amount refers to the mass of the sample used. Units are automatically copied from the Calibration Options (see step 3). In our example: *325 mg* sample had been used.

9. **Fill the dilution** that had been used ⑨.

   More Info:

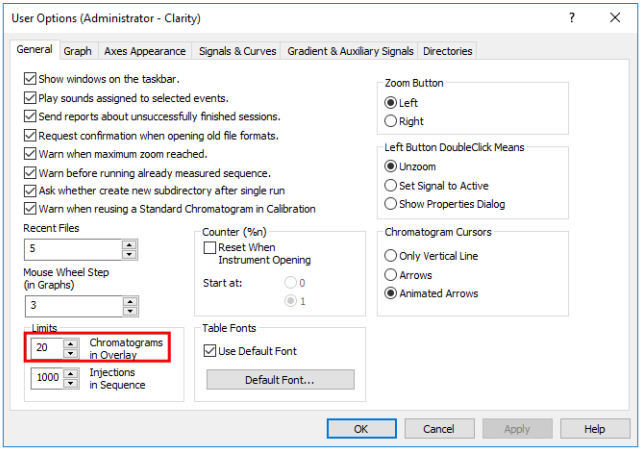
   Dilution refers to the solvent volume that has been used to dilute the sample. Dilution multiplies the values in the amount columns. In our example: *325 mg* of sample had been diluted by *100 ml* of solvent.

10. Column *Amount%* in the *Result Table* now displays the percentage amount of the compound in the sample ⑩.



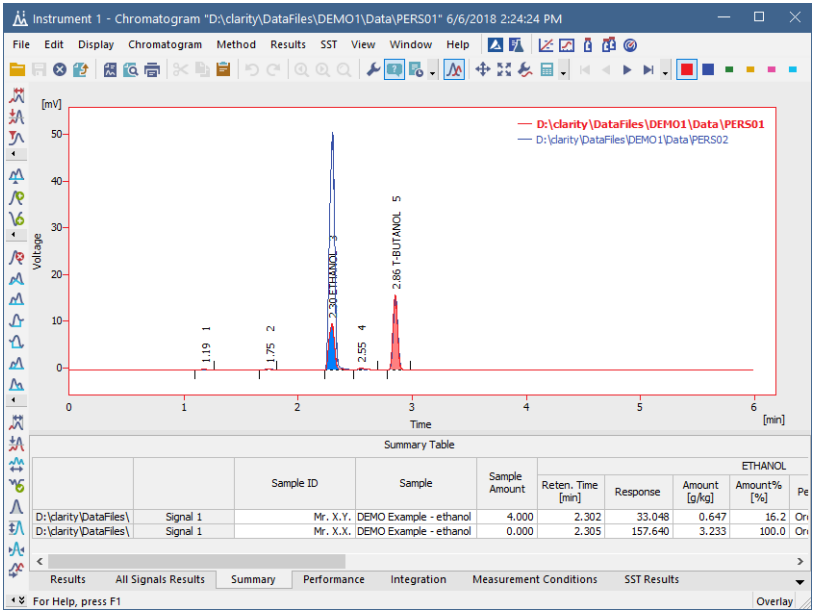
9.6 Comparing the results from several chromatograms

The default maximum number of chromatograms in Overlay is set to 20. In case summary report should include more chromatograms, this limit can be changed in the User Options window, which can be invoked from the Instrument window *Setting - User Options*.

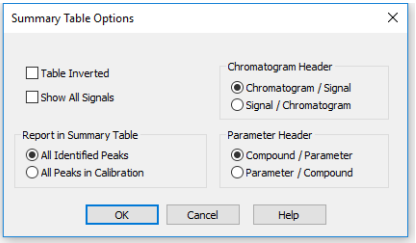


1. **Open the *Instrument* and then the *Chromatogram* window**.
2. **Disable the *Overlay Mode***, click on or un-check it from *File - Overlay Mode* and **open the first chromatogram** selecting *File - Open chromatogram….*
3. **Enable now the *Overlay Mode*** (same as above).
4. **Open the rest of the chromatograms**.
   - You can also use *File - Open Chromatograms From Sequence...* command which opens all chromatograms from sequence including Standards.
5. **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.



6. **Right click on the *Summary Table***, if you want to change the visualization of the table or add a custom column, etc.
7. To see all signals, **click on 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*.

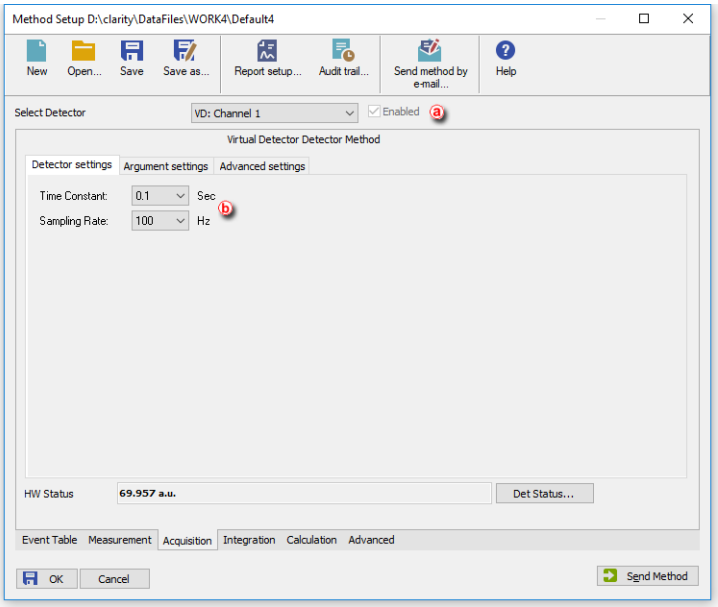


It is also possible to compare parameters from different chromatograms and check if they fall within set limits by using the SST Extension.

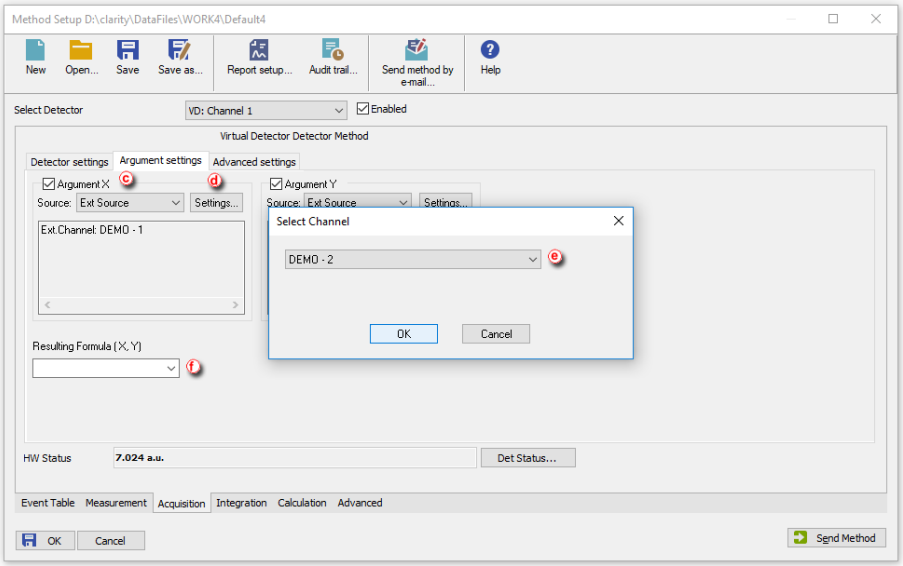
9.7 Confirming the identity of a compound by using the signal ratio

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.

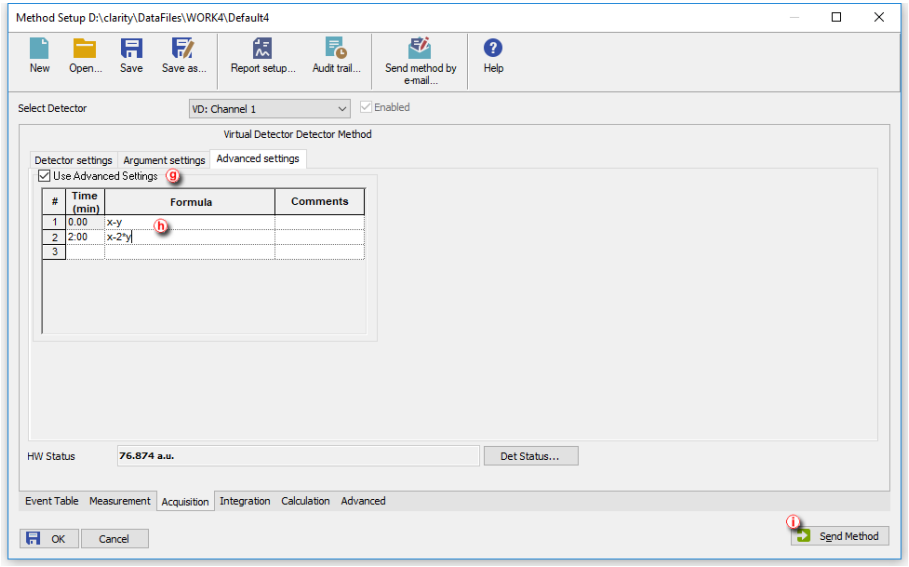
1. **Add the *Virtual Detector* as well as your dual wavelength detector,** if it has not been added already, as explained in the chapter Adding a new device**.**
2. **Open the *Method Setup - Acquisition* dialog:** select *Method - Acquisition* command.



3. **Select the *VD detector* and tick the *Enable* checkbox.** ⓐ
4. **On the *Detector Settings* tab, set the *Time Constant* to 0 to avoid distortion and type in your detector *Sampling Rate*.** ⓑ
5. On the *Argument Settings* tab**, tick the *Argument X* check box, select an *External Source*** ⓒ **and then click on the *Settings* button** ⓓ**, select the appropriate detector *Channel* and click *OK*** ⓔ.



6. **Repeat the same procedure for Argument Y.**
7. **Fill in the Resulting Formula with the Signal Ratio X/Y or a different ratio if needed.** ⓕ
8. **Alternatively, you can set a different formula for specific time intervals:**
    - Click on the *Advanced Settings* tab.
    - Tick the *Use Advanced Settings* box. ⓖ
    - Fill in the tables with the time intervals and the formulas. ⓗ



9. **Send the Method ⓘ and click OK.**

10 Data Reports

How to create a report, adjust it and print.

10.1 Setting up a report style for printing

It is possible to select what information and how you want to be 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 go to section Creating a report (example).

More Info:

- The information on the report will vary depending on which window we open it from, even if we use the same report style.

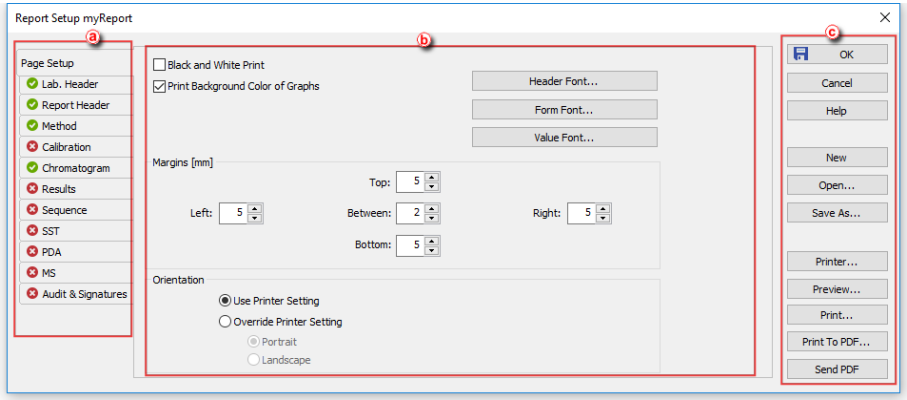
  For example, the *Chromatogram* tab in the *Chromatogram Report Setup* refers to the chromatograms opened in that specific window and the one in the *Calibration Report Setup* refers to the calibration standard opened in the *Calibration* window if any. In the *Instrument* window it will refer to the chromatograms produced after the last run or analysis.
- Only opened chromatograms will be printed.
- If you set up the report to be printed automatically from the Instrument window (from *Analysis - Batch* or from *Setting - Post run*) then Clarity will use the report style defined in the *Instrument* window. Also this report will include only the chromatograms produced after the last run or analysis.

For more info on reports go to the **Clarity Reference Guide**.

1. From the *Instrument, Calibration, Chromatogram* or *Sequence* windows, **select *File - Report Setup*.** From the *Method Setup* window **click on the *Report* button.**
2. **Click on the *New* button** if you wish to create a new report style **or on the *Open* button** ⓒ to use one created previously. Otherwise the current style will be the last used.
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.

   More Info:

   Right click on the tabs to move them or to reset to their position by default from the context menu. The first and last tabs have a fixed position.
5. **Select and configure the elements** you would like to include in that section. ⓑ
6. **Click *Preview* to see the result and repeat steps 3 and 4 if you wish to modify anything.** ⓒ
7. **Click *Save As* to save a new report style or *OK* to accept the changes** to the current style.



10.2 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.

More Info:

- 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 and the one 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.
- If you set up the report to be printed automatically from the Instrument window (from *Analysis - Batch* or from *Setting - Post run*) then Clarity will use the report style defined in the *Instrument* window. Also, this report will include only the chromatograms produced after the last run or analysis.

For more info on reports go to the **Clarity Reference Guide**.

To print a *Report*:

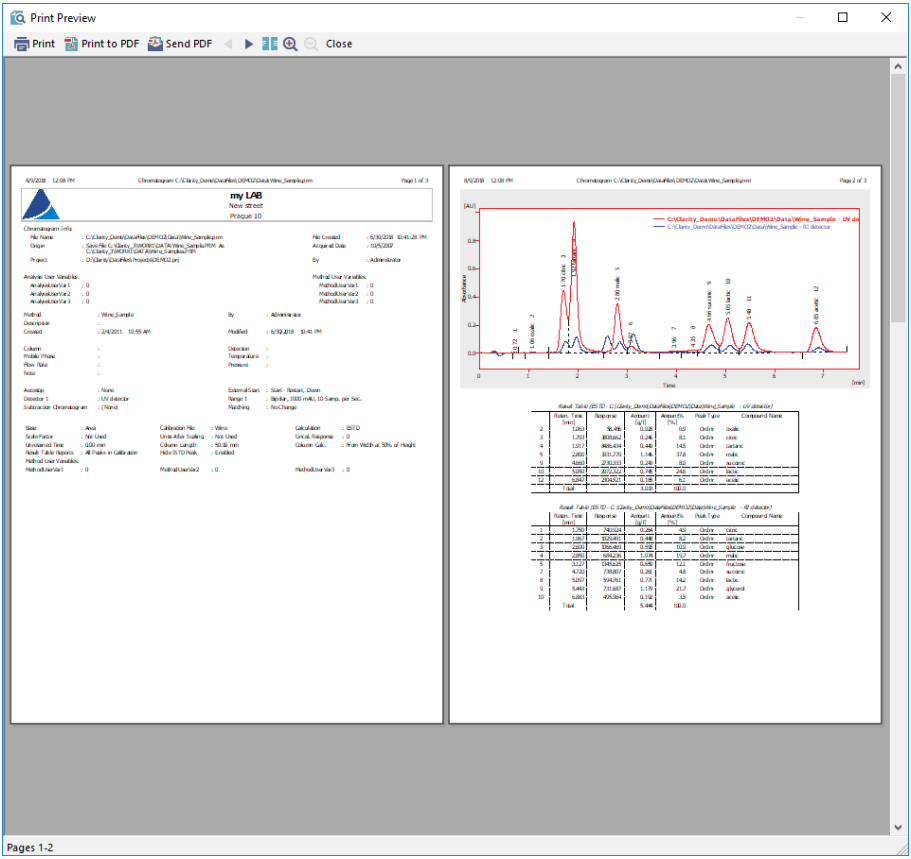
1. **Select *File - Print*** on the *Instrument, Calibration, Chromatogram* or *Sequence* windows or **click on the *Report* button** on the *Method Setup* window and then **on the *Print* button** on the Report Setup window.
2. A print dialog will open for you to setup your printing options and confirm the printout.

To *Print to PDF*:

1. **Select *File - Print to PDF*** on the *Instrument, Calibration, Chromatogram* or *Sequence* windows or **click on the *Report* button** on the *Method Setup* window and then **on the *Print to PDF* button** on the Report Setup window.
2. A Print to PDF dialog will open for you to setup your printing options and confirm the saving of the file.

To get a *Print Preview*:

1. **Select *File - Print Preview*** on the *Instrument, Calibration, Chromatogram* or *Sequence* windows or **click on the *Report* button** on the *Method Setup* window and then **on the *Preview* button** on the Report Setup window.
2. A Print Preview dialog will open. From there you can browse or print the report.



10.3 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 and in the attached **report**.

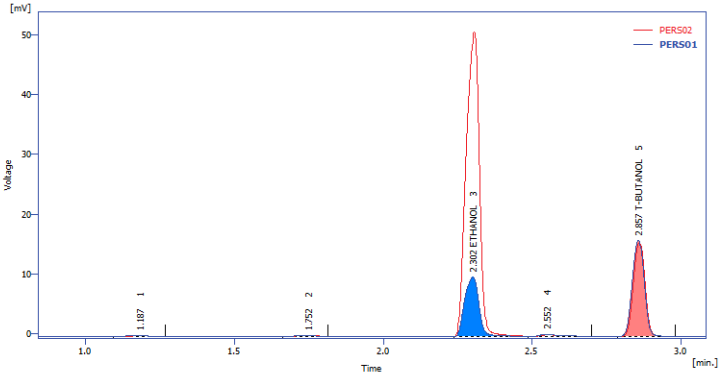
7.1.2016 15:53 Chromatogram C:\Clarity\DataFiles\DEMO1\Data\PERS01.PRM Page 1 of 2

my LAB

my LAB
New Street, 23
Prague 10

Chromatogram Info:

File Name	: C:\Clarity\DataFiles\DEMO1\Data\PERS01.PRM	File Created	: 30.12.2015 11:55:48
Origin	: Save File C:\Clarity_Alpha\DEMO1\Data\Pers01.PRMAs C:\Clarity_Alpha\DEMO1\Data\Pers01x.PRM	Acquired Date	: 16.1.1995 14:16:00
Project	: C:\Clarity\DataFiles\Projects\DEMO1PRJ	By	: DataApexLtd.

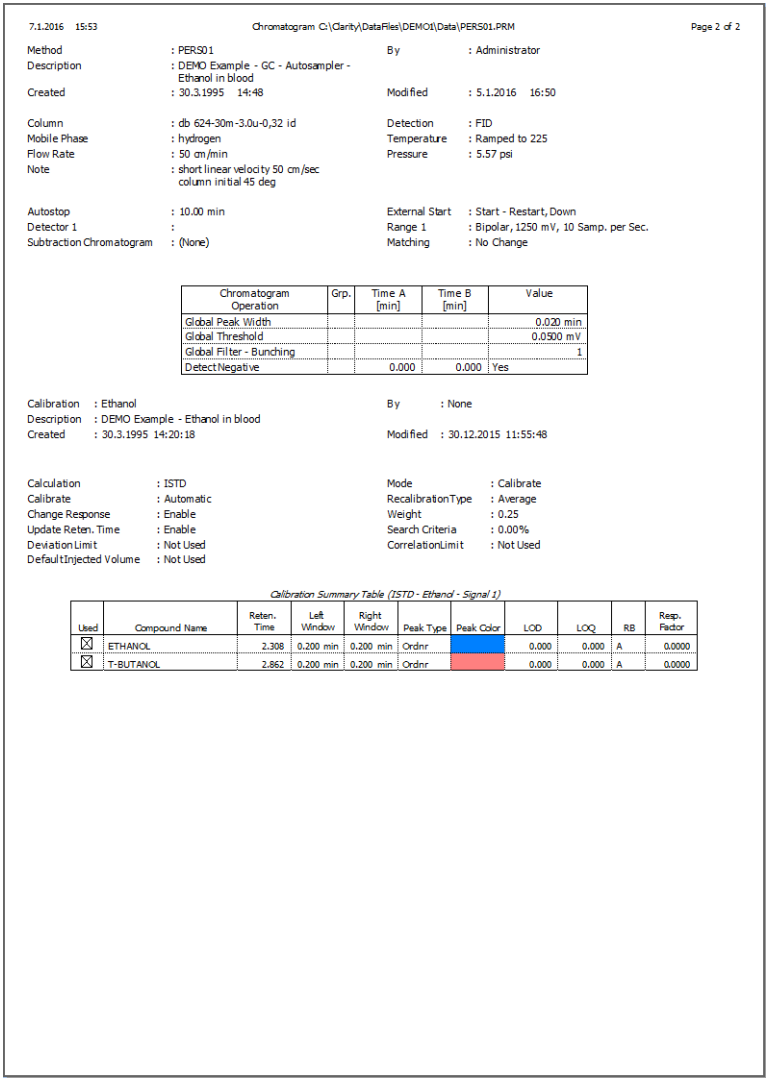


Result Table (ISTD - PERS02)

	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	2.305	157.640	3.233	100.0	Ordnr (by ISTD1)	ETHANOL
4	2.557	1.308	0.000	0.0		
5	2.860	42.530	ISTD	ISTD	ISTD1	T-BUTANOL
	Total		3.233	100.0		

Result Table (ISTD - 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		



7.1.2016 15:53 Chromatogram C:\Clarity\DataFiles\DEMO1\Data\PERS01.PRM Page 2 of 2

Method	: PERS01	By	: Administrator
Description	: DEMO Example - GC - Autosampler - Ethanol in blood		
Created	: 30.3.1995 14:48	Modified	: 5.1.2016 16:50
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
Detector 1	:	Range 1	: Bipolar, 1250 mV, 10 Samp. per Sec.
Subtraction Chromatogram	: (None)	Matching	: No Change

Chromatogram Operation	Grp.	Time A [min]	Time B [min]	Value
Global Peak Width				0.020 min
Global Threshold				0.0500 mV
Global Filter - Bunching				1
Detect Negative		0.000	0.000	Yes

Calibration	: Ethanol	By	: None
Description	: DEMO Example - Ethanol in blood		
Created	: 30.3.1995 14:20:18	Modified	: 30.12.2015 11:55:48
Calculation	: ISTD	Mode	: Calibrate
Calibrate	: Automatic	Recalibration Type	: Average
Change Response	: Enable	Weight	: 0.25
Update Reten. Time	: Enable	Search Criteria	: 0.00%
Deviation Limit	: Not Used	Correlation Limit	: Not Used
Default Injected Volume	: Not Used		

Calibration Summary Table (ISTD - Ethanol - Signal 1)

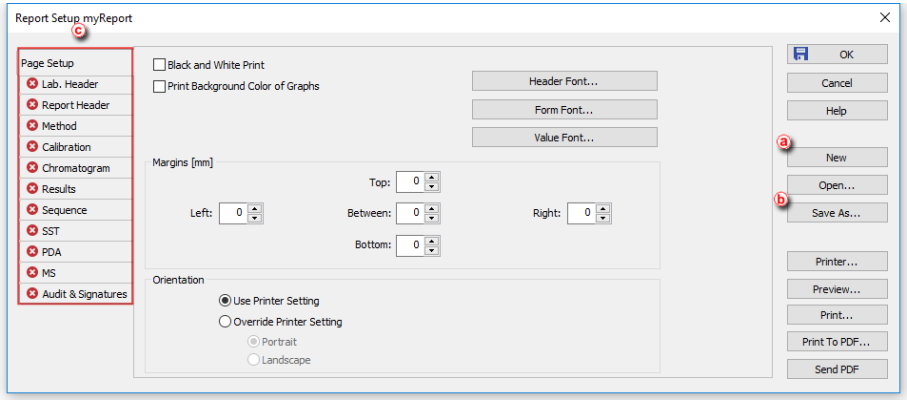
Used	Compound Name	Reten. Time	Left Window	Right Window	Peak Type	Peak Color	LOD	LOQ	RB	Resp. Factor
☒	ETHANOL	2.308	0.200 min	0.200 min	Ordnr		0.000	0.000	A	0.0000
☒	T-BUTANOL	2.862	0.200 min	0.200 min	Ordnr		0.000	0.000	A	0.0000

1. **Open one *Instrument* selecting the project DEMO1.**
2. **Open the *Chromatogram* window.**
3. **Open the chromatograms PERS01 and PERS02** in (C:\CLARITY\DataFiles\DEMO1\Data).
4. **Select the *Overlay* mode** from *File - Overlay Mode* or click on .
5. **Select the area you want to print:** click and drag the mouse pointer on the chromatogram graph.

6. **Create a new report style.**

More Info:

- 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. ⓑ



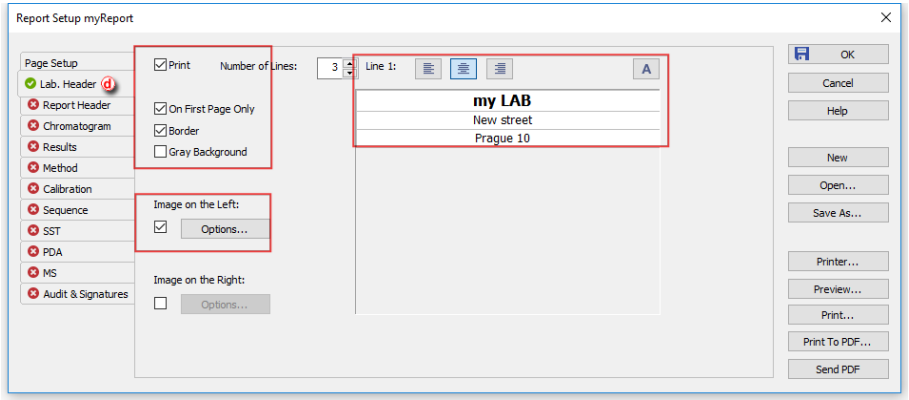
7. **Click and drag the tabs to set them in the order shown.** ⓒ This will be the order the sections will have in the report.

   You can click on the *Preview* button to see the results of your changes at any stage during the creation of the report style.

8. **Set the *Lab Header*.**

More Info:

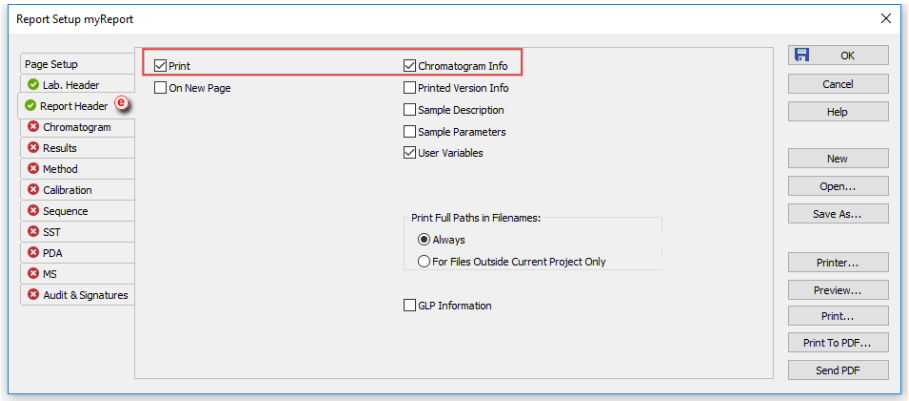
- Click on the *Lab Header* tab. ⓓ
- Check the boxes *Print*, *On First Page Only* and *Border*.
- Check the *Image on the Left* box and click on the *Options...* button to select the logo.
- Click on each line in the text box and write the text shown in the example.
- Click on the first line of text and then on the *Font* icon and select *Bold* as a *Font Style*.



9. **Set the *Report Header*.**

More Info:

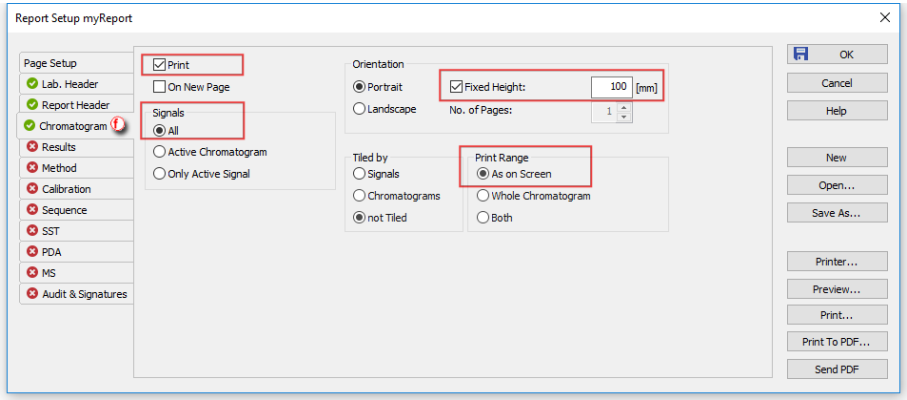
- Click on the *Report Header* tab. ⓔ
- Check the boxes *Print* and *Chromatogram Info*.



10. **Set the *Chromatogram section*.**

More Info:

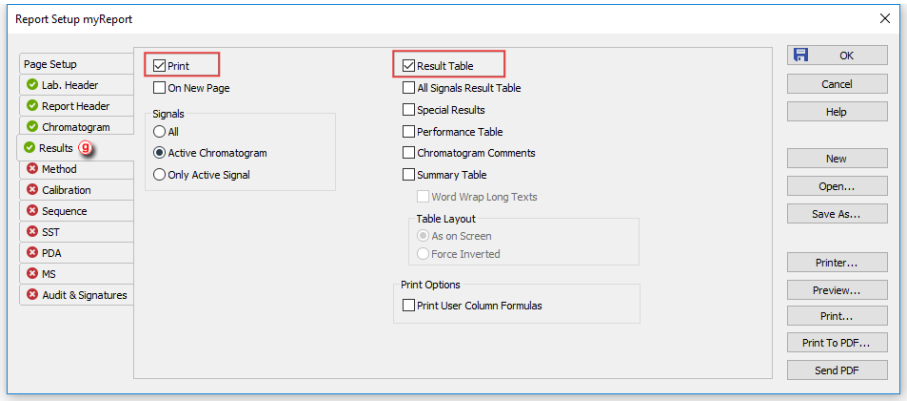
- Click on the *Chromatogram* tab. ⓕ
- Check the boxes *Print* and *Fixed Height* and set the height to 110 mm.
- Select the options *Signals - All* and *Print range - As On Screen*.



11. **Set the *Results* section.**

More Info:

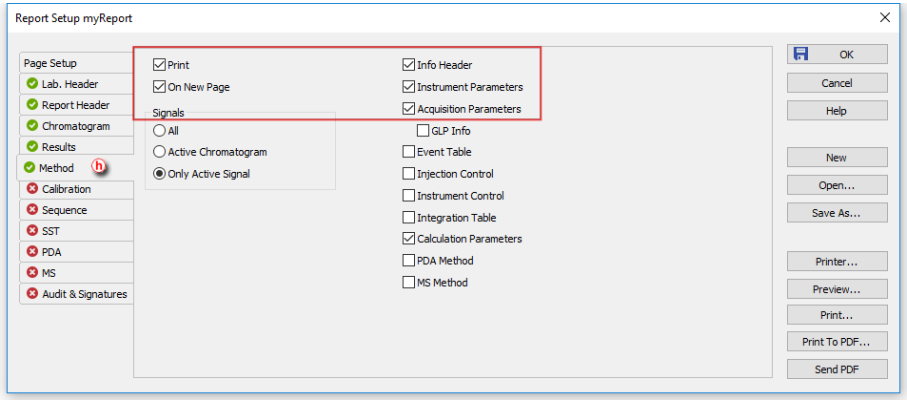
- Click on the *Results* tab. ⓖ
- Check the boxes *Print* and *Result Table*.



12. **Set the *Method* section.**

More Info:

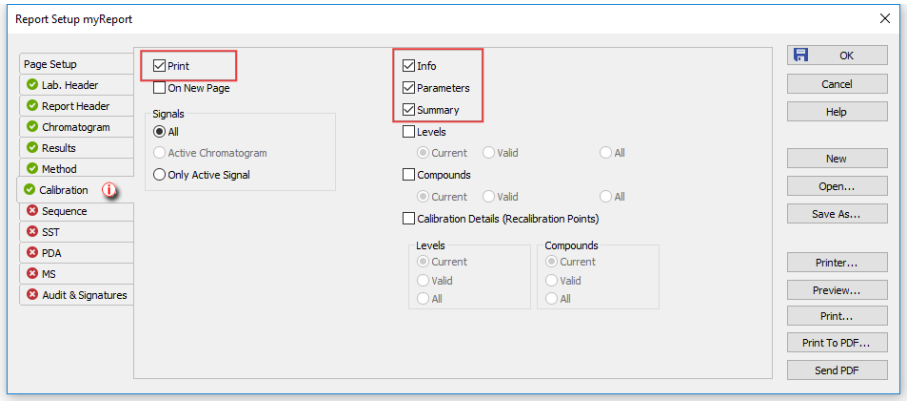
- Click on the *Results* tab. ⓗ
- Check the boxes *Print*, *On New Page*, *Info Header*, *Instrument Parameters* and *Acquisition Parameters*.



13. **Set the *Calibration* section.**

More Info:

- Click on the *Calibration* tab. ⓘ
- Check the boxes *Print*, *Info*, *Parameters* and *Summary*.

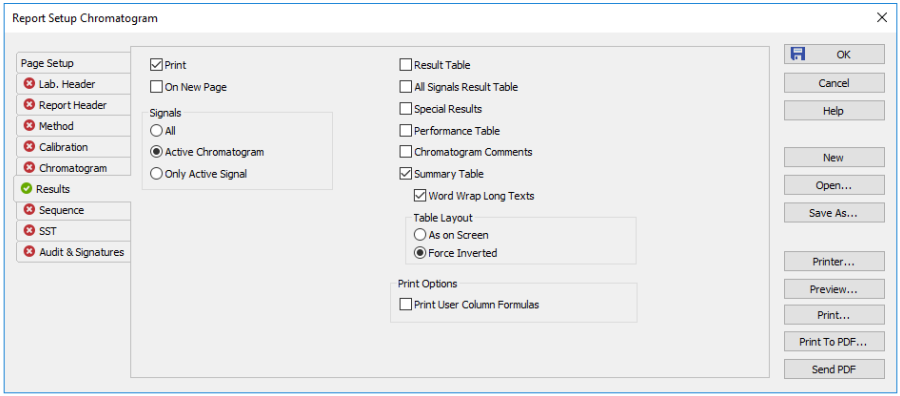


14. **Click the *OK*** button to save the report style.
15. **Print or view the report** as explained in Printing or previewing a report.

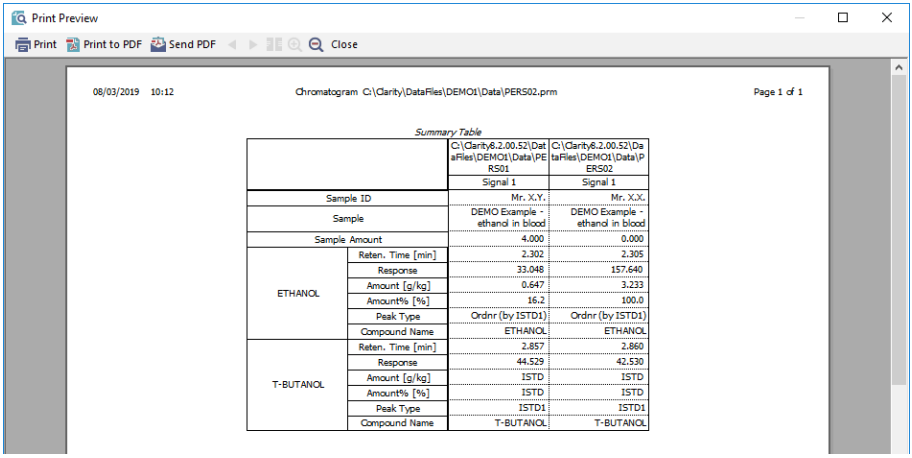
10.4 Printing the summary table

1. Open the *Summary* table in Chromatogram window. For information on how to create Summary Table, see the chapter **"Comparing the results from several chromatograms"** on pg **145**.
2. **Right click on the *Summary Table***, if you want to change the visualization of the table or add a custom column, etc.

3. Open the Report Setup Chromatogram window, click on or open it from *File - Report Setup...* and check the **Summary Table** checkbox on the *Result* table.



4. The results for all opened chromatograms will be printed (use Print, Preview for check)



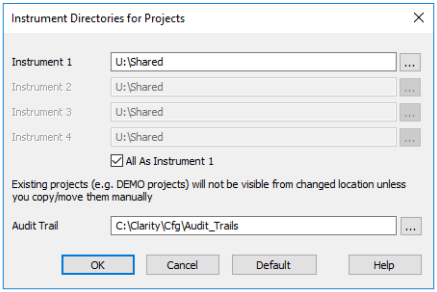
11 File Management

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

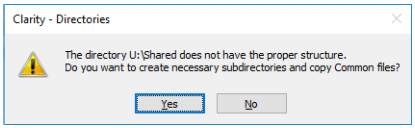
11.1 Setting up project directories

It is possible to set different directories for projects from each instrument and to set Audit Trail directory. It is useful when working with shared disk and when you need to access measured data from another **Clarity Offline**.

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 desired change the Audit Trail directory
5. When saving the changes, the following dialog may occur

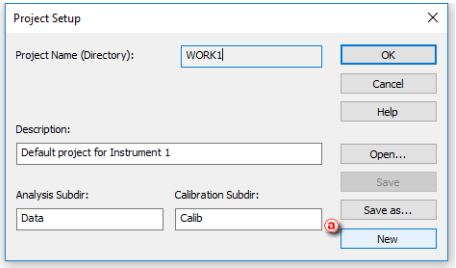


- Be aware that when updating Clarity, the Common files out of the installation directory have to be updated manually.

11.2 Creating a new project

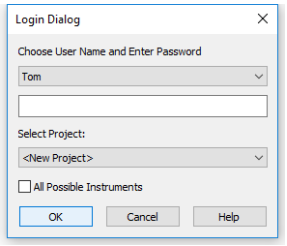
Creating a new project ensures that the measured data will be later easily found. The project itself is a directory in **Clarity's** Datafiles subfolder or selected directory where all relevant files are saved (methods, calibrations, sequences, chromatograms).

1. **Open the Project Setup dialog:** select *File - Project...* on the *Instrument* window.

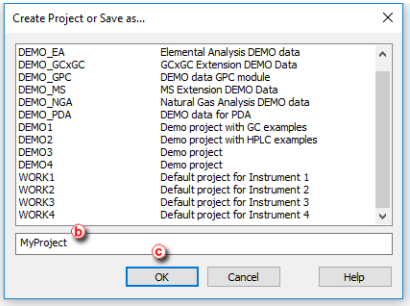


More Info:

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.

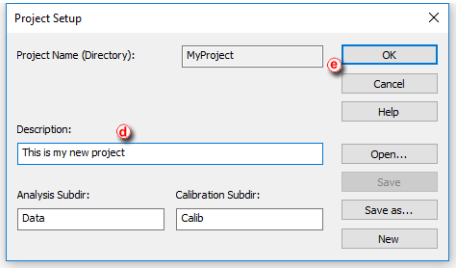


2. **Click the *New* button ⓐ to create a new project.**



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*** ⓔ.

More Info:

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

11.3 Creating customized file names automatically

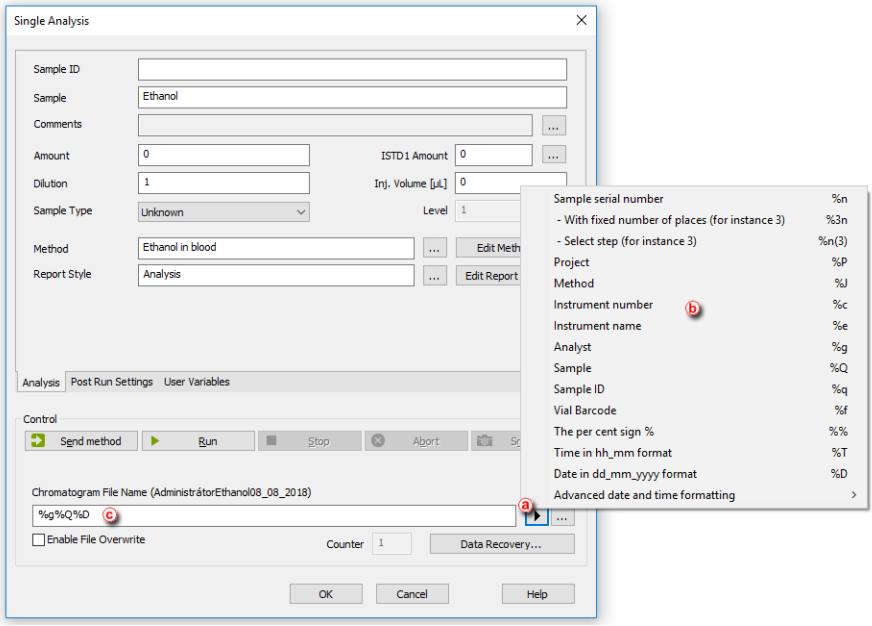
You can create customized file names automatically by appending variables to them.

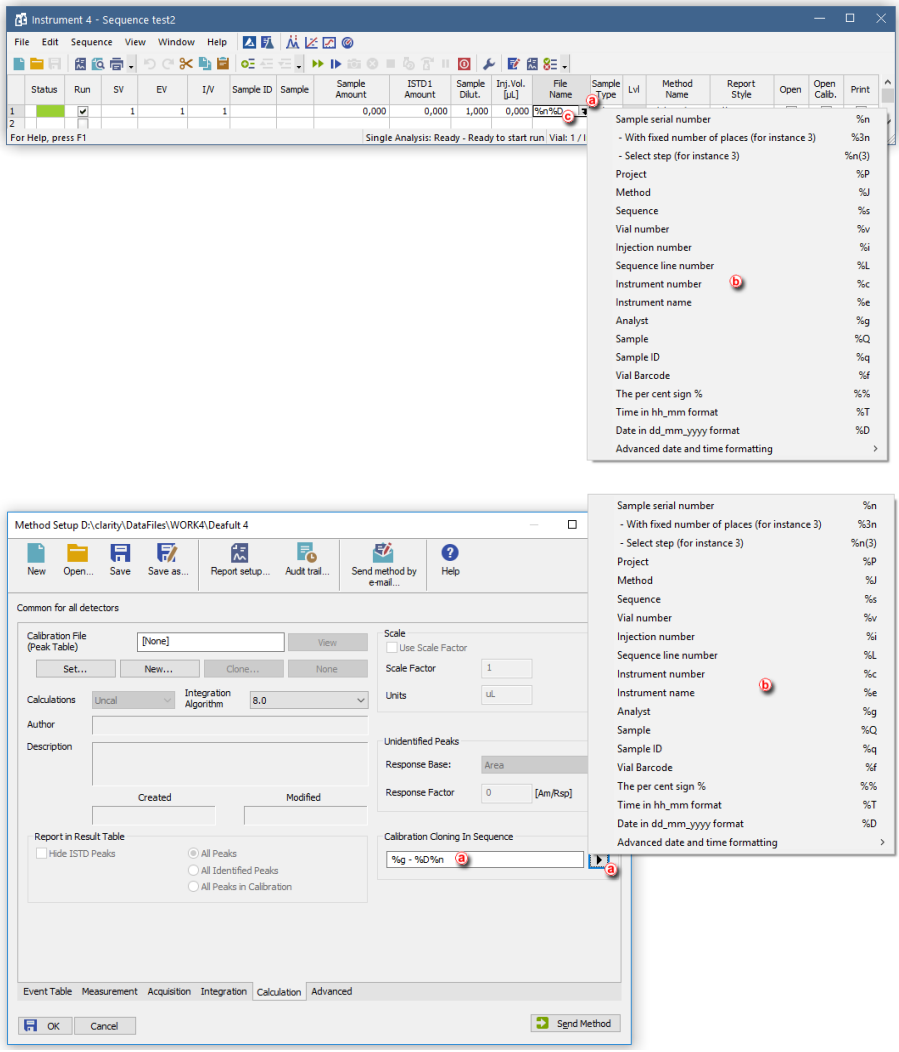
File names can be created on the *Single Analysis* window, on the *Sequence* window and on the *Method Setup - Calculation* tab.

1. **Click on the respective icons** , , on 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 ID* and the *date* it was created: "*AdministratorEthanol29-07-2016.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
Ethanol in blood
Edit Meth
Report Style
Analysis
Edit Report
Analysis
Post Run Settings
User Variables
Control
Send method
Run
Stop
Abort
Chromatogram File Name (AdministrátorEthanol08_08_2018)
%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

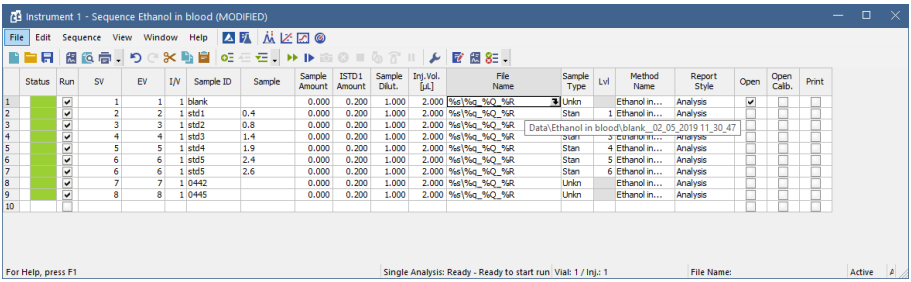


11.4 Storing files into project subfolders

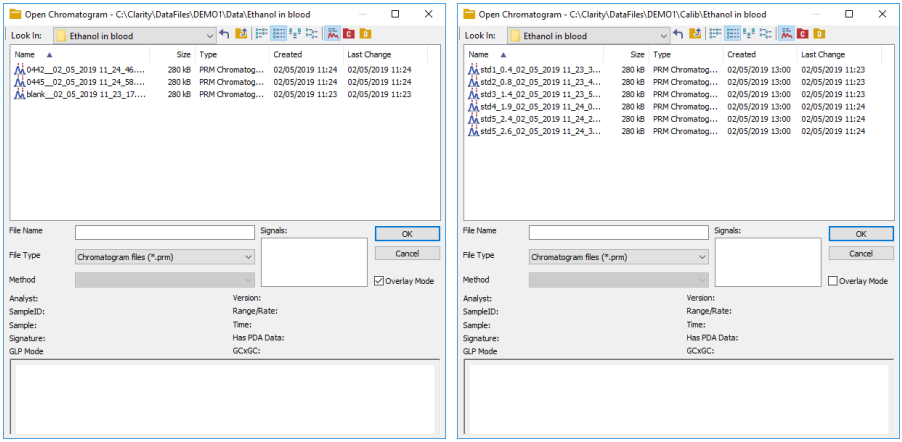
It is possible to include also the name of a subfolder in the name to store chromatograms into project's subfolder. If the subfolder doesn't exist, then it will be created when the chromatogram is stored. The directory can be set using the **"\"** character.

Here we provide an example on how to store all chromatograms of unknown samples from one sequence into one folder.

1. Login Instrument with Demo1 project
2. Open the Sequence window
3. Open ETHANOL IN BLOOD.SEQ
4. Set the File Name **%s\%q_%Q_%R** (To see detailed description on how to create the name using variables invoke help (F1))
5. Right click on the File Name column and select *Fill down/Fill series* 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.



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

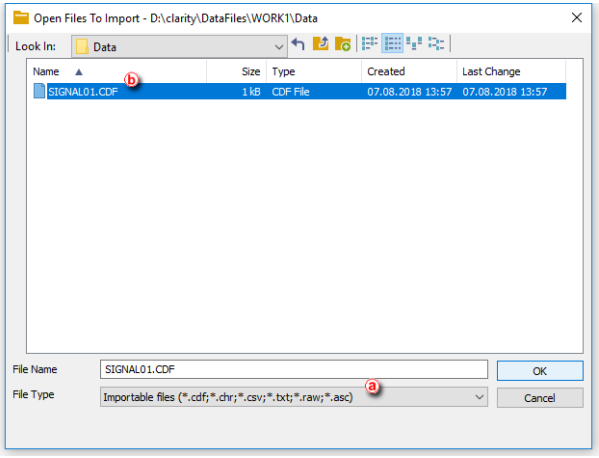
12 Import and Export Data

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.

12.1 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. **Open the *Chromatogram* window:** select *Window - Chromatogram* on the *Instrument* window or click on  .
2. **Open the Open Files To Import dialog:** select *File - Import Chromatogram….*
3. **Select the type of files which you want to import** ⓐ . By default you can see all types of supported formats.
4. **Select the file you want to import** ⓑ **and click on the *Open* button.**



5. **Set the different parameters** in the subsequent dialogs depending on the file format.

   - Import AIA File - when importing AIA file (*.CDF suffix).
   - Import Text File - when importing Text, Multidetector or EZChrom ASCII file (*.TXT, *.CHR, *.ASC and *.CSV suffixes).
   - Save As - when importing *.RAW file, as there is no need to set other parameters.

12.2 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:** select *Window - Chromatogram* on the *Instrument* window or click on  .
2. **Open the chromatogram you want to export**, then **open the *Export Chromatogram* dialog:** select *File - Export - Export Chromatogram….*
3. **Select the export format** ⓐ.

   More Info:

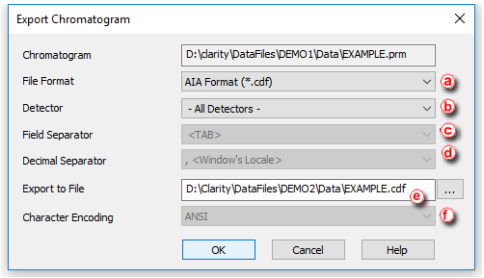
   For PDA export of 3D data only the EZChrom ASCII format is supported.

4. **Select the signals to be exported** ⓑ.

   More Info:

   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 Save 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**.

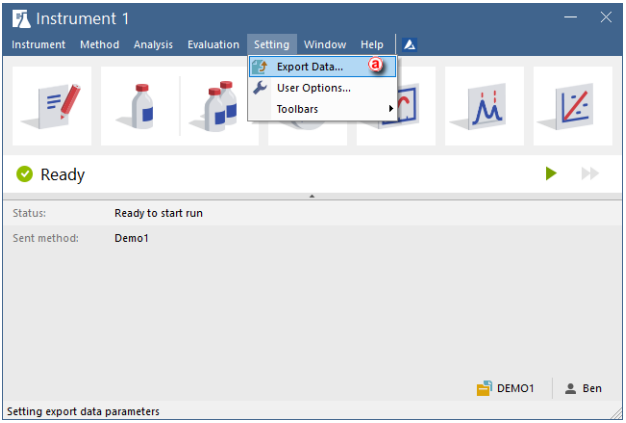


12.3 Exporting data for LIMS

Following chapter describes how to export data from Clarity to be used for LIMS. Each LIMS requires a different approach in importing external data, therefore it may be necessary to adjust your LIMS to be able to correctly process imported data from Clarity.

Export settings

1. Open Clarity Instrument window and select - *Setting* - *Export Data* ⓐ.



2. In the Export Data dialog **set the required** *Export Content* ⓑ and **select** *In Fixed Format*.

More Info:

- Otherwise the content will change according to changes on screen.

3. **Select** *Export to Text File* ⓒ.
4. **Select** *Full Format* option.

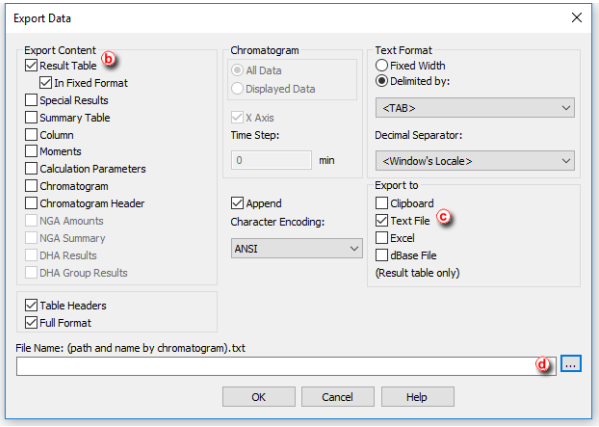
More Info:

- This will precede each result table row with a file name, date and time, thus allowing easy sorting after import.

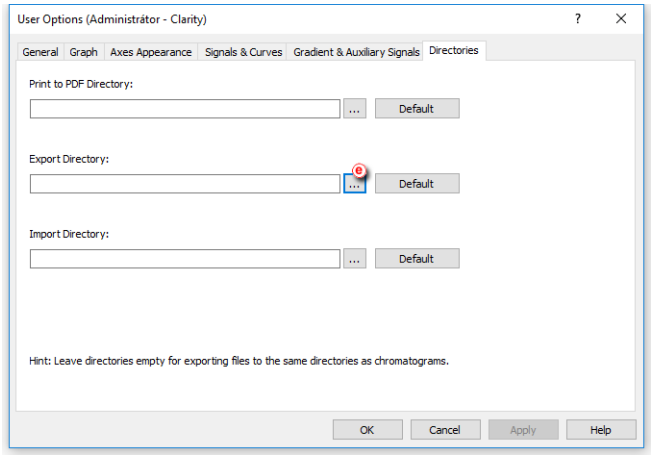
5. **Set** *File Name* ⓓ and check the *Append* option, in this way all results will be exported to a single file which can then be simply imported directly to your LIMS.

More Info:

- Leaving the field empty means that each export will be performed to a separate file. Exported files will have automatically generated file name from the chromatogram name.



- **By default**, files are exported to the same directory as the original chromatogram.
- To export to a single directory, specify it in the User Options - *Directories* tab ⓔ, accessible from the Instrument window - *View* - *Options*.



Locations to Export from

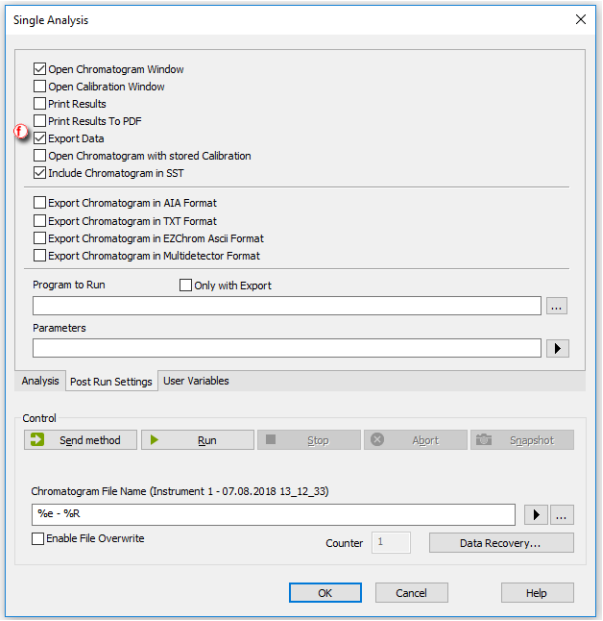
Three most common locations in exporting data to LIMS are:

Single Analysis

- In the PostRun Setting dialog, invoked from the Instrument window - *Setting - Postrun...*, **select** *Export Data* option ⓕ.

More Info:

- Export of data will be performed automatically after a single analysis is finished.

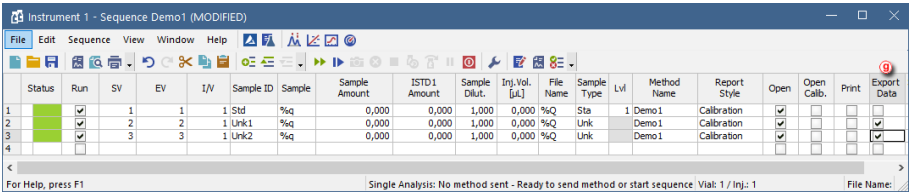


Sequence

- In the Sequence window, **select checkbox** in the *Export Data* ⓖ column for **row(s) to be exported.**
- Export of data will be performed automatically after the row has been measured.

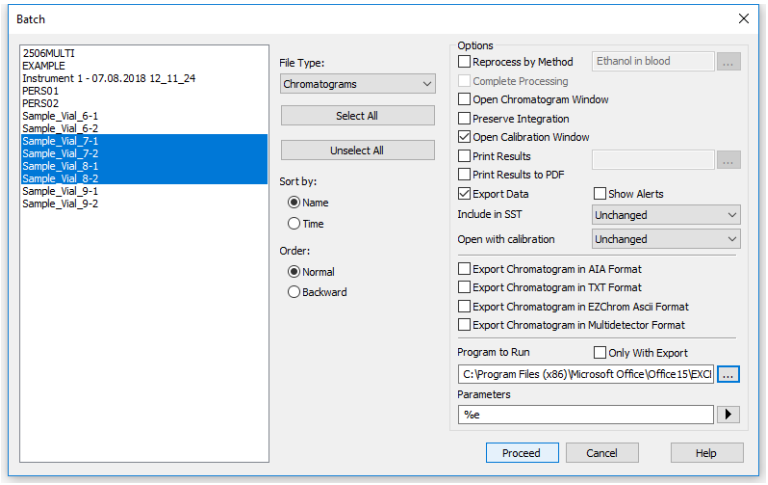
More Info:

- By default, *Export Data* column is hidden. Right mouse click in the sequence table and choose *Setup Columns...* to show it.
- From the Setup Columns dialog, choose *Export Data* from the left list and click on the *Show* button - it will be added to the show list. Once you click on the *OK* button, you will return to the Sequence window and the new *Export Data* column will be added.



Batch

- **Export multiple chromatograms** at once using the Batch dialog, accessible from the Instrument window - *Analysis - Batch...*.
- **Select chromatograms to be exported** and check the option to *Export Data*ⓗ.
- Clarity is able to start external program with a parameter ⓘ. Specify a program to run using the ... and specify a command line parameter - typically the file name of the exported text file *%e*. Once ready to export the data, click the *Proceed* button.



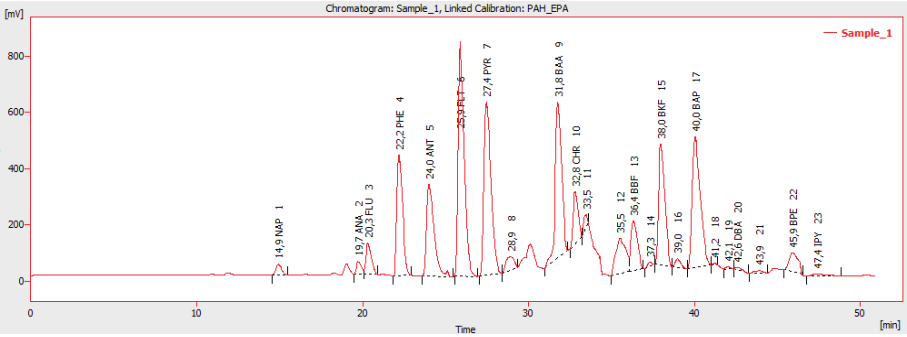
12.4 Exporting a chromatogram as a picture

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:** select *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.



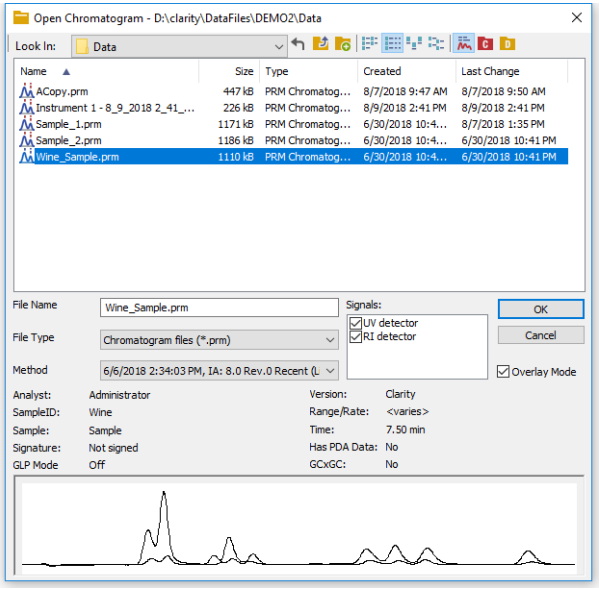
13 Mathematical Operations

This functionality was implemented into Clarity to give users a powerful tool to manipulate already measured data without modifying original raw data. Mathematical operations present a very convenient approach 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 display three examples of applications of Mathematical Operation in our web based User Guide to Clarity. Many other applications may be developed by Clarity users on their own.

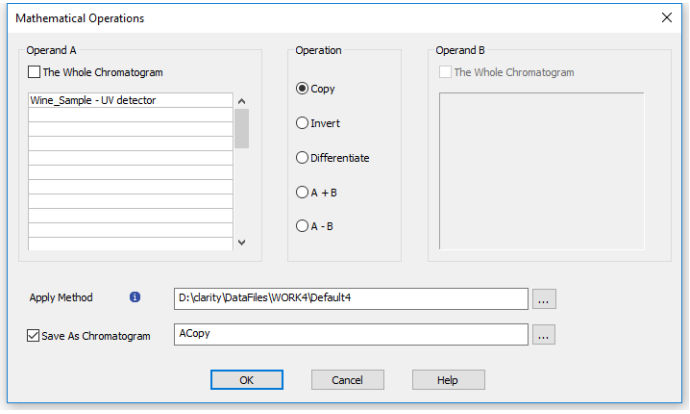
13.1 Extract chromatogram's signal using Mathematical Operations

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 the *Chromatogram* window:** select *Window - Chromatogram* from the *Instrument* window or click on  .
2. **Open your file containing the multiple signal chromatogram that you want to work with** and make sure the **Overlay Mode** checkbox is selected.



3. **Select** *Chromatogram - Overlay - Mathematics* and the **Mathematical Operations** window will open.

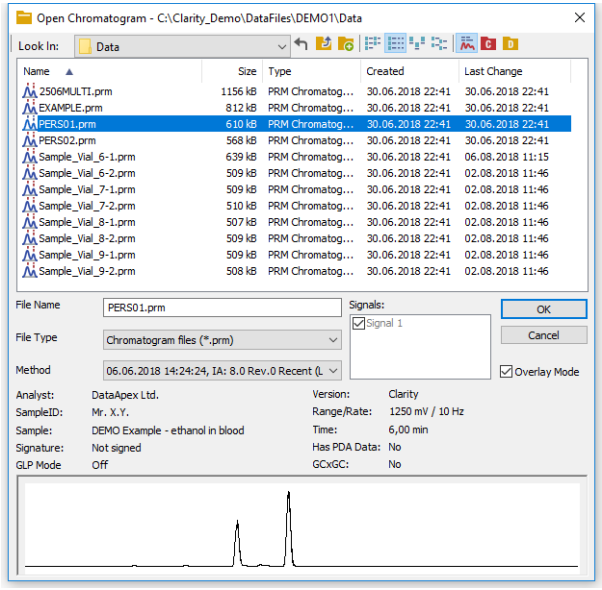


4. From the **dropdown menu** (an arrow next to the name) in the **Operand** section, **select the desired signal** of chromatogram you want to save separately. Select the *Copy* operation, fill out a name in the *Result* area and click **OK** to save the signal.

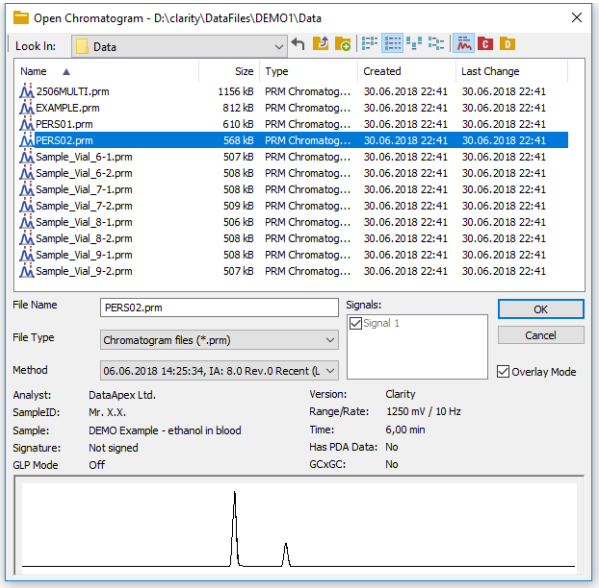
13.2 Subtraction of various chromatograms using Mathematical Operations

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. This subtraction of chromatograms may be performed using Mathematical Operations.

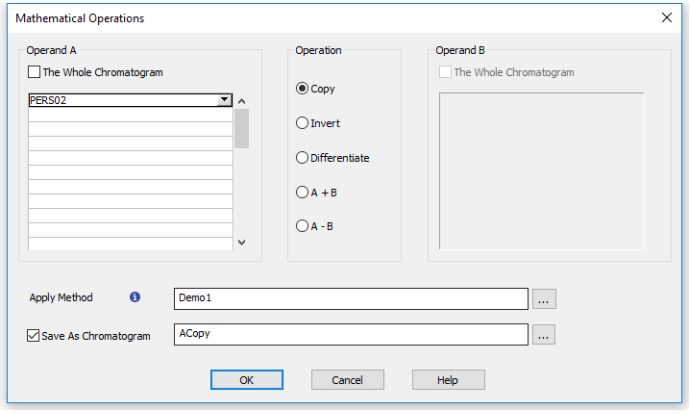
1. **Open the *Chromatogram* window:** select *Window - Chromatogram* from the *Instrument* window or click on  .
2. **Open your file containing the sample chromatogram that you want to work with.** Make sure the **Overlay Mode** checkbox is selected.



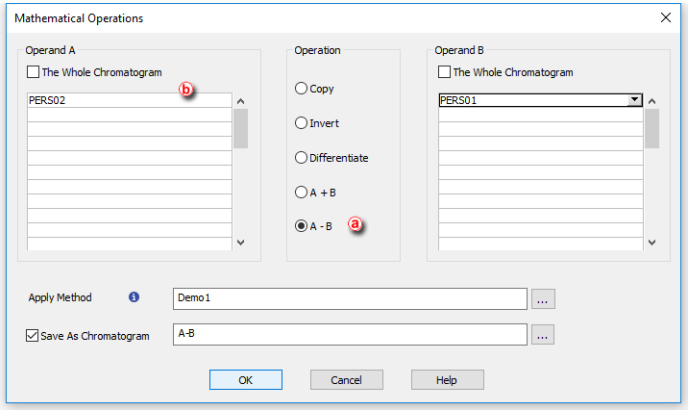
3. **Open a chromatogram you want to subtract** and make sure the **Overlay Mode** checkbox is selected.



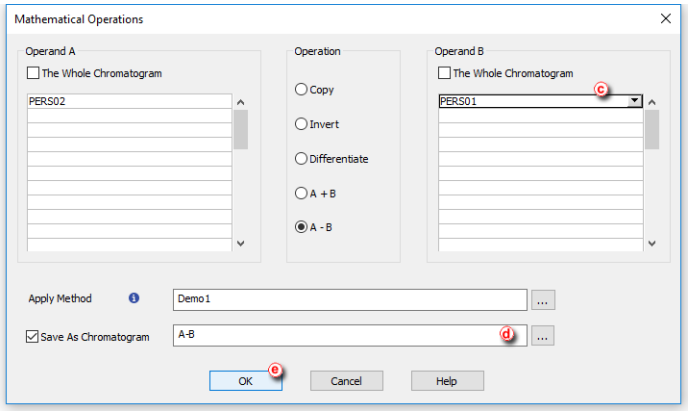
4. **Select** *Chromatogram - Overlay - Mathematics...* and the **Mathematical Operations** window will open.



5. Select operation **A - B** ⓐ. From the **dropdown menu** (an arrow next to the name) in the **Operand A** section, select the desired chromatogram you want to subtract from ⓑ.



- From the **dropdown menu** (an arrow next to the name) in the **Operand B** section, select the desired chromatogram you want to subtract ⓒ. Fill out a name ⓓ and click **OK** ⓔ to save new subtracted chromatogram.

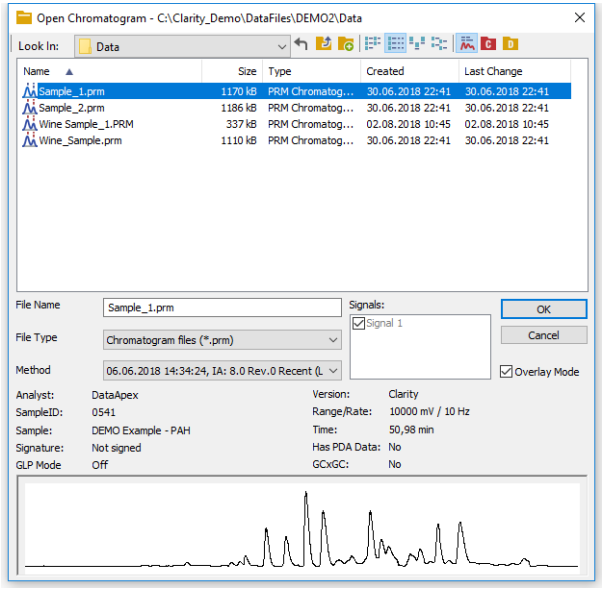


13.3 Copying of chromatogram using Mathematical Operations

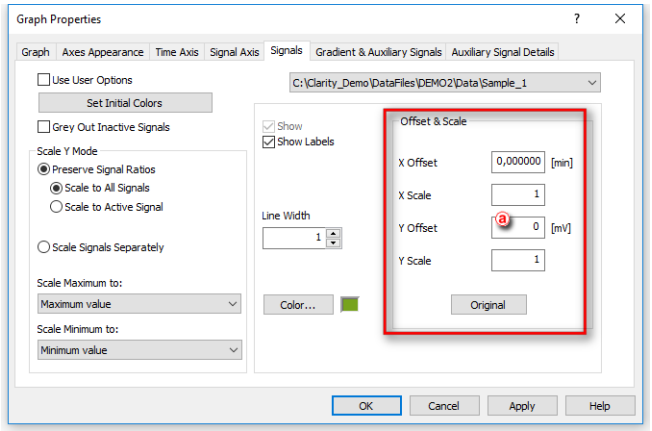
Following chapter describes how to copy a modified chromatogram into a new one without changing the original chromatogram. For example we set up new Offset of Y-axis and this modification is about to saved in new chromatogram and want to keeping the original chromatogram unchanged.

1. **Open the *Chromatogram* window:** by selecting *Window - Chromatogram* from the *Instrument* window or click on  .

2. **Open your file containing the sample chromatogram that you want to work with.** Make sure the ***Overlay Mode*** checkbox is selected.

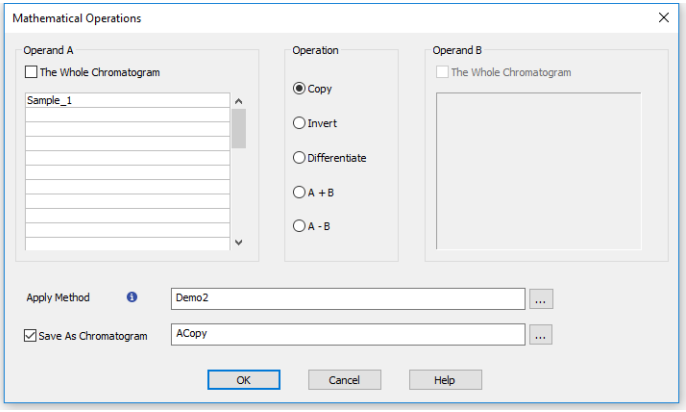


3. **Select** *Display - Properties - Signals* and the tab **Signals** will open.
4. Into Field **Y Offset** ⓐ write down value of desired offset in mV, in this case for example 333 mV, and click **OK** button.

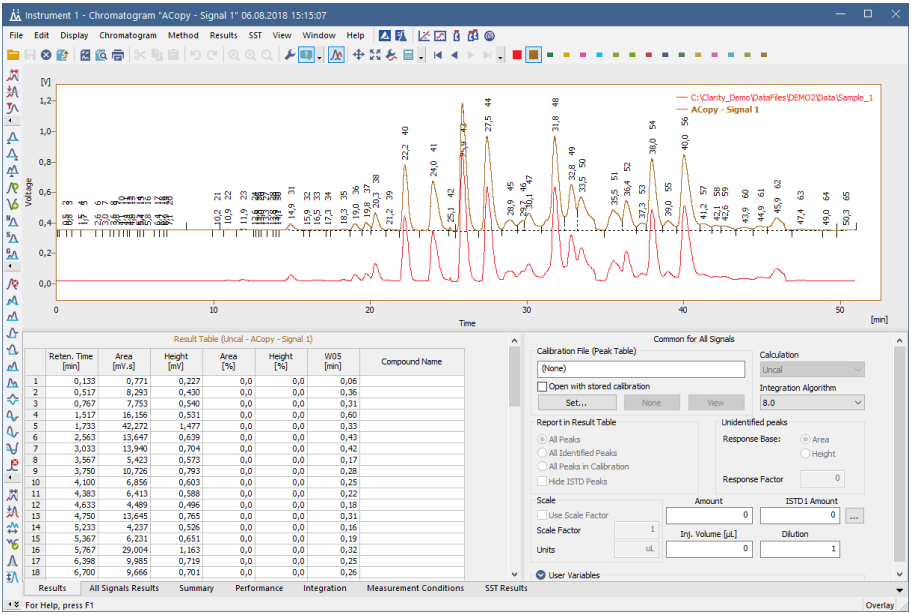


5. **Select** *Chromatogram - Overlay - Mathematics...* and the **Mathematical Operations** window will open.

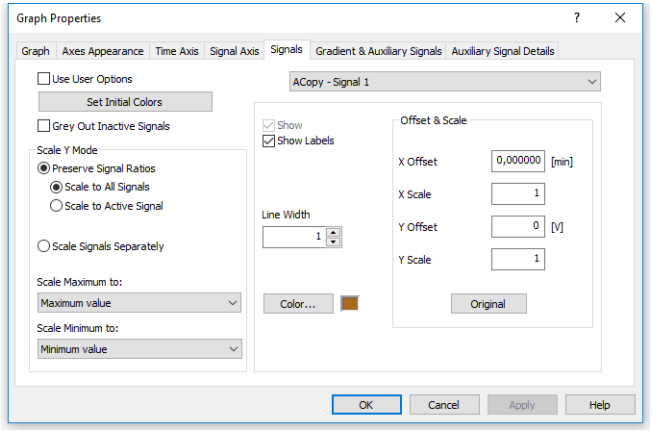
6. Check then option **Save as Chromatogram** in the *Result* panel and into Field **Result** write down the name for the new chromatogram and select the path to the directory you want to save it in and click the **OK** button.



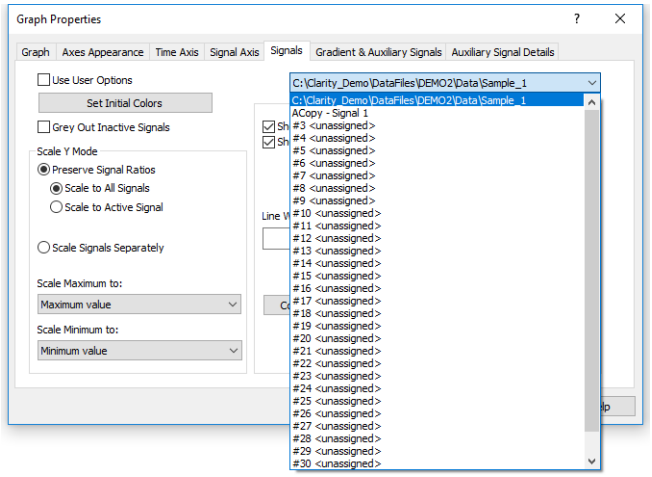
7. Both chromatograms will be displayed in overlay mode as may be seen on the next picture.



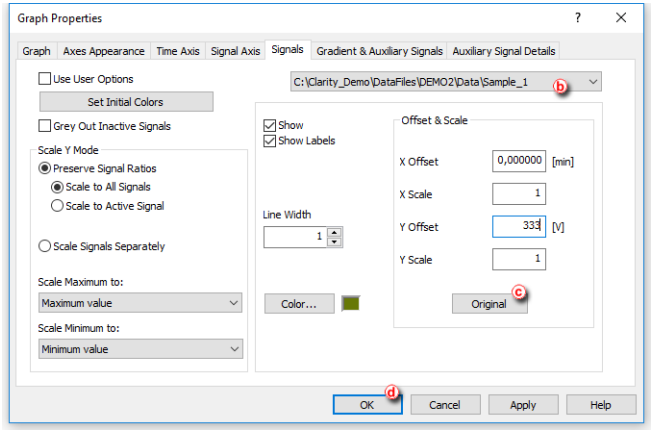
8. **Select** *Display - Properties - Signals* and the tab **Signals** will open.



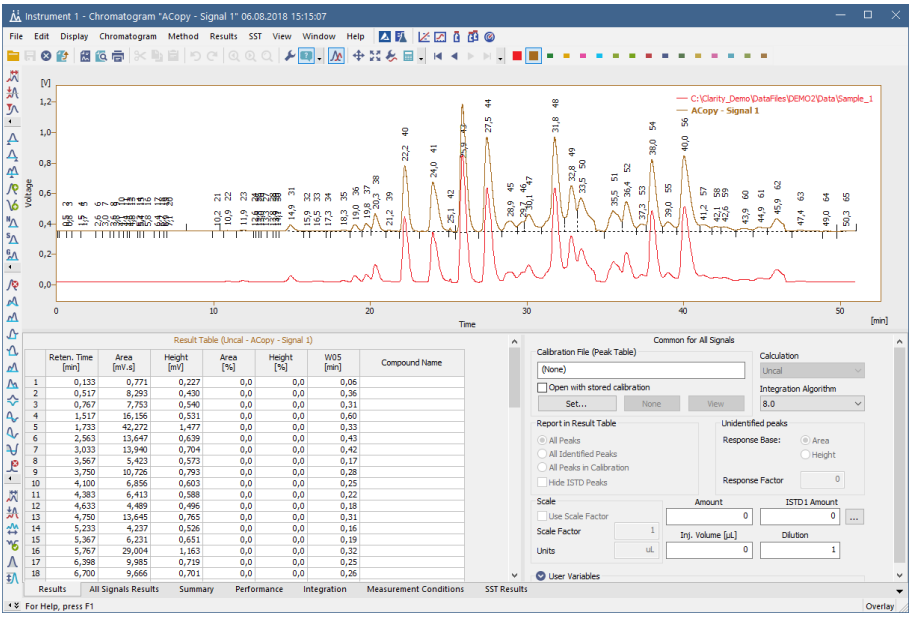
9. From the **Dropdown menu** select the original chromatogram.



10. Click button **Original** ⓒ (check if original chromatogram is selected ⓑ) click **OK** ⓓ button.



11. Both chromatograms will be displayed in overlay mode as may be seen on the next picture.



14 Back-up and Restore

Clarity allows you to backup your *Projects* (methods, sequences, measured chromatograms) and also the *Common* folder in which the print styles are stored.

14.1 Backing up a project (Creating an Archive)

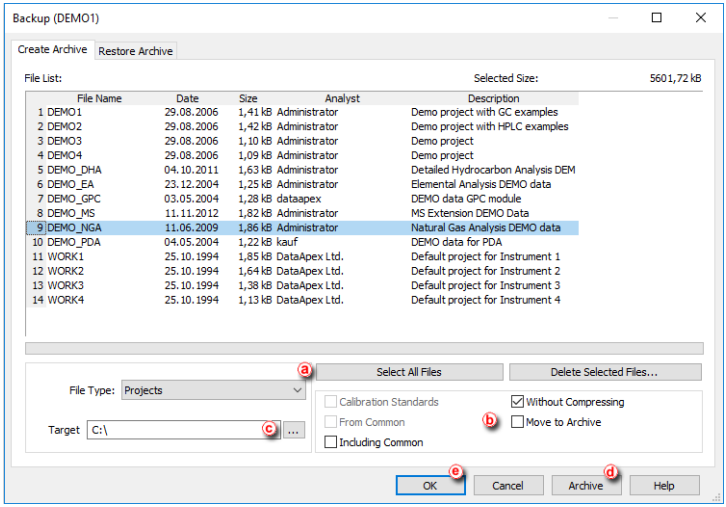
It is strongly recommended to backup the whole project folder after being shelved, but it is also possible to archive specific files only. A backup can be made by simply copying the files or by compressing them into one file (*.DGZ format).

1. **Open the Backup dialog** by selecting *Instrument- Archive...* on the *Instrument window*.
2. **Select *Projects* on 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 back up also the COMMON subdirectory.
5. **Choose the output directory and name for the archive ⓒ.**

More Info:

Compressed files will have the .DGZ extension.
Caution: If after archiving your files in a compressed archive you try to archive more files under the same archive file name, the file will be overwritten and you will loose all the files that were previously in the archive.

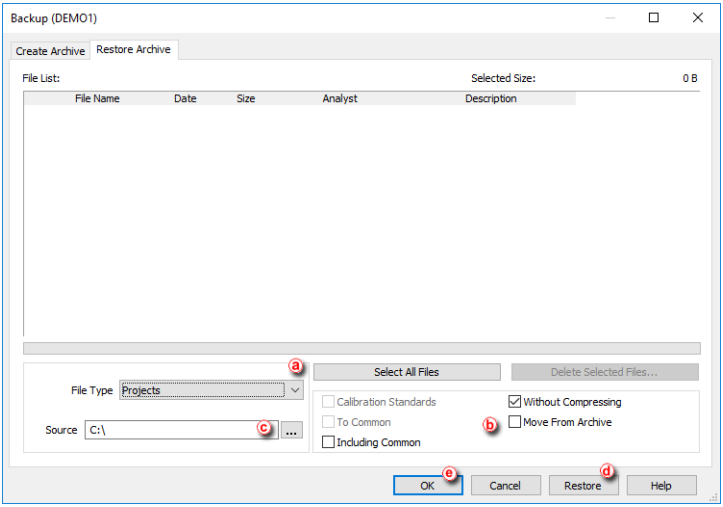
6. **Click on the *Archive* button ⓓ** to back up the project or on the ***OK* button ⓔ**, if you do not need to back up any more files.



14.2 Restoring a project from an archive

- **Open the Backup dialog** by selecting *Instrument - Restore...* on the *Instrument window*.
- **Select *Projects* on the *File Type* ⓐ option** to restore a complete project directory.
- **Select the project or projects you wish to back up from the list.** The *Select All Files* button ⓐ will select all projects.
- **Choose from the following options ⓑ:**
  - Uncheck the *Without Compressing* option to restore all files from a compressed file.
  - Check the *Move from Archive* option to have the archived files erased after restoring them.
  - Check the *Including Common* option to restore also the COMMON subdirectory.

5. **Choose the source directory and select the source file ⓒ.** Compressed files will have the .DGZ extension.
6. **Click on the *Restore* button ⓓ to restore the project** or on the *OK* button ⓔ if you do not need to restore any more files.



14.3 Backing up specific files (Creating an Archive)

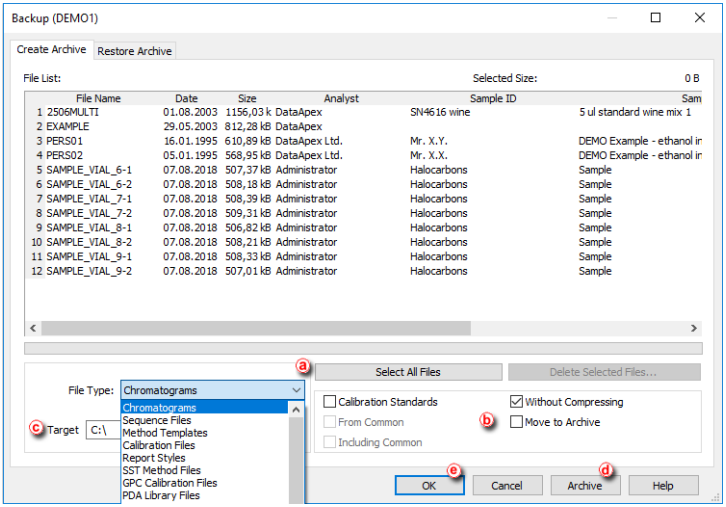
It is strongly recommended to backup the whole project folder after being shelved but it is also possible to archive specific files only. A backup can be made by simply copying the files or by compressing them into one file (*.DGZ format).

1. **Open the Backup dialog** by choosing *Instrument - Archive...* on the *Instrument window*.
2. **Select the *File Type* ⓐ option** according to the files you wish to back up.
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* checkbox for displaying the system files from the COMMON directory.
5. **Choose the output directory and name for the archive ⓒ.**

More Info:

Compressed files will have the .DGZ extension.

- **Click on the *Archive* button ⓓ to back up the file** or on the *OK* button ⓔ if you do not need to back up any more files.



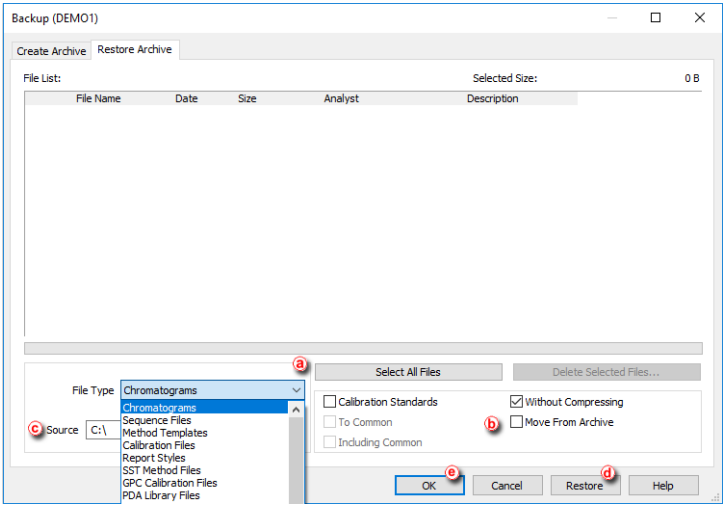
14.4 Restoring a file from an archive

1. **Open the Backup dialog** by choosing *Instrument - Restore...* on the *Instrument window*.
2. **Select the *File Type* ⓐ option** according to the files you wish to restore.
3. **Select the files you wish to restore from the list.** The *Select All Files* button ⓐ will select them all.
4. **Choose from the following options ⓑ:**
   - Uncheck the *Without Compressing* option to restore all files from a compressed file.
   - Check the *Move from Archive* option to have the original files erased after restoring them.
   - Check the *Calibration Standards* option when restoring chromatograms to the CALIB subdirectory (instead of the DATA subdirectory).
5. **Choose the source directory and select the source file ⓒ.**

   More Info:

   Compressed files will have the .DGZ extension.

6. **Click on the *Restore* button ⓓ** to restore the files **or on the *OK* button ⓔ** if you do not need to restore any more files.


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
Calibration Standards
Without Compressing
To Common
b
Move From Archive
Including Common
c
Source
C:\
e
OK
Cancel
d
Restore
Help

15 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.

15.1 Enabling instruments to be used by Clarity2Go application

Clarity enables to send specific parameters over the internet to be monitored via **Clarity2Go** application available at Android (Google Play store) and iOS (Apple store) smartphones. In this way you can monitor your analyses while outside the laboratory.
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. Press the *OK* button to save the configuration and continue with steps described in **How to set up Clarity2Go** section.

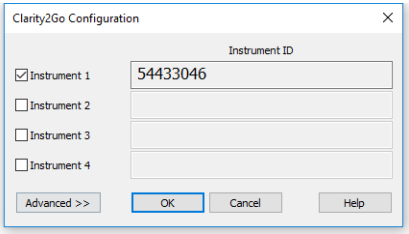


Fig 1: Clarity2Go Configuration - Basic

Options described below are optional and are not obligatory for correct functionality. They are revealed by pressing 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.
- Press the *OK* button to save the configuration and continue with steps described in **How to set up Clarity2Go**.

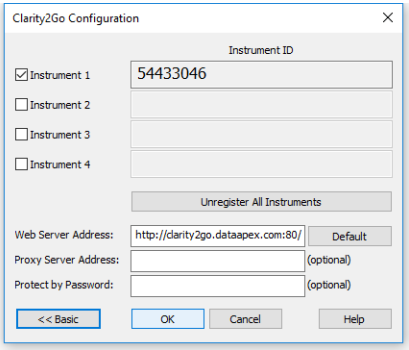


Fig 2: Clarity2Go Configuration - Advanced

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*.
    - **Clarity Demo** mode does not allow to add instruments. Stripe at the bottom serves as an information center. Changes in the

configuration or notifications are displayed here.

*Fig 3: **Clarity Demo** mode gray stripe*

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.

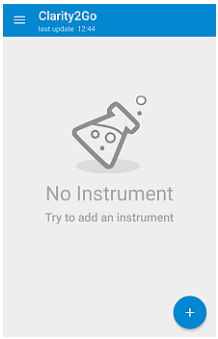


Fig 4: No Instrument screen

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.

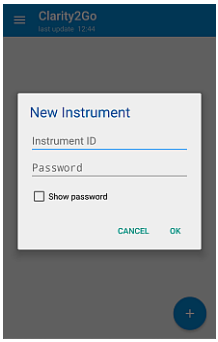


Fig 5: New Instrument screen

6. The newly configured instrument will be added to the list of instruments that are being monitored.

- Invoke the application menu by tapping on the 3 horizontal lines - the menu contains *Settings*, built-in *Help* and *About* options.

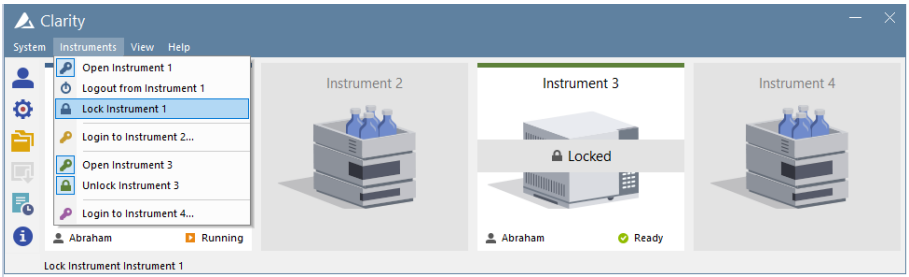
15.2 Locking/Auto Locking a Clarity Instrument

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

With Clarity running and the Instrument you want to lock opened:

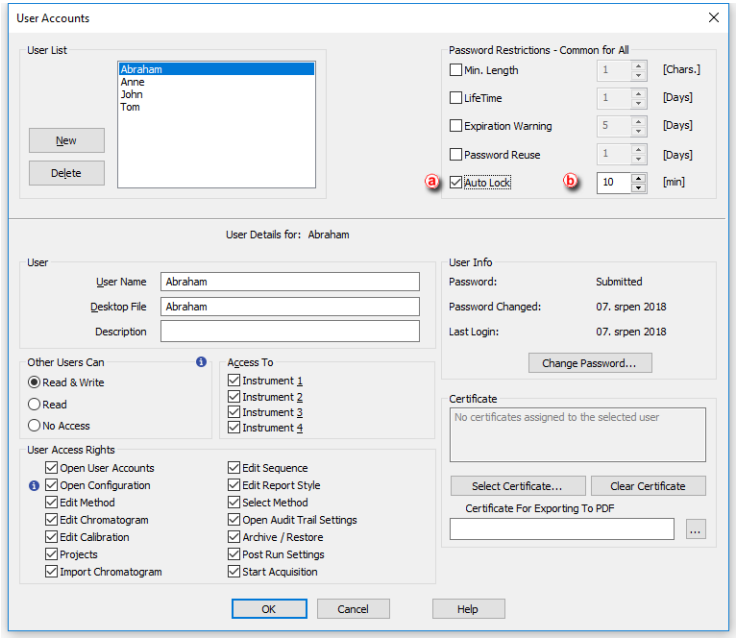
1. **Open the *User Accounts* window:** click on or choose *System - User Accounts*.
2. The *Instrument* will appear now with a lock below it.



Auto Lock

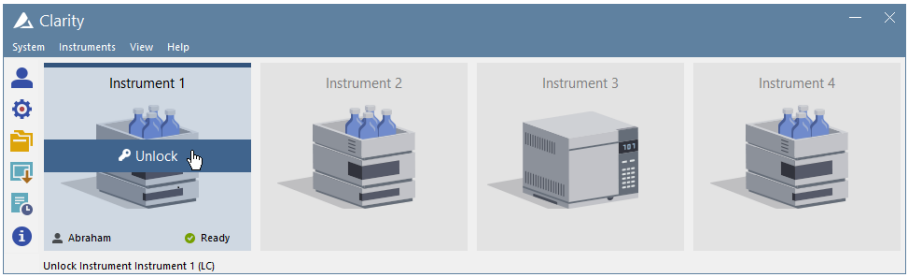
It is possible to set the Automatic Lock function so that all opened instruments will be locked after a period of inactivity.

1. **Open the *User Accounts* window:** click 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. ⓑ



15.3 Unlocking a Clarity Instrument

- **Select** *Instruments - Unlock Instrument 1* from the *Main Clarity* window **or click on the** *Instrument*.
- **Enter the password and click OK.**



Unlocking Instrument after entering wrong password three or more times:

More Info:

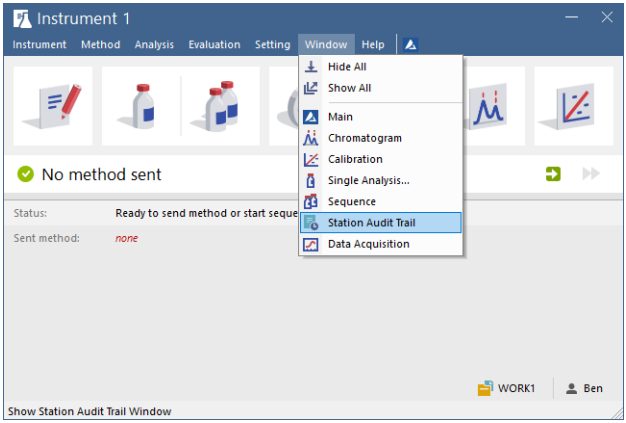
If you enter the *wrong password* three times or more, then a message will appear asking you to restart the program.

- **Unlock the *Instrument*** using credentials from a user with access to User Accounts and with administrator rights over the locked *Instrument* (to configure this, see the procedure Restricting access to Instruments).
- **Select *System - Exit Clarity* to close Clarity.**
- **Restart Clarity**. Instrument can now be opened under the previous User Name and Password.

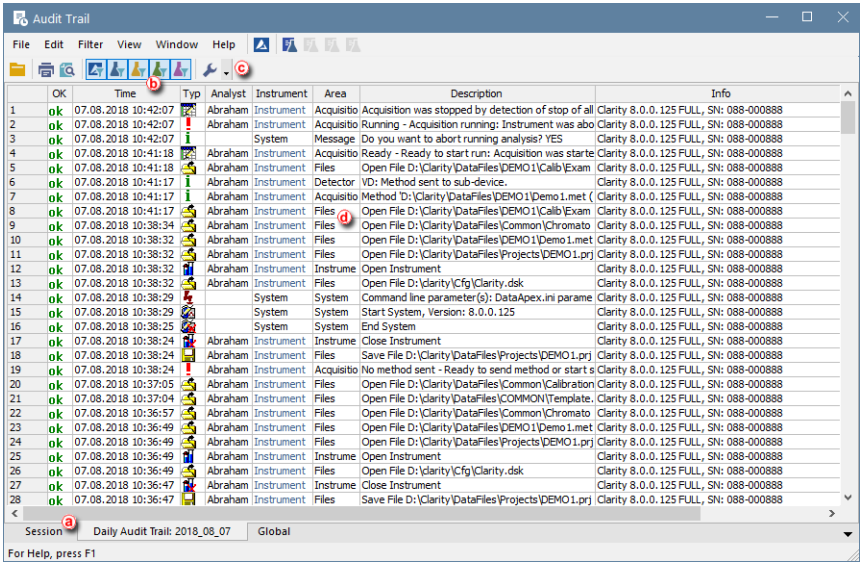
15.4 Monitoring Events and Operations in Clarity

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**.**



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.

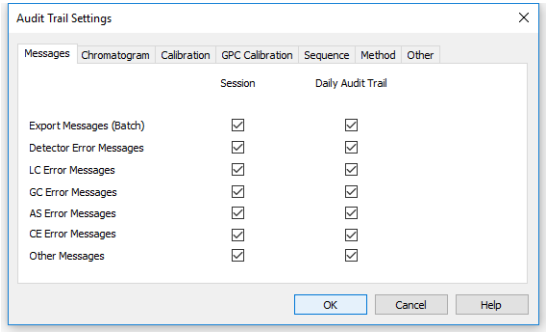


More Info:

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** ⓑ if you want to filter out events or operations.

4. **Click on the *Properties* icon** ⓒ if you want to set up which events and operations should be recorded on the *Session* or *Daily Audit Trail* on each one of the tabs.



5. **Have a look at the Description** to find out about operations and events that have taken place ⓓ.

More Info:

In this example you can see that there was a communication failure with the external A/D converter.

To access the ***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* button** on the *Method Setup* window for the *Method Audit Trail*.

More Info:

The *Local Audit Trails* are included in the corresponding *Chromatogram, Calibration, Sequence and Method* files and contain the whole local history.

15.5 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.

16 Clarity in Network

Clarity might be used in network and following chapters describe different approaches of such usage.

16.1 Clarity in network overview

Clarity is not a client-server (C/S) solution, nonetheless it can be configured for use in multi-user and multi-instrument networked environment.

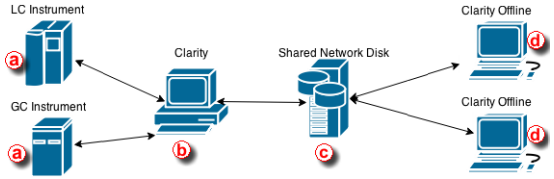
What does the solution Clarity in network offer?

- Instrument control, real-time signal monitoring and run control is possible only trough the local Clarity station, i.e. Clarity must be connected to respective chromatography instrument. Each Clarity needs to be set locally (including .cfg and .psw).
- Using the *System - Directories*, the location of the Clarity data/projects can be set anywhere within the network (typically on a shared server back upped drive). The data can be then accessed from any Clarity station on the network, including the Clarity Offline stations intended for evaluation of data from another computers.
- Clarity Offline allows users to prepare methods and evaluate acquired data.
- With Clarity Offline users are able to work with acquired data on additional computers in the laboratory or at home.
- File access conflicts may occur when accessing the same file (e.g. method) but from different Clarity stations.

What does the solution Clarity in network not offer?

- Central management of users.
- Central management of documents such as chromatograms, calibrations and methods.
- Direct control of acquisition, i.e. run/stop/abort from other Clarity stations.
- Direct control of instruments from other Clarity stations.
- Watch real time signal being acquired by detectors from other Clarity stations.

16.2 Multiple Clarity stations in a network



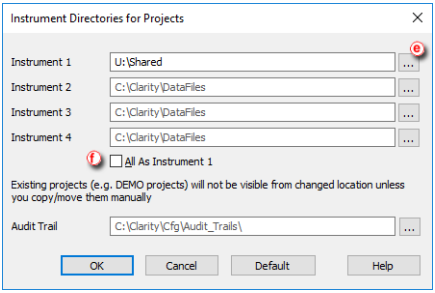
More Info:

- Note that it is possible to have more than one Clarity ⓑ in the network.
- Shared Network Disk ⓒ can be on the same PC as well and not as a separate unit as seen in the picture above.

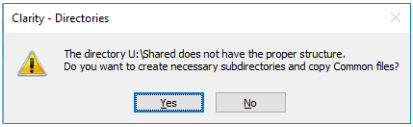
Clarity in network is a solution that consists of at least one Clarity, at least one Clarity Offline and a reliable computer network as the most basic setup.
Simplified scheme of the possible configuration is displayed in the diagram above. LC and GC instrument ⓐ is controlled via Clarity ⓑ. Chromatograms, calibrations and methods are all saved (using directory configuration) on a shared network disk ⓒ. Clarity Offline ⓓ could then be used for evaluation of acquired chromatograms and preparation of methods which are saved (using directory configuration) on the shared network disk. Clarity ⓑ is able to send those pre-prepared methods to corresponding instruments.
Note that this shared network disk is then accessible to all computers within this computer network therefore a much wider configuration can be implemented than the one described above.
Following step-by-step guide will help you configure the Clarity in network solution.

Procedure A - Firstly we will configure Clarity ⓑ which will acquire data and save them to the shared network disk.

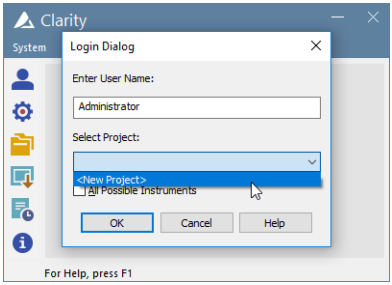
1. In the main Clarity window, go to *System - Directories* or use the icon .
2. *Instrument directories for Projects* dialog will open.
3. Choose Instrument that will share all the created files; chromatograms, calibrations, methods, sequences, reports etc..
4. Use the ... at ⓔ to browse for shared network disk. Once you locate it, click *OK*. Path to the shared network disk is now filled in the corresponding Instrument.
5. In case you want all Instruments to have the same directory, check the option *All As Instrument 1* ⓕ. This will copy the directory path for the rest of the instruments as it is set for *Instrument 1*.



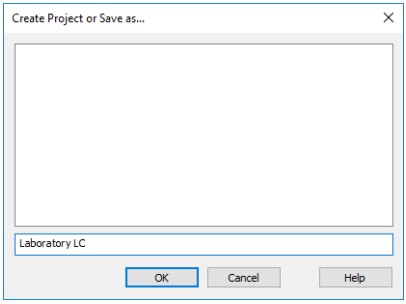
6. To save the configuration click the *OK* button.
7. Configuring the directory for the first time will result in the following message. Click *Yes* to allow the creation of necessary structure. Upon clicking *Yes*, COMMON and PROJECTS folders are created with default documents necessary for correct functionality.



8. When you try to login for the first time with the new directory configuration, you will be asked to create a new project.



9. Fill project name and click OK.

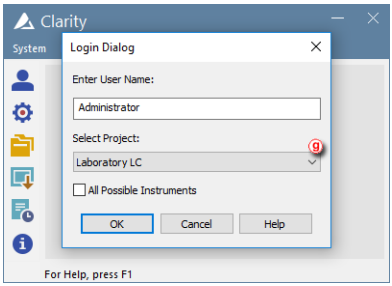


Anything created/measured within this project is saved on the shared network disk and therefore is accessible to other Clarity stations.

Procedure B - Secondly we will configure Clarity Offline ⓓ which will be used for data evaluation from shared network disk.

We need to configure directory from which Clarity Offline will open chromatograms, calibrations and methods saved on the shared network disk.

1. Configure the directory according to step *1-6*, described above.
2. When you login, select the appropriate project (the one you filled in step 9) using the drop-down box ⓖ and click *OK*.



If you have followed the steps correctly, your Clarity in network is configured. If you are not sure, you can test it by measuring some chromatogram and evaluate it on Clarity Offline. Once you see measured chromatogram in the Data directory you know it has been configured correctly.

16.2.1 Migrating Clarity Project into a Network

This step by step guide will help you to move your Clarity project with measured chromatograms, calibrations, prepared methods and other files

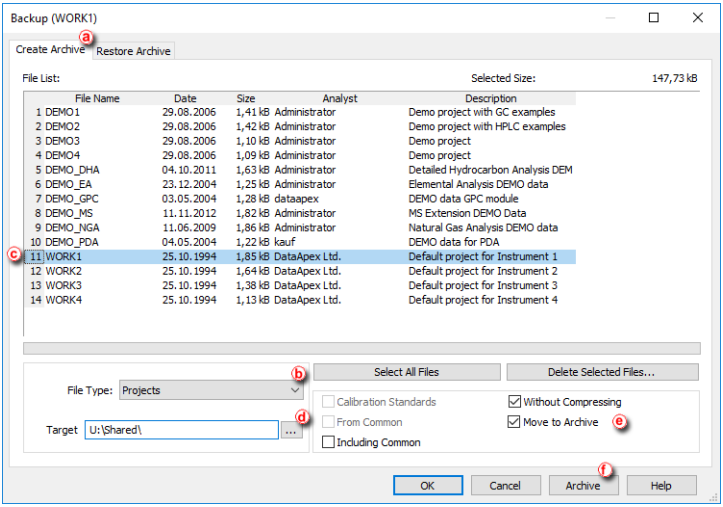
into a shared network disk or a shared server back upped drive.
This guide assumes that you have already set up directory for Clarity in network therefore you have all the necessary structure prepared - if not, refer to **Procedure A** described in the chapter **"Multiple Clarity stations in a network"** on pg **197**.

We will migrate our Clarity project into shared network disk.
Principle behind migrating Clarity project into a different location is straightforward. It is necessary to move the whole project directory (e.g. WORK1) as well as the project file itself (e.g. WORK1.PRJ). Clarity has function called *Archive* which performs this migration automatically.

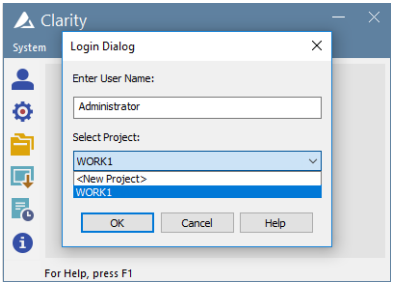
More Info:

- Note that it is possible to copy the project directory and the project file also using File Explorer.

1. In the Instrument window, go to menu *File - Archive...*.
2. Backup dialog opens on the *Create Archive* tab ⓐ.
3. Because we want to migrate whole project, change *File Type* using the drop down list ⓑ to *Projects*.
4. Section *File List* now contains all projects in Clarity. Click the project to be migrated (e.g. WORK1) ⓒ.
5. As a *Target* select the destination of the shared network disk using the ... at ⓓ.
6. Check the options for *Without Compressing* and *Move to Archive* ⓔ.
7. When everything is set as described above, you can click the *Archive* ⓕ button which migrates project WORK1 to the U:\SHARED\.

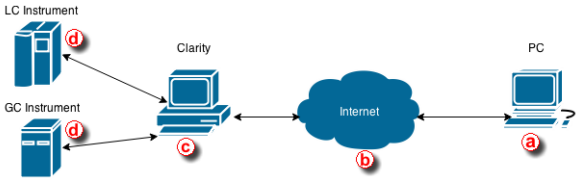


8. Now *Login* to the Instrument which has set directory in the network. Notice that in your Clarity Login Dialog the *Select Project* drop down list offers your migrated project (WORK1) only - this is because there are no other projects.



9. Your Clarity project has been successfully migrated and you can start working.

16.3 Remote control of Clarity over a network



This step by step guide will help you to connect remotely to a PC with Clarity ⓒ installed from your home or office ⓐ. It will allow you to connect

remotely to that PC and take control over the whole computer and thus control Clarity and connected instruments. The connection is realized over the internet or a local computer network. Connection over the local computer network is more secure since the transferred data never enter the internet.

Requirements:

- ⓐ PC needs to have Remote Desktop Connection installed
- ⓑ Internet connection or a reliable computer network
- ⓒ PC with Clarity needs to have Remote Desktop Connection installed

More Info:

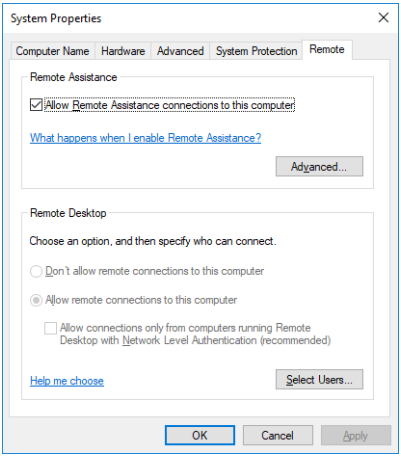
- Remote Desktop Connection is a standard application installed in Windows operating systems.

This description is for setting up a remote connection in Windows 7 Professional. Dialogs may vary depending upon the edition of Windows 7.

1. To allow remote connections on the PC you want to connect to ⓒ follow the steps below:

   More Info:

   - Open System by clicking the Start button, right-clicking Computer and then clicking Properties.
   - Click Remote settings in the left hand side of the Control panel. If you're prompted for an administrator password or confirmation, type the password or provide confirmation.
   - Under Remote Desktop, select one of the three options.
   - Click Select Users.
   - In the Remote Desktop Users dialog box, click Add.
   - In the Select Users or Groups dialog box, do the following:
     - To specify the search location, click Locations and then select the location you want to search.
     - In Enter the object names to select, type the name of the user that you want to add and then click Check Names. This will check whether the user exists. If not, it will trigger a not found dialog. Check the name once again. Note that this user must have a profile on this computer. If the user name is correct, click OK.
     - The name will be displayed in the list of users in the Remote Desktop Users dialog box. Click OK and then click OK again.
   - In case Remote Desktop options are grayed out your computer is probably in a domain and due to domain policies you may not be able to change the settings. Contact your network administrator to resolve the situation.



2. To allow Remote Desktop connections through a Windows Firewall on the remote PC ⓒ.

   If you're having trouble connecting, Remote Desktop connections might be getting blocked by the firewall. Here's how to change that setting on a Windows PC. If you're using another firewall, make sure the port for Remote Desktop (usually 3389) is open.

   More Info:

   - On the remote computer, click Start and select Control Panel.
   - Click System and Security.
   - Click Allow a program through Windows Firewall under Windows Firewall.
   - Click Change settings and then check the box next to Remote Desktop.
   - Click OK to save the changes.

3. To look up the name of the remote computer ⓒ.

   You will to provide this information in step 5.

   More Info:

   - On the remote computer, open System by clicking the Start button, right-clicking Computer, and then clicking Properties.
   - Under Computer name, domain, and workgroup settings, you can find your computer name, and its full computer name if your computer is on a domain.
   - Alternatively your network administrator might also be able to give you the name of the computer.

4. To set a password for your user account ⓒ.

   Your user account must have a password before you can use Remote Desktop to connect to another computer. This is crucial, otherwise you will not be able to connect.

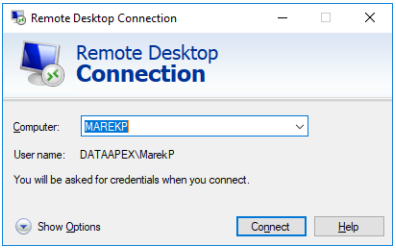
More Info:

- Click Start and select Control Panel.
- Double-click User Accounts.
- Select Change your Windows Password under User Accounts.
- Click Create a password for your account and follow the instructions on the screen.

5. To start Remote Desktop from the computer you want to work from ⓐ.

More Info:

- Open Remote Desktop Connection by clicking the Start button. In the search box, type Remote Desktop Connection, and then, in the list of results, click Remote Desktop Connection.
- In the Computer box, type the name of the computer that you want to connect to, and then click Connect. (You can also type the IP address instead of the computer name.)
- Note that the remote PC cannot be in sleep mode or hibernating.



More Info:

- This text has been taken from the How-to: "Connect to another computer using Remote Desktop Connection" created by Microsoft Windows.

Once you successfully connect to the remote PC you can work as if you were sitting in the lab and working with Clarity. The remote desktop will be presented in the normal window. To terminate the session, close the window.

This solution then enables you to:

- Control instruments that are directly connected to Clarity.
- Monitor data acquisition.
- Evaluate chromatograms in Clarity.
- Work on other projects and leave the remote session open and check once in a while if everything is running smoothly.

Possible situations that may arise using the Remote Desktop Connection:

- If you remotely connect to a PC where you are currently logged in, you will be automatically put through and you can start working.

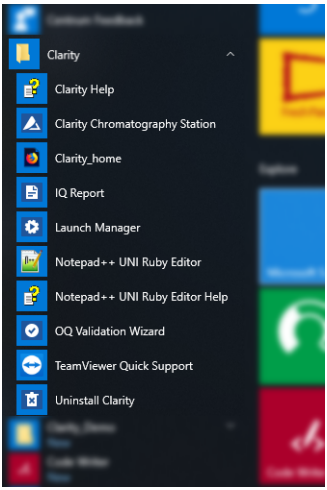
- However, if you try to connect to a PC when there is logged in someone else, e.g. another analyst, he will be asked if he allows the remote connection to put through. If he declines the remote connection you will not be able to connect.
- PC that you are connecting to must be turned on, it is not possible to connect to a PC that is off.

17 Utilities

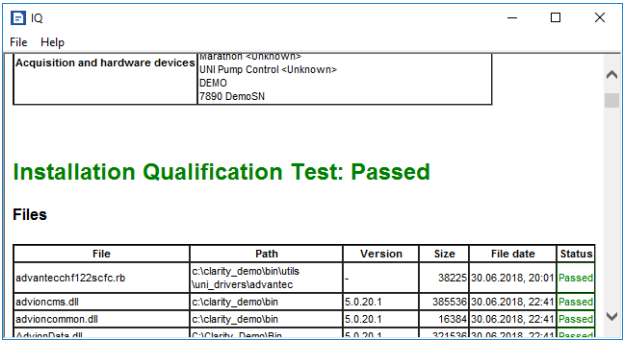
Clarity installation contains various utilities for validating the installation or predefining various Clarity profiles which helps you in using more then four configurations of laboratory instruments.

17.1 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 the files are in the correct version.



1. **Install the Clarity station** according to the instructions of the *Installation Wizard*.
2. After the installation has been completed, you can search for *IQ Report* in the search field of the Start menu.
3. **The IQ window will open.**
4. **If the installation has been correctly performed,** the status should read: "*Installation Qualification Test: Passed*".
5. **If the Installation Qualification fails**, it is recommended to uninstall and then re-install Clarity. If it fails again, contact DataApex support.



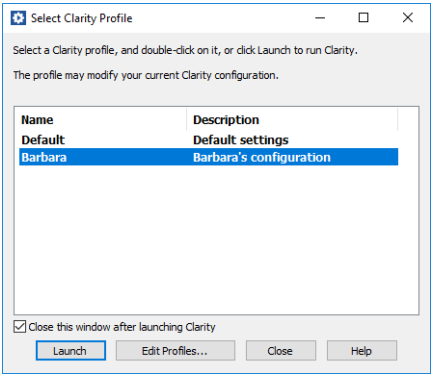
More Info:
The most common reason for a "Failed" result is the installation of an upgrade over an existing full version of Clarity. This itself does not produce any errors but since some of the files are preserved from the original installation, the checksums will not match.

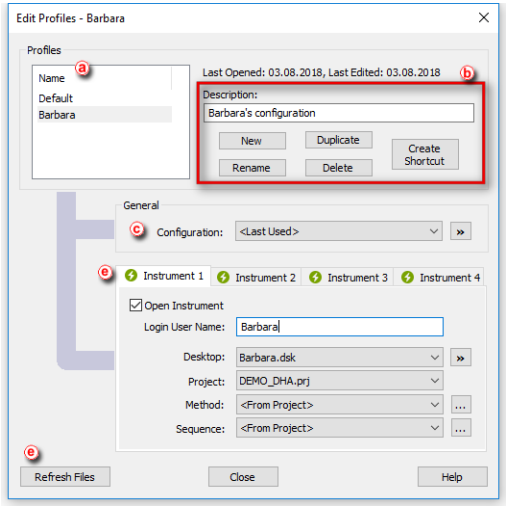
- The **Installation Qualification** report can then be printed, copied to the MS Windows Clipboard or sent as an email.

17.2 Editing Clarity user profiles using the Launch Manager

Launch Manager is an utility that allows you to start the Chromatography Station in various configurations, including predefined instruments and its projects, methods or sequences using command line parameters.

1. **Start the Launch Manager:** click on its shortcut in the Windows *Start - All Programs - Clarity* menu.
2. **Click on the *Edit Profiles* button** to create or modify the profiles.



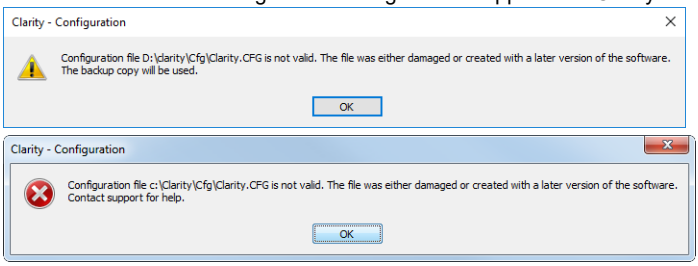


3. **Select** a profile ⓐ to modify it or click on the *New* button to **create a new profile** ⓑ.
4. **Type a name for the newly created profile**. For easier orientation it is recommended to fill in the *Description* which eases the distinguishing of different profiles.

5. **Select the configuration file that will be loaded after the start of** Clarity. ⓒ

More Info:

The list of configuration files is retrieved from the installation directory (configuration files are located in C:\CLARITY\CFG by default). If you click on [»], a menu will pop up with operations on the configuration files.
Notice that Clarity always controls the Instrument type when loading the configuration file. If *.cfg file is damaged or created in later version of Clarity, one of following error messages would appear and Clarity would be closed.



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. **Select the Desktop, Project, Method and Sequence files** that will be loaded when opening each of the instruments ⓓ. Check *Open Instrument* to open given instrument at start.
8. **Click on the *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*.

17.3 Creating a duplicate configuration using the Launch Manager

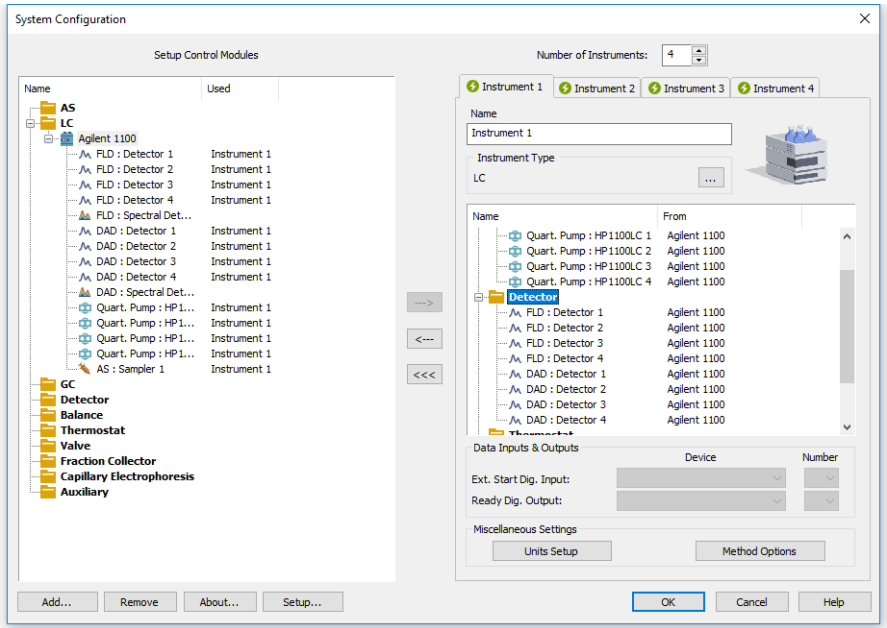
This topic describes how to create a duplicate configuration using the Launch Manager. Steps outlined below describe a situation for configuring Agilent 1100 HPLC system with FLD+DAD detectors. Nonetheless, for some type of analyzes one may require a different type of configuration, for example FLD detector alone, and this is when the Launch Manager with differently configured profiles becomes a strong tool. Note that setup described below is an example but gives the idea what needs to be done for correct functionality.

1. **Start** Clarity - open System Configuration using ⚙ or from menu *System - System Configuration...*.
2. In the System Configuration dialog **configure your station**. If your configuration is already completed, continue with the next step otherwise see

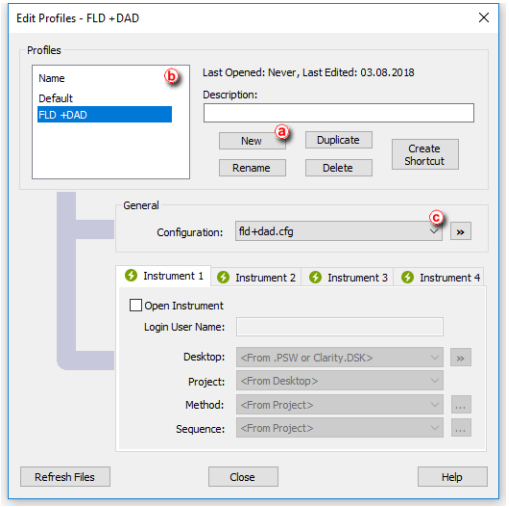
pg **22**.

More Info:

- Image below shows the configuration of the Agilent 1100 HPLC system, with configured FLD, DAD, spectral detectors, pumps and autosampler.



3. **Open** *Launch Manager* from the *Start - All Programs - Clarity* group and **click** the *Edit Profiles...* button.
4. In the Edit Profiles dialog, click the *New* button ⓐ to create a new profile and name your profile (e.g. *FLD+DAD*). Click *OK* to save the profile. Newly created profile is displayed in the small table on left ⓑ.

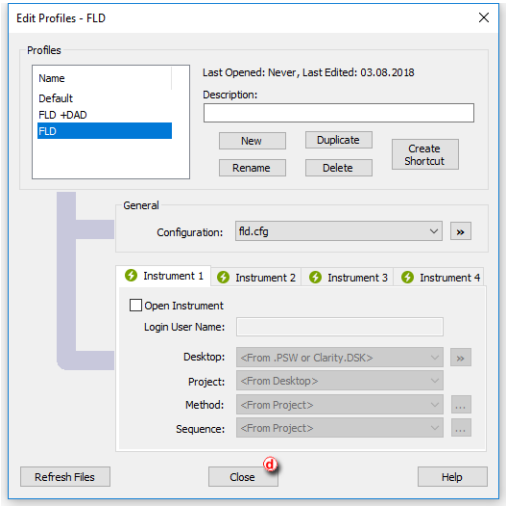


5. From the drop down list ⓒ, **select** CLARITY.CFG and click the » button, from the selection choose *Duplicate* and in the following dialog name your configuration (e.g. fld+dad.cfg).

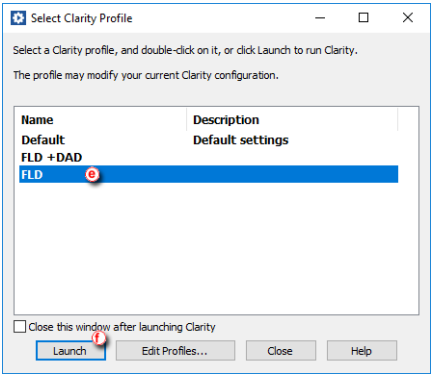
   More Info:

   - This step will create a duplicate configuration (.cfg file) based on the current Clarity setup (as described in step 2.). It prevents Clarity from overwriting a default configuration.

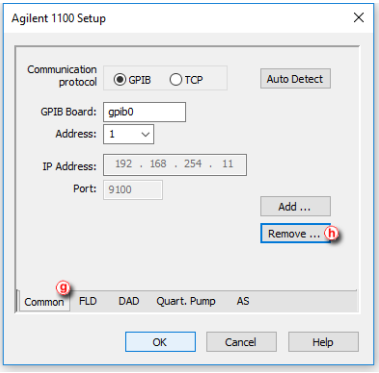
6. **Create** a new profile (FLD) with a different configuration (fld.cfg), **proceed with steps 4.-5**. Once done, your profile should look similar to the image below.



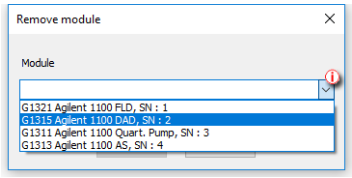
7. **Close** ⓓ this dialog to return to the main Launch Manager window.
8. In the *Launch Manager* window **select** the *FLD* profile ⓔ which has not been configured but simply duplicated and click on the *Launch* ⓕ button.



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. **Click** on the *Setup...* button to invoke Agilent 1100 Setup dialog.
10. On the *Agilent 1100 Setup* dialog **click** on the *Common* tab ⓖ and then click the *Remove* button ⓗ.



11. In the Remove module dialog, **click** on the drop down list ⓘ and select Agilent 1100 DAD, click the *Remove* button to remove it from the configuration.



12. **Click** *OK* on the *Agilent 1100 Setup* dialog and then click *OK* in the System Configuration dialog to save changes in the configuration.
13. Launch each profile using the Launch Manager to make sure that correct configuration is loaded. Make necessary changes to the configuration if needed.

18 Extensions

Chapters describing topics related to specific Extensions.

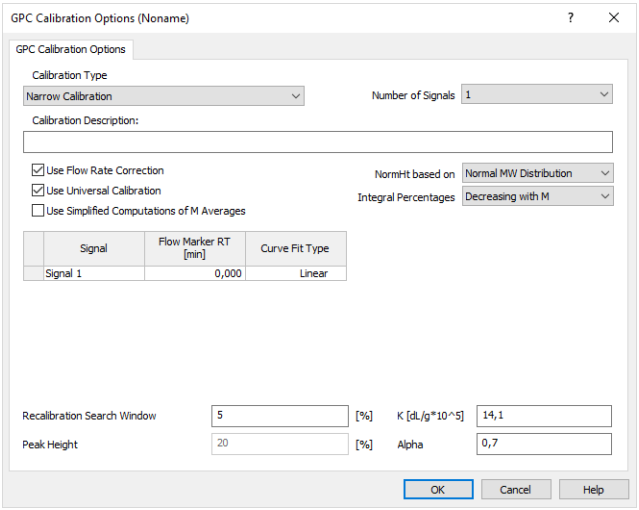
18.1 GPC operations

Following chapters describe specific procedures concerning GPC.

18.1.1 Creating a GPC calibration

To be able to create a GPC calibration, you need to have a measured and integrated GPC chromatogram of a standard sample and the instrument type of Clarity must be set to *GPC*. The *GPC* mode can be toggled on/off by selecting the *Setting - GPC Mode* in the Instrument window.

1. **Open the Calibration window:** select *Window - GPC Calibration* in the *Instrument* window or click on .
2. **Create a new calibration file:** select *File - New* or click on ⓐ.
3. Following dialog *GPC Calibration Options* will show up. Here you can **setup various options and Calibration Type**.



Caution: Once selected, the Calibration Type can't be changed later. More on GPC Calibration Options can be found in the *GPC Extension* manual, accessible on www.dataapex.com.

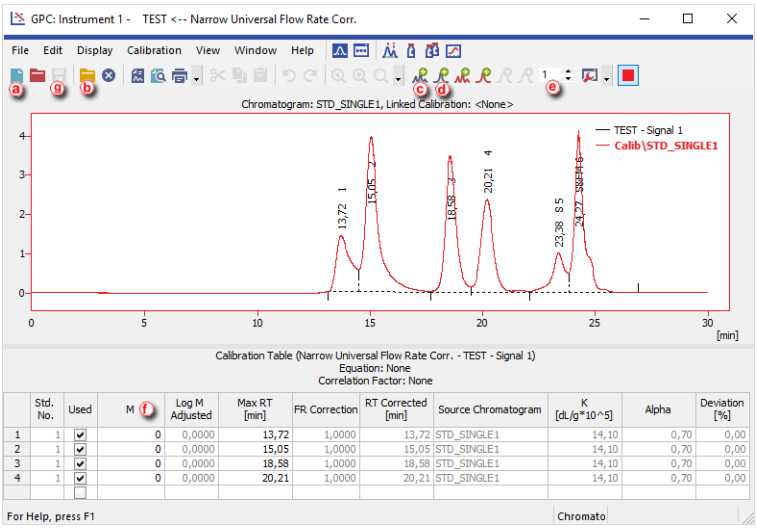
4. Click *OK* to save the calibration. To fill **calibration name** open the *File - Save As* dialog window.

5. **Open integrated chromatogram of a standard:** select *File - Open Standard…* or click on ⓑ in the *Calibration* window.
6. **Add peaks in the chromatogram of the calibration standard to the calibration file:** select *Calibration - Add All* or click on ⓒ (if you have multiple peaks in your chromatogram) or select *Calibration - Add Narrow Peak* or click on ⓓ to add desired peak from your standard.

Note: If you have multiple chromatograms of standards, you can repeat these steps to add the desired peaks: open the standard and click *Add Narrow Peak*, then open another standard and click Add Narrow Peak, repeat for all standards. The number in field ⓔ is connected to the used standard and is not connected to the concentration level. Setting a peak on already used number will overwrite the values with a newly added one.

When using any type of Broad calibration, *Add Broad Peak* will be enabled instead of *Add Narrow Peak*.

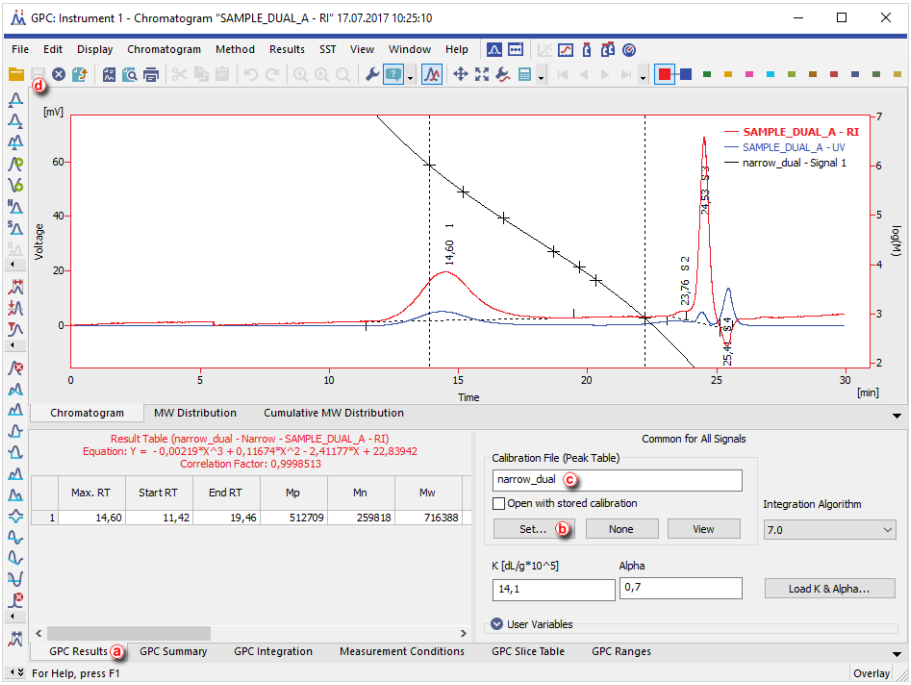
7. **Fill in the appropriate molecular weight** values for the respected peaks into the *M* column ⓕ.
8. **Save the calibration file** from *File - Save* or click on ⓖ.



18.1.2 Applying a GPC calibration to a chromatogram

If the calibration file is not assigned to the template method, the measured chromatogram will not have it linked either. To link a calibration file to a chromatogram do as follows:

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



2. **To link the calibration file to the Chromatogram**, click the *Set…* button ⓑ, so that the *Open GPC Calibration* dialog window will emerge. You can select calibration file from your current project or you can navigate to other folders.
3. **Select the correct calibration file** from the list and click *OK*.
4. **Check that the** *Calibration File (Peak Table)* field contains the name of the calibration file ⓒ.

> *Note:* When no calibration file is linked to a chromatogram, the field *Calibration File (Peak Table)* contains inscription *(None)*.

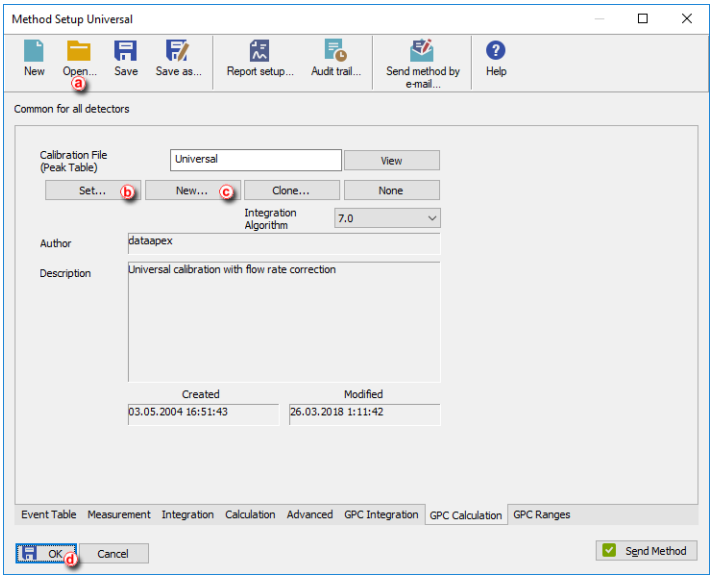
5. **Save the chromatogram:** select *File - Save* or click on ⓓ.

18.1.3 Setting a GPC calibration in the template method

Setting a GPC calibration in the template method allows you to automatically calibrate all measured chromatograms using such method during analyses.

1. **Open the Method Setup - GPC Calculation dialog:** select *Method - GPC Calculation...* in the *Instrument* window.

2. **Open the template method** by selecting the *Open...* icon ⓐ.



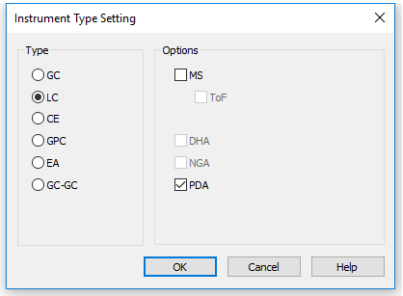
3. **Click the** *Set…* button ⓑ to set a GPC calibration file for the template method, or create a new one by clicking the *New…* button ⓒ.
4. **Click** *OK* ⓓ to apply and save the changes made to the template method.

18.2 PDA Operation

Pick the desired topic in the following chapters.

18.2.1 How to set Clarity instrument to display PDA data

- To switch an Instrument to *PDA mode*, select the **LC-PDA**, **GC-PDA**, **CE-PDA** or **GPC-PDA** option from the Instrument Type Setting dialog.
- Instrument Type Setting dialog is invoked by clicking on the ... button in the System Configuration dialog.
- Options that are technically possible and have been purchased are enabled by default. Otherwise they are automatically disabled.



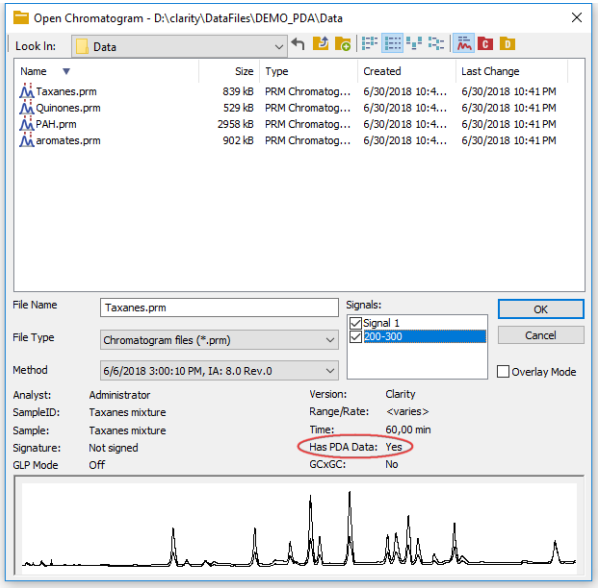
18.2.2 How to open PDA chromatogram

1. In the Chromatogram window, click the *Open Chromatogram* icon .
2. Choose a chromatogram that **has PDA data**.

   More Info:

   Notice that chromatogram containing PDA data has the flag in the *Detail Info* section, just below the list of chromatograms.

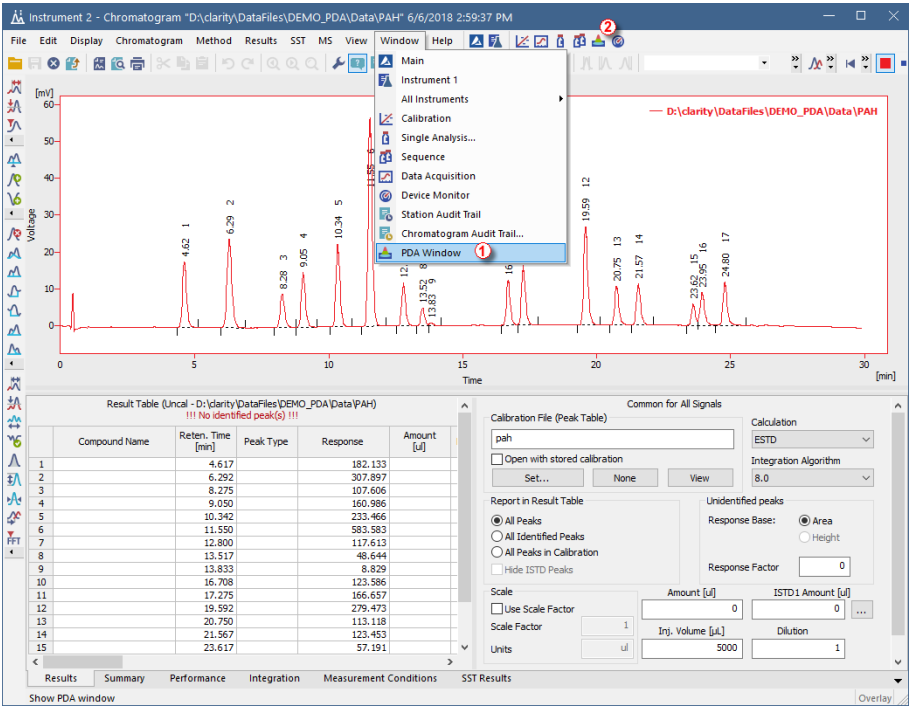
3. After choosing chromatogram(s) click *OK*.
4. Next suggested topic is: "How to work with PDA chromatogram" on the next page.



18.2.3 How to work with PDA chromatogram

Instrument Type must be set to PDA - see the chapter **"How to set Clarity instrument to display PDA data"** on pg **218**.

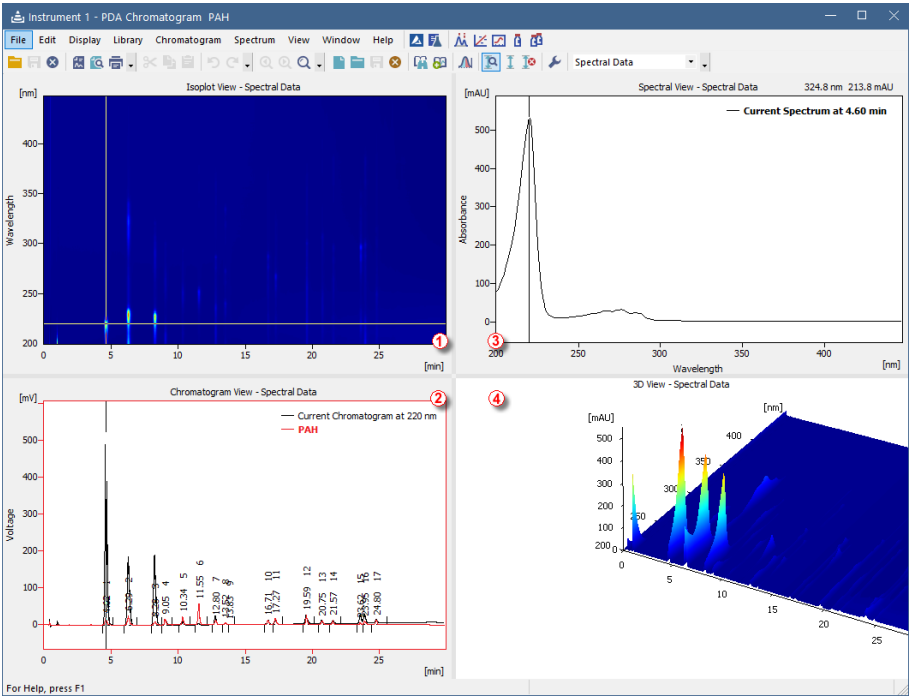
- **Open PDA window**: in the Chromatogram window go to *Window - PDA Window* ① alternatively click the **PDA** window icon ②.



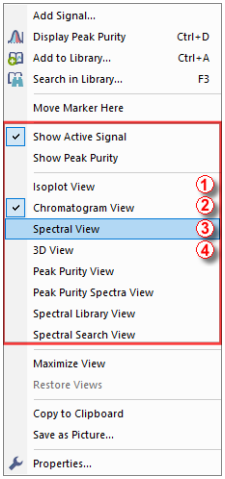
- After invoking, it will open *PDA Chromatogram* window which is covered below.

How to display PDA data

1. Spectra are automatically displayed in the PDA Chromatogram window upon opening chromatogram that contains **PDA** data.
2. By default, PDA Chromatogram is divided into 4 separate panes, each with a different information. You can change number of panes using the menu *View - Two horizontal views* for example.



3. To change a view of a pane, right mouse click and select one of the views. For a more specific example, see the chapter **"How to view specific spectra in overlay"** on pg **229**.
4. Numbers ① to ④ correspond to different views in the picture above.

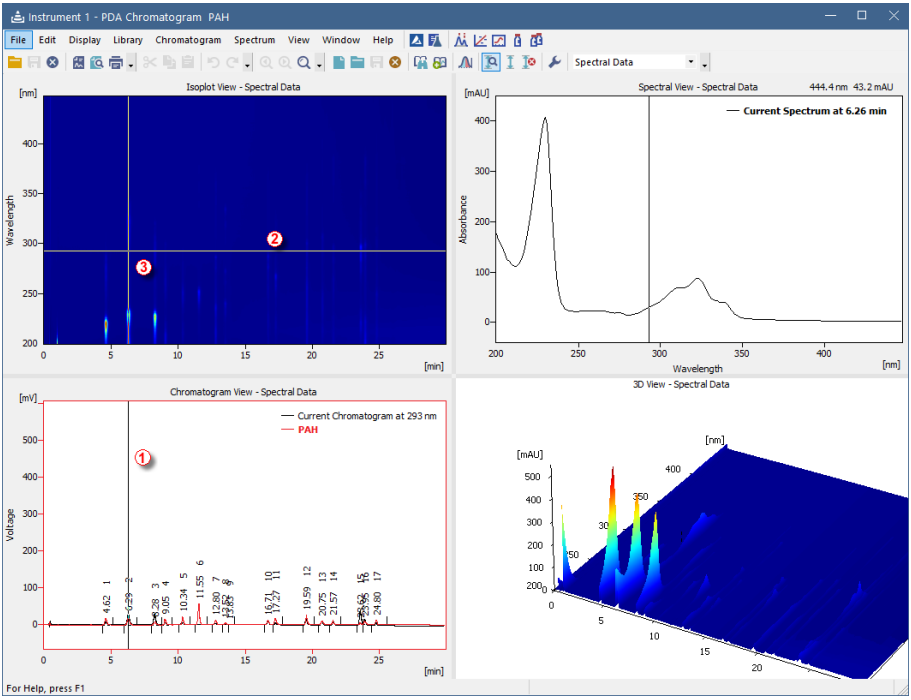


How to use markers in PDA Chromatogram

Panes in the PDA Chromatogram contain graphs with markers (thin lines of inverse color crossing the data plot ①②③). According to where the marker is positioned corresponding data are displayed.

More Info:

For example if you will be changing the wavelength in the *Isoplot View* by dragging the horizontal axis cursor, *Spectral View* will be changing relatively to it.



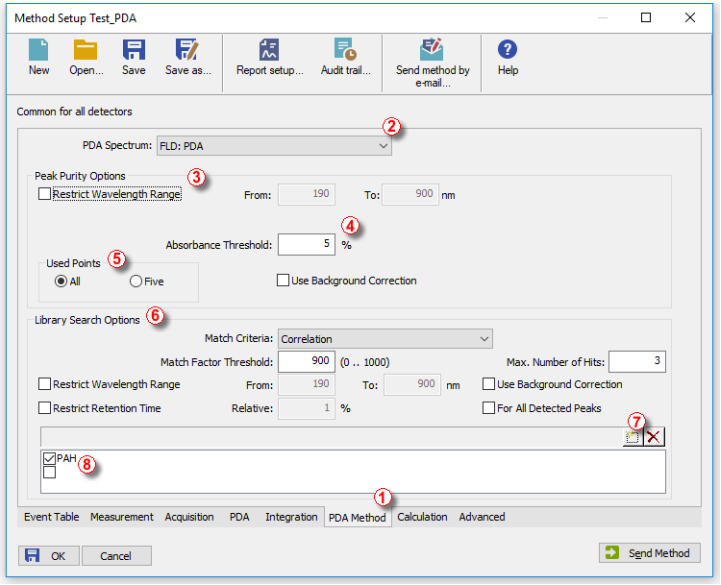
- **To change spectral data based on time**: drag the vertical marker ① to the desired time. Note that the cross cursor changes to ⟺ once the move is possible.
- **To change wavelength**: drag the horizontal marker ② to desired position. Notice that the cross cursor changes to ↕ once the move is possible.
- **To change both**, wavelength and time, move to the junction where the two markers meet ③. Once the cross symbol changes to ✥, left mouse click + hold + drag to your desired position.

- In the *3D View* you can move the whole graph to your area of interest - simply left mouse click + hold + drag. Note that markers in other panes will change accordingly to the moved area.
- Increasing the zoom may cause that the markers may be out of the current view. **To locate them** on the current zoom, right mouse click in the pane - *Move Markers Here*.

18.2.4 How to set PDA method

This section deals only with method setup related only to **PDA options**. For a method setup see "Setting up a method"

- *PDA Method* tab ① is available only when **PDA** Extension is configured on the given instrument.
- From the drop down ② box select *PDA Spectrum* - if chromatogram contains more than one (typically DAD and FLD).
- For the *Peak Purity Options* there are several settings which can restrict the evaluation of peak purity. It can be restricted based on the *Restrict Wavelength Range* ③ check-box and filling the range of wavelength in which it will be evaluated.
- Another restriction can be made using the *Absorbance Threshold* ④.
- *Used Points* ⑤ specifies the number of points peak purity will be evaluated, either from the *All* the points or from the *Five* most significant.
- In the *Library Search Options* ⑥ select criteria according to which the *Search in Library* command, described in see pg **227**., will be performed.
- To add another **PDA library** to search in, click the  icon ⑦ and then click ..., from the dialog choose a library.
- List of libraries that will be searched in is listed ⑧. Alternatively enable/disable the search for specific library using the check-box.



18.2.5 How to display peak purity

Displaying peak purity is one of the fundamental tasks when ensuring that no co-eluting or co-migrating impurities contribute to the peak's response.

1. Used views: **Chromatogram View**, **Peak Purity Spectra View**, **Peak Purity View** and **Isoplot View**.

   More Info:

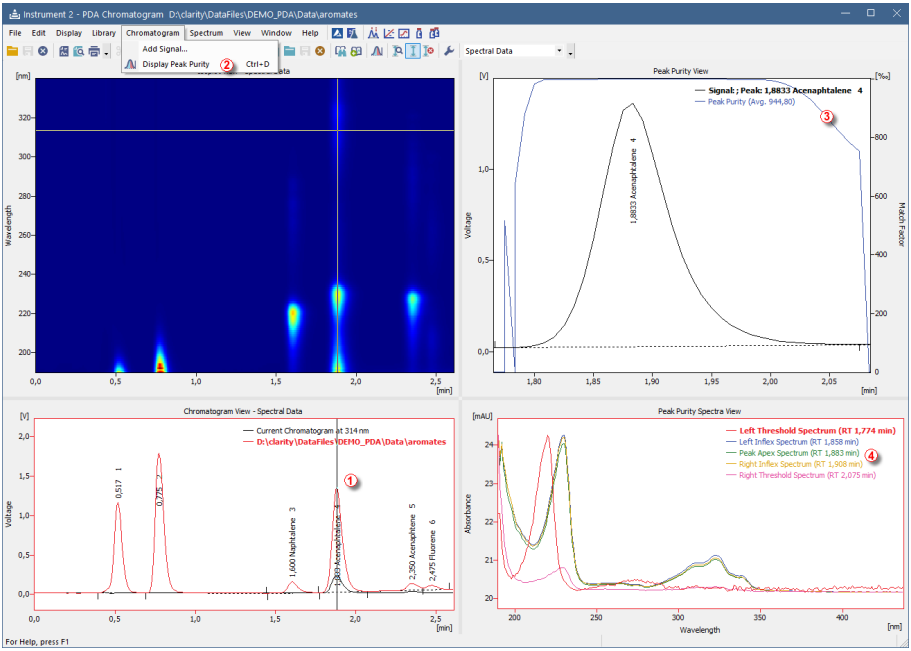
   See "How to work with PDA chromatogram" on page 220

2. Move the marker ① to the peak for which you want to display peak purity.
3. In the menu *Chromatogram* - click the *Display Peak Purity* ② command or click the icon in the toolbar.

   More Info:

   If you get *No peak selected* in the **Peak Purity View** the reason is that you have not applied point number 3.

4. **Peak Purity View**: displays signal for selected peak and its calculated **Peak Purity** ③.
5. **Peak Purity Spectra View**: displays spectra in several significant points ④ of the peak selected in the **Peak Purity View**.



18.2.6 How to work with PDA library

PDA Library serves for storing compounds along with their PDA data such as spectrum.

More Info:

It works on a similar basis as calibration. *Search In Library* command, searches the **PDA library** for similar spectrum as defined by your cursor axis in the chromatogram.

PDA library can be managed either from the menu *Library* or using the toolbar which is shown below:

Manage libraries:

- **Create a new library**: click the *New Library* icon.
- **Open existing library**: click the *Open Library* button and in the dialog choose your desired library.

Add compounds:

1. **Add a spectrum into the library**: click the *Add Spectrum* icon which opens Spectrum Property. In the dialog you can specify compound name and additional comment.
2. **Add all identified peaks**: click the command from the menu *Spectrum - Add All Identified Peaks*.

Note: Identified peaks are those that correspond to peaks identified and named in the calibration file. Peaks are added into the currently opened library.

3. **Save library**: to keep any changes made in the library, click the *Save Library* icon.
4. **Close library**: click the *Close Library* icon. If you have unsaved changes you will be prompted to either save the changes or discard them.

View library:

1. **Spectral Library View**: to view contents of your library, right mouse click in any pane and choose *Spectral Library View*.

More Info:
It contains a table with spectrum name, retention time and other parameters.

18.2.7 How to search in PDA library

To search for a matching compound in the PDA library, there is number of ways.

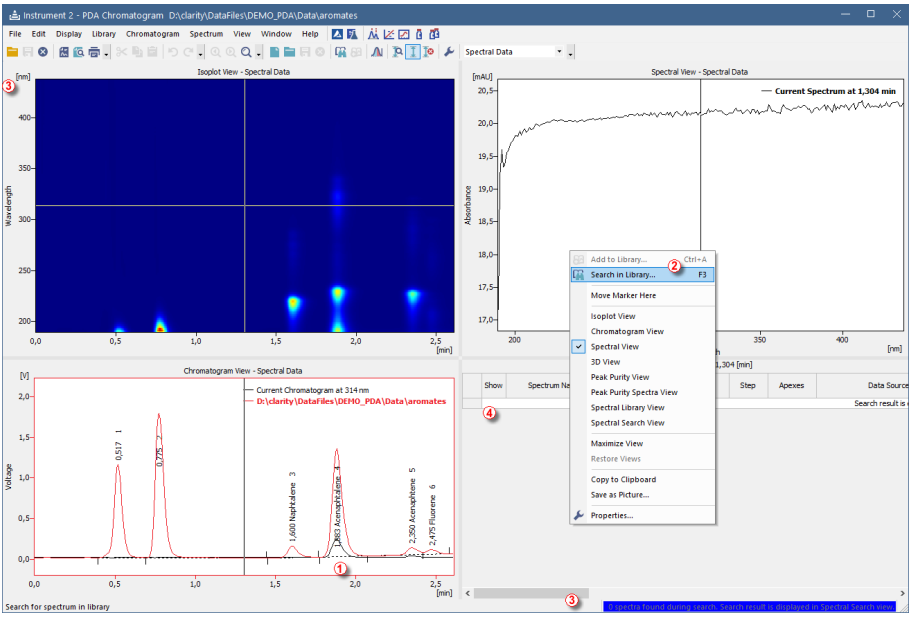
Most common ways to search in library:

1. **Move marker** ① to peak for which you want to search in library.
2. **Right mouse click** in the *Chromatogram View*, *Isoplot View* or *Spectral View* and from the menu choose *Search in Library...*.
3. Use the **Search in Library** icon from the toolbar.
4. **Press** the *F3* on your keyboard.
5. **Go to menu** *Spectrum* and choose the *Search in Library...* or alternatively use the keyboard shortcut *CTRL + F*. Upon invoking this command - Spectral Library Search Options dialog will pop-up where you can further refine match criteria as well as searching across multiple libraries.

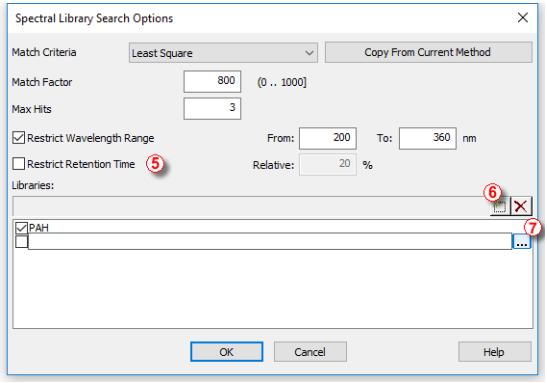
Caution: Search results are displayed in the Spectral Search View pane, therefore make sure that you have this pane visible.

Problems arising while using Search in Library

Search in library is based upon multiple requirements, if any of the requirements fails, the compound will not be displayed in the result of the search.



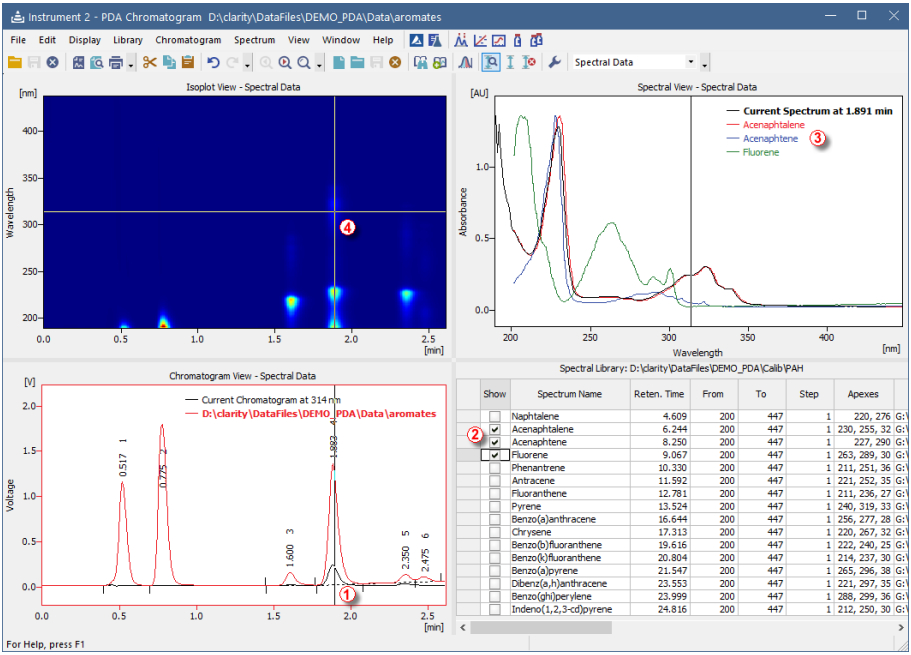
- After you **Search in Library** ② for corresponding spectrum, you may notice that the blue ribbon ③ at the bottom of the window informs you that *0 spectra found during the search*.
- **Library Search View** is also empty ④.
- Possible reason for such behavior can be that the *Library Search Options* are incorrectly set up.
- In the menu click the *Spectrum - Search in Library...* command. Below dialog will open.



- Note that *Restrict Retention Time* check-box ⑤ should be enabled only when the **PDA library** has been created under same conditions as the chromatogram measured.
- **Add another** library using the ⑥ which may contain spectrum you are looking for.
- **Choose** ⑦ library using the ...
- Once criteria are set up, click *OK* to apply them.

18.2.8 How to view specific spectra in overlay

To view specific spectra from **PDA library** in overlay and thus have the opportunity to compare current spectrum against spectra from the **PDA library**, follow the steps below.



1. Used views: **Chromatogram View**, **Spectral Library**, **Spectral View** and **Isoplot View**.

   More Info:

   See "How to work with PDA chromatogram" on page 220

2. Move the **marker** to your desired position ①.
3. In the **Spectral Library View** check the *Spectrum Name* for each ② spectrum that you want to show in the **Spectral View**.
4. **Spectral View** displays current spectrum along with other spectra ③ checked in the **PDA library**.
5. Move the marker ④ in the **Isoplot View** to change only the spectrum or spectrum and retention time.

   Note that those steps can be also performed on results from the *Search in Library* - thus having spectra from the search in overlay.

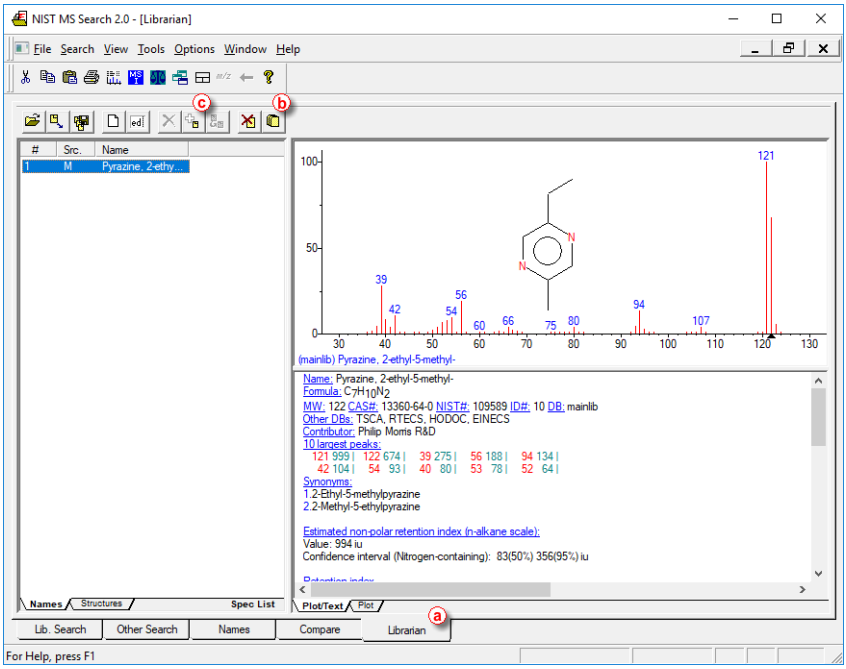
18.3 MS Operation

Pick the desired topic in the following chapters.

18.3.1 Creating and filling your own MS library

Own **MS Library** can be created using external program **NIST MS Search** accessed either from the *MS toolbar* or from the *MS* menu in the MS Chromatogram window:

- Use the *Manage Libraries* button to open the **MS Search**.
- Switch to the Librarian tab ⓐ.
- Use the *Create Library* button ⓑ to create your own library, and *Add to Library* button ⓒ to add the selected compounds into it.



To be able to add selected compounds (or spectra) to own library, such compounds must be selected in the Librarian tab. To do so, you can either perform the *Single Compound Search* or use *Add Spectrum to Library* icon or command from the MS Chromatogram window.

Add Spectrum to Library

After clicking the *Add Spectrum to Library* icon or command, the view will lock in the graph and will let you select the spectrum. After selecting the spectrum the Add MS Spectrum to Library dialog for inserting that particular **MS Spectra** appears:

- Set the *Averaging Time Range* field to perform averaging and smoothing of the spectra inserted into the library – if not selected, the actual spectra as clicked into the graph will be stored.
- Set a *Compound Name* under which you want to add the spectrum into the library.

- Press the *OK* button.
- The **MS Search** program will open, which allows you to add the spectrum into the library upon switching to the Librarian tab and using the *Add to Library* button.

Single Compound Search
After clicking the *Single Spectrum Search* icon or command, the view will lock in the graph and will let you select the spectrum. After setting the desired parameters and clicking the *Search* button the **MS Search** program will open. Switch to the Librarian tab and using the *Add to Library* button add the spectrum into the library.

Note: For more details on *Single Search Compound* please see the chapter "MS Libraries".

18.4 SST operations

Following chapters describe specific procedures concerning SST.

18.4.1 Using SST for quality control

The optional SST Extension allows to set up limits for selected parameter. It compares measured values against those preset limits and perform actions based on the result. The SST works with calibrated chromatograms and the evaluation is based on the compound name in Chromatogram.
Here we provide an example on how to create SST method which can be used to check if the control samples are within expected limits and how to set up sequence to be checked by different SST methods.

Caution: In order to get desired reactions to passed or failed limits it is necessary to have chromatogram **Overlay Mode switched off**.

1. On a chromatogram **create a SST method** in the Chromatogram window using the:
   - *SST - SST Result* to display the SST tab
   - *SST - New* to create a new SST method
   - *SST - Update from Calib* to load the list of peaks from a calibration file (There has to be calibration linked to the chromatogram on the Results tab)
   - Than the screen will look similar to this:

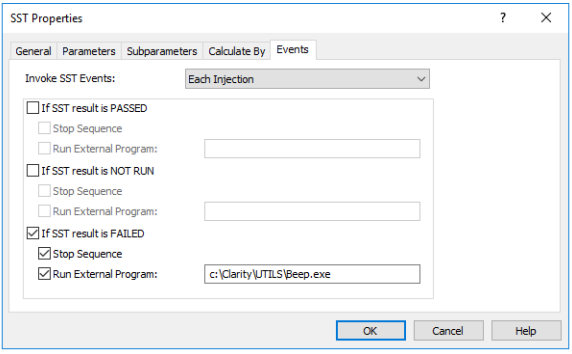
2. As a second step, **fill in the necessary parameters for the limits**.*(In this case Tetrachlormethane peak is the one used to check actual against expected value in Control sample., Expected Amount is 1.2, lower limit is 1.1, upper limit 1.3.)*
    - Select the checkbox of the Tetrachlormethane in the table on the left
    - Double-click the Amount Column in the table on the right to activate it
    - Set the 1.1 value in the Lower Limit cell of the column, 1.3 into the Upper Limit cell
    - Right-click the table and select the SubParameters item. On it uncheck the *%RSD Limit* item (as you do not need it) and select the *Each Individual Value*.

      More Info:
        - When the SST Result is based on *Each Individual Value* than it compares each evaluated value with the Upper Limit or Lower Limit.
        - When the SST Result is based on *Mean of All Values* than it compares average value of all opened chromatograms with linked calibration with the Limits. So pay attention to all opened chromatograms.

    - You may hide the inactive rows and columns by using the SST - Show All Columns and SST - Show All Rows items in the menu
    - The result of the check is displayed by the green tick mark or red cross. You can validate several different parameters at the same time this way.

- You will see similar result now:

3. In another step you can **set reaction to the test result:**
   - Use the *SST - Events* command to open the dialog again.
   - Set the tab as on next picture:



   - It is possible to trigger any external program wanted, set different events on failed check or passed check etc.
4. Save the created method by using the SST - Save item (I used HighControl.sst file name).

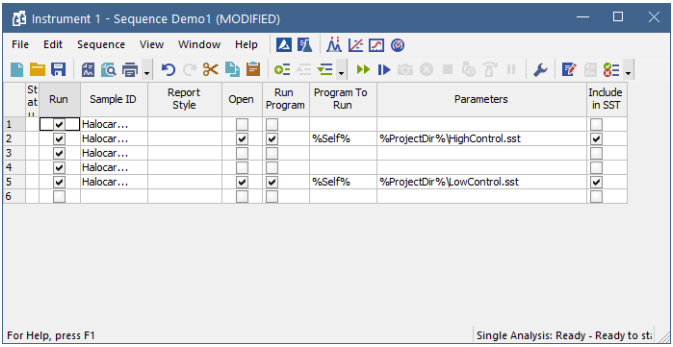
5. You can create other SST methods in the same manner.

More Info:

- For example if you use multiple calibration levels it is possible to create methods which control each level against its own limits.

How to set up sequence to be checked by different SST methods

- Set the sequence accordingly:
  - Right-click the sequence table and select the Setup Columns item.
  - Set the columns Open, Run Program, Program to Run, Parameters and Include in SST as visible.
  - Set the columns for the rows with *High Control* and *Low Control* samples as shown on the next picture:



	Stat	Run	Sample ID	Report Style	Open	Run Program	Program To Run	Parameters	Include in SST
1		☑	Halocar…		☐	☐			☐
2		☑	Halocar…		☑	☑	%Self%	%ProjectDir%\HighControl.sst	☑
3		☑	Halocar…		☐	☐			☐
4		☑	Halocar…		☐	☐			☐
5		☑	Halocar…		☑	☑	%Self%	%ProjectDir%\LowControl.sst	☑
6		☐			☐	☐			☐

  - This will force Clarity to open the correct SST method for the row and perform the check.