

REFERENCE GUIDE

Clarity Software

ENG

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Sections of the manual connected only to the **Clarity Full** version are marked with the  icon.

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Author: DM

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

Open File (italics) describes the commands and names of fields in **Clarity**, parameters that can be entered into them or a window or dialog name.

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

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

Chromatogram (blue underlined) marks clickable links referring to related chapters.

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

Note: Notifies the reader of relevant information.

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

Marks the problem statement or trouble question.

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

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

1 Clarity Full version

The main window of the **Clarity** station contains Instrument icons as well as a menu for the configuration of the station, opening and closing Instruments etc.

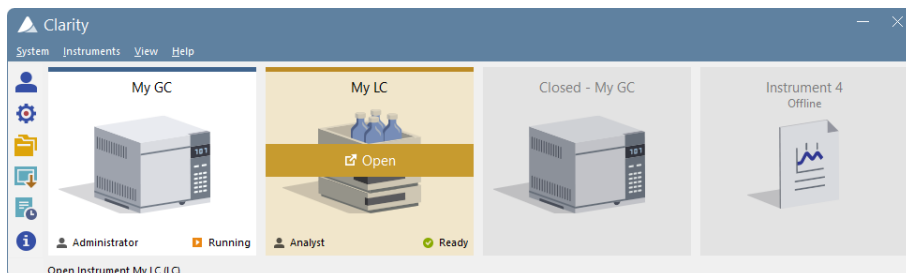


Fig. 1: Main Clarity window

Moving mouse cursor over the image of the Instrument highlights card of the Instrument and displays possible action (Login, Open, Unlock). Clicking the image of the Instrument opens the [Instrument](#) window.

In the screenshot above, there are two logged on Instruments (My GC and My LC), the first is used by the user *Administrator* whereas the second one by the user *Analyst*. The other two instruments are logged off, additionally Instrument 4 is Offline meaning that it has not sufficient license to be used for data acquisition, i.e. only data processing can be performed.

On the logged on instruments status info can be found in the right bottom corner. The first instrument is in *Running* state and the second one is in *Ready* state.

Above the chromatograph is the name of the Instrument and colour which is used throughout the station for easier navigation among multiple opened instruments.

Note: To quickly view the configuration of the specific instrument, simply point mouse cursor over the picture of the chromatograph, name and its configuration will be displayed in the status bar. Type of configuration is located in the parenthesis, (LC) for the above image.

While trying to open **Clarity Instruments** or some other dialogs ([User Accounts](#), [System Configuration](#) and others) or to invoke certain commands, the [Login Dialog](#) appears. This dialog is described in detail in the chapter "**Login**" on pg. 39..

Starting and closing Clarity

While the **Clarity** is starting or closing, the starting or closing splashscreen is visible instead of the main *Clarity* window. This might be important mainly with some of the control modules because of the quite long times when **Clarity** loads or unloads the necessary drivers.

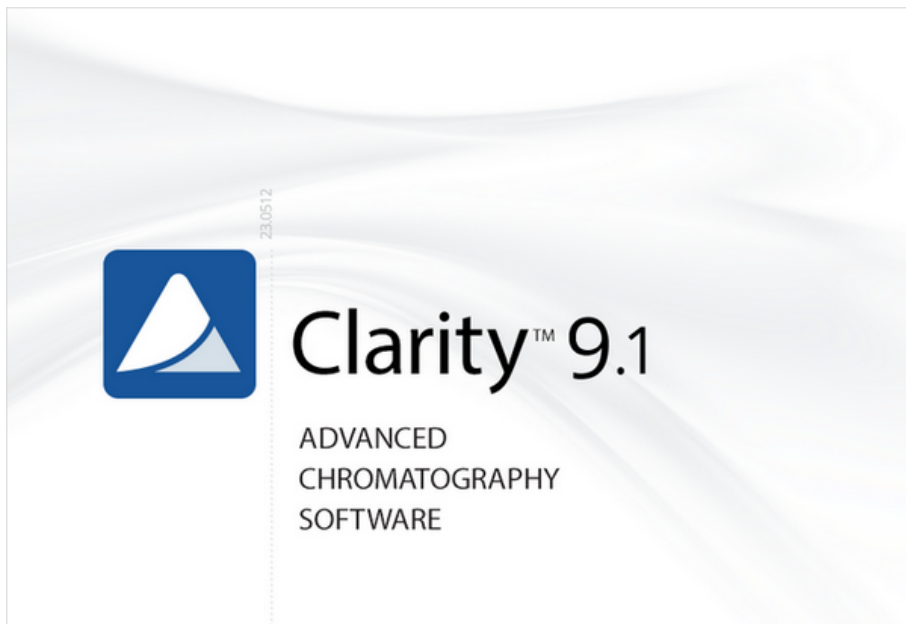







Fig. 2: Clarity starting and closing splashscreens

1.1 System

Submenu with system commands:

	User Accounts	Sets the access rights and passwords particularly for the administration of user accounts.
	User Details	Shows the details of user account settings even to the users that don't have the access to the User Accounts dialog.
	Configuration	Sets the station HW configuration.
	Units Setup	Opens a dialog for specific instrument to set units.
	Directories	Sets directories for individual Instruments.
	Clarity2Go	Sets the communication with server for watching instruments in your iPhone or Android phone.
	GLP Options	Sets the global regulated-environment connected options.
	Digital Outputs	Sets the outputs control.
	Audit Trail	Displays the records of selected station tasks and sets their logging.
	Exit Clarity	Exits the program. If the measurement is active on any Instrument, you will be notified. You will also be prompted to save changed files.

Invoking commands from the *System* menu or the *Help - User Code...* command requires all instruments to be closed. The user has to Logout all instruments. In case the *Logout All Now* button is disabled, an **Instrument** is locked. Unlock the **Instrument** manually (for more details see the chapter **Lock** on pg. 42)..

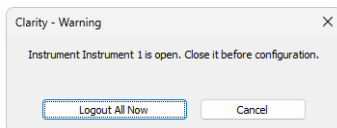


Fig. 3: Logout all instruments

1.1.1 User Accounts


Administration of user accounts, access rights and passwords. When the *System - User Accounts...* command or  icon is invoked, the *User Accounts* dialog will appear. Such dialog is used to define all users working with the station and to set their access rights. User accounts settings are saved in the CLARITY.PSW file.

Fig. 4: User Accounts

Note: Setting access rights is used predominantly to prevent intervention by untrained persons. This is not conceived as data protection against theft - such protection would require setting access rights in **MS Windows**. If any file is modified outside the **Clarity** station environment, it would be identifiable due to built-in security features.

User List

Provides a complete list of previously defined users. The name of the user to whom the content of all displayed fields relates will be displayed in inverse mode (i.e. white text on the blue background). Other users are selected by using arrow keys or clicking your mouse on the desired user name.

New

Adds a new user. During this operation, the new *User name* is checked against existing user names for possible collision.

Duplicate

Duplicates a selected user account from the user list. Rights from section "Other Users Can", "Access To" and "User Access Rights" are copied from the original

user.

Delete

Erases a selected user from the user list. If all users are deleted the station automatically switches to “all users” mode. In such mode the password is no longer required.

Password Restrictions

Caution: *Password Restrictions* parameters are common to all users.

Min. Length

Refers to the minimum length of the password entered. A password shorter than the prescribed number of characters will not be accepted.

Life Time

Refers to the period of a password's validity. After its expiration the user must select a new password.

Expiration Warning

Alerts the user specified number of days prior to a password's expiration.

Password Reuse

Relates to the period from which an already used password can be used again.

Auto Lock

If the user doesn't have any activity in Windows, all opened Instruments will be locked after specified time in minutes. All windows opened on instruments will be hidden and the user has to unlock the [Instrument](#) by clicking on its picture in the [Clarity](#) window.

Caution: When an Instrument is Auto Locked, all eventual unsaved changes in modal dialogs (Method Setup, Single Analysis, Report Setup, etc) are discarded and those dialogs are closed.

User Details for:

The fields displayed in the lower part of the window always relate to the user whose user name is selected from the *User List*. Only a user with adequate access rights can change the settings of those access rights (i.e. such user has selected *Open User Accounts* in the *User Access Rights* section).

User

User Name

User name will automatically be placed in all headers of files that are created while working in the station. The user name will be displayed along with the *Created by* or *Analyst* phrase when a file is selected. It is compulsory for a user to fill in this field and forbidden for two users to have the same user name.

Desktop File

Refers to the name of the file (*.DSK) in which the desktop settings are saved. The file contains settings regarding size, location and visibility of the Instrument windows as well as all the amendable Instrument parameters which are not part of

system files. If this field is left empty, it will be filled in automatically according to the *User Name* field.

This setting is common to all Instruments available for the user.

Note: If you wish to share the same settings for several users, you can link them to the same desktop file. To do so, simply fill in the name of the user with desired settings.

Description

Provides a user's detailed description.

Note: *User Name* and *Description* are part of signature during electronic signing.

Other Users Can

This section serves for setting what other users can do with files created by selected user.

Read & Write

Other Clarity users can view and edit files created by selected Clarity user.

Read

Other Clarity users can view files created by selected Clarity user but cannot edit or otherwise modify them.

No Access

Other Clarity users does not have any access to files (even for reading them) created by selected Clarity user.

For example three Clarity users exist - Alice, Bob and Cameron. Alice's account is set to *No Access* option, Bob's account is set to *Read* option and Cameron's account is set to *Read & Write* option. Alice and Cameron will be able to open files (chromatograms, methods, calibrations...) created by Bob but will not be able to modify them. Alice and Bob will be able to open and modify files created by Cameron (because of his *Read & Write* option). Bob and Cameron will not be able to read nor modify files created by Alice (because of her *No Access* option).

Access To

Instrument X

Defines which Instruments the user may access within a station.

User Access Rights

Open User Accounts

A user with access to user accounts can add, delete or change the access rights of other users. A selected checkbox is essentially equivalent to allocating administrator rights. It also allows the user to use the *System - GLP Options...* command to change the rules for files overwrite. User without such rights can't even open the *User Accounts* dialog.

Open Configuration

Checking this field allows specific user to access following dialogs: "Configuration" on page 11, "Units Setup" on page 25, "Directories" on page 27 and "Digital

Outputs" on page 37.

Edit Method

Enables the user to create, delete or edit a method. A user with no rights to edit method still can *Send Method* to Instrument.

Note: If the method is changed by any reason (the MODIFIED inscription is shown in the [Instrument](#) window header) and the user without the *Edit Method* privilege should leave the [Instrument](#) window, all changes to the method are automatically discarded.

Edit Chromatogram

Enables the user to edit chromatograms.

Edit Calibration

Enables the user to create and edit calibrations.

Projects

Enables the user to switch among all available projects directly from the [Instrument](#) window without need to perform log-off and log-in steps. When enabled the respective user will have access to [Project Setup Dialog](#) from [Instrument](#) window. When disabled the user will still possess an option to switch to any different project via [Login Dialog](#). This item does not control privilege for creation of new project or assignment of project to respective Clarity users at all.

Note: It is not possible to prevent any Clarity user from creating new project via [Login Dialog](#) and [Project Setup Dialog](#).

Import Chromatogram

Enables the user to import chromatograms.

Take Control of Locked Instrument

Enables the user to take control of instrument from another user. The instrument has to be locked by the previous user using Auto Lock or by using *Instrument - Lock Instrument X* command in *Main* or *Instrument* window. All actions will be logged into *Audit Trails* under the newly logged user. If the new user does not have *Start Acquisition* rights, running analysis or sequence will be finished but next analysis will not be started.

Caution: All eventual unsaved changes in files not saved by the previous user will be discarded.

Note: It is recommended to set one common *Desktop File* for all users with this option enabled. Otherwise desktop of the first logged user will be used for all users that take control over the Instrument, until the Instrument is closed again.

Note: It is also recommended to set the same *Edit...* rights for users that plan to take over Instruments as different rights may limit the options of second user.

Note: It is possible to take control of locked Instrument using the "Command line parameters" on page 482. Always include the user (*user=...*) and password (*p=...*) parameters for each command, because the instrument is kept locked.

Edit Sequence

Enables the user to create and edit sequences.

Edit Report Style

Enables the user to create and edit report styles.

Select Method

Enables the user to select a method for Single Analysis. This feature does not apply to Sequence and Batch.

Note: To disable it in sequence, please refer to Edit Sequence.

Open Audit Trail Settings

Accesses the setting changes in station task logs.

Archive/Restore

Permits the user to archive/delete/restore files and projects in the **Clarity** software.

Post Run Settings

Enables the user to change the post run settings in the [Single Analysis - Post Run Settings](#) tab, [Sequence](#) window and the [Batch](#) dialog.

Start Acquisition

Permits the user to start the sequence or single analysis. This right also allows the user to use *Skip Vial* and *Repeat Injection* commands.

User Info**Password**

Notifies whether a user has already selected a password or not. Possible conditions are either *Submitted* (password already entered) or *Blank* (password not entered yet).

Password Changed:

Date of last password change.

Last Login

Date of last login.

Change Password

Changes password. After the prompt a [New Password](#) dialog appears. Here you may enter a new password.

Certificate

Sets a certificate which will be available as a default option while using the electronic signature - the *Sign* function in the [Chromatogram](#) window. If certificate is not selected, the *No certificates assigned to the selected user* note is shown.

Note: More information on working with certificates and electronic signatures can be found in manual *M132 Clarity in Regulated Environment*, chapter 3.9 Electronic Signatures, accessible on *DataApex website* in the *Documentation - Manuals* section of the *Download* page.

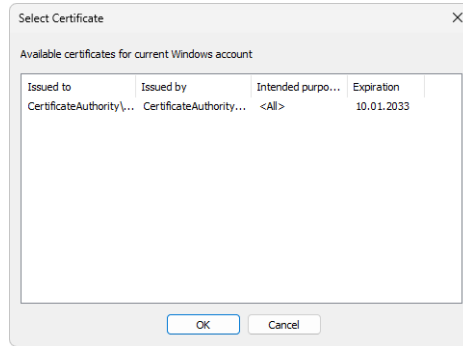


Fig. 5: Select Certificate

Select Certificate

In the *Select Certificate* dialog one of the certificates installed on computer can be selected.

Clear Certificate

Cancels the assigned certificate.

Certificate For Exporting To PDF

Invokes the *Open* dialog for selecting the PKCS#12 private key. Documents exported from **Clarity** are then signed automatically with this certificate.

Note: DataApex does not issue certificates nor can mediate their purchase. Certificates are issued by independent companies (for example Thawte or Verisign), list of other companies issuing certificates can be found *online* (accessed on 2nd August 2017).

1.1.2 User Details

In the *User Details* dialog (accessible from [Clarity](#) window using the *System* menu) can users without the authorization to enter the [User Accounts](#) dialog view their own user account settings and enter or edit the password to their own account. Here they may also select a certificate for digital signing.

Note: If there are no users defined, the *User Details* command will not be accessible.

The description of individual fields of this dialog is identical to the corresponding fields in the [User Accounts](#) dialog

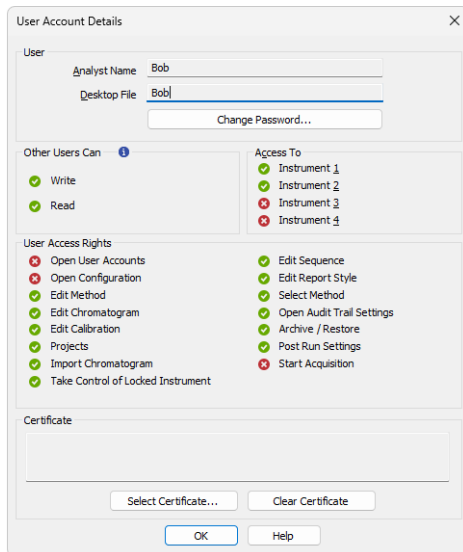



Fig. 6: User Account Details

1.1.3 Configuration

Serves for the setting of the station's configuration, which is saved in CLARITY.CFG file.

After prompting the *System - Configuration...* command or pressing the  icon, the *System Configuration* dialog will be opened. Access to the *System Configuration* dialog is permitted only to users with adequate access rights settings. Access is also denied if any of the **Clarity Instruments** is not closed (you will be prompted to close opened [Instruments](#)).

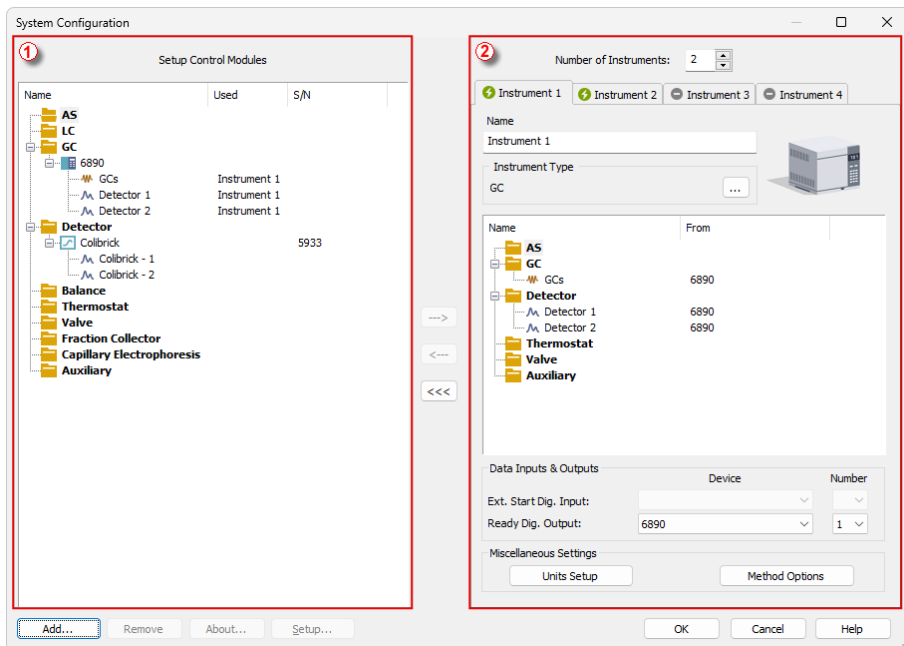


Fig. 7: System Configuration

The left section of the dialog ① is used to configure equipment in the **Clarity** station, while the right section ② is where the equipment is allocated to individual Instruments.

Note: Step by step procedure of configuration is described in **Clarity Getting Started** manual. The configuration of individual Control modules can be found in corresponding **Clarity Control** manual.

1.1.3.1 Left section of the System Configuration dialog

Setup Control Modules

Lists the configured equipment (e.g. internal or external A/D converters for data acquisition, directly controlled chromatographs, autosamplers, LC pumps, etc.).

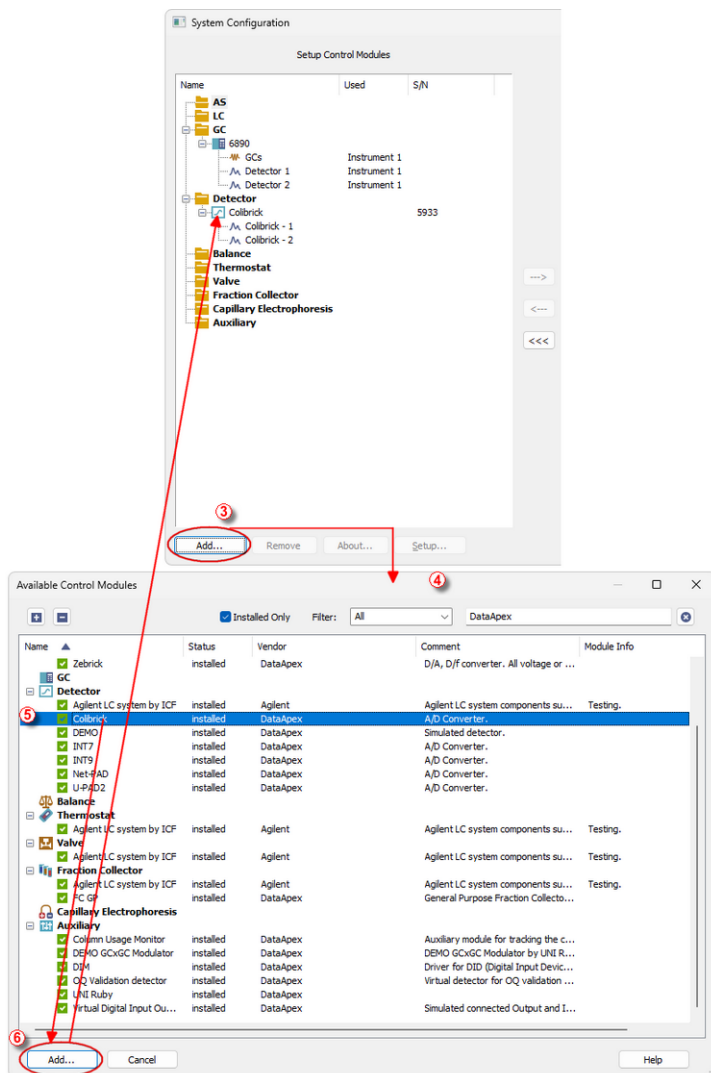


Fig. 8: System Configuration - left part and Available Control Modules dialogs

Add ③

Adds and configures drivers for any available equipment. After prompting, the *Available Control Modules* dialog ④ will appear with a list of all available drivers for data acquisition and chromatographic equipment control (for more details see the chapter **Available Control Modules** on pg. 14).

Note: If you wish to use one control module for two various Instruments, you have to add it to the **Clarity** station twice.

Select the required item (name of the driver) ⑤. By clicking the *Add* ⑥ button or double clicking on the item you can add the selected driver to the *Setup Control Modules* list. *X Driver Setup* dialog (where X stands for the device name) will appear, enabling you to fill in the exact configuration of the device (for more details see the chapter **A/D Converter Setup** on pg. 17).

Note: Drivers correspond to CSW???.DLL files, which are present in the station's main station directory. The physical presence of these files in the directory is not sufficient. Files must be "registered", which is done automatically by the installation program. Files both registered and present can be checked in the station's main window using *Help - About* command. The list can be found on the *System Files* tab. Reinstalling the station easily resolves all file registration problems.

Remove

Removes the selected configured equipment from the **Clarity** station.

About

Displays the information regarding the selected equipment's driver.

Setup

Sets driver parameters for selected equipment in *X Driver Setup* dialog, where X is the equipment name, e.g. INT7, U-PAD, HP6890, etc.

Note: The *X Driver Setup* dialog can be also called up by double clicking on the name or icon of the device and is automatically displayed while adding the device to the **Clarity** station.

1.1.3.2 Available Control Modules

The *Available Control Modules* dialog allows to add the particular control module driver into the [System Configuration](#) dialog. Try to search the driver by its name using the *Filter* function or select it manually in the list of the devices section.

Note: OEM versions of various instruments can be usually set both under their original name or the OEM names.

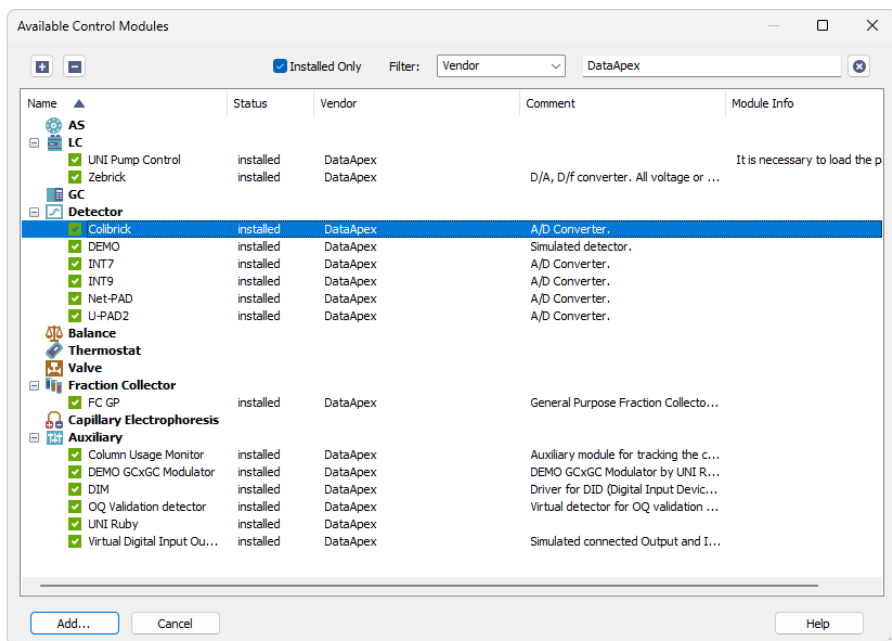


Fig. 9: Available Control Modules

+ / - Buttons

Click the button to unfold all sections in the *Available Control Modules* dialog or click the button to fold all sections.

Installed Only

Serves for the simplification of the driver selection. When checked there are listed installed control modules only.

Filter

Serves for the simplification of the driver selection. Simply enter any text string in the second field to search all columns for this string, or restrict the search to any desired column by selecting the column name from the drop down list in the *Filter* field. The **Fig. 9** on pg. 14. shows all drivers containing the "DataApex" keyword filtered.

Add

Opens the setup dialog for the device selected in the list of the drivers (as the Colibrick is in the **Fig. 9** on pg. **14.**). After selecting the desired driver and clicking this button the setup dialog for the driver is displayed (for more details see the manual of the appropriate control module or hardware). When correctly configured, the driver is added to the [left section of the Configuration Dialog](#) and the *Available Control Modules* dialog is closed.

Cancel

Exits the dialog without any action taken.

List of the drivers:

The content of the driver's list section is dependent on the *Filter* used. All available drivers are displayed only in case no filter has been used. In order to sort (either in the ascending or descending order) the listed drivers, simply click on the name of the column according to which you want to sort; to sort in the other direction simply click the column name again. Small arrow in the respective column indicates the sort order.

Name

Contains the names of the drivers grouped in sections, sorted alphabetically (see the small arrow next to the *Name*).

Status

Informs the user if the control module is installed on the system or not. In the list you can see all the control modules and hardware which are controlled by **Clarity**. In typical **Clarity** Installation, not all drivers are installed on the system. By clicking on the *Add...* button an information how to install the driver will be displayed.

Vendor

Holds the information on the device vendor.

Comment

This column may hold some other type of driver description (e.g. for what sub-versions of instruments is the driver suitable and so on).

Module Info

Contains the information on the control module state (e.g. whether it is an Alpha or Beta version) and the author of the device driver. Items with the Module Info column empty are both in the Release version (had been thoroughly tested) and have been developed by the **DataApex** company.

1.1.3.2.1 Control Module Is Not Installed

This dialog is displayed in case you tried to add a control module to [System Configuration](#) which is not installed in **Clarity** yet. You can find here an information how to install the module. Mostly it is necessary to reinstall **Clarity** and select the *Full* installation or select the specific module to install. In other cases, you must contact the control module vendor to obtain it, etc.

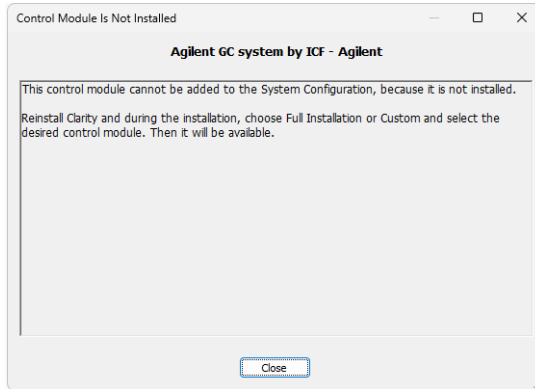


Fig. 10: Control module is not installed dialog

1.1.3.3 A/D Converter Setup

Signal Names and *Units* are stored for individual signals according to the configuration of the detector. For **DataApex A/D Converters** the signal units can be configured in the *Setup* dialog accessible from [System Configuration](#) dialog.

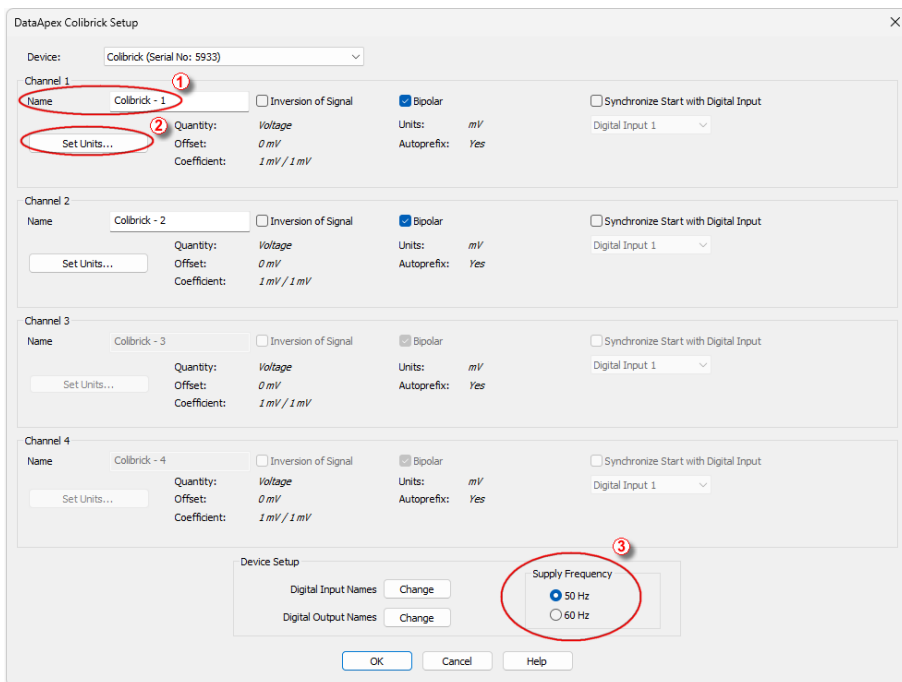


Fig. 11: DataApex A/D Converter Setup dialog

For each channel provided by the A/D Converter, the name of the signal can be edited in the Name ① field of the corresponding *X Device Setup* dialog (where X is the name of the device). The Set Units... ② button can be used to change other signal parameters.

Note: In *X Device Setup* dialog of some **DataApex A/D Converter** types, desired **Supply Frequency** ③ can also be selected.

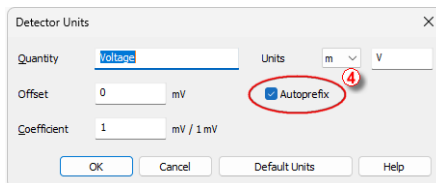



Fig. 12: Detector Units

When the unit prefix in *Graph* window should be adjusted automatically, enter the units and prefix separately and check the *Autoprefix*  box. In tables, the units with the prefix entered will be used.

1.1.3.4 Right section of System Configuration dialog

Sets the number of displayed Instruments and allocates equipment to the relevant Instruments.

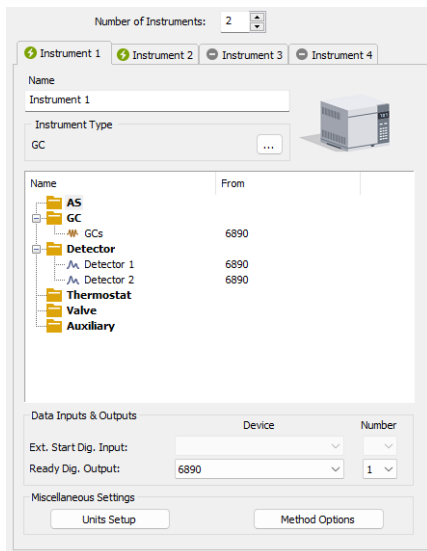







Fig. 13: System Configuration - right section

Allocate the configured equipment (displayed on *Setup Control Modules* pane in the left section) to the relevant Instrument (in the right section) by “drag and drop” with the mouse or using the following buttons located in the center of the window:

Button	Description
	Allocates selected equipment to an active Instrument.
	Removes selected equipment from an active Instrument.
	Removes all equipment from an active Instrument.

Number of Instruments

Provides the possibility to set the number of displayed Instruments. 1 to 4 Instruments can be displayed at a time, but you are only allowed to measure with as many Instruments as you have purchased (these are so called “online Instruments”). However, you can display more Instruments and use them for “offline” preparation of sequences and evaluation of chromatograms. Online Instruments have  icon in their tab header, while offline ones have  icon. The tab(s) of any offline Instrument(s) will have the “Offline” inscription on them.

In the following image there are three Instruments set for display. The first two are online and the third is offline.

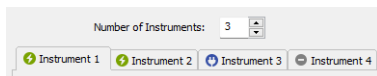




Fig. 14: Tabs of individual Instruments


Tabs of Instruments 1 - 4

Tabs of individual Instruments. You can enter an Instrument name and Instrument type on each tab and connect drivers which will enable the measuring of a signal and directly control the chromatograph and other devices.

Tabs are indicated in the header with icons:

 icon indicates an online Instrument, which is usable for the data acquisition (as well as to evaluate chromatograms, prepare methods, etc.).

 icon indicates an offline Instrument, which cannot be used to acquire data, but can be used to prepare sequences or evaluate already measured chromatograms.

 icon indicates an Instrument that has been switched-off. The corresponding chromatograph symbol is not displayed in the main [Clarity](#) window.

Note: The tab of a switched-off Instrument is accessible only to allow for the removal of modules previously installed on it.

Name

Holds any arbitrary Instrument description and will be displayed in the main [Clarity](#) window above the picture of the chromatograph.

Instrument Type

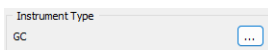




Fig. 15: GC Instrument Type

Use the  button to select type of analysis that will be performed on this **Clarity** Instrument. In addition to standard GC and LC types, optional **Clarity Extensions** provide additional Instrument Types (CE, GPC, EA, GC-GC and appropriate combinations with MS, MS-ToF, DHA, NGA and PDA).

Left mouse click on the  button invokes the *Instrument Type Setting* dialog where the user can select a combination of instruments.

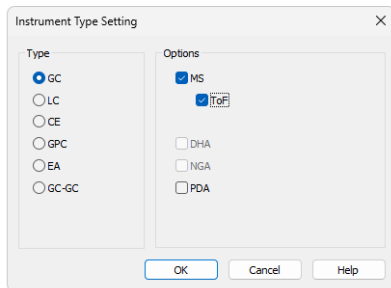


Fig. 16: Instrument Type Setting dialog

For convenience the selected combination is displayed in the **Instrument Type** section.

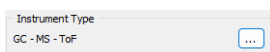


Fig. 17: GC-MS-TOF Instrument Type


Note: Description of these Instrument types can be found in separate **Clarity Extensions** manuals.

Depending on the selected Instrument Type, the station's main window displays an implicit symbol of a LC or GC chromatograph (if you have not set your own image) and the **List of Equipment** connected to the Instrument (see below) displays only the sections relevant to selected **Instrument Type**.

Name

Holds any arbitrary Instrument description and will be displayed in the main [Clarity](#) window above the picture of the chromatograph.

Instrument Image Setup

Apart from default pictures of Instruments, it is possible to insert a custom picture. Click the picture of the chromatograph to open *Instrument Image Setup* dialog. To load a custom picture check the *Custom Image* checkbox and using the  button you can browse for your own image.

Custom Image checkbox can be used to permit or forbid use of a user's image.

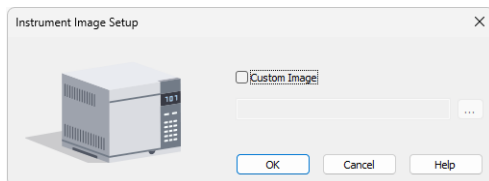


Fig. 18: Instrument Image Setup dialog


To select other than default image, *Custom Image* checkbox has to be checked. At that moment the  button can be used to select an image file. There is only one

image file for both the closed and opened Instrument image, the difference is provided by color overlay (closed image is darker). It is recommended to use preferably *.PNG or *.JPG image files.

If the custom image is not available, the preview will display a symbol of missing bitmap and in the main [Clarity](#) window the default image will be used.

List of the Equipment Connected to the Instrument

Name	From
AS	
Sampler 1	Alias
GC	
GCs	6890
Detector	
Detector 1	6890
Detector 2	6890
Thermostat	
Valve	
Auxiliary	

Fig. 19: List of equipment connected to an Instrument

Detectors

List of data sources for the **Clarity** station.

GC/LC

Sets direct control of the used chromatograph, detector or pump.

AS

Sets direct control of the used autosampler.

Note: Other categories may appear, including Valves, Fraction Collectors, Thermostats and other miscellaneous directly controlled equipment.

Setting of digital inputs/outputs for external Start/Stop:

Data Inputs & Outputs	Device	Number
Ext. Start Dig. Input:	Colbrick	1
Ready Dig. Output:	Colbrick	1

Fig. 20: Digital Outputs for external Start/Stop

The START synchronization between Clarity and the autosampler (eventually other devices such as Detectors, LC Pumps, etc.) is governed via cable pins for inputs and outputs (A/D Converter) or by serial port communication. The most common connections are described in **Getting Started** manual in the chapter "Connecting Autosamplers (AS)"

External Start Digital Input is assigned to the device and its specific pin that gives Clarity information about injection being performed. Subsequently Clarity starts Data Acquisition.

Ready Digital Output defines the device and its specific pin through which Clarity informs other parts of the system that sequence can be run.

If you are measuring on multiple instruments using a single A/D converter, each independent instrument must have separate *Ext. Start Dig. Input* and *Ready Dig. Output* pins configured.

If you have more than one A/D converter installed, in the *Device* combobox you can choose the one, whose digital inputs/ outputs you want to use. In the *Number* field of the *Ext. Start Dig. Input* line you can define which digital input the selected Instrument will use to start or stop the measuring. Similarly, it can be set which digital output the selected Instrument will use to permit sampling in an active sequence in the *Number* field of the *Ready Dig. Output* line. The option "--" (*None*) is enabled for selected devices. It can be used in the case when the START synchronization is ensured by other means (e.g. with directly controlled autosamplers over digital line).

In case no A/D converter is used and the devices are not offering digital inputs and outputs, it is suggested to use the DataApex Virtual Digital Input Output Loop (auxiliary device, requires A24 LC or A23 GC Control license) to simulate inputs/ outputs needed.

Miscellaneous Settings

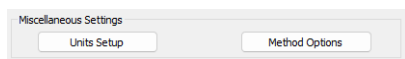


Fig. 21: Miscellaneous Settings

Units Setup

Units Setup button invokes the *Units Setup* dialog for respective instrument. Instrument 1 to 4 can each have set a different units and thus allowing a large variability.

See [Units Setup](#) for further instructions.

Method Options

Method Options button invokes the *Method Sending Options* dialog.

This setting is individual for each **Clarity** Instrument.

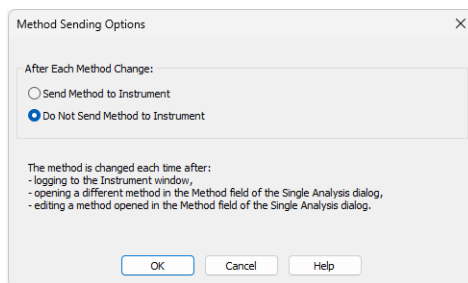


Fig. 22: Instrument Method Sending

This dialog sets whether the LC/GC/AS method has to be sent to the instrument (device) at each change of the *Single Analysis* method.

Note: Method Options button is not accessible for instruments with modules that send method automatically every time when is changed. Such modules are A/D converters Colibrick, INT7, INT9 or DEMO detector.

After Each Method Change in the Single Analysis dialog

Method changes by:

- Opening the [Instrument](#) window which automatically loads last used method from the given project.
- Changing the currently opened method in the *Single Analysis* dialog.
- Modifying method that is opened in the *Method* field of the *Single Analysis* dialog.

There are two possible regimes available:

Send Method to Instrument - **Clarity** will send the LC/GC/AS method to the instrument (device) automatically without prompt.

Do Not Send Method to Instrument - **Clarity** will **not** send LC/GC/AS method to instrument (device) each time a change occurs. Prior to running analysis, method must be sent manually.

Regardless of the setting, the LC/GC/AS method will be sent:

- From the running **Active Sequence** according to the **Sequence Table**.
- Manually using the **Send Method** button from the [Single Analysis](#) dialog and [Device Monitor](#).

Caution: Be aware that once a method is sent to the instrument, it can clear error that should stop the system (typically for LC system errors like overpressure or leak). When the method is sent to the Instrument without fixing of the error's cause it may cause the system run again. At the end the system could run and leak (for example) for very long time without anyone noticing the spilling. Therefore option *Send Method to Instrument* is not recommended for LC systems.

1.1.4 Units Setup

Instrument units are set globally from this window only and affect gradient table, tabs of auxiliary pumps, monitors of auxiliary pumps, device monitor and tabs of other controlled devices in *Method Setup* and [Chromatogram](#) windows.

Basic Units and *Auxiliary Signal Units* can be set from the predefined. In case of the *X-Axis Units*, *Custom Units* are a possible choice.

Note: *Custom Units* may result in incorrect calculations, since there is not a conversion table specified. Recommended for advanced users only.

Instrument 1 - Units

Basic Units

Units

Flow Rate Units: mL/min

Pressure Units: MPa

Temperature Units: °C

Injection Volume Units: µL

Auxiliary Signal Units

Units

Voltage Units: V

Power Units: W

Current Units: mA

X-Axis Units

Title	Units	Custom Units
Time	Time - minutes	

Replace Retention Time with: Retention Time

Replace Start Time with: Start Time

Replace End Time with: End Time

Display Area in: Time - seconds

Display W05 in: Time - minutes

Display Drift in: Time - hours

OK Cancel Default Help

Fig. 23: Instrument Units dialog

Basic Units

Flow Rate Units

Sets *Flow Rate* units - default unit is mL/min.

Pressure Units

Sets *Pressure* units - default unit is MPa.

Temperature Units

Sets *Temperature* units - default unit is degrees Celsius.

Injection Volume Units

Sets *Injection Volume* units - default unit is µL.

Auxiliary Signal Units

Set units for auxiliary devices.

Voltage Units

Sets the *Voltage* units - default unit is V.

Power Units

Sets the *Power* units - default units is W.

Current Units

Sets the *Current* units - default unit is mA.

X-Axis Units

Allows to set a different unit on the X-Axis than the default unit which is *Time* in minutes. *Title* can be changed to a custom value as well as the units. Once *Custom* unit is chosen *Retention Time*, *Start Time* and *End Time* columns of the *Result Table* can be renamed to a user defined value. *Area*, *W05* and *Drift* columns of the *Result Table* will be displayed in *Custom* defined units.

Default

Upon clicking the *Default* button all units will be changed to the default units specified above.

Cancel

Cancels all changes made to the instrument units.

Note: Chromatograms measured with custom defined units and then opened on Instrument with a default units set, will always display units according to the settings of the instrument.


Restrictions of the X-Axis Units:

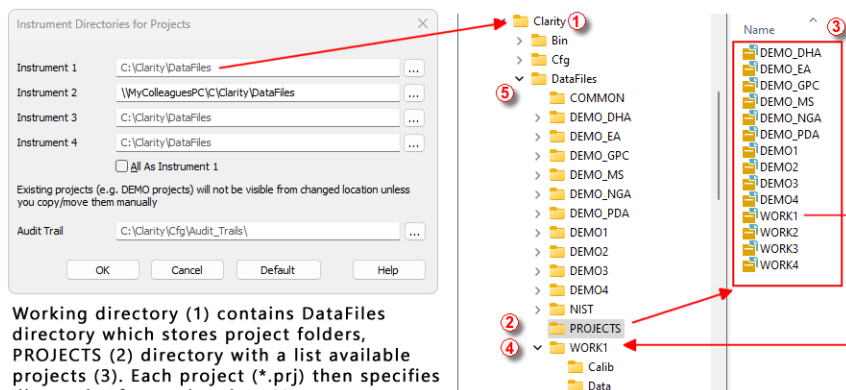
- *X-Axis Units* section is disabled (grayed out) for the following instrument types: LC-MS, GC-MS, GC-MS-ToF, GC-MS-PDA, DHA, NGA, GPC, GPC-PDA, EA and GCxGC.
- Further settings of the *X-Axis Units* section apart from *Custom* option is allowed for CE and CE-PDA instrument types.
- Full customization of *X-Axis Units* is allowed for LC, GC, LC-PDA and GC-PDA instrument types.

1.1.5 Directories

Clarity installation folder contains 4 directories:

- BIN - directory storing supporting *.DLL files and other programs necessary for correct functionality.
- CFG - directory storing configuration files, such as *.CFG, *.DSK, *.INI, *.PSW and *.SNO file. It also contains AUDIT_TRAILS directory for storing daily logs, BACK, BUG_REPORTS, DEBUG_LOGS and IMAGES directories.
- DATAFILES - directory storing project folders, PROJECTS directory and COMMON directory. All your measured data will be stored here by default.
- DOCUMENTATION - directory storing documentation such as manuals and datasheets (all in PDF form) as well as WHATSNEW.TXT and ABOUT.TXT files.

Sets the working directory ① that contains C:\CLARITY\DATAFILES\PROJECTS subdirectory ② with the list of available projects ③. Each project specifies the subdirectory for saving data by its name ④. A working directory is the directory where existing projects are sought and new projects established; it can be set independently for each Instrument. The *Directories...* command or the  icon opens *Instrument Directories for Projects* dialog containing four **Instrument 1** to **Instrument 4** fields.



Working directory (1) contains DataFiles directory which stores project folders, PROJECTS (2) directory with a list available projects (3). Each project (*.prj) then specifies directories for storing data (4). All projects from the same working directory share report styles stored in the COMMON (5) directory.

Fig. 24: Instrument Directories

Note: In the above image the **Instrument 2** shares projects with another **Clarity** station that has been installed on a networked computer named **MyColleaguesPC**.

Each field specifies the working directory for the corresponding Instrument. Field left blank is pre-filled with the working directories set during **Clarity** installation (C:\CLARITY\DATAFILES by default). The *Default* button restores the default

directory for Audit Trails (...Bin\Audit_Trails\)) and the working directories for all the instruments according to directory set as Data Location during **Clarity** installation.

Use the button to find the required directory. The *All As Instrument 1* checkbox sets a single directory for all Instruments.

Note: When defining a new directory, user is asked whether he wants to create the directory (two directories with identical name cannot exist) or whether he wants to create the COMMON sub-directory too and fill it with the default files.

Note: The Directory name cannot contain following characters / : * ? " < > | and also cannot end with a space or a dot.

The *Audit Trail* field specifies the directory to which the files with all logged activities of the station are stored. If the cell is left blank, the log files will be stored by default in the AUDIT_TRAILS subdirectory in the installation folder (C:\CLARITY\CFG by default).

Pre-set directories are stored in the CLARITY.CFG configuration file, thus being common for all users, even in the protected mode.

Opening of a project on [Instrument](#) is described in the chapter "**Project**" on pg. 71.

In case there is an error during opening a project, [Error Opening Project](#) dialog is displayed.

Caution: If you reinstall or update **Clarity** station, you should consider that the installer updates files in the COMMON directory located in the **Clarity** installation directory only. It is necessary to update the content of COMMON directories in your custom project directories manually.

1.1.6 Clarity2Go Configuration

Allows you to set the communication with the **Clarity2Go** server.

Clarity2Go is a tool for remote monitoring of state of **Clarity Instrument**. It consists of three independent parts: **Clarity** station sending the information to the server, server dispatching the information, and client on the target device (smartphone, tablet or PC) receiving the information. The client application is currently available for smartphones with iOS and older versions of Android OS and can be downloaded free of charge on Google Play or App Store (named **Clarity2Go**).

Note: Application might not be available from Google Play on devices with the latest versions of Android OS while using Google account that has not used Clarity2Go previously. The application could still be installed directly using the apk, it can be provided by DataApex upon request, if you are interested, please contact support@dataapex.com.

DataApex is providing public server for this use on following address: <http://clarity2go.dataapex.com:80/>

How to set it up:

- Check the checkbox of **Instrument 1..4** you want to monitor. After successful registration every checked Instrument will get its unique *ID*, displayed right to the name of the *Instrument*.
- Enter this *ID* into **Clarity2Go** client on your smartphone to access it for monitoring.

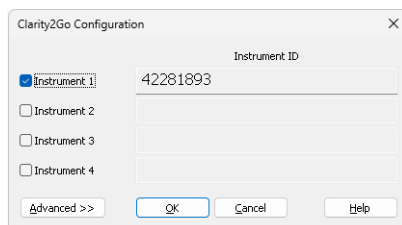


Fig. 25: Clarity2Go Configuration dialog

Instrument 1..4

Turns On/Off the sending of the status of particular Instrument. When Instrument is not registered, checking this checkbox will connect Clarity2Go server and register the Instrument.

Advanced/Basic

Show/Hide advanced settings, which has no use for most users.

Close

Close the *Clarity2Go Configuration* window.

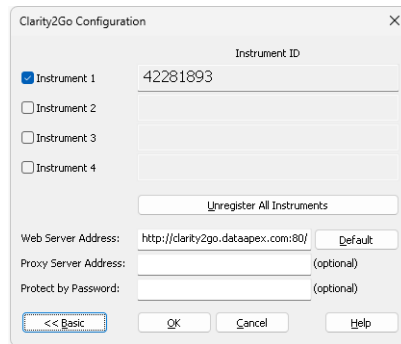


Fig. 26: Clarity2Go Configuration - Advanced dialog

Unregister all instruments

Unregister all registered Instruments on **Clarity2Go** server.

Web server address

Set the address of **Clarity2Go** server.

Default

Set the default address of **Clarity2Go** server.

Proxy server address

When proxy server is used for connecting the Internet, set its address.

Protect by Password

By entering a password here, protection is enabled and the same password needs to be filled in on a mobile client.

1.1.7 GLP Options

This dialog is used to set the global regulated-environment connected options. After prompting the *System - GLP Options...* command, the user is asked to enter the password for the **Clarity** station. Only users allowed to modify the User Accounts (for more details see the chapter **User Accounts** on pg. 4). are allowed to enter this dialog. All changes performed in this dialog are logged into the station audit trail.

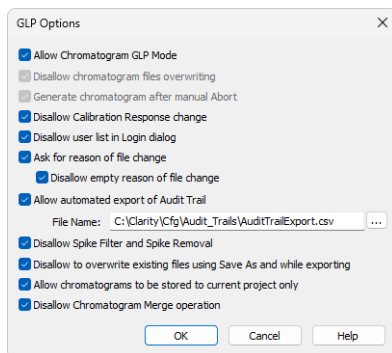


Fig. 27: GLP Options dialog

Allow Chromatogram GLP Mode

This checkbox ensures that settings preventing the possibility of losing the data from chromatograms are correctly set. If checked, both the *Disallow Chromatogram Files Overwriting* and *Generate Chromatogram After Abort* checkboxes will be checked. Chromatograms acquired by an Unauthorized Control Module or by a Development version of Control Module, will contain record in the *Chromatogram Audit Trail* about the fact that they were acquired by such a device in order to comply with GLP.

Note: If you open a chromatogram created in *GLP Mode* in [Clarity](#) without enabled *GLP Mode*, it will be always opened as read-only.

Disallow chromatogram files overwriting

This checkbox cancels the possibility to overwrite the chromatogram if a file with the same name already exists in the selected directory. The behavior differs according to the action that should cause the chromatogram to be overwritten - when it is a user action (using the *Save As* command for example), the user will be prompted to change the file name to any still unused file name. If the overwriting should be caused by the **Clarity** data acquisition (e.g. creating new chromatograms caused by **Single Analysis** or **Sequence** measurement), a unique 4- to 6- digit number is added at the end of the original filename. In the improbable case that all of these combinations are already taken, the **Clarity** will ask the user to change the file name personally so it is unique.

Generate chromatogram after manual Abort

This feature will cause the generation of the chromatogram in case the analysis is aborted manually by user.

Note: If the analysis is aborted by an error, [Chromatogram](#) is always generated, regardless the checkbox settings.

Disallow Calibration Response change

When checked, the manual change of the response in the [Calibration](#) window is disabled.

Note: The manual change, if allowed, is still marked in the [Calibration Audit Trail](#), but it breaks the link between the calibration standard and the calibration itself and is not recognizable in the chromatogram linked to the calibration file.

Disallow user list in Login dialog

This checkbox disables the display of all available **User Names** in the [Login](#) dialog. The user is then required to enter two unique identification components to successfully log in.

Ask for reason of file change

The *Ask for Reason of File Change* checkbox sets the possibility to fill in the reason for a change. When saving a chromatogram, method, sequence, calibration or GPC calibration file, the *Reason for Chromatogram (Method, Sequence, ...) Change* dialog will appear. The user can (but is not obliged to) fill in the reason for the change.

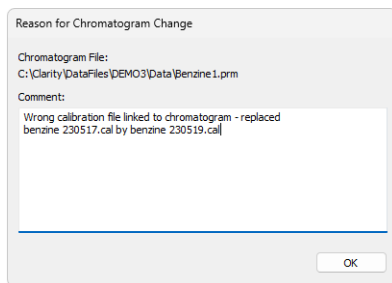


Fig. 28: Reason for Chromatogram Change

Note: The reasons of changes are displayed in the **Audit Trails**, separated by a dash from the „file has been saved“ event.

Disallow empty reason of file change

By checking this checkbox the user becomes obliged to fill in the reason of the change. No empty reason field nor reasons solely composed from spaces are now allowed.

Allow automated export of Audit Trail

By checking this checkbox the station audit trail file will be automatically exported to the file and location specified in the *File Name* field. To set the appropriate location,

use the  button to browse to the desired directory.

Changes to this export file will be made continuously and the exported file will be marked as read-only for as long as the **Clarity** is opened.

Disallow Spike Filter and Spike Removal

By checking this checkbox the *Spike Filter* and *Spike Removal* functions from the [Chromatogram](#) window will be disabled. These are potentially dangerous operations to work with in respect to the GLP practice. The operations are only available in **Clarity** version 4.0 or higher.

Disallow to overwrite existing files using Save As and while exporting

By checking this checkbox users are prohibited to overwrite any existing file. This feature applies to any file (method, calibration, chromatogram, etc.) created by **Clarity**, as well as exporting a file over an existing one - the user must save it under a different filename. Exporting in form of appending to the existing file is still allowed.

Allow chromatograms to be stored to current project only

Option *Allow Chromatograms to Be Stored to Current Project Only* allows storing any newly generated chromatogram within one of working directories (typically *Data* or *Calib*) of current project only.

This feature disables:

- storing any newly generated chromatogram outside of working subfolders (typically *Data* or *Calib*) of current *Project*,
- storing any newly generated chromatogram directly into root of current *Project*,
- automated creating of new subfolders directly in root of current *Project*.

This feature is intended as support of data integrity because it will disallow creating data in destinations where might not be applied measures against uncontrolled data deletion or alteration.

During defining destination for newly generated chromatogram **Clarity** essentially constantly evaluates user's input where to store new chromatogram and provides feedback to user. The feedback provided to user in *Single Analysis* is done through the text above *Chromatogram File Name* field. When given destination is allowed it is in standard black color, if it is prohibited it is displayed in red.

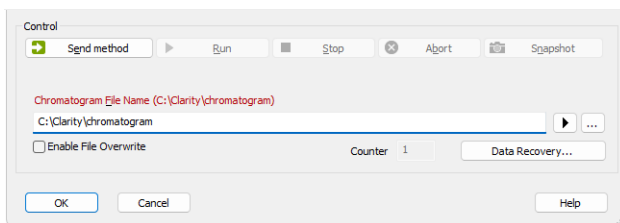


Fig. 29: Single Analysis - Allow Chromatograms to Be Stored to Current Project Only - Prohibited Destination

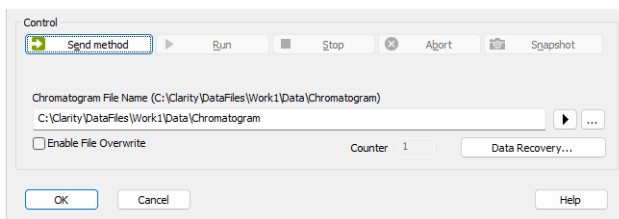


Fig. 30: Single Analysis - Allow Chromatograms to Be Stored to Current Project Only - Allowed Destination

When user tries to start analysis with prohibited destination defined, **Clarity** will deny to start analysis and will display related error message. The user has to adjust currently defined destination to allowed one in order to run measurement in **Clarity**.

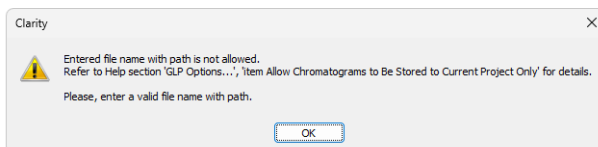



Fig. 31: Single Analysis - Allow Chromatograms to Be Stored to Current Project Only - Prohibited Destination - Error Message

The feedback provided to user in **Sequence** about prohibited destination is done through  indication in the **Status** column for incorrect input. If currently defined location for new chromatogram directs outside allowed destination in current project **Clarity** will prevent user from triggering any new analysis and will display respective error message. This event will be also recorded in **Audit Trail**.

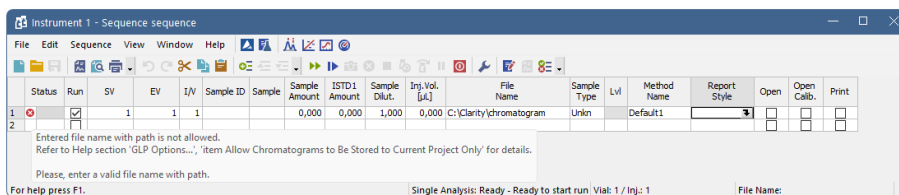


Fig. 32: Sequence - Allow Chromatograms to Be Stored to Current Project Only - Prohibited Destination

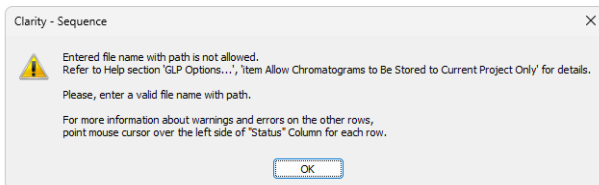


Fig. 33: Sequence - Allow Chromatograms to Be Stored to Current Project Only - Prohibited Destination - Error Message

Following image provides review what are allowed destinations and what is prohibited destination within current project folder.

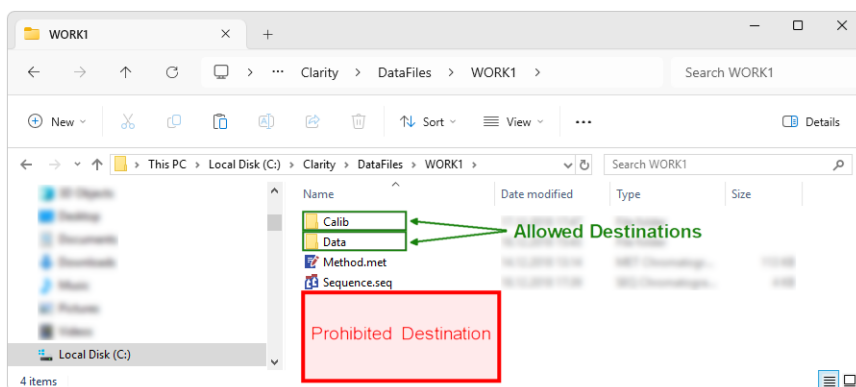


Fig. 34: Allow Chromatograms to Be Stored to Current Project Only - Destinations

In case of unexpected external start of analysis when there is incorrect location defined **Clarity** will apply internal fallback mechanisms and will try to store new chromatogram within subfolder (i.e. *Data* or *Calib*) of current project. This exceptional case will be specifically recorded in *Audit Trail* as well.

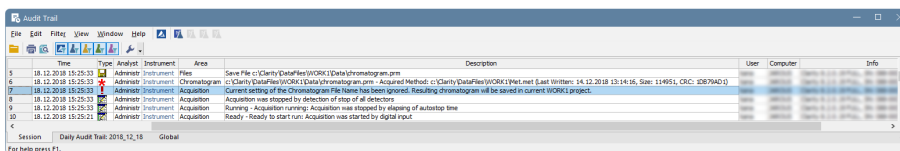


Fig. 35: Audit Trail - Allow Chromatograms to Be Stored to Current Project Only - Fallback Mechanism

The option *Allow Chromatograms to Be Stored to Current Project Only* should also be used if it is planned to transfer given [Project](#) among various computers. This option will ensure that all related files are stored in the project folder, meaning that no data will be lost during the transfer.


If the option *Allow Chromatograms to Be Stored to Current Project Only* is not used, it is possible to define basically any (local or networked) location for a newly

generated chromatogram. However, sticking to the Clarity project structure and avoiding using absolute paths for storing chromatograms is recommended. If it is still desired to save a new chromatogram to a specific location, keep in mind that Clarity (and Windows user) needs write access to the location. Typical examples of problematic destinations are root folder of the system hard drive (e.g., C:\) or root folder of server (e.g., \\server\).

Disallow Chromatogram Merge operation

By checking this checkbox users are prohibited to use "Merge" on page 274 operation.

1.1.8 Digital Outputs

This dialog, accessed through the *System - Digital Outputs...* command or by  icon, is used to control the digital outputs of the installed A/D boards. These TTL outputs can control, via the **Event Table** (for more details see the chapter **Event Table** on pg. 85), the external measuring devices during the analysis. The command enables one to set up the initial and current state of these outputs by means of the displayed *Digital Output Control* dialog. Any changes performed in the dialog will be saved at the moment of the dialog closing.

Note: If more than one board has been installed, the [Select Control](#) dialog containing a list of all boards will open first. If a converter has not been installed or is not functional, the *Digital Outputs...* command will not be active (dimmed).

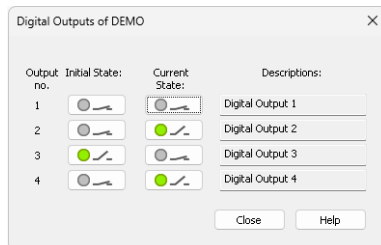


Fig. 36: Digital Output Control

Output no.

Lists the numbers of individual outputs.

Initial State

Selects the **Initial** status of the digital output when the station starts. The status is indicated in two halves: first shows the digital output (*Output*) and second its usability as a relay (*Relay*). Where no relay contact can be used, only the state of the output is shown.

Current State

Displays and enables modification of the current status of outputs. The status is indicated in two halves: first shows the digital output (*Output*) and second its usability as a relay (*Relay*). Where no relay contact can be used, only the state of the output is shown.

Change in these columns takes effect immediately. To change the status click the corresponding field with the inscription *HIGH* or *LOW* indicating the output value. The output status is also indicated by color, where gray corresponds to logical zero (*LOW*) and green to logical one (*HIGH*).

Descriptions

Outline description indicating the meaning of individual outputs. The names of individual digital outputs can be edited in the [System Configuration](#) dialog for the actual device providing the outputs.

Note: It is not possible to access the *Digital Outputs* dialog of the device that is configured solely on the Instrument you do not have the access to. The access to particular Instruments for different users may be set in the [User Accounts](#) dialog.

Note: Access to the *Digital Outputs* dialog can be controlled through the [User Accounts](#) dialog by checking or unchecking of **Open Configuration** item in the *User Access Rights* section.

1.1.8.1 Select Control

If more than one board is installed the *Select Control* dialog containing a list of all boards opens first.

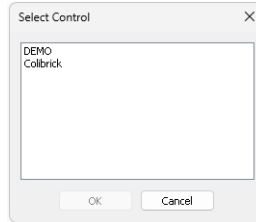


Fig. 37: Select Control

Note: If a converter has not been installed or is not functional, the [Digital Outputs](#) command will not be active (dimmed).

1.2 Login

Command for opening respective Instrument. Opened Instruments are checked.

The [Instrument](#) window can also be opened by clicking directly on the Instrument's picture in the main [Clarity](#) window or using a **Ctrl + 1** shortcut (2, 3, 4 for further Instruments).

If you have user account, the *Login Dialog* will be displayed after the prompt. Here you select your username from the drop-down list. Choose the user name and fill in the password to log to the **Clarity Instrument**. For heightened security, asterisks ("**") are displayed on your screen when entering a password instead of characters.

Note: After the password has been entered erroneously three times, it is necessary to restart the **Clarity** station.

If the station is in "not restricted" (no password) mode, and therefore no user account exists, the dialog for entering your name will be displayed. The entered name will be saved in all files which you create during your session. You can quickly change the current project or create a new project in *Select Project* combobox. Project offered by default is the last one used by selected user (as saved in user's desktop file) or the last one used in default desktop file (where no user's are created). In case Clarity's command line parameters are used, it is possible to choose project offered through these parameters, either by directly selecting appropriate project or by selecting user with particular project in his desktop file.

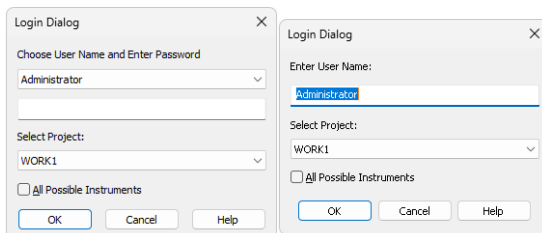


Fig. 38: Login dialog and Username dialog

All Possible Instruments

If you have checked *All Possible Instruments* box, then all available Instruments that you have access to will be opened.

Note: A modification of the *Login Dialog* also appears when configuring, setting user accounts or creating electronic signatures.

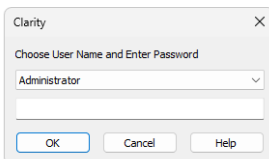


Fig. 39: Login dialog when opening System Configuration or User Accounts

Initial password

After receiving your username from the administrator and logging in to the station for the first time, you will receive a verification notice and be prompted to enter your password.

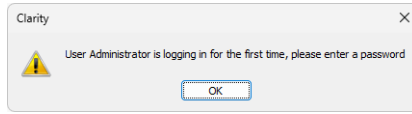


Fig. 40: Initial password warning

To prevent keying mistakes during the initial login process, you will be prompted to enter your password two times.

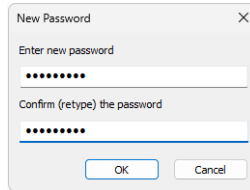


Fig. 41: New Password dialog

The administrator can set and control the conditions of a password, allowing for a minimum number of characters and/or the time limit of a password's validity. After a password expires, you will be prompted to enter a new password.

1.3 Logout

Command for closing respective Instrument. The names of Instruments that are already closed will be dimmed. The user will be notified of an analysis or sequence in process as well as of all modified files that have not yet been saved. Modifications not yet saved will always be marked after the filename by the MODIFIED inscription.

Close All Instruments

Closes all opened Instruments at once. Command is visible only when it is possible to close all instruments, i.e. all configured instruments are opened and none is locked.

1.4 Lock

Command for locking and unlocking of respective Instrument in the protected mode. This enables the user to prevent against unauthorized actions on the Instrument during user's absence. Locked Instruments are denoted with gray stripe and titled **Locked**. A name of the user who is logged on the locked instrument is displayed in the left bottom corner of the respective Instrument. Locking an Instrument affects neither the proceeding data acquisition nor a running sequence. An Instrument can be unlocked by entering the password of the user who has locked it.

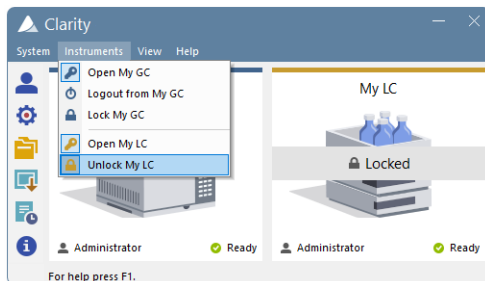


Fig. 42: Opened "My GC" and locked "My LC" Instruments

Note: If the Instrument has been locked by a user, it can be also unlocked by the **Clarity Administrator**. This action is recorded into the [Station Audit Trail](#) and the person that unlocked the locked Instrument becomes logged on this Instrument. The **Clarity Administrator** is any user with access to User Accounts dialog and the given Instrument (for more details see the chapter **User Accounts** on pg. 4).

1.5 View

This is a submenu for setting up the appearance of the main [Clarity](#) window. Similar ones can be found in all major **Clarity** windows.

Note: If the main [Clarity](#) window covers any of the dialogs, the workstation will look as if it has not reacted to any of your commands. In this case it is important to shift the main window aside and react to the covered dialog report.

Hide All Minimizes (hides) all open windows.

Show All Displays all open and minimized (hidden) windows.

Tablet Mode Switches Tablet Mode on/off. Tablet Mode represents a special windows layout in Clarity dedicated to simulate one window application. It is designed for devices with small tablet size monitor that enables their control. In default layout, Instrument window is narrower than in standard Clarity and is positioned to the upper left corner of the monitor, other windows are opened one over another and fill the remaining space on the monitor. All windows remain fully resizable and customizable. Default layout can be restored by reactivating the Tablet Mode. Tablet Mode allows use at higher general scales in Windows (up to 200 %) which improves handling of the software and parameters readability.

Tablet Mode is not accessible in Clarity Lite.

Toolbars Displays commands for toolbars.

- **Standard:** Hides/shows the standard toolbars.
- **Customize...:** Customization of items in the toolbars.
- **Reset All:** Sets all default toolbars and menus back to their initial state.

Note: *Reset All* does not display hidden toolbars. To show them invoke *Customize... - Toolbars* menu.

Note: In case you accidentally move the menu bar out of the screen, you can return it back by using the shortcut **Alt + V**.

1.5.1 Customize...

Customize... dialog is invoked either from the menu - *View - Toolbars - Customize...* or mouse-right click in the toolbar and select *Customize...*

It allows the customization of toolbars. It is possible to customize the content, position and define user specific toolbars.

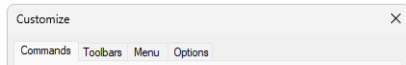


Fig. 43: Title bar of the Customize dialog

By default, toolbars are locked and cannot be customized. After invoking *Customize* dialog, small dots will appear in all the toolbars, meaning that toolbars are unlocked and in the editing mode and can be customized.



Fig. 44: Toolbar available for customization

1.5.1.1 Commands

The *Commands* tab enables the user to arrange, at will, available icons of individual toolbars. Available icons will be arranged in categories that roughly correspond to menu items. Add/remove an icon to/from the toolbar by dragging it with the mouse.

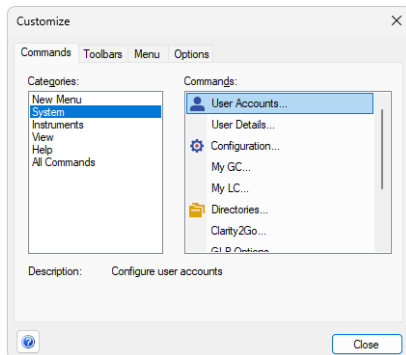


Fig. 45: Customize - Commands

Note: Toolbars are set separately for each window and for each user (except the main [Clarity](#) window). The set of available icons differs from window to window.

1.5.1.3 Menu

The *Menu* tab serves for the customization of menus.

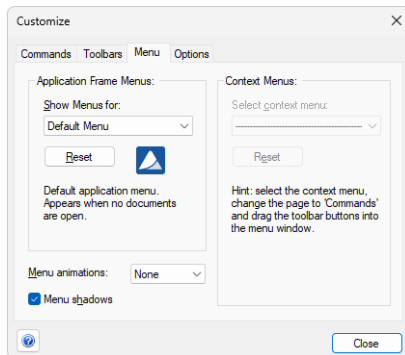


Fig. 48: Customize - Menu

- *Show Menus for* displays default menu.
- *Reset* command restores the original settings. Confirmation dialog appears once this command is invoked.
- *Menu animations* combobox offers selection of different styles of (un)foldering menus. Default setting is *None*.
- When *Menu shadows* checkbox is checked, menus will create shadows in the background.

1.5.1.4 Options

Options tab displays options for toolbars.

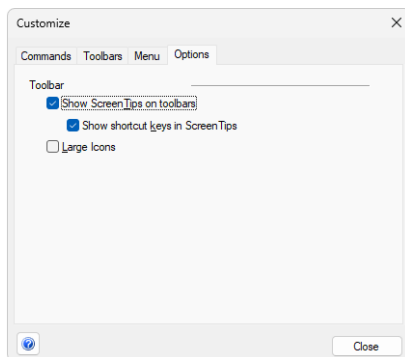


Fig. 49: Customize - Options

- When *Show Screen Tips on toolbars* checkbox is checked, help in the form of a tooltip will be displayed when mouse pointer is positioned over the icon in the toolbar.

- When *Show shortcut keys in Screen Tips* checkbox is checked, keyboard shortcuts will be displayed along with the screen tips in the tooltip - only if the shortcut exists.
- When *Large Icons* checkbox is checked, all icons found in Clarity will be by default larger (24x24 px instead of 16x16 px) - for better readability.

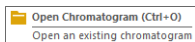


Fig. 50: Customize - Options - Screen Tip & Shortcut

1.6 Help

This is an entry point to a submenu of commands that displays fundamental information about the **Clarity** chromatographic station. An analogous menu is available in all basic station windows.

Help	Displays the introductory help item concerning the main Clarity window.
Register...	Allows to register your workstation online.
Check for Updates...	Automatically determines the presence of new versions of Clarity from the Internet.
Languages	Allows you to select the language. You will have to restart Clarity for the change to have an effect.
User Code...	Provides the possibility to enter a user code.
Trial Prolongation...	It opens a dialog that allows you to extend the trial period (available only in Clarity TRIAL).
Send Report by Email	Sends information regarding the state of Clarity to the DataApex user help.
Clarity Online	Invoking this command opens your default web browser and connects to the DataApex website. Your computer must be connected to the Internet to be able to do so.
TeamViewer QS	Invoking this command opens download link for TeamViewer QuickSupport utility in your default web browser. TeamViewer QS can be used for remote support by DataApex . Your computer must be connected to the Internet to be able to do so.
About...	Displays information about Clarity .

1.6.1 Register

Online registration of your **Clarity** station. Registration is voluntary and it automatically allows you to download updates from the **DataApex** website directly from the **Clarity** station environment using the *Check for Updates* function.

The selected username and password is also used to gain access to our protected website sections at www.dataapex.com, which are reserved for registered users only. If you have already registered on our website, simply log in with your username and password to add serial number into your existing user account in the *Clarity Registration* dialog.

In case your computer is not connected to Internet, after pressing *Register...* menu item an offline registration form will be opened. You have to fill it, print it and send it to us by mail.

The screenshot shows a web browser window with the URL <https://www.dataapex.com/registration.php?SN=011-10...>. The page content is as follows:

Software registration

SW registration enables features as **download** and **update** chromatography software.

Log in

Add serial number into your existing user account.

Username *

Password *

Must have 6 characters or more.

 [Reset password](#)

Don't have a user account yet?

Create a user account and register your chromatography software.

Fig. 51: Clarity Registration dialog

Continue

Sends the registration data to **DataApex** through the Internet. Your computer must be connected to the Internet in order to register successfully.

Note: The next screen allows you to check and correct all the information before pressing the *Submit* button. After processing the information on the server a confirmation screen is displayed. To complete your registration, you will need to verify your email address by clicking on the link in the email we sent you after submitting the registration form.

Caution: After you finish the registration, activate it from your e-mail. Otherwise the regular updates will not be available.

1.6.1.1 Register Clarity question

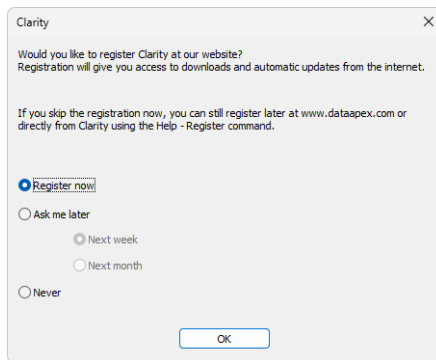


Fig. 52: Clarity registration message

This dialog allows you to register your **Clarity** station online at the **DataApex**. Registration is voluntary and it automatically allows you to download updates from the **DataApex** website directly from the **Clarity** station environment using the *Check for Updates* function.

Select the *Register now* and click the *OK* button to open the [Clarity Registration](#) dialog (and proceed with the registration) or skip the registration for a time set by the *Ask me later* option. You will be notified of the registration once the set time has passed. You can select the *Never* option and click the *OK* button to skip the registration whatsoever.

The registration may be performed anytime by invoking the *Help - Register* command from the main [Clarity](#) window. If you have already registered on our website, log in using the same username and password in the [Clarity Registration](#) dialog.

1.6.2 Check for Updates

If your computer is connected to the Internet, **Clarity** connects to an updating server and checks whether there is a new software update available. When the update program determines that your version is older than that available on the server, it will offer you an automatic download of the newer version from the Internet. Newer software update is indicated by the *Update available* command in the bottom right corner.

Note: Automatic update feature can be used only if you have registered your **Clarity** workstation via the *Register* command.

Caution: Change in the first part of the version number equals to paid upgrade and requires a new user code. Make sure you have a new user code for such version before proceeding with the update.

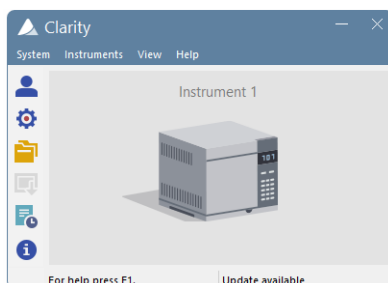


Fig. 53: Update available in the main Clarity window

If the station is not connected to the Internet, the following dialog shows up. In that case check your Internet connection by opening any web page in your browser or try checking the LAN cable or WIFI connection.

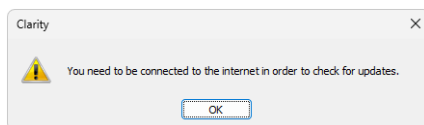


Fig. 54: No connection during the Check for Updates action

Clicking on the *Update available* command triggers the *Check for Updates* dialog. The *Check for Updates* dialog opens and displays the phrase “Connecting to server”. When a successful connection is established, the program for updating compares the number of your version to the last available version on the server. If you have the newest available version, the message “No updates available at this time” will be displayed.

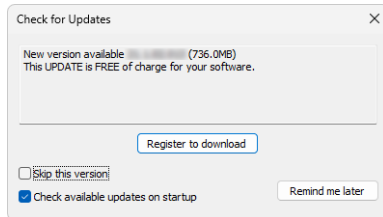


Fig. 55: Check for Updates dialog - Register to download

Register to download

Download of **Clarity** update is available for registered users only. By clicking on this button a registration web page will be opened in your default web browser. For more details see the chapter **Register** on pg. 49.. Once you switch back to Clarity, you will be notified that you have to confirm your registration from your email.

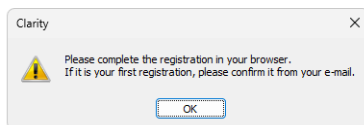


Fig. 56: Confirm your registration from your e-mail

Caution: The update will not be available until you activate your registration from your e-mail.

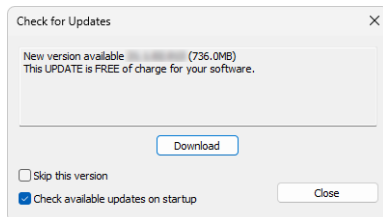


Fig. 57: Check for Updates dialog

Caution: Whether the new available version is free update or paid upgrade is noted by the text in the dialog.

Download

If you registered your **Clarity** installation and confirmed the registration from your e-mail, by clicking on this button a download of a new version will start.

Skip this version

Checking of this option skips update for the newer version and unless next update is available, *Update available* command will not be displayed. Update can be performed manually from the main **Clarity** window - *Help - Check for Updates....*

Check available updates on startup

Leaving the option checked means that it automatically checks for updates upon every start of **Clarity**. This option is recommended to keep your software updated. Unchecking this option means that checking for updates is performed manually from the main **Clarity** window - *Help - Check for Updates...*

Close

Closes *Check for Updates* dialog.

Note: If the user who performs the download does not possess appropriate rights to install applications in Windows system, a warning message will be displayed. It will offer the possibility to download the update and save it on the local hard disk.

After pressing the *Download*, the *AutoUpdate* dialog will appear. Here you can see the rate and progress of downloading of the update file from the Internet.

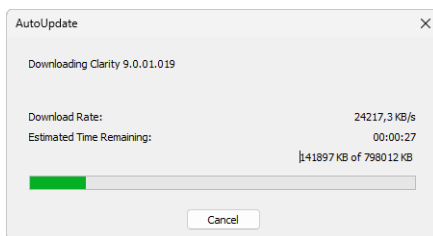


Fig. 58: AutoUpdate dialog

While downloading the update from the Internet, you will not be able to use the **Clarity** workstation for measuring and processing of analyses. After completion of the download from the updating program, the **Clarity** workstation automatically switches off and runs an Installation program. This will take you step-by-step through the update of the workstation.

1.6.3 User Code...

Enters, displays and edits the **User Code**. The user code is the encoded form of the Serial Number of your **Clarity** station.

Note: The **Serial Number (S/N)** is a unique number, that is linked to the specific HW key. It can be found on the back of the plastic card provided with the installation USB or in the [About](#) dialog in **Clarity**.

The **User Code** is saved in the CLARITY.SNO text file in the **Clarity** installation group (implicitly C:\CLARITY\CFG).

The **User Code** also defines the number of **Clarity Instruments** available for measurement and which **Control Modules** you are allowed to use.

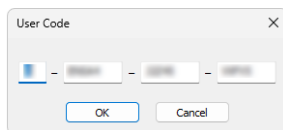


Fig. 59: User Code dialog

Trial Mode

If you do not enter the **User Code** (accomplished by hitting *Skip* in the *User Code* dialog during the installation), **Clarity** will be able to run 30 days or 100 starts (whatever comes first) in **Trial Mode**. **Trial Mode** is indicated in the header of the main [Clarity](#) window.

1.6.3.1 Language Selection

This dialog is displayed in case the **Clarity** is set to a language which is not available for your licence (User Code). Please, contact **DataApex** to consult the languages availability.

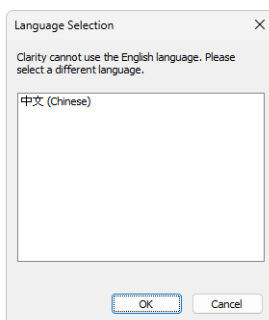


Fig. 60: Language Selection dialog

After you select one of the listed languages, restart of the **Clarity** Chromatography Station is performed to change the environment into selected language.

1.6.4 Trial Prolongation...

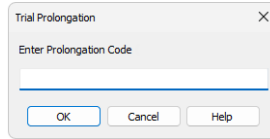


Fig. 61: Trial Prolongation dialog

This dialog allows user to extend the **TRIAL** version of **Clarity**. Paste or type the *Code* you received for prolongation and **Clarity** will change its behaviour to the **TRIAL** version. This dialog is accessible only in **Clarity TRIAL**.

1.6.5 Send Report by E-Mail

Sends the information on the state of the **Clarity** workstation to the user help desk of **DataApex**. Use this command in the case that you have problems with the functionality of the **Clarity** workstation. The command creates a new e-mail message addressed to our technical support.

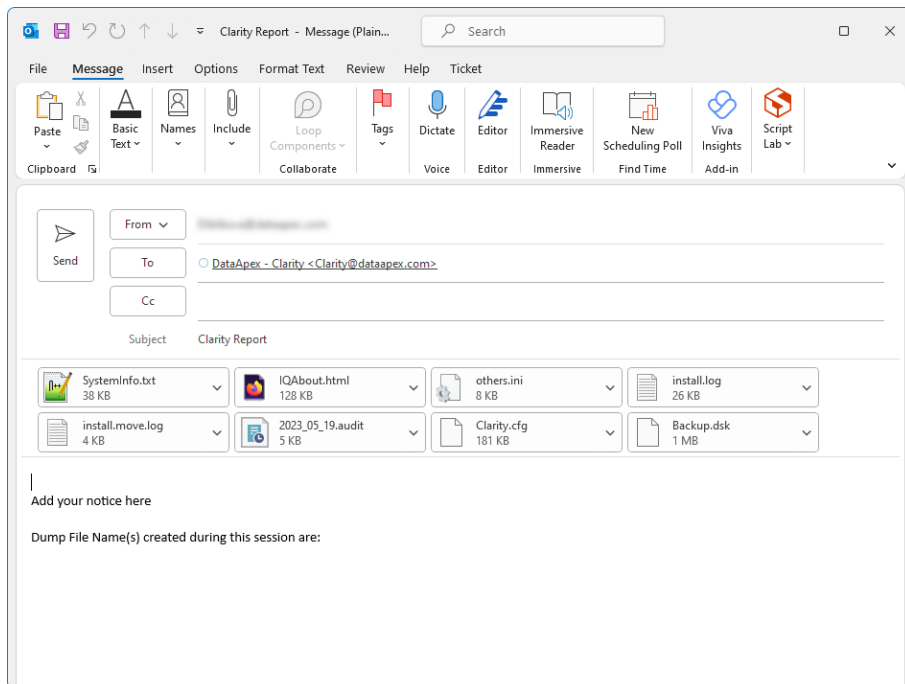


Fig. 62: E-mail message with information about Clarity

In the appendices are the SYSTEMINFO.TXT, BADTRACE.TXT files, current desktop, current configuration and two last files of the station audit trail. All these files contain information describing the state of the **Clarity** workstation at the time when the problem(s) occurred.

Note: The SYSTEMINFO.TXT and BADTRACE.TXT files can be found in the CLARITY installation group (implicitly C:\CLARITY\CFG). The content of the SYSTEMINFO.TXT file is also displayed in the [About - System](#) dialog. You may read through the files of the log in the [Audit Trail](#) window by using the *Open* command (for more details see also chapter [Audit Trail](#) on pg. 413).

Should the work with the **Clarity** workstation have been terminated improperly, an offer to send an e-mail with the error description will automatically be displayed on the next start up. The data will be send under no circumstances until you approve it.

Note: You can deactivate the automatic offer to send the error description by checking the *Send Reports About Unsuccessfully Finished Sessions* checkbox on the [General](#) tab of the [User Options](#) dialog described on pg. 148.

1.6.6 About...

Displays the version number and date of the release, serial number and other system information.

Clarity tab

Displays the name of the release followed by its topical number in the format W.X.Y.Z followed by the date when the *Build* was compiled. The *S/N* abbreviation prefaces the serial number of your station such as 011-123456.

What's new tab

The tab shows the contents of the WHATSNEW.TXT text file from the installation directory of the **Clarity** station (C:\CLARITY\DOCUMENTATION by default). The file contains a chronological list of all changes made in each new version of the station.

Readme tab

Displays a brief description of the station.

System Files tab

The tab shows the contents of the IQ.HTML text file from the installation directory of the **Clarity** station (C:\CLARITY\BIN by default). This file presents fundamental information about both the station and the computer and is updated each time the station is run. If you encounter any problems, send the file to your vendor or directly to **DataApex**. This tab also displays the number of Instruments allowed, purchased extensions and lists available control modules.

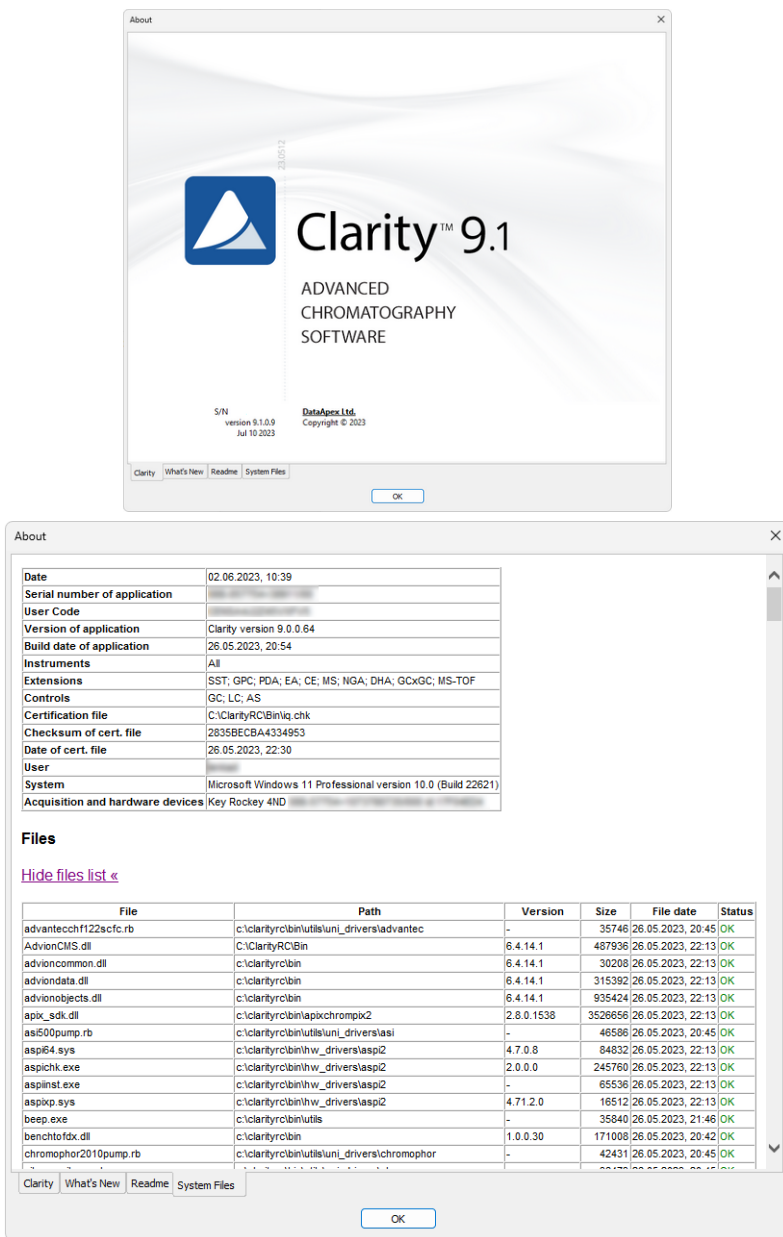


Fig. 63: About - Clarity & System Files

2 Instrument

Caution: In **Clarity Lite**, this window is also called the (Main) *Clarity Lite* window and supplies some of the properties of *Clarity* window. Any differences between **Clarity Instrument** window and *Clarity Lite* window will be discussed later, most notably on pgs. **66.**, **67.** and **161.**








This chapter describes the commands of the *Instrument* window - the fundamental window for chromatogram measurement and evaluation.

To open or display an Instrument window, invoke the command *Login to Instrument* from the *Instruments* submenu or click on corresponding icon in the main [Clarity](#) window. The Instrument name is taken from the configuration, where you can set it (for more details see the chapter **Right section of System Configuration dialog** on pg. **20**). The station allows for up to four *Instrument* windows to be displayed at one time. The number of displayed Instruments may exceed the number of Instruments actually purchased, but the excess Instruments may not be used for data acquisition.

Note: Users commonly utilize these so called **Offline Instruments** for method development or evaluation of already measured analyses.

The *Instrument* window displays a logical sequence of operations and commands necessary for the comprehensive processing of an analysis with icons. This **simplified workflow** consists of navigation icons and starts from method preparation, sample injection, through data acquisition until evaluation of chromatograms. Each Instrument has a different colour of the header to easily distinguish between them.

Simplified workflow

Icon	Name of Window	Description
	Method Setup	Open Method Setup dialog to create a new method or modify existing. <i>Note:</i> <i>Method Setup</i> dialog remembers and opens previously opened method on the last closed tab.
	Single Analysis	Open Single Analysis dialog to set specific parameters related to the measurement.
	Sequence	Open Sequence window to prepare or measure multiple samples using sequence table.
	Device Monitor	Open Device Monitor window to display parameters of directly controlled chromatograph and other controlled instrumentation.
	Data Acquisition	Open Data Acquisition window to display signals from detectors.
	Chromatogram	Open Chromatogram window to evaluate measured data.
	Calibration	Open Calibration window to create a calibration which is then used for data evaluation.

Note: In Tablet Mode, when general scale in Windows is higher than 100 %, workflow icons are divided into two rows to remain easy touchable.

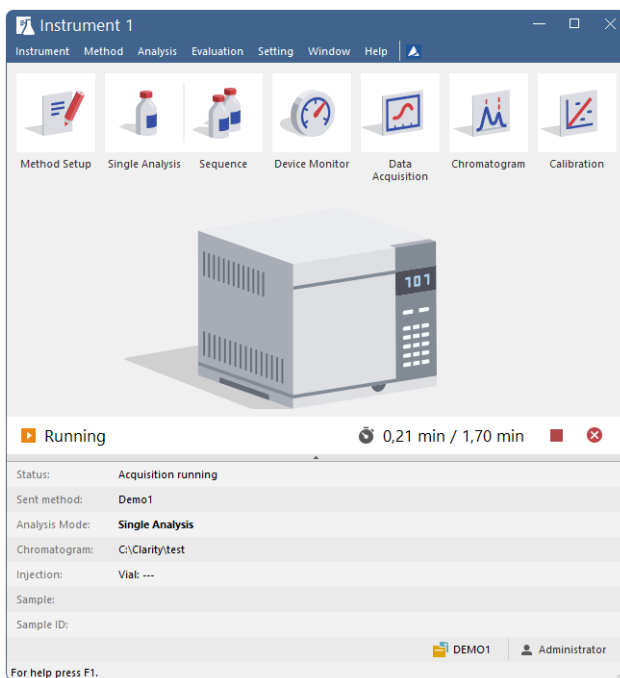


Fig. 64: Instrument

Analysis status

In addition to the menu and the navigation icons the Instrument window contains **Analysis status line** providing information about state of the instrument such as elapsed time during a Running analysis or sequence and current measurement status. Status line also contains acquisition control buttons that change dynamically depending upon the possible action:



Fig. 65: Analysis statuses

- **Send Method:** sends method that is selected in the [Single Analysis](#) dialog to connected hardware.
- **Run Sequence:** starts measuring of sequence opened in the [Sequence](#) window.
- **Stop Acquisition:** stops running acquisition.
- **Abort Acquisition:** immediately aborts running acquisition.

Note: In Tablet Mode, when general scale in Windows is higher than 100 %, analysis status line is divided into two rows to remain legible.

Information table

Below the status line is the **information table** which provides information about currently running analysis.

Status	Displays complementary information to the status displayed above it.
Sent Method	Displays which method was sent to the instrument and thus will (once the analysis is started) or is being used for the current acquisition.
Analysis Mode	Displays information what mode is running, whether Single Analysis or Sequence (in case of sequence it displays the name).
Chromatogram	Displays the name of the resulting chromatogram.
Injection	Displays information about <i>Row</i> , <i>Vial</i> and <i>Injection</i> . In <i>Single Analysis</i> mode, the number of information will be limited.
Sample	Displays name of the <i>Sample</i> (as it was inserted).
Sample ID	Displays name of the <i>Sample ID</i> (as it was inserted).

Note: The information table can be hidden using the small arrow below the status line. To view the hidden table, simply click the arrow again.

Note: When analysis is not running only *Status* and *Sent Method* fields are displayed, the rest is hidden.

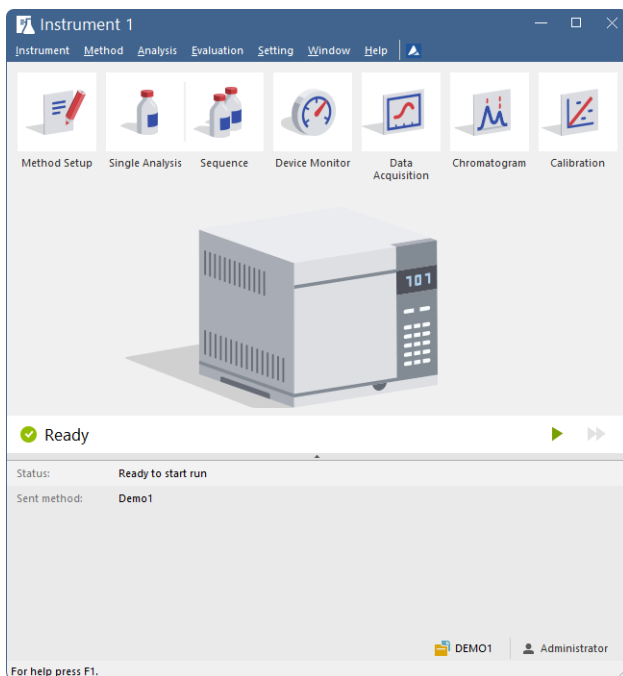


Fig. 66: Instrument Ready

Project and user

The lower end of the *Instrument* window displays the information on how to invoke the context help and the information on the **Project** opened and the name of the **User** who is logged to the **Instrument**.

Resizability

Instrument window is resizable in both the horizontal and vertical directions:

- In the horizontal and vertical direction it can be resized by clicking and dragging the left/right or top/bottom window edge - release it when desired size is achieved.
- Moreover, in the vertical direction it can be achieved by clicking the small arrow button that separates the *Status* bar from the *Information Table* which either displays or hides the *Information Table*.

Note: In Tablet mode, *Instrument* window cannot be fully maximized. Its width can be expanded up to a maximum of 50% of the monitor width.

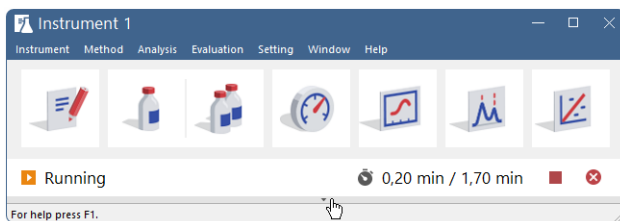


Fig. 67: Vertically resized Instrument window

2.1 Clarity Lite window specifics

In the **Clarity Lite** version, after starting the software, the dialog for entering your name will be displayed. The entered name will be saved in all files which you create during your session.

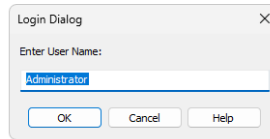







Fig. 68: Username dialog

Then the *Clarity Lite* window (in all important respects same as [Instrument](#) window) will open.

2.2 Instrument

This is a sub-menu of commands for setting up projects, working with system files and exiting an Instrument.

	Project...	Selects project directory.
	Archive... <small>✓ Full version</small>	Backs up files and projects of Clarity station.
	Restore... <small>✓ Full version</small>	Restores files and projects of Clarity station.
	Lock <NameOfInstrument> <small>✓ Full version</small>	Locks respective instrument.
<p><i>Note:</i> Instrument can be locked only in protected mode, meaning that users are defined in the <i>User Accounts</i> dialog.</p>		
	Logout from <NameOfInstrument>	Terminates work with an Instrument and closes all its windows. A warning is issued if an analysis is in progress. The user is also notified of modified files that are unsaved. In the full version <small>✓ Full version</small> , an Instrument can also be closed by using the <i>Logout</i> command from the main Clarity window or gained by right-clicking on its icon.

2.2.1 Select Method

Enables to select a method when invoked from [Sequence](#) or [Single Analysis](#) dialog or select, open and edit a method when invoked from [Method Setup](#) dialog.

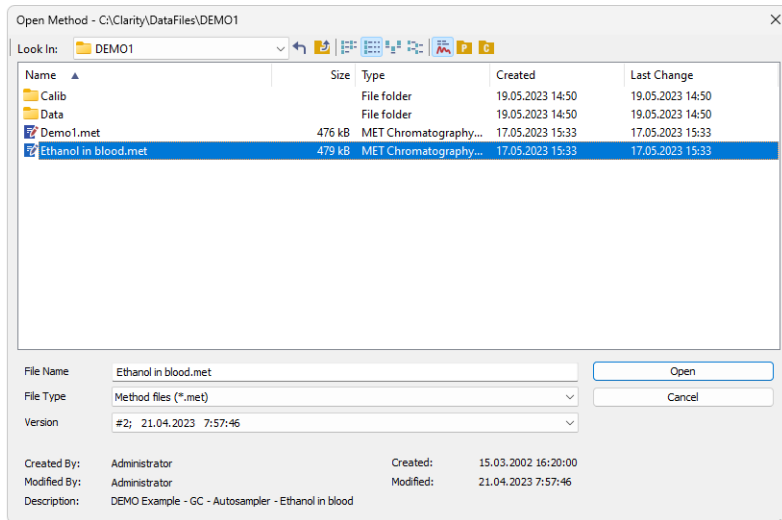


Fig. 69: Select Method

Version

Enables an option to open specific version of method. The most recent version of the method is always automatically preselected. The method file maintains a history of adjustments as a list of versions. A new version is created anytime when saving is invoked and the method contains some modification compared to previous version.

If a version from history (not the latest one) is selected it will be opened as *READ ONLY* preventing any modifications to it. Such method can still be printed. For its modifications it is necessary to save as a new method using the *File - Save As...* command under new unique filename.

Text in the *Version* dropdown list such as *#1; 25.11.2019 9:59:10* stands for version of the file, date and time when the version was saved. In this case the method *Ethanol in blood* there is about to be open version # 1 which was saved on 25th November 2019 at 9 hours 59 minutes and 10 seconds. Time and date is displayed according to current *system locale* settings in *Windows*.

Note: In some places in **Clarity** the *Version* dropdown may be missing - certain actions such as reprocessing a chromatogram in the [Batch](#) dialog can only be performed according to the latest method version, so the dialog in fact only serves to select the method according to which such action will be performed.

Created By

A name of Clarity user who created the method. The name originates from the *User Name* entered in [Login Dialog](#) during logging to [Instrument](#).

Description

Description of the method as given in *Method Description* field in the [Measurement](#) tab of the [Method Setup](#) dialog.

Note: To display the method used in the measurement in progress, invoke the *Method* command from the [Single Analysis](#) dialog or the *Sequence - Edit Current Method* command from the [Sequence](#) window.

2.2.2 Send Method by Email

Sends the displayed method file as an email attachment.

The command will create a new email message in your default e-mail client.

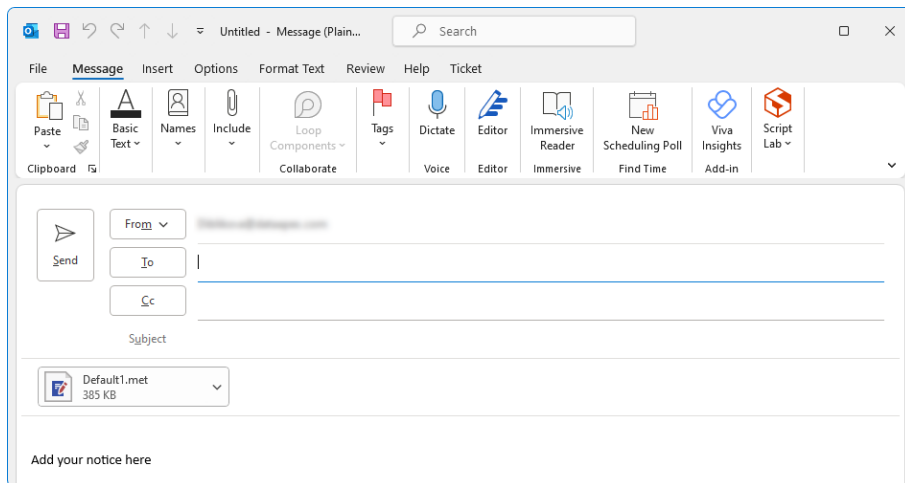



Fig. 70: Send method by email

Caution: The proper function of this command is conditional upon having a working email account.

The command is used in all major **Clarity** windows and serves for sending the respective files handled in these windows (e.g. *Send Calibration by Email*, *Send Chromatogram by Email*, etc.)

2.2.3 Project

Use the menu *Instrument - Project...* command (icon ) when working with project directories.

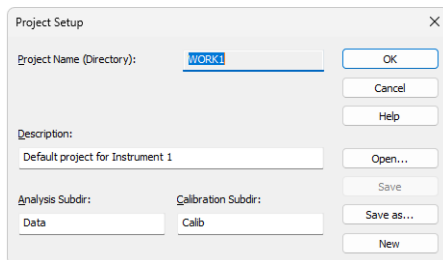


Fig. 71: Project Setup

Invoking this command will open the *Project Setup* dialog. Here the setup of the current project can be updated or another project opened or created.

Project Name (Directory)

Contains both the project name and the project directory. Only methods and sequences will be stored in the project directory (chromatograms and calibration files are stored in the corresponding subdirectories).

Description

Description of the project (this field serves for information only).

Analysis Subdir


Subdirectory for storing data (chromatograms).

Calibration Subdir

Stores calibration standards and calibration files.

Note: More information on the project directory structure can be found in the chapter "**Directories**" on pg. 27.

Open...

Selects a new project from a list of existing ones. In the full version , the same project can be opened in two different Instruments. This configuration can be useful, for example, when preparing a new sequence during measurement.

Caution: Although the same **project** can be opened in two **Clarity** Instruments within one station, the same **file** cannot. However, with multiple **Clarity** (Lite) stations running in a PC network, this limitation does not apply and the same file can be displayed on any number of stations.

Note: The list of existing projects corresponds to the list of *.PRJ files in the PROJECTS directory.

Save

Saves the displayed project parameters.

Save as

Copies the current project and saves it under another name. The project description and the name of data subdirectories are copied automatically. Copies of all files are created only after confirmation.

New

Creates a new project. Invoking the command displays a list of existing projects where the name of the new project can be entered. Two data subdirectories are offered with the default names DATA and CALIB.

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

2.2.3.1 Error Opening Project

This error dialog is displayed if there is an error during opening a project, it also allows you to decide, what will **Clarity** do in this type of the situation.

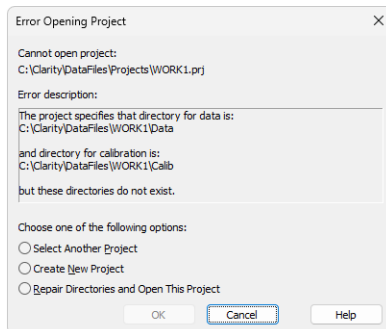


Fig. 72: Error Opening Project

Select one of the option below and click the **OK** to perform the action and continue.

Select Another Directory

Set this option in case the directory with your projects has moved.

Select Another Project

Allows to select another project within the projects directory.

Create New Project

Allows to create new project in existing the projects directory.

Repair Directories and Open This Project

Allows to create required subdirectories in the project's directory.

2.2.4 Archive ✓ Full version

Archives or erases selected files or entire projects in the **Clarity** station. The command opens the *Backup - Create Archive* dialog. Files from the current project can be backed up to any directory on any disk either as simple copies of individual files or as a single compressed *.DGZ file.

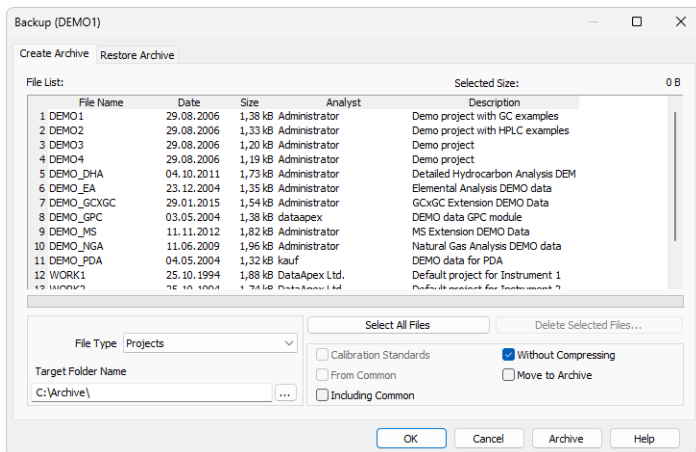


Fig. 73: Backup - Create Archive

File list

Lists all selected files from the current project. Click on files to select them, click again to deselect the file. Any number of the displayed files can thus be selected. In addition to the filenames, the list contains the date when it was last saved, file size, and the name of the user who created the file. *Sample ID* and *Sample Columns* will be shown for chromatograms. *Description* will be displayed for the other files and projects.

Selected Size

Indicates the size of the selected files (in kB).

File Type

Selects the type of file: *Chromatograms*, *Sequence files*, *Method Templates*, *Calibration Files*, *Report Styles*, *SST Method files*, *GPC Calibration files*, *PDA Library files*, *Projects* (meaning all files of a given project), *Audit Trail Files*, *PetroCal Files* and *NGA Method Files*.

Note: Archiving the whole project will also archive all files from the common directory (C:\CLARITY\DATAFILES\COMMON by default) that contains for example report styles.

Select All Files

Rapidly selects all files in a list.

Delete Selected Files

Deletes selected files. Once deleted, files cannot be restored from within the **Clarity** station!

Calibration Standards

Determines whether chromatograms from the DATA or from the CALIB directory will be listed.

Without Compressing

If checked, the selected files will be copied or moved, otherwise a single compressed *.DGZ file will be created.

Note: Previously existing files of identical names will be rewritten and not extended!

From Common

Displays system files only from the common directory COMMON. This checkbox is active only for system files.

Move to Archive

After a successful backup, the files will be deleted from the current directory.

Including Common

While this checkbox is checked, the COMMON subdirectory will be also archived with other files of the archived project. This option can only be checked while archiving whole projects.

Target Folder Name / Target File Name

The field changes name and behavior according to the *Without Compressing* setting. When the *Without Compressing* checkbox is checked, *Target Folder Name* field defines the folder to which the selected files will be archived. With the checkbox unchecked, *Target File Name* field defines the location and name of resulting *.DGZ archive into which files will be copied.

Be aware it is not allowed to save files to root folder of operating system (typically "C:\") usually because of commonly predefined *UAC - User Account Control* settings in *Windows 7* and newer. In this case is necessary to select other location for storing of resulting *.DGZ archive than *Windows* root folder.

OK

Saves any modifications made in the archive settings and closes the *Backup* dialog.

Cancel

Closes the *Backup* dialog without saving any of the modifications made in the archive settings.

Archive

The proper command for backing up (copying or moving) selected files. A warning is given if files with identical names exist in the target directory.

2.2.5 Restore ✓ Full version

Restores or deletes files and projects in the **Clarity** station. This command invokes the *Backup - Restore Archive* dialog. The *Restore* command restores files from any directory to the current project.

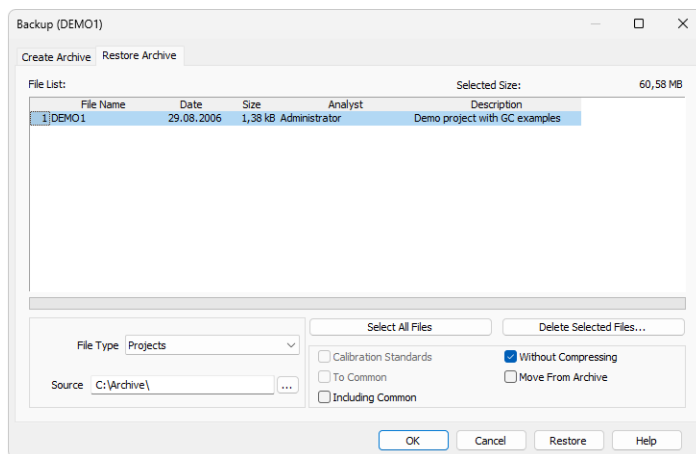


Fig. 74: Backup - Restore Archive

File list

All files of the selected type from the directory selected by *Source* command. Files are selected by clicking once and deselected by clicking a second time allowing for any number of displayed files to be selected this way. The list that is displayed contains file names, size, the date on which they were last saved, and the name of the user who created the file. The *Sample ID* and *Sample* columns will be shown for chromatograms. The *Description* column will be displayed for other files and projects.

Selected Size

Indicates the size of the selected files (in kB).

File Type

Selects the type of file: *Chromatograms*, *Sequence files*, *Method Templates*, *Calibration Files*, *Report Styles*, *SST Method files*, *GPC Calibration files*, *PDA Library files*, *Projects* (meaning all files of a given project) and *Audit Trail Files*.

Note: Restoring the whole project will also restore all files to the common directory (C:\CLARITY\DATAFILES\COMMON by default) that contains for example report styles.

Select All Files

Rapidly selects all files in a list.

Delete Selected Files

Deletes selected files. Once deleted, files cannot be restored from within the **Clarity** station!

Calibration Standards

Determines whether the chromatograms will be restored to the DATA or CALIB directory.

Without compressing

If checked, the selected files will be simply copied or moved, otherwise the content of a single compressed *.DGZ file will be displayed.

To Common

Restores system files to the COMMON directory. This checkbox is active only for system files.

Move from Archive

Files successfully restored will be deleted (the *Restore* command functions similarly to the *Move* function).

Including Common

While this checkbox is checked, the project will be restored including the COMMON subdirectory (if it is included in it). The option is only available for restoring whole projects. Note that files restored from the project will try to overwrite the actual content of the COMMON subdirectory.

Source

Identifies the source directory (of the *.DGZ file) where selected files will be sought.

OK

Saves any modifications made in the settings of the *Backup - Restore* dialog and closes the *Backup* dialog.

Cancel

Closes the *Backup* dialog without saving any of the modifications made in the settings of the *Backup - Restore* dialog.

Restore

The proper command for restoring (copying or moving) the selected files. A warning dialog is shown if files with identical names exist in the target directory.

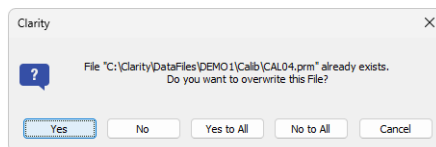


Fig. 75: Warning message when the filename already exists

2.2.6 Open Dialog (Sequence, Chromatogram, Calibration, Method)

This is a universal dialog for selecting files. As it differs somewhat in appearance from the standard window for file selection of the **Windows** operating system, it is described in more detail below:

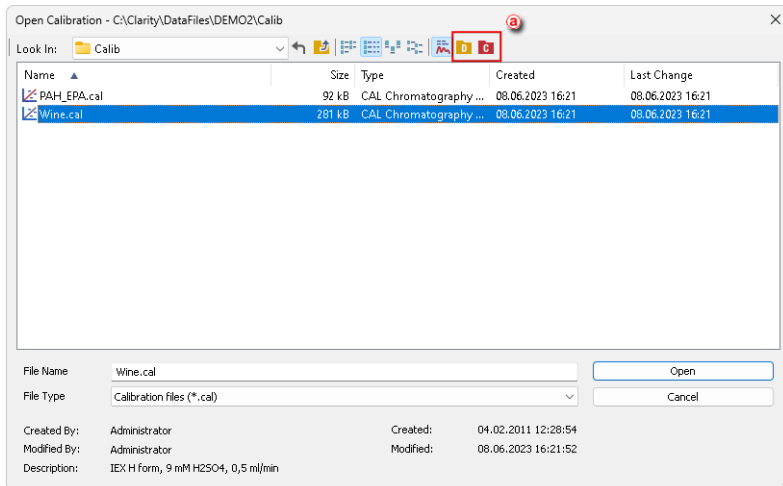



Fig. 76: Open Calibration

Icons in the right upper corner **a** serve for quick navigating through useful folders, e.g. DATA, CALIB, COMMON. What folders are shown is dependent on the currently opened dialog, as stated in the following table:



Tab. 1: Icons for navigating through folders

Icon	Description	Appears in dialog
	Displays files from the current Project	Open Sequence, Select Method
	Displays files from the COMMON directory	Open Calibration, Open Sequence, Select Method
	Displays files from the CALIB folder within the current Project	Open Calibration, Open Chromatogram
	Displays files from the DATA folder within the current Project	Open Chromatogram
	Transfers you up to the parent directory	Any File Open dialog
	Returns you to the previous directory	Any File Open dialog

Note: There are some other open dialogs, which do not contain any of the specified icons in the right upper corner .

List of files

Displays all files of the selected *File Type* from the previously opened directory.

Files are sorted and displayed in conformity to their previous setting. The layout can be changed by using the  button to access the *Detailed View* menu. In the *Detailed View* layout you can change the sorting order by clicking on the heading of the desired column. A second click reverses the order. The type and method of file sorting is indicated by a small  arrow next to the column name.

The mode in which files are displayed and the ordering method are automatically saved in the current desktop file (*.DSK).


Note: In the non-protected mode all settings are the same for the entire station. However, in the protected mode each user may have a dedicated *.DSK file.

File Name

This field contains the name of the selected file. The name can be entered directly or selected from the list of filenames. When the name is being entered directly, only files whose names begin with the characters already entered will be displayed. The files and directories that match the so-far entered letters in the given actual directory will be shown in the listbox on the *File Name* row.

Note: If you search for files containing only some characters, enter an asterisk (* - which stands for any number of characters) or several question marks (? - substitutes for a single character) before those characters.

Detail Info

Use the  button to display/hide the following **detailed information** about the selected file. Detailed information are dependent on the particular dialog in which they are displayed.

Created by

Indicates the name of the user who created the file. Each file contains the name of the user who created it by use of either the *New* or *Save As* commands. The name of the user originates from the *User Name* entered in [Login Dialog](#) during logging to [Instrument](#).

Description

A supplementary file description that enables to fill in or update the information in the corresponding editing window of the file (this field serves for information only).

Version

Displays file format information related to station in which the file was last saved.

2.2.7 Save As Dialog (Sequence, Chromatogram, Calibration, Method)

This is a universal dialog for saving files where the new name can be entered or a new directory selected. As it differs somewhat in appearance from the standard window for file selection of the **Windows** operating system, it is described in more detail below.

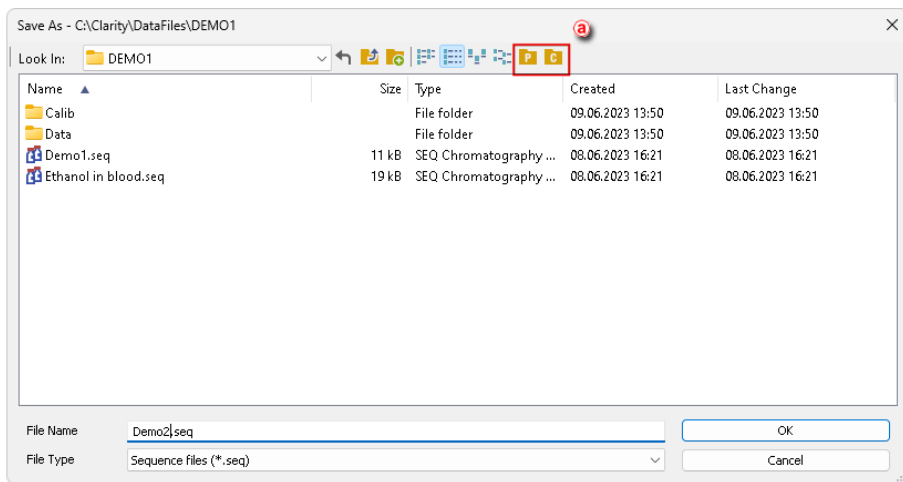



Fig. 77: Save As Dialog

Icons in the right upper corner a serve for quick navigating through useful folders, e.g. DATA, CALIB, COMMON. What folders are shown is dependent on the currently opened dialog, as stated in the following table:



Tab. 2: Icons for navigating through folders

Icon	Description	Appears in dialog
	Displays files from the current Project	Save Sequence As, Save Method As
	Displays files from the COMMON directory	Save Calibration As, Save Sequence As, Save Method As
	Displays files from the CALIB folder within the current Project	Save Calibration As, Save Chromatogram As
	Displays files from the DATA folder within the current Project	Save Chromatogram As
	Transfers you up to the parent directory	Any File Save As dialog
	Returns you to the previous directory	Any File Save As dialog

Note: There are some other save as dialogs, which do not contain any of the specified icons in the right upper corner .

List of files

Displays all files of the selected *File Type* from the previously opened directory.


Files are sorted and displayed in conformity to their previous setting. The layout can be changed by using the  button to access the *Detailed View* menu. In the *Detailed View* layout you can change the sorting order by clicking on the heading of the desired column. A second click reverses the order. The type and method of file sorting is indicated by a small  arrow next to the column name.

The mode in which files are displayed and the ordering method are automatically saved in the current desktop file (*.DSK).

Note: In the non-protected mode all settings are the same for the entire station. However, in the protected mode each user may have a dedicated *.DSK file.

File Name

The name under the file is saved is entered here. The name can be entered directly or selected from the list of file names. When the name is being entered directly, only files whose names begin with the characters already entered will be displayed. The files and directories that match the so-far entered letters in the given actual directory will be shown in the listbox on the *File Name* row.

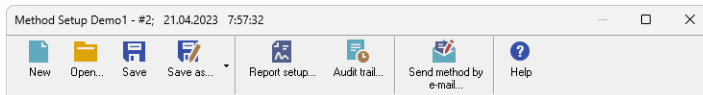
Note: If a file of that name already exists and has been opened on other Instrument or window, the name cannot be used. Moreover, in the protected mode (full version  only), a user may not overwrite a file he/she is not entitled to modify (see the *User Account* command).

Note: If you search for files containing only some characters, enter an asterisk (* - which stands for any number of characters) or several question marks (? - substitutes for a single character) before those characters.

Note: In Clarity there are some other types of *Save As* dialogs where the file type of the file is different from the typical Clarity file types (*.PRM, *.MET, etc.) , for example when *Print to PDF* dialog is invoked data are saved as PDF document, when in *Print..* the *Print To File* checkbox is checked the data are saved as *.prn file type.

2.3 Method Setup

Displays and updates the measuring method through a set of commands. Upper part of *Method Setup* features a set of commands which can be applied to the current method.



Dialog Header



Method Setup header provides information about name and version of currently opened method. Date and time informs when the current version was created (ie. saved).

Text *Demo1 - #2; 21.04.2023 7:57:32* stands for method name 'Demo1', version number '2' which was saved on *21st April 2023 at 7 hours, 57 minutes and 32 seconds*. Time and date is displayed according to current *system locale* settings in *Windows*.

If there is opened any method created in older version of Clarity without method versioning the method will be transferred to version 1.



New

Creates a new (**Ctrl** + **N**) method. When invoked, a *Method Setup* dialog opens on the [Measurement](#) tab of the new method called NONAME. User will be notified if the previously opened method was modified and yet not saved. The modification of the method is indicated in the Method Setup window next to the filename by the "(MODIFIED)" inscription. *Save As* dialog pops up upon pressing *OK* or *Cancel*.



Open...

Selects and opens (**Ctrl** + **O**) an existing method.

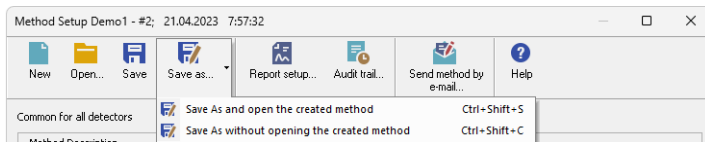


Save

Saves (**Ctrl** + **S**) existing method.



Save as...



The commands open the Save As dialog. Here a new name can be entered or a new directory selected.

Save As and open the created method Saves current method (**Ctrl** + **Shift** + **S**) with all its modifications in the as new method and loads the new method to *Method Setup* dialog.

Save As and without opening the created method Saves current method (**Ctrl** + **Shift** + **C**) with all its modifications in the as new method but keeps current method loaded *Method Setup* dialog with its modification unsaved.

If a file of a particular name already exists and has been loaded in some other window, the name cannot be used. Moreover, in the protected mode a user may not modify or a file he/she is not entitled to modify (see the [User Accounts](#) item *Edit method*). Filename *NONAME* is reserved for newly created file and thus no file may be saved under the filename *NONAME*.

Note: For existing filenames, message box about file overwriting pops up.



Report setup...

Opens the [Report Setup](#) (**Ctrl** + **Alt** + **P**) dialog on the [Method](#) tab. When there are some changes performed in the *Method Setup* dialog prior to using the *Report* button, the user is asked to either apply the changes or not. The report will then be made according to changed or unchanged method



Audit trail...

✓ Full version

Opens the [Method Audit Trail](#) window, a window holding an audit trail of the current method. When there are some changes performed in the *Method Setup* dialog prior to using the *Audit Trail* button, the user is asked to either apply the changes or not.

Note: The [Method Audit Trail](#) is, unlike other local audit trail windows, modal. That means that it is necessary to close it in order to be able to work with any other **Clarity** windows and dialogs.



Send Method by Email

Sends method file (displayed in the header of the instrument window) as an email attachment.



Help...

This button calls the online context help for the tab being currently opened.

Lower part of the *Method Setup* contains tabs which are dependent on added control module - each will have its own sub-menu command here (e.g *Thermostat Control*, *Valve Control*, *Fraction Collector Control*, ...).

Tab. 3: List of common tabs in the *Method Setup* dialog

Tabs	Contents of the tab
Event Table	Enables to trigger actions during analysis.
Measurement	Parameters that specify the measurement conditions.
Acquisition	Parameters that decide the method used to measure the detector signal.
Integration	Parameters that define the method of integration and baseline modification.
Calculation	Parameters that define the method of results calculation.
Advanced <small>✓ Full version</small>	Contains <i>Subtraction Chromatogram</i> function, <i>Column Calculation</i> and <i>User Variables</i> parameters.
GC (LC) Control <small>✓ Full version</small>	Parameters that define direct control of the chromatograph.
AS Control <small>✓ Full version</small>	Parameters that govern the method of an injection when using direct autosampler control.

Aside of the particular tabs the *Method Setup* dialog also contains a series of buttons. These buttons are present on every tab of the *Method Setup* dialog, in truth the tabs are only laid into the main frame which holds the buttons.




Fig. 78: *Method Setup* - buttons

These buttons, when invoked, perform the following actions:

OK

Applies and saves changes performed in the method setup dialog to the opened version of the method. If the acquisition is running, only the change in the *Autostop* and *Run Time* parameters from the [Method Setup - Measurement](#) tab can be modified, the rest of the tabs are locked against changes.


Upon pressing the *OK* button, for newly created method (*New*  command), *Save As* dialog pops - save it with a valid file name.

Cancel

Discards all changes performed in the *Method Setup* dialog and leaves the dialog.

Send Method

When invoked, sends the method (that is displayed in the header of the *Method Setup* dialog) to all connected control modules/hardware. By clicking the *Send Method* button, currently opened method is also set to [Single Analysis](#) dialog into the *Method* field. This button is not available during the data acquisition (during a running analysis).

Note: It is not possible to send a method which has the “(MODIFIED)” inscription or which has not been saved yet (Noname method). *Send Method* command is disabled directly after pressing *New*  command - pressing the *OK* button invokes *Save As* dialog. Once the method is saved, the *Send Method* command is enabled again.

Note: In Tablet Mode, the *Method Setup* dialog is maximized by default. The user can shrink and position the window, as well as outside the Tablet Mode, and Clarity will remember the settings until the next restart of Tablet Mode.

2.3.1 Event Table

The *Event Table* enables to trigger action with specified Output based on events from selected Input. *Event Table* tab is common to all devices on the same **Clarity** Instrument.

Inputs:

- Acquisition and Idle events - Time, signal level, digital input state
- Events from Control module - Auxiliary signal level
- System events - Begin and end of sequence, acquisition etc.

Outputs:

- Digital Output control - **DataApex** A/D Converters, selected Control modules (for more details see the chapter **Events used in Active Sequence** on pg. **91**).
- Acquisition and Sequence control commands (*Stop, Abort, Skip Vial, etc.*).
- Run program - Launching an external program, with/without start parameters. Basic set of external tools is supplied with **Clarity**.
- None - Nothing will happen, suitable for development and testing of the method.

Each row in the table represents an independent event. When several events controlling the same output collide, the subsequent event masks the preceding one. When two events occur simultaneously, the event listed as last in the **Event Table** prevails.

Some events occurs in *RUNNING* or *IDLE* state only, these are coined with **Run** or **Idle** words in the event name.

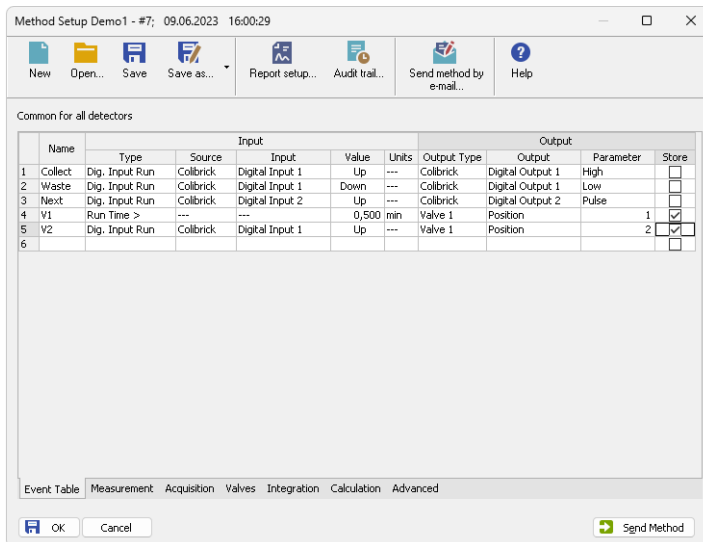


Fig. 79: Method Setup - Event table

Individual lines or the entire table of events may be erased by right clicking the mouse on the available context menu above the table and using *Delete Row* or *Delete All Rows* commands. When a line becomes invalid, it will be highlighted with red background. Such row may be edited and must be repaired prior to saving the method. It is possible to select and copy the whole rows, paste them in the table and modify them. This is useful for creating sets of similar events.

Name

Arbitrary name to describe the event.

Input

The set of columns describing the Input that will trigger the action specified in *Output* columns.

Type

Sets the type of the input. Available options are shown in the **Tab. 4** on pg. **87.**:

Tab. 4: List of events available in the Event Table

Name of the event	Condition on when the event is triggered
<i>Run Time</i> >	Duration of acquisition (Instrument in <i>RUNNING</i> state) exceeds adjusted value (reset by every start of acquisition).
<i>Input Run</i> >	Measured quantity (e.g. input voltage or AU) exceeds adjusted value (works in <i>RUNNING</i> state only).
<i>Input Run</i> <	Measured quantity (e.g. input voltage or AU) drop below adjusted value (works in <i>RUNNING</i> state only).
<i>InpRel Run</i> >	Measured quantity (e.g. input voltage or AU) exceeds adjusted value+offset (works in <i>RUNNING</i> state only, offset is locked in the moment of acquisition start).
<i>InpRel Run</i> <	Measured quantity (e.g. input voltage or AU) drop below adjusted value+offset (works in <i>RUNNING</i> state only, offset is locked in the moment of acquisition start).
<i>Time Idle</i> >	Duration of idle time (Instrument in <i>WAITING</i> or <i>READY</i> state) exceeds adjusted value (reset by every sending of method and by the end of the acquisition).
<i>Input Idle</i> >	Measured quantity (e.g. input voltage or AU) exceeds adjusted value (works except <i>RUNNING</i> state only).
<i>Input Idle</i> <	Measured quantity (e.g. input voltage or AU) drop below adjusted value (works except <i>RUNNING</i> state only).
<i>InpRel Idle</i> >	Measured quantity (e.g. input voltage or AU) exceeds adjusted value+offset (works except <i>RUNNING</i> state only, offset is locked in the moment of method sending).
<i>InpRel Idle</i> <	Measured quantity (e.g. input voltage or AU) drop below adjusted value+offset (works except <i>RUNNING</i> state only, offset is locked in the moment of method sending).
<i>Dig. Input Run</i>	Digital input changes its state (works in <i>RUNNING</i> state only).
<i>Dig. Input Idle</i>	Digital input changes its state (works except <i>RUNNING</i> state only).
<i>Aux Run</i> >	Auxiliary input level exceeds adjusted value (works in <i>RUNNING</i> state only)
<i>Aux Run</i> <	Auxiliary input level drop below adjusted value (works in <i>RUNNING</i> state only)
<i>Aux Idle</i> >	Auxiliary input level exceeds adjusted value (works except <i>RUNNING</i> state only)
<i>Aux Idle</i> <	Auxiliary input level drop below adjusted value (works except <i>RUNNING</i> state only)
<i>Ready</i>	All connected hardware becomes ready.
<i>Run Begin</i>	Run has begun, i.e. start of acquisition, start of the sequence row (before injection and after injection), but not the restart.

Name of the event	Condition on when the event is triggered
<i>Injection</i>	Start of the sequence row, Instrument is waiting for carrying out the injection.
<i>Bypass Injection</i>	Start of the bypassed sequence row (row with <i>Sample Type = Bypass</i> value set).
<i>Acq Begin</i>	Acquisition has begun, i.e. start of acquisition, start of the sequence row (after injection or bypass), but not the restart.
<i>Restart Acq</i>	Restart of acquisition (by wire or manually by button).
<i>Acq End</i>	Correct completion of acquisition (<i>Autostop</i> or <i>Stop</i> button).
<i>Run End</i>	Completion of acquisition (<i>Autostop</i> , <i>Stop</i> button, <i>Abort</i> button).
<i>Control Elapsed</i>	Completion of acquisition and all programs on controlled devices (e.g. gradient program on pump or temperature program on column oven).
<i>HW Error</i>	Hardware error occurred (e.g. error on communication, device firmware error or physical failure).
<i>User Abort</i>	Abortion of acquisition by <i>Abort</i> button.
<i>User Shut Down</i>	System was shut down by user (using button on <i>Device Monitor</i> , command is available with controlled device connected only).
<i>Close Instrument</i>	Instrument was closed.
<i>SST OK</i>	On the end of acquisition, when SST resulted with OK.
<i>SST Unknown</i>	On the end of acquisition, when SST resulted with Unknown.
<i>SST Failure</i>	On the end of acquisition, when SST resulted with Failed.

Notes: *WAITING FOR INJECTION* state is considered as *IDLE* from event table's point of view, so for correct launching of e.g. *Stop Seq* command on any circumstances is necessary to create two events with the same command, one for *RUN* and one for *IDLE* state.

Notes: SST events occurs only when acquisition is finished.

Notes: User Shut Down event is available with controlled device connected only and after removing corresponding device from configuration particular event table row must be removed too.

Notes: In the event table, controlled devices are listed under names entered in their configuration dialogs, after change of name of the device, particular event table row must be corrected or removed.

Source

Sets the device which should be used as Input (e.g. detector, A/D converter, ...).

Input

Applies only for Digital Inputs, where it sets the input number.

Value

Indicates the value that is to be compared during the acquisition with current values (time, voltage on detector, digital input state etc.).

Note: When using Events evaluating Input values (Input Run, InpRel Run, Input Idle, InpRel Idle), please note that event will be triggered only when the change of input signal will be greater than EventThreshold value set in [OTHERS.INI](#) file.

Note: When triggering Events based on Auxiliary Signals (Input Run, Input Idle, Aux Run, Aux Idle), please note that event will be triggered only when the change of input signal will be greater than specific EventThresholdAux value set in [OTHERS.INI](#) file.

Units

Units of the *Value* (if applicable). For detectors, these are the units set in the [Device Setup](#) dialog of the [System Configuration](#) dialog. This field is not editable.

Output

The set of columns describing **Output** triggered by the action specified in *Input* field.

Output Type

Selects from the available output options:

- A/D converter (Colibrick) - digital outputs
- Controlled device (Agilent 6890, etc.) - digital outputs
- Run Program - runs external program, command line parameters can be set.
- None - Nothing will happen, suitable for development and testing of the method. (e.g. when it is needed to log event in the chromatogram)

Note: There are two auxiliary software utilities in the \BIN\UTILS subdirectory. SENDCOM.EXE for sending simple commands over serial line and BEEP.EXE for acoustic signaling, check the text files in the \BIN\UTILS subdirectory for detailed description.

- Command - commands for internal controlling of the software run (for more details see the chapter **Sequence** on pg. 402).

Output

Meaning of this field varies according to the *Output Type* used:

- A/D converter - sets the number of the controlling output to be set to the value indicated in the *Parameter* field.
- Controlled device - sets the name/number of the controlling output to be set to the value indicated in the *Parameter* field.
- Run Program - sets the filename of the software to be run (including the full path).
- Command - sets the command for internal controlling of the software run:

Tab. 5: List of possible outputs for the Command output type

Name of the command	Meaning of the command
<i>Start Seq</i>	Start of the Sequence . Sequence file must be properly filled and saved in order to execute this command.
<i>Start Acq</i>	Start of the acquisition. When launched in <i>RUNNING</i> state, restarts the acquisition only with <i>Start-Restart</i> option checked (for more details see the chapter Measurement on pg. 92). .
<i>Snapshot</i>	Creates a snapshot of currently running analysis. Snapshot processes and saves the data from currently measured sample without terminating the measurement.
<i>Stop Acq</i>	Stop of the acquisition. In sequence run, current acquisition is halted, the Sequence continues on the next row.
<i>Stop Seq</i>	Stop of the Sequence . Current acquisition will be finished, then the sequence will stop.
<i>Repeat Injection</i>	Acquisition of current row in Sequence is halted immediately, the same sample is injected and analysed again.
<i>Skip Vial</i>	Acquisition of current row in Sequence is halted immediately, the Sequence continues on the next row.
<i>Abort</i>	Aborting of Single Analysis or the Sequence (chromatogram is always saved, regardless of setting in GLP options).
<i>Shutdown</i>	Shutting down all the devices connected (command is available with controlled device connected only).
<i>LC Hold/Resume</i>	Holds or Resumes the execution of the Gradient Table at the actual flow and mobile phase composition. Type of action depends on current state of the device.

Note: For more details see the chapter **Sequence** on pg. **385**.

Parameter

Its meaning varies according to the **Output Type** used:


- **A/D Converter:** The level to be set on the corresponding output specified in the *Output* field:

High - High level (output voltage 3 to 5 V) - corresponds to an opened contact.

Low - Low level (output voltage 0 to 1 V) - corresponds to a closed contact.

Pulse - Inverts the current level of the output for a given time and then returns back. Implicit length of the pulse is 1 sec.

Note: The duration of the pulse can be adjusted in the OTHERS.INI file (for more details see the chapter **others.ini file** on pg. **506**).


- **Run Program:** Adds command line parameters to be applied to the program specified in the *Output* field. Parameters can be input manually or can be chosen from the menu after clicking the  button.

%Q - Sample name.
%q - Sample ID.
%s - Sequence name.
%J - Method.
%K - Chromatogram.
%v - Vial number.
%i - Injection number.

Store

Sets whether the performed event should be stored within the chromatogram file. Stored events can be displayed in the [Chromatogram](#) window.

2.3.1.1 Events used in Active Sequence

The control outputs are also used in *Active Sequence* to enable the autosampler to inject the next sample. In full version , these inputs are assigned in the [System Configuration](#) dialog.

Caution: Do not use these inputs and outputs in the **Event Table**.

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

2.3.2 Measurement

The *Method Setup - Measurement* tab describes in detail the measuring conditions and determines the duration of an analysis.

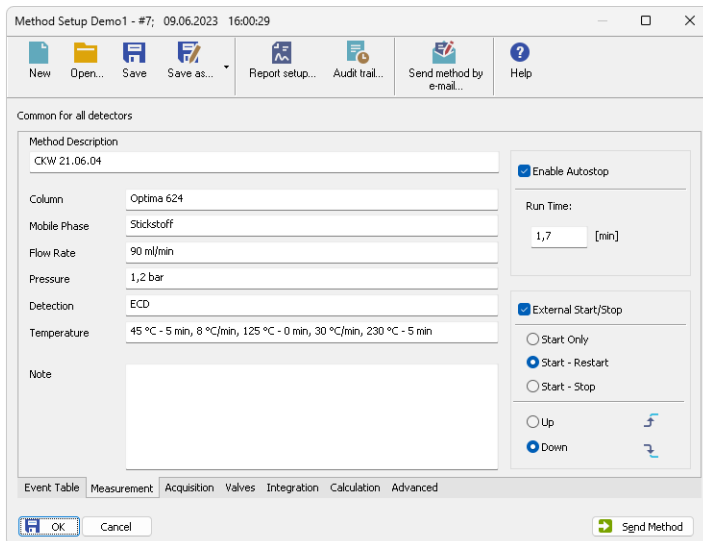


Fig. 80: Method Setup - Measurement

The *Method Setup - Measurement* dialog will open with the method name displayed in the title bar when invoked from the [Instrument](#) or [Single Analysis](#) window. While performing a multi-detector measurement, this tab is common for all signals.

Method Description

Contains the description of the method. When opening the method, the content of this field is displayed in the *Description* field of the [Open Method](#) dialog after the method is selected.

Column

Describes (informational purposes only) the column being used.

Mobile Phase

Describes (informational purposes only) the mobile phase used.

Flow Rate

Indicates (informational purposes only) the mobile phase flowrate.

Pressure

Indicates (informational purposes only) the mobile phase pressure.

Detection

Contains (informational purposes only) the detector characteristics.

Temperature

Describes (informational purposes only) temperature parameters.

Enable Autostop

Sets automatic termination of an analysis after the time set in the *Run Time* field.

Run Time

Specifies the duration of analysis. After the appointed run time has been reached, the analysis will automatically be terminated and processed. The possible time interval is between 0.2 - 9999 minutes. *Enable Autostop* option must be checked for this field to be editable and functional.

Note: The *Run Time* field must be set for all methods used in an active sequence since the time determines the cycle duration.

Note

An optional note (for informational purposes only).

External Start/Stop

Enables external start synchronization using an external signal from Digital Input on the A/D converter. Three types of the *External Start/Stop* operation are possible:

- *Start Only* - The external signal only starts analysis. Any external signals coming during the analysis will be ignored.

Note: The *Start Only* operation mode is automatically preselected upon creating a new method.

- *Start - Restart* - The external signal terminates the analysis in progress and at the same time starts a new one. The first signal starts the analysis, the second signal terminates it and at the same time starts a new one. This is known as “the continuous measurement”.

Note: The *Start/Restart* operation mode can not be performed for majority of directly-controlled instruments.

- *Start - Stop* - The external signal starts and stops an analysis. The first signal starts the analysis, the second signal stops it, third signals starts a new analysis etc.

The externally synchronized instrument may react on contact closure or contact opening. **Clarity** allows both options.


Up

The station reacts to a voltage change in the relevant controlling input from low (< 0.7 V) to high (> 3 V), or in other words, to an opened contact.

Down

The station reacts to a voltage change in the relevant controlling input from high (> 3 V) to low (< 0.7 V), or in other words, to a closed contact.

2.3.3 Acquisition

Sets the measuring conditions. When the menu command or  icon is invoked, the *Method Setup - Acquisition* dialog will be opened. The type of items displayed depends, in part, on the type of A/D converter that has been installed (or the type of chromatograph used while using direct digital acquisition). Be aware that parameters cannot be changed during analysis! The type of the A/D converter along with the name of the detector can be seen in the upper part of the tab.

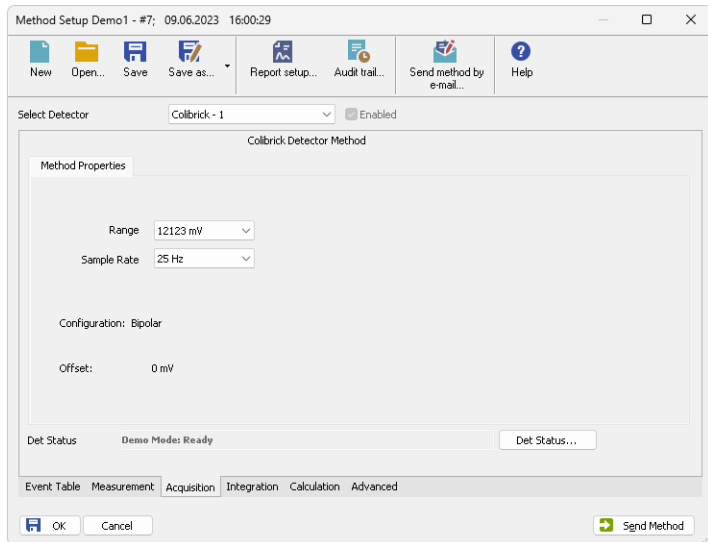


Fig. 81: Method Setup - Acquisition

Note: At the beginning of the acquisition **Clarity** performs calibration of the A/D converter. Depending on the type of the converter (INT9, U-PAD2, Colibrick, etc.) and *Sample Rate* the first 20 - 200 ms of the chromatogram will not contain valid data.

Select Detector

Selects between the individual detectors in case several detectors are configured on the same Instrument (multi-detector configuration).

Caution: When using a multi-detector configuration, it is necessary to set the parameters individually for each detector.

Enabled

Enables/disables signal selected in the *Select Detector* field.

Range


Selects the voltage input range (in mV) and defines the maximum output voltage of the detector that the A/D converter can process.

Sample Rate

Specifies the sample rate (ranging from 6,3 to 480 samples per second, depending on the converter used) of a chromatogram. The selected sample rate will affect the ability to measure very narrow peaks. Sufficient number of samples (about 20) is a prerequisite for successful peak detection. This parameter decides on the size of the resulting chromatogram and the speed of its processing.

Note: Available sampling speeds may change with the acquisition equipment used (INT7, INT9, U-PAD, U-PAD2, Colibrick, Net-PAD, digital collection directly from the chromatograph, etc.).

2.3.4 Integration

Sets the integration parameters. When invoked by the menu command or by the  icon, the *Method Setup - Integration* dialog will be opened.

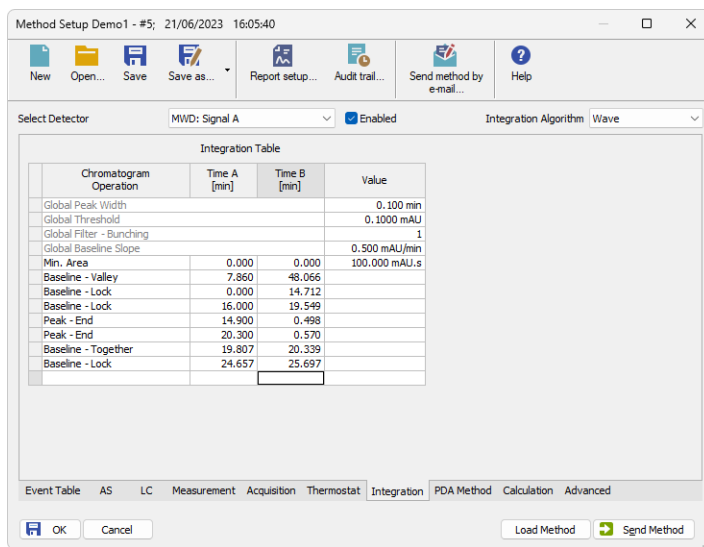


Fig. 82: Method Setup - Integration

Select Detector

Selects between integration tables for the individual detectors when using a multi-detector configuration. In such case each detector will have its own integration table.

Integration Algorithm

Selects the integration algorithm to be applied to new chromatograms measured according to this method or reprocessed according to this method. Some functions of the integration algorithm may be only present in particular versions of integration algorithm. Selected integration algorithm is common to all signals.

Currently **Clarity** offers two different integration algorithm lines - *Wave* and *Legacy*. Both lines differ in the approach to the automated integration and both have their strong sides and drawbacks. The default algorithm for newly created methods is *Legacy*.

Note: In case the selected integration algorithm fails to solve the integration of your chromatograms, we suggest to try the other one to see whether the situation will be better.

Integration Table

The integration table defines the sequence of baseline operations to be conducted with a chromatogram that will be measured according to the displayed method.

Chromatogram Operation

Selects the operations to be performed on the chromatogram. Clicking the right border of the field displays a list of all possible operations. (This is identical to the list of commands in the *Chromatogram - Baseline, Peak, Integration, Separation* and other sub- menus of the [Chromatogram](#) window).

Grp.

Group identifier for the *Add Group* and *Delete Group* commands.

Time A

- a) Indicates the starting time of the operation (for interval commands).
- b) Indicates the peak retention time (for commands that modify the peak start, peak end, etc.).

Time B

- a) Indicates the final time of the operation (for interval commands).
- b) Indicates the position of a new start, end, etc. relative to the peak apex (for commands that modify the start, end, etc.).

Note: Zero entered in the *Time B* will set the end of the interval to the end of the chromatogram.

Note: Indicating the relative position (i.e. time) is more suitable than indicating a mere absolute value, since in using the **Integration Table** the peak with the most similar retention time is then found and the peak start/end is shifted to the point calculated from the relative shift on the actual retention time. This substantially diminishes the differences in actual retention time of the same peak in different chromatograms.

Value

Value (if relevant for the operation) with appropriate units.

Paste (CTRL+V) into the Integration Table

Inserting into the **Integration Table** using the *Paste* command or using the keyboard shortcut *CTRL+V* is possible with some limitations - it is only possible to copy non-global lines of the **Integration Table** as a whole. It is not possible to paste global lines, overwrite only particular lines or just selected values. When the *Paste* operation is invoked for the **Integration Table**, **Clarity** evaluates the content of the clipboard on correctness. Incorrect clipboard content is announced by an error message and *Paste* operation fails, while on correct evaluation the focus in the **Integration Table** is moved to the empty edit line and the rows from the clipboard are added to the end of the **Integration Table**.

Note: Typical fails in evaluation of the correctness of the **Integration Table** may be too few columns in the clipboard, global operations in the clipboard or units inside of the value cells of some rows while copying from text file or Excel.

You may consider using one of the alternative approaches of copying the **Integration Table**, as described in the section **Method on pg. 276** - more

specifically the *Set Model*, *Copy from Model* and *Copy from Chromatogram* commands.

2.3.4.1 Integration table items

Several first lines of the integration table contain a default settings of basic integration parameters - *Global Peak Width*, *Global Threshold*, *Global Bunching* and *Global Baseline Slope*. These settings apply everywhere where no values for *Local Peak Width*, *Local Threshold* and *Local Baseline Slope* have been entered.

Global Peak Width / Local Peak Width [min]

This parameter defines the smallest peak width, which is to be detected. The value range is between *0,001* and *100* minutes.

The value is not critical, so even narrower peaks than the entered value will be detected, but if set incorrectly, the beginning and end of a peak may be inaccurately determined and the baseline could be incorrectly inset.

The *Global Peak Width* parameter is always displayed in the first row of the integration table and is applied to the whole chromatogram.

It is possible to set a different peak width for individual sections by adding the *Local Peak Width* parameters into further rows of the integration table which then override the *Global Peak Width* settings in the given area of chromatogram.

Global Threshold / Local Threshold [mV]

Determines the sensitivity the integration algorithm has to noise. The height of all peaks (measured from the baseline to the top) that should be detected has to be at least double this parameter. The value range must be *1 μ V - 10 V*.

The *Global Threshold* parameter is always displayed in the second row of the integration table and is applied to the whole chromatogram.

It is possible to set a different noise threshold for individual sections by adding the *Local Threshold* parameters into further rows of the integration table which then override the *Global Threshold* parameter in the given area of the chromatogram.

Note: In the *Wave* integration algorithm, peaks that are lower than twice the threshold may still appear in the chromatogram if they are on the same baseline with valid (higher) peaks not to influence the course of the baseline. Such peaks can be hidden using the *Peak - Hide* function or the baseline can be modified to remove them using the *Integration - Minimal Height* operation set to twice the threshold value (baseline changes in the latter case).

Global Bunching

Sets the averaging of data points for the signal displayed (and calculated with) in the chromatogram. *Global Bunching* serves as a filter and reduces the high frequency noise. The value must be between *1* (no averaging performed) and *250* (for each 250 data points measured, only 1 is displayed). Applying higher *Global Bunching* values will significantly change the signal course.

The *Global Bunching* parameter is always displayed in the third row of the integration table and is applied to the whole chromatogram.

Global Baseline Slope / Local Baseline Slope

Determines the position of the peak starts and peak ends on peak sides. The value must be between 0 and infinity, the higher the value the higher on the peak slope the starts and ends will be. If the value is set to 0, default peak start and peak end position is used (the value is considered to be $8 \times \text{Global Threshold}$). The slope on peak ends is considered as a negative value of the value entered, target slopes for negative peaks are using negative value for starts and positive one for peak ends.

Global Baseline Slope parameter is always displayed in the fourth row of the integration table and is applied to the whole chromatogram. It is only present for *Wave* algorithm.

It is possible to set a different slope for peak starts/ends for individual sections by adding the *Local Baseline Slope* parameters into further rows of the integration table which then override the *Global baseline Slope* parameter in the given area of the chromatogram.

Integration Interval

Limits the time period over which the chromatogram will be integrated. This means that the chromatogram profile will be ignored beyond the set time interval. This is the main difference compared to *Lock* command, which cancels already integrated peaks only in defined sections and does not reintegrate the whole chromatogram. If the parameter is not defined, integration is done on the whole chromatogram.

Rejection section

Consists of several integration parameters which specify the conditions for including/excluding peaks in/from the integration. The peak parameters must be larger than the specified values, otherwise the peak will not be displayed.

Min. Area

This parameter sets the minimum peak area in mV.s. Peaks whose area is smaller than the specified value are not displayed.

Min. Height

This parameter gives the minimum peak height in mV. Peaks whose height is smaller than the specified value are not displayed.

Half Width [min]

This parameter gives the minimum peak half-width in minutes. Peaks whose *W05* is smaller or equal to the specified value are not integrated.

Separation section

Several parameters defining the integration of non-separated peaks.

ValleyToValley Slope

Specifies the maximum slope of the baseline. If the baseline slope is smaller than the specified value, the separating perpendicular line is canceled and the baseline passes through the valley.

The default value of 0 prevents the baseline from passing through the valley.

Tangent Area Ratio

Constitutes the first condition imposed on tangential separation. The condition is satisfied if the ratio of areas of the main and the separated peak exceeds the specified value.

The default value of 0 prevents tangential separation. If there is no *Tangent Slope Ratio* item defined in the **Integration table**, its value is considered to be 1.5.

Tangent Slope Ratio

This is the second condition imposed on tangential separation. The condition is satisfied if the ratio of slopes of the second and the first peak exceeds the specified value. The slope ratio is defined as the tangent to the first peak at its end point divided into the slope of the line connecting the beginning and end of the second peak.

The default value of 0 prevents tangential separation. If there is no *Tangent Area Ratio* item defined in the **Integration table**, its value is considered to be 0.1.

For the description of the other items in the table see the chapter "**Chromatogram**" on pg. 217., namely topics [Baseline](#), [Peak](#), [Separation](#) and [Noise & Drift](#).


The evaluation process

The evaluation process does not proceed exactly in the same order as the parameters in the integration table are shown. The process is:

- Primarily initiated with the *Global (Local) Peak Width*, *Global (Local) Threshold* and *Integration Interval* parameters.
- Secondly the *ValleyToValley Slope* parameter will be applied. After all groups of non-resolved peaks have been tested by this parameter the remaining two parameters *Tangent Area Ratio* and *Tangent Slope Ratio* are applied to all remaining non-resolved groups. Tangential separation is used whenever the relevant criteria are met.
- Only then is the **Integration Table** used, followed by the *Rejections* parameters.

It thus follows that the separation parameters are not applied (e.g. to manually added peaks) and can be suppressed by the *Together* and *Valley* commands included in the **Integration table**.

2.3.5 Calculation

Sets the method of calculation. When invoked by the menu command or via the  icon, the *Method Setup - Calculation* dialog will open. When utilizing a multi-detector chromatogram, the tab will be common to all signals.

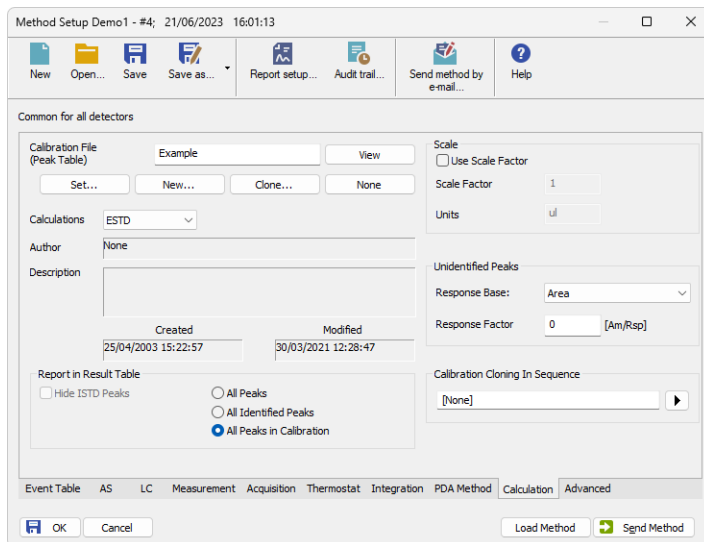


Fig. 83: Method Setup - Calculation

Calibration File (Peak Table)

Name of the calibration file to be used in the chromatograms measured with this method. The chromatograms will be automatically calibrated with this calibration file.

Note: When the selected calibration file is located in the current project (stored in the CALIB subdirectory), the relative file path is used. Otherwise, the absolute file path is used. After changing or copying a method file to a different location (e.g., a different Project), its necessary to update the path to the used calibration file.

View

Opens the calibration file in the [Calibration](#) window.

Note: The *View* command is contained in what is known as the modal window and, therefore, the [Calibration](#) window is displayed only under the [Method Setup](#) dialog. For a full display, you must close the [Method Setup](#) dialog using the *OK* or *Cancel* button.

Set...

Selects a calibration file.

New...

Creates a new empty calibration, invoking the *Save As* dialog to select the name and location of the new calibration file.

Clone...

Creates a copy of the current calibration file. Using the *Save As* dialog, you can select the name and location of the cloned calibration file. The created calibration clone will then be linked to the method.

Note: Suppose the new calibration should not contain responses from the original calibration (e.g., only the compound names and retention times are to be kept). In that case, the responses can be deleted using the *Clear Responses* checkbox in the *Save As* dialog.

None

Removes the calibration from the method. The calculation type is changed to uncalibrated - *Uncal*.

Calculations

Selects the calculation type:

Uncal

Uncalibrated calculation, no calibration file is used. The integration result is a percentage share of the individual compounds in the chromatogram.

ESTD

External standard method. The result (in the *Amount* column) is calculated using the calibration equation of the particular compound from the *Response* value of that compound.

ISTD

Internal standard. The result (in the *Amount* column) is calculated using the calibration equation of the particular compound from the *Response* value of that compound, adjusted by the ratio of responses of the internal standard in the unknown sample and in the standard.

NORM

With this calculation mode, the calculations are performed identically to the **ESTD** calculation mode according to the actual calibration settings with an added validity check: it is verified that all integrated peaks in the chromatogram are calibrated or have *Amounts* calculated in other way, and that the *Amount* values in the whole chromatogram are be empty (0). If these criteria are not fulfilled, no results are calculated, a warning message appears in the *Result Table* header, the *Peak Type* is set to *ERROR*, and the *Amount%* is empty.

STDADD

Standard Addition calculation. The resulting compound amounts in the unknown sample are calculated based on the standard addition calibration curve by extrapolating the calibration curve to point with the Y coordinate equal to zero. The results are displayed in absolute values.

Caution: Each new unknown sample will need a new calibration file - using the *Calibration Cloning In Sequence* function is highly recommended when the *STDADD* calculation is performed.

Author

Name of the user who created the calibration.

Description

Informative description of the calibration.

Created

Date of the calibration creation in the respective directory.

Caution: When copying or moving an arbitrary file, the **Created** field contains the date of this copy or move operation.

Modified

Date of the last modification.

Report in Result Table

Determines which peaks will be displayed in the Result table when using a calibration.

Note: When the *Calculations* item is set to *Uncal*, this section will be inactive (disabled).

Hide ISTD Peaks

The peaks identified as internal standards will not be present in the Results table.

All Peaks

All chromatogram peaks will be displayed.

All Identified Peaks

Only the peaks identified in the calibration file will be displayed.

All Peaks in Calibration

All peaks from the calibration file will be displayed regardless of how many peaks the chromatogram contains and which of them are identified. This is known as the fixed table format as its size is given by the number of peaks in the calibration file.

Scale

Auxiliary calculation parameters section. To utilize these options, the *Use Scale Factor* checkbox must be checked.

Note: When the *Calculations* item is set to *Uncal*, this section will be inactive (disabled).

Use Scale Factor

Permits the use of *Scale Factor* and *Units* parameters.

Scale Factor

All values in the *Amount [x]* column in the result table will be multiplied by this value.

Units After Scaling

Units of the amounts after the scaling is performed. In the result table the original units adapted from the calibration file will be replaced by the units defined here.

Unidentified Peaks

Handles the behavior of unidentified peaks present in the chromatogram.

Note: When the *Calculations* item is set to *Uncal*, this section will be inactive (disabled).

Response Base

Selects the response base (*Areal/Height*) for unidentified peaks.

Response Factor

Coefficient for calculating the *Amount* of unidentified peaks. The quantity is determined as the *Response Base* of a peak multiplied by this coefficient. This is basically an artificial single-point calibration.

Calibration Cloning In Sequence

Sets the name for cloned calibration files used in the Standard Addition calibration method, during Calibration Bracketing, or created when the *Clone on first recalibration (safe calibration usage)* option is selected in the *Sequence Options*. The field enables the use of any text, however it is recommended to use variables (accessible via the button) to create unique name for each clone, appropriate to the calibration method. For more details on the variable types and functions, see the chapter "**Chromatogram File Name**" on pg. 124.

Note: It is advantageous to use the *Sample ID (%q variable)* as a part of calibration clone name for the Standard Addition measurements, where all lines belonging to one sample (i.e., *Unknown*, possibly *Blank*, and all *Standards* on other levels of the same sample) share the same *Sample ID* in the [Sequence](#) window. For Calibration Bracketing, the use of *Date* and *Time* (in any format) as a part of the *Calibration Cloning In Sequence* field may be advantageous. For Safe Calibration Usage, the use of *Date (%D variable)* as a part of the cloned calibration name is advantageous.

2.3.6 Advanced Full version

Sets other parameters of the method, most notably the *Subtraction* and *Auxiliary Signals*. When invoked by the menu command, the *Method Setup - Advanced* dialog will open. The tab is common to all signals while performing multidetector measurement.

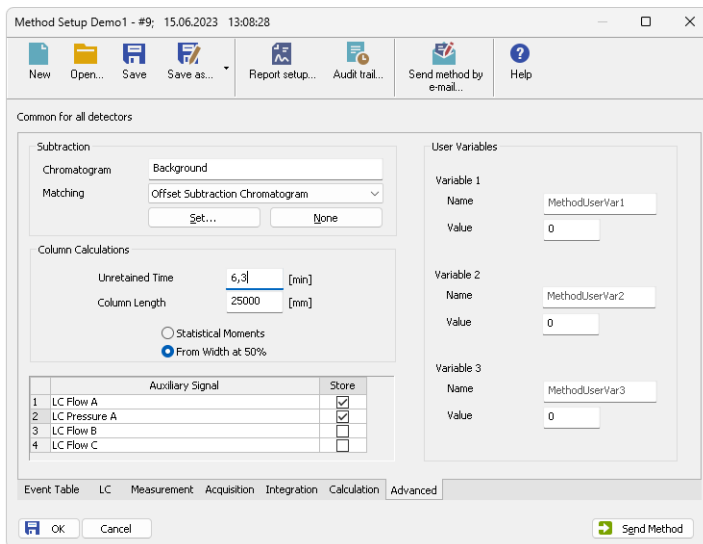


Fig. 84: Method Setup - Advanced

Subtraction

Sets an automatic subtraction of a previously measured chromatogram from the currently measured chromatogram. The subtraction will be indicated in the printout with the “*mathematics*” inscription. Use of automatic subtraction is also shown in the Chromatogram Audit Trail.

The subtracted chromatogram is saved into the measured chromatogram, it is not simply linked to it. The changes occurring with the subtraction chromatogram thus do not influence the measured chromatogram from which the background is subtracted. The subtraction, however, does not hold its history - only last subtracted chromatogram's data is saved when it is changed, all older subtraction chromatograms are discarded.

If the chromatogram being subtracted has different number of signals than the method, only the signals present both in the method and in the subtracted chromatogram will be subtracted.

Note: The subtracted chromatogram may be displayed during a measurement in the [Data Acquisition](#) window. It will appear in the background as a grey chromatogram.

Chromatogram

A dialog for specifying the subtracted chromatogram.

Matching

Sets the method of the background chromatogram subtraction.

No change - The subtraction chromatogram will be subtracted from the measured chromatogram without any additional amendments.

Offset Subtraction Chromatogram - The **Clarity** workstation attempts to “offset” the measured chromatogram with the subtraction chromatogram by shifting it on the axis X (time axis) before the actual subtracting.

Scale Subtraction Chromatogram - The **Clarity** workstation attempts to “offset” the measured chromatogram before subtracting by scaling the subtraction chromatogram on the time axis.

Note: Offsetting of chromatograms is designed according to the largest peaks in the chromatogram (i.e. either the highest peak or the peak with the greatest area).

Set...

Opens the [Open Chromatogram](#) dialog for selecting the file to be subtracted.

None

Cancels subtraction of the chromatogram.

Note: Should you wish to display e.g. the solvent only on the background of the [Data Acquisition](#) window without automatic subtraction, use the *File - Set Background Chromatogram...* command in the [Data Acquisition](#) window.

Column Calculations

Parameters affecting calculations on the [Performance](#) tab in the [Chromatogram](#) window.

Unretained Time

Determines the unretained peak time of used column in minutes. This parameter is used to calculate the capacity ratio.

Column Length

Determines the column length in millimeters. This parameter is used to calculate relative column efficiency.

Statistical Moments

Calculation runs based on statistical moments.

From Width at 50%

Calculation runs based on peak width at half the height and corresponding half-lengths.

Auxiliary Signals

This section of the *Method Setup - Advanced* tab is used for setting the auxiliary signals storing and possible display.

Note: The presence of auxiliary signals is dependent on the directly controlled device. Some of these have auxiliary signals, some do not.

Auxiliary signal

List of available auxiliary signals.

Store

Check the checkbox to save the particular auxiliary signal to the measured chromatogram.

Note: To display the auxiliary signals in the graph it is necessary to set their display in the [Graph Properties](#) dialog of the particular graph. It is, however, necessary to have the particular signal stored in order to be able to display it.

User Variables

Sets *Method User Variables* which can be used for *User Columns* calculations. Up to three independent variables can be set.

Name

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

Value

Sets the numerical value of the variable.

2.3.7 GC (LC) Control ✓ Full version

Direct instrument control pages. When prompted, the *GC (LC, LC Gradient or other)* tab of the *Method Setup* dialog will be displayed. The command is functional only if the respective control module is installed and some type of such directly controlled instrument is configured on the **Clarity** Instrument. Detailed information is included in corresponding **Clarity** Controls manual.

2.3.7.1 LC Gradient

The *Method Setup - LC Gradient* dialog serves for setting up the LC instrument method.

	Time [min]	A [%]	B [%]	C [%]	Flow [mL/min]
1	Initial	10,0	20,0	70,0	1,000
2	1,00	10,0	20,0	70,0	1,000
3	3,00	50,0	30,0	20,0	1,000
4	4,00	50,0	30,0	20,0	1,000
5					

Fig. 85: Method Setup - LC Gradient

Gradient Table

A table for setting the composition of the mobile phase and the overall flow rate as a function of time. Operation is analogous to that of spreadsheets (Excel, Quatro Pro, etc.). To prepare the cell to receive values, click it by the left mouse button; the cell will highlight by dots. A cell that fails to highlight is not available for editing.

Time [min]

Sets the time at which the ratio of flow rates and the overall flow rate correspond to the values entered in the corresponding row. (These values vary continuously from one time to the next in a manner ensuring that the conditions specified in the next row are satisfied).

XXX1(..4) [%]

Represents the percentage of a component. The designation **XXX1-4** is in fact replaced by the name of the component (items *Solvent 1 - 4* in the

[Gradient Options](#) dialog). Should you enter a component value such that the sum of all values exceeds 100 %, the percentage in the last column is automatically adjusted; if the percentage of the last compound is already zero, the value of the currently entered component is adjusted instead. The flow rate of a compound is calculated by multiplying the overall flow rate (indicated in the *Flow* column) by the corresponding percentage divided by 100.

Flow [ml/min]

Indicates the overall flow rate through the column. The entered value applies to the time specified in the corresponding row.

Graph

The graph depicts the percentage of components as a function of time together with the overall flow rate. Data are taken over from the **Gradient Table**. Changes effected in this table are immediately reflected in the graph. Legend in the header of the graph indicates the assignment of colors to individual components. The assignment is fixed and individual components are displayed in the graph from bottom to top. The flow rate is displayed as a black line.

The graph has two vertical axes: the axis on the left refers to the mixing ratio, the one on the right to the overall flow rate.

Parameters

Standby Flow

Sets the overall flow rate through the column in the *STANDBY* state reached after the last row of the table has been performed and the time period defined in the *Time to Standby* field has passed. The duration of this state is defined by the *Standby Time* item. The ratio of individual components in the respective *STANDBY* and *IDLE* states is given by the first row of the **Gradient Table** (the *Initial* row).

Time to Standby [min]

Indicates the time during which the flow rate and mobile phase composition changes continuously between the last values entered in the table and the values defined by *Standby Flow* field and the *Initial* row mobile phase composition.

This time is included in the analysis time (the Instrument is in the *CONTROL* state). In case when the *Time to Standby* is zero, there is step change from flow and components percentage specified on the last row of gradient table to that specified for *STANDBY* state.

Standby Time [min]

The time during which the flow rate is maintained at *Standby Flow*. This time is included in the analysis time (the Instrument is in the *CONTROL* state).

Idle State

An item specifying the overall flow rate through the column outside the instrument method. The following options are possible:

Pump Off

The flow rates of all components are zero.

Caution: Be careful as this setting may damage the column in some cases.

Initial

The flow rate is defined by the first row of the gradient table (the *Initial* row).

Standby

The flow rate is the same as in the *STANDBY* mode and, accordingly, corresponds to the value entered in *Standby Flow* field.

Initial - Standby

When the Method is sent to pump or the analysis has started, the flowrate is defined by the first row of the *Gradient Table* (the *Initial* row). After the last row of the table has been performed and the *Time to Standby* has passed, the overall flowrate is set to value entered in the *Stand By Flow*.

The *IDLE* state comes into effect each time an Instrument is opened, at the end or after abortion of an analysis by the *Abort* command, and is also maintained after the **Clarity** program is shut down.

The mixing ratio of individual components in both the *IDLE* and *STANDBY* states is given by the first row of the **Gradient Table** (the *Initial* row).

Note: There is a step change in the flow and components percentage from the values specified for the *STANDBY* state to those specified for the *IDLE* state if the *Idle State* field is not set to *Standby*.

Options...

Opens the [Gradient Options](#) dialog that allows the setting of minimum and maximum pressure limits and solvent names.

2.3.7.1.1 Gradient Options

Invoke the *Options...* button in the [Method Setup - LC Gradient](#) dialog to open the *Gradient Options* dialog. This dialog allows to set the custom name for particular solvents, to switch whether they are used or not in the gradient and to set the warning levels for pressure to prevent the damage to hardware.

Fig. 86: Gradient Options

Min. Pressure

Sets the minimum pressure for the given pump. When pressure drops to the set value, the pump will shut down. This prevents the solvent leakage.

Max. Pressure

Sets the maximum pressure for the given pump. When pressure reaches the set value, the pump will shut down. This serves to prevent the damage to the pump when the column is blocked.

Max. Pressure for Set Flow

Sets the maximum pressure to be used in the *Set Flow...* dialog in the "Device Monitor" on page 135.

Solvent 1 (.4)







It is possible to enable/disable particular solvent, as well as to set custom name to it.

2.3.8 AS


Selection of autosampler sampling program. When prompted, the AS tab of the [Method Setup](#) dialog will be displayed. The command will only be functional if the respective control module has been installed and a directly controlled autosampler is configured on the given Instrument. Detailed information on AS tab can be found in the manual of respective control module.

2.4 Analysis

This is a submenu containing commands for measurement control:

	Single	Prepares and measures a single analysis.
	Sequence	Prepares and measures a series of analyses.
	Batch <small>✓ Full version</small>	Processes previously performed analyses.
	Data Acquisition	Displays the signal of the connected detectors. Displays the signals of connected detectors. After selection, the Data Acquisition dialog described on pg. 369. appears. You may also select this dialog by using the  icon located in the Instrument window.
	Device Monitor	Monitors chromatograph status.

2.4.1 Single Analysis

Prepares and runs a single analysis. Invoking this command opens the *Single Analysis* dialog, which can also be opened using the  icon in the [Instrument](#) window. The dialog provides commands for controlling a measurement and its fundamental description. It contains tabs of individual sections:

- "Single Analysis - Analysis tab" on the next page
- "Single Analysis - Post Run Settings" on page 120
- "Single Analysis - User Variables" on page 123

Note: If the *Analysis* tab contains other fields than described here, then you are probably using one of the **Extensions** (such as **GPC** or **EA**), refer to the corresponding manual.

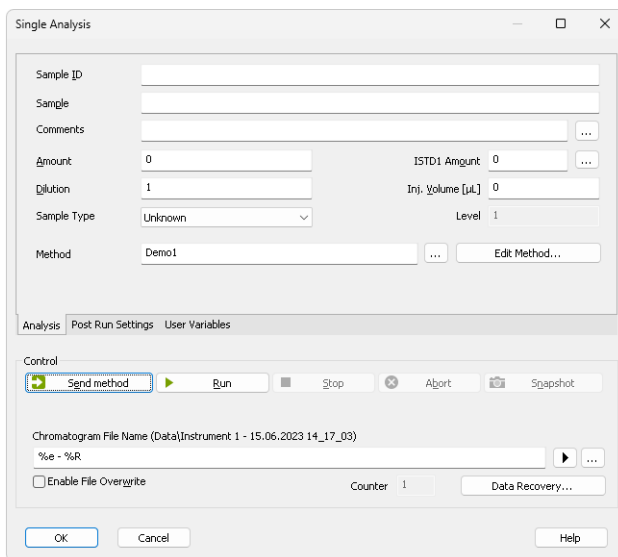


Fig. 87: Single Analysis - Analysis tab

Analysis

Comprises the description and parameters of single analysis. All entered values will be transferred to the chromatogram header after completion of the analysis.


Sample ID

Sample identification field used for information purposes only. Maximum number of characters in this field is limited to 64. Variables that can be used are described in the *Chromatogram File Name* field (for more details see the chapter **Chromatogram File Name** on pg. 124).

Sample

Sample description used for information purposes only. Maximum number of characters in this field is limited to 64. Variables that can be used are described in the *Chromatogram File Name* field (for more details see the chapter **Chromatogram File Name** on pg. 124).

Comments

Serves for adding some information about the chromatogram created by current method. Comments can be edited in the [Comments](#) dialog accessible through the  button.

Amount

Sample amount. The value is used in calibration calculations of individual components percentage in the *ESTD* and *ISTD* methods. In *ISTD* enter the sample amount without the addition. Enter values using the same units that were used in the calibration file (*Units - Compound* parameter in [Calibration Options](#) window). The default value is 0.

ISTD Amount

An added amount of the internal standards for the ISTD method - the amount of the ISTD1 can be directly edited in the *Single Analysis* dialog, the amounts for ISTD2 - ISTD10 can be set using the [Edit ISTD Amounts](#) dialog accessible through the button next to it. Always state this parameter in the same units that are used in the calibration file (*Units - Compound* parameter in [Calibration Options](#) window). The default value is 0.

Dilution

A sample dilution factor. This value is used to multiply each calibrated amount in the *Amount* column of the *Result Table*. Dilution factor is the total number of unit volumes in which the sample was dissolved. In other words, dilution represents the total volume of solute + solvent. The default value is 1.

Inj. Volume

An injected volume of the sample. The responses of all compounds will be corrected by the ratio of this value and the *Default Injected Volume* parameter from the calibration file in recalibration or calibration calculations. The default value is 0. The units are set in the [Instrument Units](#) dialog (described in the chapter "**Right section of System Configuration dialog**" on pg. 19.).

Sample Type

Sets the type of the sample being measured. This option cannot be changed during running analysis. Possible options are:

Unknown - denotes an unknown sample and resulting chromatograms will be stored in the data sub-directory.

Standard - measured chromatogram will be used to create a calibration which needs to be specified (*Calibration File*) in the method on the [Calculation tab](#). Resulting chromatograms will be stored in the calibration sub-directory.

Blank - in fact a calibration standard with no amount of added sample. The *Blank* is thus one point of a calibration curve (with the *Amount* of 0). Calibration file needs to be specified (*Calibration File*) in the method on the [Calculation tab](#).

Level

Sets the calibration level for calibration or recalibration. This field is active only when *Standard* option is selected.

Method

Displays method which will be used to acquire chromatogram. Name of existing method can be directly inserted into the row or it can be chosen via the button. To view or edit method which is displayed, simply press the *Edit Method...* button which will open corresponding method in the [Method Setup](#) dialog. During a running analysis another method may still be opened (will not be sent) in the Method Setup.

Control


Section with commands and parameters for controlling an analysis.

Send Method

Sends method, that is displayed in the *Method* row, parameters to controlled modules, regardless on the setting of the LC/GC/AS method.

Note: The *Send Method* button is visible only when the instrument is configured with a control module.

Run

Runs an analysis. Analysis in progress is indicated by the inscription *RUNNING* in the **Status Line** below the  icon. The parameters of the current measurement method in the [Method Setup - Acquisition](#) dialog cannot be changed while an analysis is in progress.

Invoking Run command during analysis is possible only when *External Start* setting in [Method Setup - Measurement](#) dialog is set to *Start-Restart*. Clicking the command terminates running analysis and at the same time starts another one - this operation procedure is often called continuous measurement.

If you enter the *Chromatogram File Name* including a subfolder, for example *%B_%Y%e - %R%e - %R*, then the *Clarity - Directories* dialog will be displayed.

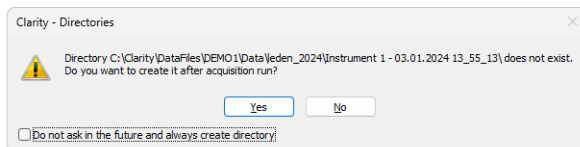


Fig. 88: *Clarity - Directories* dialog when the subdirectory doesn't exist

Click *Yes* if you want to allow Clarity to create the subfolder after the acquisition is finished. If you press *No*, then you must delete the directory and the backslash from the *Chromatogram File Name*. In the dialog you can see that it is also possible to use the parameters in the subfolder name as in the chromatogram name.

Note: Invoking the command during analysis is possible only when there are only analog detectors (INT7, Net-PAD,...) configured on Instrument. If there is one or more digital detectors on Instrument, invoking the command during analysis is not possible.

Stop

Terminates the running analysis and processes the results - a chromatogram is created with the name entered in the *Chromatogram File Name* field. The method used in its processing is the measurement method (its name is found in the **Information Table**). Events following the completion of an analysis are specified by items from the "Single Analysis - Post Run Settings" on page 120 tab. The Instrument returns to the *STOP* or *WAITING* state. While the program controlling the chromatograph is running, *CONTROL* is displayed.

Abort

Aborts an analysis without storing or processing the data. The instrument will return to either the *STOP* or *WAITING* state, the chromatograph controlling program, if any, is aborted.

Snapshot

Processes the existing part of the analysis without its termination. A chromatogram is created using the name specified in *Chromatogram File Name* field. The processing mode is the same as with the *Stop* command, the Instrument, however, remains *RUNNING*. If you are about to replace an already existing file, you will receive a warning, but only upon the first use.

Use Autosampler

This checkbox enables to perform injection using directly controlled autosampler. Once checked, this option renames *Run* button to *Inject & Run*. Incorrect *Inj. Volume* will prevent you from starting the acquisition. The checkbox will remain checked until the user unchecks it again.

Note: Only an autosampler configured in the *System Configuration* can be used to perform the injection. If an autosampler is not configured, option to *Use Autosampler* will be hidden and thus not possible to use.

Vial

Specifies vial number from which one injection will be performed. Incorrect vial number triggers an error and must be solved otherwise it is not possible to perform an injection. Autosamplers supporting graphical interface for inserting vial number, display - clicking this button invokes *Select Vial* dialog for selecting a vial.

Chromatogram File Name

Sample name for created chromatograms. The name can be composed of fixed expressions, as well as variable parameters (e.g. adding time, date and/or sample ID and many other parameters). Fixed part may be combined with the variable part in a single chromatogram name.

Chromatogram File Name is checked for correctness of the name. Upon clicking the *Run* button, invalid name triggers a message with a description of the problem.

After clicking the button a list of available parameters and a brief description of their functions is displayed. You may stepwise compose the title of the file by selecting the required variables (for more details see the chapter **Chromatogram File Name** on pg. 124).

It is possible to include also the name of a subfolder in the name to store chromatograms into subfolders of the [Data Subdirectory](#). E.g. the *MySubProject\MyFileName* in the DEMO1 project will result in the MYFILENAME.PRM stored in the C:\CLARITY\DATAFILES\DEMO1\DATA\MYSUBPROJECT folder. If the subfolder doesn't exist, then it will be created when the chromatogram is stored.

Note: *Chromatogram File Name* field content can be changed when the analysis is running and will influence the name of its resulting chromatogram, when the change is accepted by pressing the *OK* button afterwards.



Selects a chromatogram location that is different from the current project. After clicking on this button the *Save As* dialog will appear. Here you may select a folder for saving the chromatogram.

Note: It is not particularly suitable to save chromatograms outside of their project folder.

This button is most often used for determining the titles of previously existing files in the folder and helps to avoid the use of identical titles. It is also possible to create a new file on the basis of an already existing title.

Enable File Overwrite

Enables the overwrite of existing chromatograms without giving notice. It is necessary to close the *Single Analysis* dialog and open it again for this setting to take effect.

In case the file overwriting is not allowed and the chromatogram with the same name already exists, a chromatogram with the same name and suffix *_001.PRM* is created instead. The number of such suffix is then incremented in case the necessary file name is already taken. This is applied when an acquisition is restarted and following conditions are set in the method: *External Start/Stop* is chosen and *Start - Restart* mode is selected.

Counter

Shows the current value of the sample counter. If automatic numbering is used for naming chromatograms in the *%n* format, the current value may be changed here.

Data Recovery...

Rescues data from an interrupted analysis. If an analysis has been interrupted for any reason (power failure, computer breakdown, invocation of the *Abort* command, etc.) a portion of the measured chromatogram may still be rescued.

Invoking the command opens the *Rescue Data* dialog where you select from the **LAST.RAW* and **RUN.RAW* files. If no data can be rescued, the items will be dimmed.

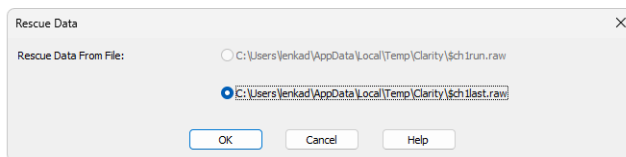


Fig. 89: *Rescue Data*

The **LAST.RAW* and **RUN.RAW* files are stored in the *TEMP* subdirectory located on local disk in Windows User's account directory (*C:\USERS\<USER NAME>\APPDATA\LOCAL\TEMP\CLARITY* by default).

Note: The AppData folder is hidden in Windows by default.

The *RUN.RAW file will be created only when **Clarity** station has crashed while measuring data (e.g. after a power failure). Otherwise the last measured chromatogram will always be saved to the *LAST.RAW file.

Pressing the *OK* button invokes the *Save As* dialog.

During a running analysis data are saved to the hard disk with various period and duration of this period is dependent on used instrumentation (detector).

2.4.1.1 Single Analysis - Post Run Settings

Settings found on the "Single Analysis - Post Run Settings" below tab serve for post-processing of a chromatogram. Selected actions are always executed following the completion of each **Single Analysis** measurement.

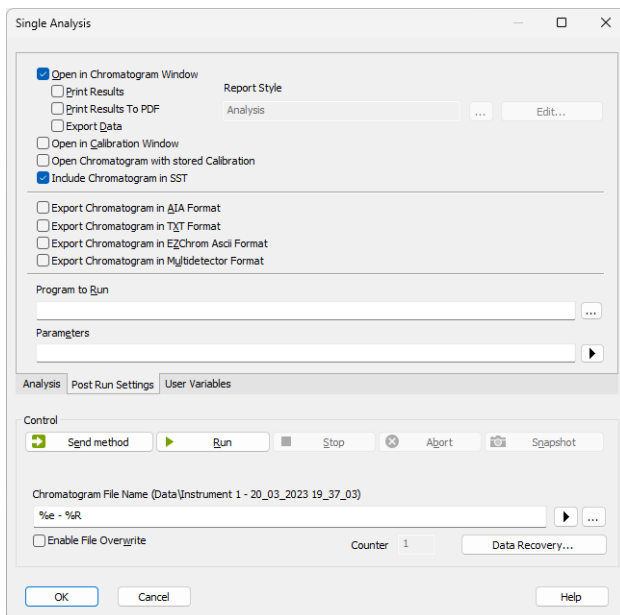


Fig. 90: Single Analysis - Post Run Settings

Open in Chromatogram Window

The created chromatogram will be automatically opened in the [Chromatogram](#) window. If the [Chromatogram](#) window is minimized it will not maximize once a new chromatogram is created.

Note: When there is a running acquisition with automatic opening of acquired chromatogram enabled and there is open chromatogram in [Chromatogram](#) window containing unsaved changes and the *OVERLAY MODE* is switched off the automatic opening of new chromatogram is suppressed. There is also a record of this suppressed opening of new chromatogram in [Station Audit Trail](#).

Note: When there is a running acquisition with automatic opening of acquired chromatogram enabled and there are opened chromatograms in [Chromatogram](#) window in *OVERLAY MODE* at maximum number governed by limit in [General tab](#) of [User Options](#) dialog and at least one of opened chromatograms contains unsaved changes the automatic opening of new chromatogram is suppressed. There is also a record of this suppressed opening of new chromatogram in [Station Audit Trail](#).

Report Style

Displays selected report style according to which results will be printed - for *Single Analysis* the default report style is ANALYSIS.STY. Name of existing report style can be directly inserted into the row or it can be chosen via the button. To view or edit report style which is displayed, simply press the *Edit...* button which will open corresponding method in the [Report Setup](#) dialog.

Print Results

A report will be printed according to the print style set in the *Report Style* field.

Print Results To PDF

A report will be printed to *.PDF file according to the print style set in the *Report Style* field.

Export Data

The created chromatogram will be exported according to settings made in the [Export Data](#) dialog (for more details see also chapter **Export Data** on pg. 141).

Open in Calibration Window

The created chromatogram will be automatically opened in the [Calibration](#) window.

Include Chromatogram in SST

Sets whether the created chromatogram will be included in the SST calculations or not.

Open Chromatogram with Stored Calibration

Chromatogram will be opened with the recent stored version of the calibration file, as opposed to the linked calibration when not checked.

Export Chromatogram in AIA Format

Exports a chromatogram in AIA format. This corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window. The exported chromatogram will be saved under the same name as the source chromatogram (with the *.CDF suffix) and located in the same directory (for more details see also chapter **Export Chromatogram** on pg. 182).

Export Chromatogram in TXT Format

Exports a chromatogram in the TXT format. Corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The exported chromatogram will be saved under the same name as the source chromatogram (with the *.TXT suffix) and located in the same directory.

Export Chromatogram in EZChrom ASCII Format

Exports a chromatogram in the ASC text format, which is used by the EZ CHROM program. This corresponds to *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The exported chromatogram will be saved under the same name as the source chromatogram (with the *.ASC suffix) and located in the same directory.

Export Chromatogram in Multidetector Format

Exports a chromatogram in the TXT format. Multiple signals will be stored in separate columns of the resulting file. Corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The exported chromatogram will be saved under the same name as the source chromatogram (with the *.TXT suffix) and located in the same directory.

Program to Run

Sets the program which will be run after the completion of the measurement.



Searches for the program which should be entered in the *Program to Run* field.

Only with Export

This item has two functions:

- The program specified in the *Program to Run* field will only be run if the *Automatic Export* checkbox has been selected.
- While manually exporting from the [Chromatogram](#) window using **Ctrl + E** shortcut this item enables the simultaneous running of the program specified in the *Program to Run* field.

Parameters

Parameters of the run program, which are normally entered in the command line behind the program name (e.g. name of loaded file, macro, etc.).

The following variables can be used in the *Parameters* field:

- Variable %f will be substituted by the name of the chromatogram at the moment of processing.
- Variable %e will be substituted by the name of the file to be exported at the moment of processing. (This does not apply when exporting multidetector chromatograms in TXT or AIA formats.)

Click the button next to the *Parameters* field to enter the variables automatically.

For facilitating of exported chromatogram files copying you can use COPYFILES.EXE utility, located in UTILS subfolder. It allows you to copy all the exports from one chromatogram (.TXT, .PDF) at once. An utility is thoroughly described in COPYFILES.TXT file in the same folder.

2.4.1.2 Single Analysis - User Variables

Settings found on the "Single Analysis - User Variables" below tab serves for setting *Analysis User Variables* which can be used for *User Columns* calculations. Up to three independent variables can be set.

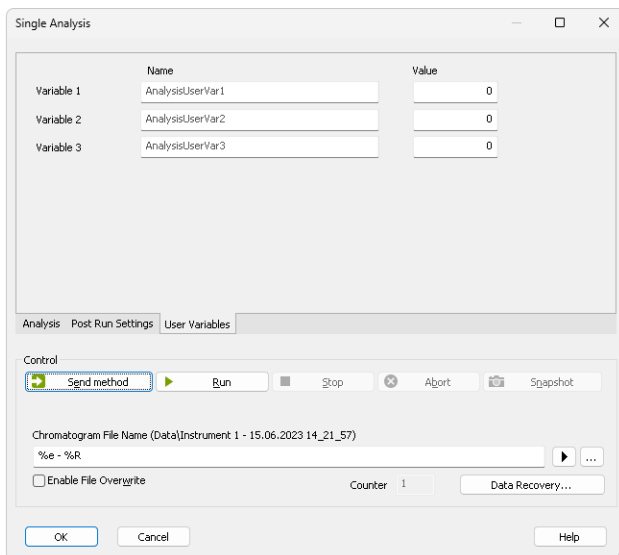


Fig. 91: Single Analysis - User Variables


Name


Enables to name the variable. If the field is left empty, default name *AnalysisUserVar1 - AnalysisUserVar3* will remain filled in.

Value

Enables to set numeric value for the specific variable.

2.4.1.3 Chromatogram File Name

This field contains a template for creating chromatogram names. Up to 254 characters may be entered including spaces and international characters, the following characters are, however, forbidden: 

Note: If the current value of the variable contains a forbidden character it is replaced by 

The automatic filename composition option is a powerful tool. The station uses a set of variables preceded by the "%" character as described below. After an analysis is terminated each variable is replaced by its current value. Variables may be combined at will. The current value is displayed in parentheses above the editing field and in the **Information table** of the [Instrument](#) window.

Tab. 6: List of common file name variables

Variable	Meaning	Example of use
%n	Sample serial number, also called <i>Counter</i> , which is automatically incremented every time the chromatogram is created (when multiple <i>Snapshot</i> functions are used during the same acquisition, and the resulting chromatogram is either created or not, the counter is incremented only once). The value may be modified depending on the place - for single measurements in the Single Analysis dialog, the <i>Counter</i> field or for sequences in the <i>Counter value</i> field in the Sequence Options dialog of the particular sequence. The counter values for single analysis and sequence are separate. Alternatively, the counters may be set automatically to 0 or 1 each time the Instrument is opened by the <i>Reset when Open Instrument</i> checkbox from the <i>Counter</i> section of the User Options - General dialog (for single analysis) or through <i>Counter</i> section in the Sequence Options for sequence counter.	
%P	Name of the project.	Pollutants
%J	Name of the method (without .MET suffix).	DDTInWater
%s	Name of the sequence (without .SEQ suffix).	BalticSea
%V, %v	Vial number (Only for the sequence table or when an autosampler is used in single analysis).	
%I, %i	The number of the injection taken from a given vial (Only for the sequence table).	
%L, %l	The Sequence Line Number is a number of the row in the Sequence Table (Only for the sequence table).	

Variable	Meaning	Example of use
%c	Number of an Instrument.	
%e	Name of an Instrument.	
%g	Analyst name/ User name.	
%Q	Sample (contents of the Sample field).	
%q	Sample ID (contents of the Sample ID field).	
%f	Vial barcode.	BarCode-00001
%%	The sign for percentage.	%
%T	Time of the analysis start (in the format hh-mm).	%T=13-41
%D	Date (in the format dd_mm_yyyy).	%D=24_02_2009

Additionally, some of the above variables allow for special formatting - namely variables for counter (%n), vial number (%v or %V), sequence injection number (%i or %I), sequence line number (%l or %L) and Instrument number (%c). These allow for defining the particular number of places used, counter in addition allows to define step by which the counter will be incremented.

Variable	Meaning	Example of use
%xn	Selects fixed number of places for the variable. The number is formatted using preceding zeroes where needed (e.g. for x=3:).	%3n = 001-999
%n(x)	Selects step for the counter, (e.g. for x=5:).	%n(5)=1, 6, 11

Note: Sometimes vial number variable may be noted in alphanumerical values rather than simple numerical values (e.g. vial B1), in such case special number formatting is not used and the alphanumerical value is used as it is.

Advanced date and time formatting

Submenu with advanced date and time formatting functions.


Tab. 7: List of advanced file name variables

Variable	Meaning	Example of use
%H	Hours (24-hour format).	00 - 24
%h	Hours in the (12-hour format).	00 - 12
%p	Designation a.m./p.m.	AM/PM
%M	Minutes.	0 - 59
%S	Seconds.	0 - 59
%a	Day of the week (abbreviated).	Mo, Thu, ...
%A	Day of the week.	Monday, ...
%b	Month (abbreviated).	Jan, Feb, ...
%B	Month name.	January, ...
%R, %r	Date and time of the analysis start as set in the current Windows format.	
%o	Day of month.	01 - 31
%j	Day in calendar year.	1 - 366
%m	Month.	01 - 12
%U	Week of calendar year beginning on Sunday.	00 - 53
%u	Day of week beginning on Sunday.	1 - 7
%W	Week of calendar year beginning on Monday.	00 - 53
%w	Day of week beginning on Monday.	1 - 7
%x	Date as set in the current Windows format.	
%X	Time as set in the current Windows format.	
%y	Last two digits of calendar year.	00 - 99
%Y	Full calendar year.	2001
%Z	Name of the time zone.	

The above variables may also be used in *Sample* and *Sample ID* fields both for individual injections and in a sequence table. In order to use the variables in *Sample* and *Sample ID* fields you must also use it in the filename.

Note: Some parameters (e.g. %p) may depend on the settings in the **Windows** system and may thus be shown in different format than in the table above.

2.4.1.4 Comments

The *Comments* dialog allows the user to enter any description of the method. The description can be formatted using the classical functions of text processors (Bold, Italics, Underlined text, text alignment, text color, text font, text size, bulleted text). This dialog is accessible (and the method description can be edited) prior to the analysis from the [Single Analysis](#) or [Sequence](#) dialog using the  button or after the analysis has ended from the [Chromatogram](#) window using the *Edit...* button in the *Chromatogram* section of the [Measurement Conditions - Instrument](#) tab.

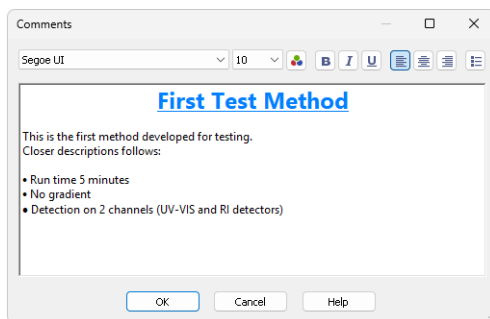


Fig. 92: Comments

2.4.2 Sequence

Command for the preparation and measurement of a series of analyses using sequence file. The [Sequence](#) window is displayed at the prompt. The major component is a **Sequence Table**, where each line describes the method of processing for one or more samples. Detailed information on [Sequence](#) window can be found in in the chapter "**Sequence**" on pg. **385**.

2.4.3 Batch Full version

Batch processes single chromatograms, automatically and simultaneously executes selected actions with numerous chromatograms or reprocesses whole sequences. When invoked, the *Batch* dialog will be displayed.

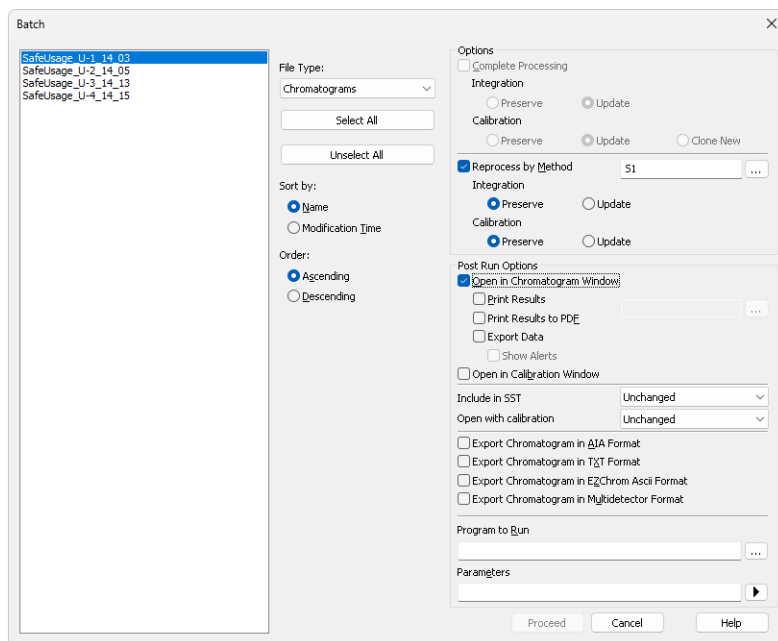


Fig. 93: Batch

List of files

Lists all chromatograms or sequences from the current project according to the settings in the *File Type* field. Left click the mouse while holding the **Shift** or **Ctrl** key to select and deselect multiple files. This will enable you to progressively mark any arbitrary number of displayed files.

File Type

Selects the type of files to be batch processed.

Chromatograms - The list will display all chromatograms from the data subdirectory and its subdirectories.

Calibration Standards - The list will display all chromatograms from the calibration subdirectory and its subdirectories. (i.e. calibration standards).

Sequence Files - Sequences from the current project will be displayed. You can change information on several columns (*Run*, *Sample Type*,

Lvl, *Report Style* and *Postrun functions*) of the already measured sequence file to define which rows should be reprocessed and how.

Note: Each sequence file remembers chromatograms, which were measured last and, therefore, it is not necessary to update the *File Name* column. Chromatograms not found are ignored.

Caution: When a sequence is run repeatedly, the list of measured files in that sequence will be reset and the original files cannot be processed using the *Batch* command.

Select All/ Unselect All

Quickly selects or deselects all files in the list.

Sort by

Sorts files by *Name* or by the *Time* upon which they were last saved.

Order

Sorts files in *Ascending* or *Descending* order based on *Sort by* setting. As files are processed in the order in which they appear in the list, the order of processing can be changed this way.

Options section

Options section is divided to two halves - one for *Complete Processing*, the other for *Reprocess by Method*. These sections are mutually exclusive.

Complete Processing

This command is active only for processing chromatograms according to the sequence file (the *File Type* field must be set to *Sequence Files*). In this case, all chromatograms will be processed according to the current sequence table contents and methods used, including the eventual recalibration. This means that you can batch change headers of already measured chromatograms and reintegrate them, if you modify the integration parameters in used methods, etc.

Note: The *Post Run Options* section is disabled as the Post Run activities will be performed exactly according to the sequence settings on a particular sequence row during the reprocess.

Caution: Only the last set of measured chromatograms will be processed (if the same sequence was used more than once and reset in between uses).

Integration

Governs the behavior of the integration tables contained within chromatograms that originated from the given sequence. With *Preserve* option the Integration tables will not be changed during the reprocess, with *Update* option (default) the Integration tables of chromatograms will be replaced by the integration tables of signals as they are in the method used on a given sequence table row.

Calibration

Governs the behavior of calibration handling in the sequence being reprocessed. With *Preserve* option the calibrations connected to the

particular chromatograms will be left as they are (see note below), for sequence rows with calibration standards and calibration level filled in the calibration will not be recalibrated. With *Update* option (default), the calibrations that are currently connected to the chromatograms will be used for potential recalibration (if the sequence contains samples marked as calibration standards with level filled in) and the latest version of the calibration available at that moment will be connected to the chromatogram being reprocessed. In case the sequence used calibration cloning, the original clone will be used. With the *Clone New* option, in case the sequence used calibration cloning, a new set of calibrations will be cloned, calibrated and the chromatograms will be reconnected to these new clones. In case the sequence does not use calibration cloning, the option behaves same as *Update* option.

Note: The *Open with stored calibration* checkbox in the *Sequence* controls how the chromatogram is opened - if checked, it is opened with the version of the calibration last stored in the chromatogram (in case of *Update*, the version after reprocessing), and any subsequent changes do not affect it. Otherwise, the chromatogram opens with the linked "live" calibration - any calibration change is immediately propagated to the chromatogram results.

Reprocess by Method

Reprocesses all selected chromatograms according to the selected method. By default, displayed method matches method in the [Single Analysis](#) dialog. This option can be used with both chromatograms and sequences - in case of sequences, selected sequence only serves as a source of selection of the used chromatograms, e.g. no recalibration will be performed no matter the settings.

Integration

Governs the behavior of the integration tables contained within selected chromatograms. With *Preserve* option the Integration tables will not be changed during the reprocess, with *Update* option (default) the Integration tables of chromatograms will be replaced by the integration tables of signals in the method used for reprocessing.

Calibration

Governs the behavior of calibration handling in the chromatograms being reprocessed. With *Preserve* option the calibrations connected to the particular chromatograms will be left as they are (see note below), with *Update* option (default), the calibrations in the chromatograms will be replaced by the calibration set in the method used for reprocessing.

Note: The *Open with Calibration* drop-down list controls how the chromatogram is opened, when *Unchanged* is selected, the setting in the chromatogram itself is used. If *Stored*, it is opened with the version of the calibration last stored in the chromatogram (in case of *Update*, the version after reprocessing), and any subsequent changes do not affect it. Otherwise, the chromatogram opens with the linked "live" calibration - any calibration change is immediately propagated to the chromatogram results.

Post Run Options section

This section allows to perform the post-run action same as if set in [Single Analysis](#) dialog or [Sequence](#) window. The actions will be carried out on selected chromatograms or chromatograms measured from selected sequence. The actions can be performed standalone or in a combination with *Reprocess by Method* option.

Open in Chromatogram Window

Chromatogram will be opened in the [Chromatogram](#) window. Opening of the chromatogram in [Chromatogram](#) window is necessary for several further actions (printing or exporting result tables) so these further options are available only if the *Open in Chromatogram Window* checkbox is enabled. Chromatograms are opened in the window according to the current display options there (*Overlay* mode on/off, number of chromatograms opened at the same time, table layouts) which may influence printed results (e.g. contents of a printed Summary table).

Print Results

Prints a report according to the selected report style. Each report style is adjustable in the [Report Setup](#) dialog which is accessible from different windows and dialogs, such as *Single Analysis* and *Method Setup* dialogs, *Sequence*, *Chromatogram* and *Calibration* windows and others.

Print Results to PDF

Prints a report to the *.PDF file according to the selected report style.

Export Data

Each chromatogram will be exported according to the settings in the [Export Data](#) dialog (for more details see also chapter **Export Data** on pg. 141).

Show Alerts

Sets the display of system alerts possibly appearing during the export - if checked, the alerts are displayed in user interface in addition to saving them in the log (which happens no matter the setting).

Open in Calibration Window

Chromatogram will be opened in the [Calibration](#) window, no further actions are performed with it.

Include in SST

Selects whether the batch-processed chromatograms will be included in SST calculations. Available options are *Exclude*, *Include* and *Unchanged*.

Open with calibration

Selects the type of calibration with which the chromatogram will be opened. Available options are *Linked*, *Stored* or *Unchanged*. *Linked* and *Stored* values influence how the chromatogram will be opened for particular other actions set in the *Batch* dialog (such as print or export) and are then saved to the chromatogram itself, so that after the reprocess the chromatogram will be opened by default from the file manager in the same manner as well. *Unchanged* value leaves the same parameter in the chromatogram untouched.

Note: The setting also influences calibration handling in case *Preserve* option is selected in *Reprocess by Method* section - with chromatograms opened using the *Stored* option the calibration will stay exactly as it was before reprocessing, with *Linked* option the latest version of the same calibration will be used within chromatogram.

Export Chromatogram in AIA Format

Exports a chromatogram in AIA format. Corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The CDF format file will have the same name as the chromatogram and will be saved in the same (data or calibration) subdirectory of the current project as the exported chromatogram.

Export Chromatogram in TXT Format

Exports a chromatogram in TXT format. Corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The TXT format file will have the same name as the chromatogram and will be saved in the same (data or calibration) subdirectory of the current project as the exported chromatogram.

Export Chromatogram in EZChrom Ascii Format

Exports a chromatogram in ASC text format, as it is used by the EZ-Chrom program. Corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

A file with the ASC suffix will have the same name as the chromatogram and will be saved in the same (data or calibration) subdirectory of the current project as the exported chromatogram.

Export Chromatogram in Multidetector Format

Exports a chromatogram in CHR text format so that all signals of multidetector chromatogram are exported to a single file (for more details see also chapter **Export Chromatogram** on pg. 182).

A file with the CHR suffix will have the same name as the chromatogram and will be saved in the same (data or calibration) subdirectory of the current project as the exported chromatogram.

Program to Run


Allows to select the program that should be started as part of the chromatogram reprocess (e.g. EXCEL.EXE).



Searches for the program to be run. Standard **MS Windows** window will be displayed for program search.

Parameters

Sets the parameters of an initiated program; these parameters are generally entered in the command line after the program name (e.g. name of loaded file, etc.).

The following variables can be used in the *Parameters* field (the  button allows to select them interactively):

- *%f* will be replaced by the name of the chromatogram after export.
- *%e* will be replaced by the name of the file after export. This does not apply when exporting multidetector chromatograms in the .TXT or .AIA formats.

Proceed

Runs batch processing.

2.4.4 Device Monitor

Displays the current status of a directly controlled chromatograph and other controlled modules. Invoking this command opens the *Device Monitor* window, which accommodates monitors from multiple devices.

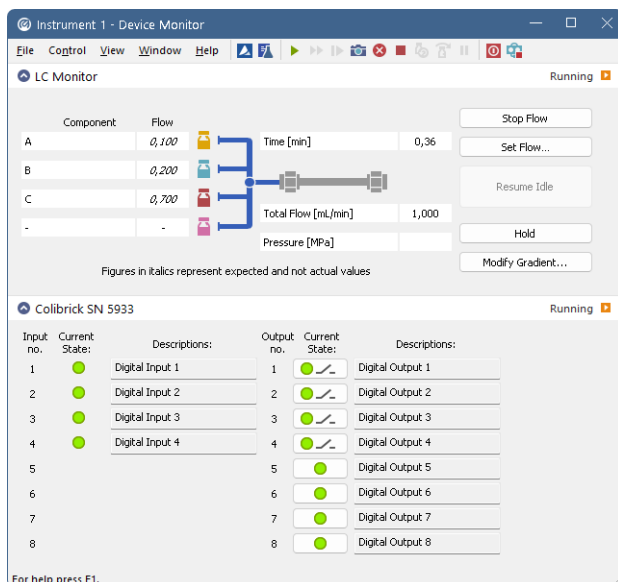


Fig. 94: Device Monitor

Menu

File	Submenu for controlling the <i>Device Monitor</i> window.
Control	Submenu for controlling the device.
View	Submenu of commands for setting up the appearance of the <i>Device Monitor</i> window.
Window	Submenu containing commands governing the appearance of base windows.
Help	Submenu of commands that displays help.

Toolbar

The toolbar includes buttons that can be used for controlling the analysis process (*Run Single*, *Run Sequence*, *Resume Sequence*, *Snapshot*, *Abort*, *Stop*, *Shutdown*, etc.) (for the description of these functions see the chapter "**Single Analysis**" on pg. 113. and the chapter "**Sequence**" on pg. 385.). Additionally the (*Stop Flow*, *Set Flow...*, *Resume Idle*, *Hold* and *Modify Gradient...*) functional

buttons will be available in selected monitors after the appropriate control module has been installed and configured in the [System Configuration](#) window. A detailed description of the particular sections of the *Device Monitor* window can be found in corresponding manuals for Control modules.

Use [Customize...](#) dialog to add icons/commands to toolbars.

Individual panels - monitors

Context menu in *Device Monitor* window (right mouseclick) enables to change the order of individual device monitor panes.

Individual monitor panes can be collapsed/expanded using the checkbox in the header of the pane (left to the Device Name). In the collapsed form only the state is displayed.

2.4.4.1 File

Close Window Closes the [Device Monitor](#) window.

2.4.4.2 Control

Send Method Sends method, that is displayed in the [Single Analysis](#) dialog on the *Method* row, to controlled modules, regardless on the setting of the LC/GC/AS method.

Shut Down Function is individual for each device. Detailed description is in a separate manuals for Control modules.

LC Control

- **Stop Flow** : Function is individual for each device. Detailed description is in a separate manuals for Control modules.
- **Set Flow...** : Command for flushing/purging the pump outside a run.
- **Resume Idle** : Resumes back to *IDLE* state after flushing/purging the pump using the *Purge* command.
- **Hold** : Pauses the execution of the **Gradient Table** at the actual flow and mobile phase composition. The same flow and composition will be maintained until the *Resume* button is pressed.
- **Resume** : Resumes the execution of the **Gradient Table** after the *Hold* button has been pressed.
- **Modify Gradient...** : Opens the [LC Control Manual Flow](#) dialog allowing to set custom flow and mobile phase composition, disregarding the **Gradient Table** set in the method.

Note: Availability of *Resume / Hold* and *Modify Gradient* commands depend on the capabilities of pumps used in the gradient. The commands are only available while an analysis is running.

2.4.4.2.1 LC Control Manual Flow

The *LC Control Manual Flow* dialog accessible through using the *Modify Gradient...* button from [Device Monitor](#) window allows the user to set a custom mobile phase composition and flow while the analysis is running. It resembles the [Method Setup - LC Gradient](#) tab in functionality.

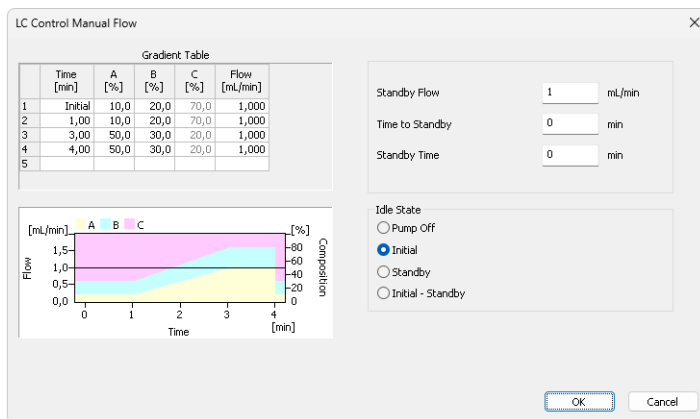


Fig. 95: LC Control Manual Flow dialog



The *LC Control Manual Flow* dialog is only available while an analysis is running. When it is invoked and the *OK* button is pressed, the original **Gradient Table** from the acquisition method is discarded and replaced by the **Gradient Table** from the *LC Control Manual Flow* dialog. Any such operation is recorded in the audit trail of the measured chromatogram.

Caution: After the analysis run which used manual flow changes ends, the original method is automatically sent to all controlled devices to make sure **Clarity** station returns to the original method.

2.4.4.3 View

Fit to Content	When selected, the window changes its size according to its content. When not selected, the window can be re-sized according to individual preferences - the size will be automatically saved into corresponding desktop (*.DSK) file.
Toolbars	<p>Displays commands for toolbars. The command is analogous to that shown in the Clarity window (for more details see also chapter View on pg. 43).</p> <ul style="list-style-type: none"> • Customize...: Customization of items in the toolbars. • Reset All: Sets all toolbars and menus back to their initial state - that which the Clarity workstation was in when you installed it. <p><i>Note:</i> <i>Reset All</i> does not display hidden toolbars. To show them invoke <i>Customize...</i> - <i>Toolbars</i> menu.</p>
Reorder Monitors	Opens a dialog where you can reorder monitors.
Component Flow in %	Display the component Flow in % of the <i>Total flow</i> instead of the volume units.

2.4.4.4 Window

 Main	Displays the main Clarity window (for more details see also chapter Clarity on pg. 1).
 Instrument	Displays the Instrument window (for more details see also chapter Instrument on pg. 60).

2.4.4.5 Help

Help	Displays the help item concerning the Device Monitor window.
-------------	--

2.5 Evaluation

This is a submenu containing commands for evaluation and processing of measured chromatograms:



Chromatogram

Displays the [Chromatogram](#) window.





Calibration

Displays the [Calibration](#) window.

2.6 Setting

Sub- menu with commands for setting export and post- processing of chromatograms.

 Export Data	Opens the Export Data dialog which sets the method of automatic results export.
 User Options...	Sets up Instrument properties.
Toolbars	Displays commands for toolbars. The command is similar to the <i>View - Toolbars</i> command in the main Clarity window but with different command options. <ul style="list-style-type: none">• Acquisition Controls: Hides/shows toolbar with preset icons for controlling acquisition.• Customize...: Customization of items in the toolbars.• Reset All: Sets all default toolbars and menus back to their initial state. <p><i>Note:</i> <i>Reset All</i> does not display hidden toolbars. To show them invoke <i>Customize... - Toolbars</i> menu.</p>

Note: In case you accidentally move the menu bar out of the screen, you can return it back by using the shortcut **Alt + V**.

2.6.1 Export Data

Sets the automatic results and chromatogram export parameters. When prompted, the *Export Data* dialog will be displayed. The same dialog can be called up using the *File - Export - Export Data* command from the [Chromatogram](#) window, where the command is intended for manual export of the active chromatogram and its results. Remember that this is the same window, so changes made in one place also apply to the other window. Selected data can be exported to a file or clipboard. Automatic export can be activated in the [Single Analysis - Post Run Settings](#) tab.

Note: User columns may be exported only from the **Result Table** and / or from the **Summary Table**.

Using the **Ctrl + E** shortcut it is possible to export data directly from the [Chromatogram](#) window without opening the *Export Data* dialog.

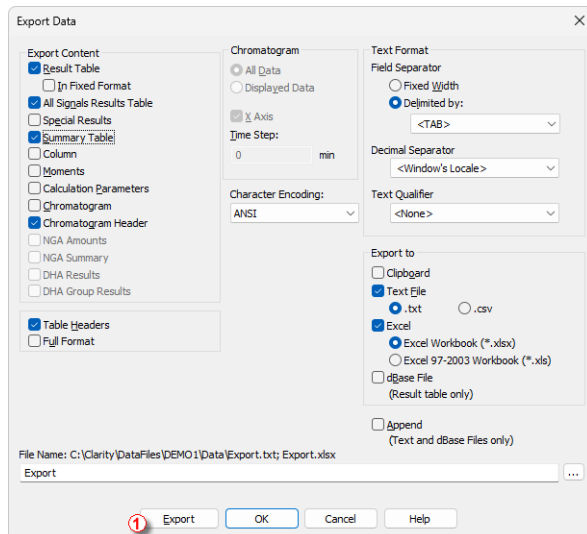


Fig. 96: Export Data

Note: Besides exporting using *Export Data* command, a chromatogram can also be exported by *Export Chromatogram in AIA (TXT, EZChrom) Format* command (for more details see the chapter **Export Chromatogram** on pg. 182).

Export Content

Determines the type of exported data.

Result Table

Exports integration results table.

Caution: Hidden columns will not be exported.

In Fixed Format

When checked the data will be exported always in the same format regardless of the setting on the screen. This means it will not be WYSIWYG format.

It is useful to check this option when the exported data should be automatically processed by other program. However, user columns will not be exported while the *In Fixed Format* checkbox is checked.

Note: Changes made in the [Units Setup](#) dialog will be omitted and exported data will be in default units.

All Signals Results Table

Exports all signals results table.

Note: Exported all signals results table is always sorted by retention time.

Special Results

Exports any data given by control modules (e.g. fraction table in case of fraction collector, ...).

Summary Table

Exports summary table.

Column

Exports *Column Performance* table counted from the half height. This table is exported in fixed format.

Moments

Exports *Column Performance* table counted from statistical moments. This table is exported in fixed format.

Calculation Parameters

Exports calculation parameters (parameters from the [Method Setup - Calculation](#) tab).

Chromatogram

Exports actual chromatogram according to specifications in the *Chromatogram* section.

Chromatogram Header

Exports chromatogram header.

NGA Result Table

Exports the Result Table from the *NGA Results* tab in the **NGA** Extension. Available only if the *Instrument Type* is NGA.

NGA Summary Table

Exports the Summary Table from the *NGA Summary* tab in the **NGA** Extension. Available only if the *Instrument Type* is NGA.

Table Headers

Exports all table headers with exported tables.

Full Format

Exports full format of all tables. Each line is extended by the file name, date and time of creation.

Chromatogram

Section determining the format of exported chromatogram. It will be active only when the *Chromatogram* checkbox in the Export Content group is checked.

All Data

Exports whole chromatogram regardless of selection.

Displayed Data

Only the displayed time period of chromatogram will be exported.

X Axis

Determines, whether or not will the data contain time in the first column.

Note: The time axis is exported with 5 decimal places precision (other data with 4 decimal places).

Time Step

Determines the length of time interval (in minutes) from which will be each exported value calculated (using arithmetic mean of the highest and lowest point). Value lower than chromatogram sampling rate (including zero value) will not change anything, thus the export of the chromatogram will have same the number of datapoints as original chromatogram. Entering a time step larger than the length of the chromatogram will result in a single value corresponding to the mean value for the whole chromatogram.

Caution: The highest and lowest points equal to the highest and lowest Y-axis values within each *Time Step* interval. *Time Step* is performed on data with [Global Bunching](#) setting applied. *Time Step* is not performed on raw data.

Character Encoding

Selects the encoding type of the chromatogram while exporting. *ANSI* or *Unicode (UTF-8)* encoding format is available.

Text Format

Output format selection:

Field Separator

Defines how the exported items will be separated.

Fixed Width

Items will be separated by an adequate number of spaces to maintain alignment (this occurs only for disproportional letter types).

Delimited By:

Items will be separated by: *Comma*, *Semicolon* or *Tabulator*.

Decimal Separator

Chose decimal separator: *Window's Locale*, *Dot* or *Comma*.

Text Qualifier

Used to distinguish beginning and end of contents of a text field. If exported item (e.g., Compound Name) contains character which is used either as Field Separator or Text Qualifier, then such item is enclosed in characters defined in *Text Qualifier*. Possible options are: *None*, *Single Quotation Marks*, and *Double Quotation Marks*.

Export To

Clipboard

Automatically exports to clipboard.

Text File

Automatically exports to text file. It is possible to choose suffix of the exported file. Options are *.txt* or *.csv*.

Excel

Automatically exports to Excel file. Settings of *Text Format* are not applied to exporting to Excel. Decimal separator is always based on Windows settings. It is possible to choose between *.xlsx* (default) or *.xls* formats.

Caution: For exporting to *.xlsx* format it is required to have Excel 2016 or newer installed. Export to *.xls* format is supported with Excel 97 or newer.

Note: Exporting to Excel is not supported in any **Starter** edition of MS Office.

dBase File

Automatically exports to database file of dBase format. Only the results table is exported in database format.

If you select export only to the *dBase File*, the entire window will be grayed and *Results* and *Full Format* checkboxes will be checked.

Caution: Export to *dBase File* with the *Append* option enabled is limited. See [File is not compatible](#) for more information.

Append

When the *File Name* field in *Export Data* dialog is set, then *Append* checkbox will:

- append data to existing file or
- create new file if it did not exist.

Note: If the *File Name* field is empty, it will always create separate file for each chromatogram.

Caution: Excel files cannot be appended, a new file is always created instead.

Caution: Clipboard content cannot be appended, it is always overwritten instead.

File Name


Filename for export to a file. Above the edit field a full path including the file name is displayed. If the edit field is not filled, a file with the same name but a different file extension as the exported chromatogram will be created and located either in the location where exported data are placed (as set in the [User Options - Directories](#) dialog) or, if the export folder setting is empty, in the same directory as the chromatogram is in. It is possible to manually override either the file name, path or both. This override is valid for just a single export (when export path in [Directories](#) is set) or until Clarity [Instrument](#) window is closed.



Searches for a file or directory that is to be entered to the *File Name* field.

Export

Performs the export to destinations selected in *Automatic Export To* area.

Note: The *Export* button  is only available if you open this dialog from the [Chromatogram](#) window.

OK

Saves the current settings.

Cancel

Leaves the dialog without saving any changes.

2.6.1.1 File is not compatible

Export to *dBase File* utilizing the *Append* option is limited. If the file with the set *File Name* already exists, the export settings in [Export Data](#) dialog must be set the way it was for the existing file. The export will fail when the settings is changed. In such case, following message, stating that the file is not compatible, is displayed.

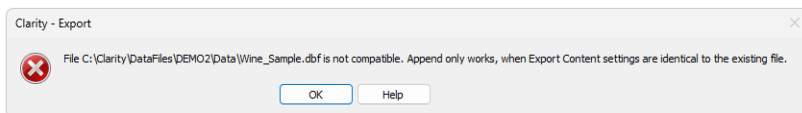


Fig. 97: File is not compatible

Caution: Export to *dBase File* with the *Append* option enabled is sensitive specifically to the option *Export Content - In Fixed Format* ①. This means that when the first export is done with the option enabled, following export cannot be appended if the option is disabled. Other options, in this case *Full Format*, can be change between exports, without influencing their functionality.

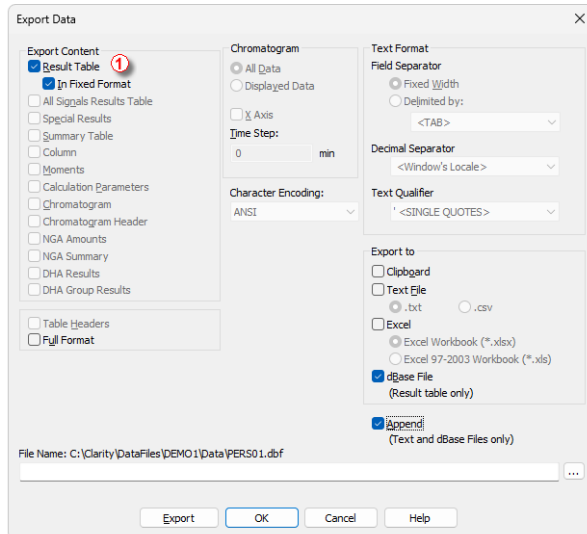



Fig. 98: Export Data - Export to dBase File

Note: The *Export Data* dialog provides more options for export to *dBase File* in the **GPC** extension. These are specifically options *Slice Table* and *Ranges Table*. Each of these options can be changed between exports without influencing export functionality. For more information refer to **Export of data** chapter in **GPC Extension** manual.

2.6.2 User Options...

Sets [Instrument](#) window properties. When prompted, the *User Options* dialog will be displayed.

Settings are saved in the appearance settings file (*.DSK). This means that when "all user" mode is being used (no password entered) these settings are common to all users. These settings are common to all [Instrument](#) windows in the **Clarity** station.

 If the station is used in "login" mode (i.e. all users have a password), settings are derived from the settings file of the respective user.

Note: Location of the *.DSK file can be set in the [User Accounts](#) dialog in the *Desktop File* field (for more details see also chapter **User Accounts** on pg. 4).

Currently logged user and his desktop file name is shown in the title bar of the dialog. In the **Fig. 99** on pg. **148**. is example of "all user" mode configuration, when *Administrator* is the default user and *CLARITY* is the default desktop file name.

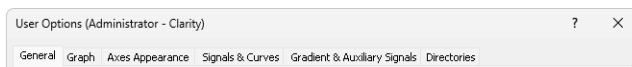


Fig. 99: Title bar of the User Options dialog

2.6.2.1 General tab

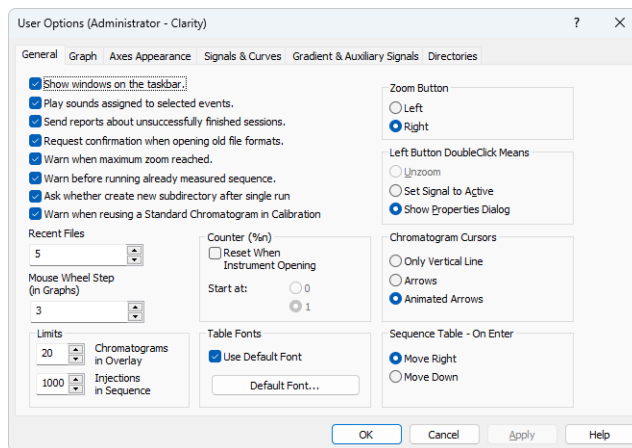


Fig. 100: User Options - General

Show windows on the taskbar

All open windows can be displayed as icons on the taskbar or in the reverse case, it is possible to choose to have only the opened [Instrument](#) and the station's main [Clarity](#) window displayed on the taskbar.

Play sounds assigned to selected events

Permits sounds to be played with selected actions: *Start, Stop, Abort, Snapshot, Open Chromatogram, Close Chromatogram*. Other sounds can be selected on the *Sounds* tab of the *Control Panels Windows* dialog in the *DataApex - Clarity* section.

Send reports about unsuccessfully finished sessions

Allows the automatic delivery of a report which is used by **DataApex** technical support to troubleshoot the nature of the problem. A message box will automatically appear on the very next start-up after an error has occurred that has caused an improper shutdown of the system. This message box will inquire whether or not you would like to e-mail error information directly to the **DataApex** technical support.

Request confirmation when opening old file formats

When selected, while opening any file saved in a previous format the informative dialog will show up, saying that the file is in an obsolete format and will be converted to a new format upon saving. When not selected, the station will automatically convert all opened obsolete format files to the new one upon saving. When *Save As* command instead of *Save* command is used, the *File Format* combobox in the *Save As* dialog offers the obsolete format to be used, too.

Warn when maximum zoom reached

Activates/deactivates the warning message display when attempting to exceed the maximum zoom of the graph.

Warn before running already measured sequence

Activates/deactivates the warning message display when attempting to run already measured sequence.

Note: Only the data from the last measurement of a given sequence may be reprocessed by the *Batch* command with *Sequence Files* parameter.

Ask whether create new subdirectory after single analysis

Enables/disables the confirmation message for creation of subdirectories after the single analysis measurement, if the subdirectory defined in the file name is not present. Similar feature is present in the Sequence measurements too, but the creation of the subdirectories is always silent.

Warn when reusing a Standard Chromatogram in Calibration

Activates/deactivates the warning message display when attempting to use already used Standard Chromatogram in a calibration.

Recent Files

Sets the number of recently opened files that will be displayed in the *File* menu. This setting is common to the [Instrument](#), [Sequence](#), [Chromatogram](#) and [Calibration](#) windows.

Mouse Wheel Step (in Graphs)

Sets the mouse wheel sensitivity on zooming the graphs.

Limits

Sets the general limits in **Clarity**.

"Chromatograms in Overlay"

Limits the number of chromatograms that can be simultaneously displayed in the [Chromatogram](#) window. The chromatogram displayed longest will be closed when the newer chromatogram is opened. 10,000 is the maximum number, the preset default is 20.

Injections in Sequence

Limits the maximum number of analyses measured from a single sequence. When the number of measurements reaches the set limit, the check of the sequence prevents from running it. This limit is set to prevent the lowering of the **Clarity** performance - sequence check may be unnecessarily long when there are several thousands of injections there.

Whole chromatograms are always counted regardless of the number of signals in the multi-detector chromatogram(s).

Counter (%n)

Allows for automatic reset of the %n counter used in the [Single Analysis](#) dialog. After checking, the counter will reset to 0 or 1 (according to further setting) at each [Instrument](#) window start.

The setting is common for one user, but the counter of each Instrument increases its value independently.

Note: Similar setting for sequential measurement can be found in the [Sequence Options](#) dialog (for more details see also chapter **Sequence Options** on pg. 405).

Table Fonts

Selects default fonts for all **Clarity** station tables.

Use Default Font

When selected, the station will use the font set by the *Default Font...* button in all tables. If the box is checked and filled with gray color (instead of black), it means that at least one column in one table contains a different font.

Default Font...

After clicking this button the *Font* dialog will appear where you may choose the font, style, color and size of the table text font.

Note: If you wish to use a different font in any table, right click the mouse on the table and select the *Setup Columns...* command. This will open the [Setup Columns](#) dialog where it is necessary to deselect the *Use Default Font* checkbox in favor of desired font for specific column by using *Font* button.

Zoom Button

Selects which mouse button should be used for selection from the graph.

Left - It is the new standard. If you use the left mouse button, the right button will be used to open a local menu.

Right - As it was used in station **CSW17**.

Left Button Doubleclick Means

Defines what will occur when doubleclicking the left button in graph:

Unzoom - The graph returns to the appearance before zooming.

Set Signal to Active - If more chromatograms than one are displayed, doubleclicking over a specific chromatogram will set it as active.

Show Properties Dialog - Double-clicking on the graph opens the [Graph Properties](#) dialog for setting graph and chromatogram properties.

Chromatogram Cursors

Sets the cursor style for chromatogram modification. Cursor is shown as:

Only Vertical Line - A vertical line throughout the whole graph.

Arrows - Vertical line with two arrows at the point where this line intersects the chromatogram curve.

Animated Arrows - Animated arrows that function as those listed above.

Sequence Table - On Enter

Defines where will the focus move in Sequence table after pressing Enter.

Move Right - Default behaviour.

Move Down - Convenient to use with the barcode reader that emulates keyboard to fill in the Sequence table.

2.6.2.2 Graph tab

Sets the appearance of the default graph. This selection applies to all graphs when the local setting in the [Graph Properties - Graph](#) dialog has the *Use User Options* checkbox selected.

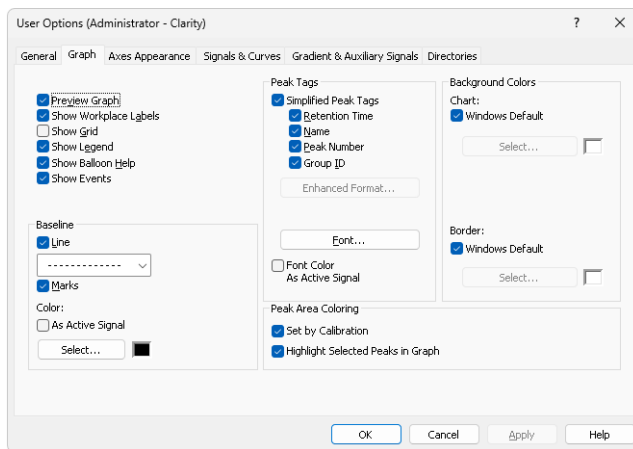


Fig. 101: User Options - Graph

Preview Graph

Shows/hides a preview graph.

Show Workplace Labels

Shows/hides all labels and lines created using the *Create Label* command.


Show Grid

Shows/hides a grid for simplified graph reading.

Show Legend

Shows/hides a legend that displays chromatogram names and their signals.

Show Balloon Help

Displays balloon help next to the cursor lines when user performs interactive modifications of the chromatogram. This feature can also be switched on/off using the  icon on the toolbar in the [Chromatogram](#) window.

Show Events

Permits the display of events from the [Event Table](#) tab of the [Method Setup](#) dialog.

Baseline

Line - Shows/hides the baseline.

Marks - Shows/hides auxiliary marks of peak starts and ends.

Color

As Active Signal - Determines whether baseline color will be the same as the chromatogram color. If not, it will be the color set by the *Select* button.

Select - Button for color selection.

Peak Tags

Allows to shows, hide peak tags or set enhanced format of tags. The format of fields and values is defined by the format set for the **Result Table**.

Simplified Peaks Tags

Enables/disables checkboxes concerning simplified peaks tags. Simplified tags follows the changes of retention time caused by *Scale* and *Offset* parameters of *Time Axis* settings.

Retention Time - Retention time.

Name - Peak names made according to calibration file.

Peak Number - Peak serial number.

Group ID - Name of group to which a peak pertains.

Enhanced Format...

Displays the [Peak Tags Format](#) dialog which allows to set custom format of peak tags. Available only if the *Simplified Peaks Tag* checkbox is unchecked. Enhanced peak tags are derived from the result table, thus changes on *Time Axis* does not influence them.

Font...

Sets font for peak tags. When prompted, the standard *Font* dialog will be displayed.

Font Color As Active Signal

Determines whether the peak tag color will be the same as the chromatogram color. This overrides the color set by the *Font...* button.

Peak Area Coloring

Set by Calibration - The area of peaks will be colored based on the color specified in **Calibration Summary Table** (*Peak Color* column).

Highlight Selected Peaks in Graph - Peaks selected in the chromatogram graph will be highlighted in the *Result Table* and *All Signals Result Table*. Cleared checkbox highlights peak in the *Result Table* and *All Signals Result Table* but not in the chromatogram graph.

Background Colors

Selects the background color - *Chart* section - and border color - *Border* section - of a graph.

Windows Default - Color will automatically be adopted from the **MS Windows** appearance scheme. If deselected, the color will be set according to the *Select* button.

Select - Color selection button.

2.6.2.2.1 Peak Tags Format

Peak Tags Format dialog allows custom setting of the peak tag. The values are formatted according to the **Result Table**.

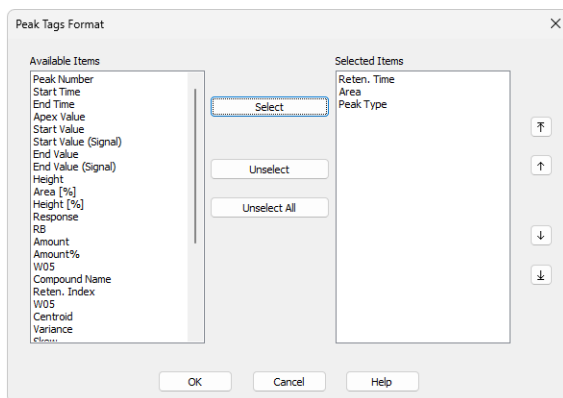


Fig. 102: Peak tags format dialog

Available Items

Allows to select an item from the list.

Select

Moves the selected item from the *Available Items* list to the *Selected Items* list.

Unselect

Moves the selected item from the *Selected Items* list to the *Available Items* list.

Unselect All

Moves all items from the *Selected Items* list to the *Available Items* list.

Selected Items

List the items those will be displayed in the peak tag. To change their order, use the arrows on the right side of the dialog.

2.6.2.3 Axes Appearance tab

Axes appearance in the graph.

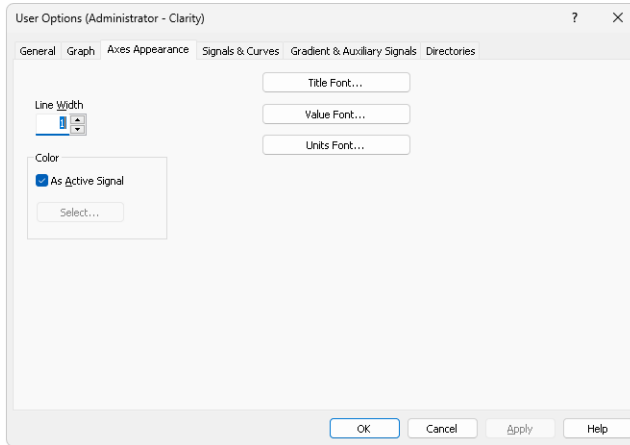


Fig. 103: User Options - Axes Appearance

Line Width - Axis width in pixels.

Color - Axes color selection.

As Active Signal - Color will be the same as the color of the active signal.

Select... - Color selection button.

Title Font... - Selects font for axes graph titles.

Value Font... - Selects font for axes numerical values.

Units Font... - Selects font for axes units.

2.6.2.4 Signals & Curves tab

Sets the default curve properties.

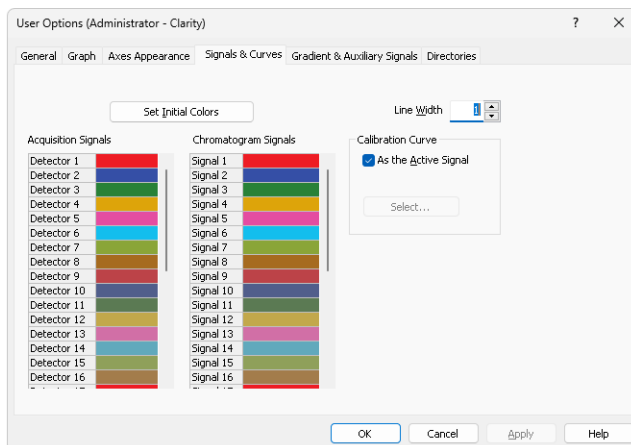


Fig. 104: User Options - Signals & Curves


Line Width

Selects the default curve width.

Set Initial Colors

Resets to initial colors (the default setting returns colors to the state they were in after the initial installation of the **Clarity** station).

Acquisition Signals and Chromatogram Signals

Actual settings of colors for particular signals can be seen in these sections. Select appropriate color and click on  button to set the color from a pre-set palette. Additionally, it allows user to create a newly defined color.

Calibration Curve

Section for changing the calibration curve color.

As the Active Signal

Sets the color of the calibration curve to the color of the active signal.

Select...

Button for the color selection.

2.6.2.5 Gradient & Auxiliary Signals tab ✓ Full version

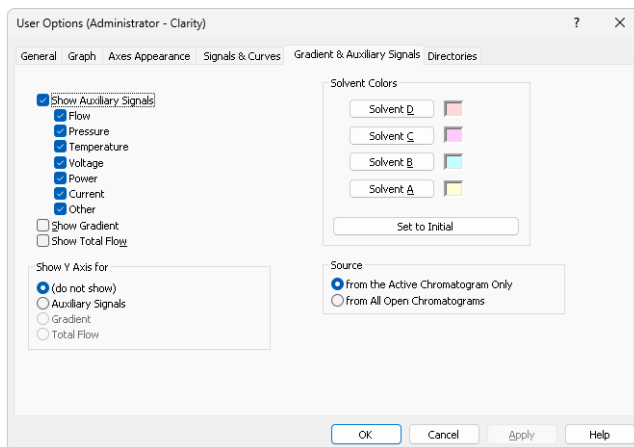


Fig. 105: User Options - Auxiliary Signals

This tab determines which auxiliary signals will be displayed in the graph and selects the gradient graph display (in the [Chromatogram](#) and [Data Acquisition](#) windows) when utilizing direct control of HPLC pumps.

Show Auxiliary Signals

Switches the display of the auxiliary signals on/off and activates the possibility to select the auxiliary signal as Y-axis. Each auxiliary signal is included in one of the following categories: *Flow*, *Pressure*, *Temperature*, *Voltage*, *Power*, *Current* and *Other*. The display of all signals in each category is allowed together.

Show Gradient

Switches the display of the gradient on/off and activates the possibility to select the gradient as the right Y axis.

Show Total Flow

Switches the display of the total flow on/off and activates the possibility to select the total flow as Y axis.

Show Y Axis for

Determines the appearance of the right (second) Y axis. Available options are:

(do not show) - Not visible.

Auxiliary Signals - Shows the axis for auxiliary signals. The right Y axis of checked auxiliary signal will be displayed automatically in the graph. In case that several auxiliary signals are in the same chromatogram, the axis of first auxiliary signal (based on Show Auxiliary Signal list) will be displayed. The right Y axis always corresponds to the active auxiliary signal in the graph.

Gradient - The percentage share of individual solvents.

Total Flow - Flow rate in units set in the [Instrument Method Sending](#) dialog accessible from the [System Configuration](#) dialog.

Solvent Colors

Selects colors for the display of individual gradient components.

Set to Initial

Returns to default colors.

Solvent D-A

Selects the colors of each of four possible gradient components. Buttons are arranged in the same order as in the graph (i.e. from the bottom).

Source

This section governs which auxiliary signals will be shown.

from the Active Chromatogram Only

Selected types of auxiliary signals will be displayed only in the active chromatogram.

from All Open Chromatograms

Selected types of auxiliary signals will be displayed in all opened chromatograms.

2.6.2.6 Directories tab

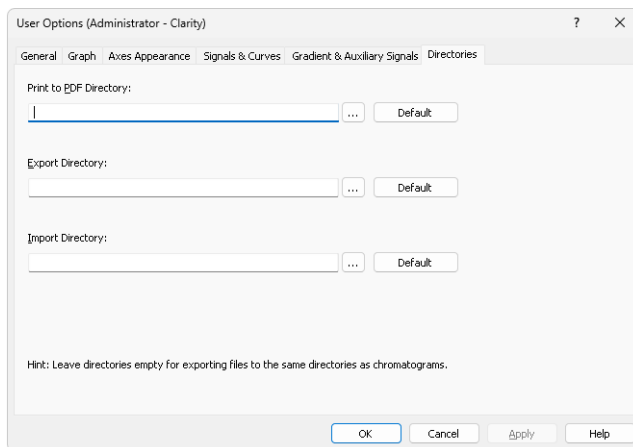











Fig. 106: User Options - Directories

Sets the directories that will be used for the automatically created *.PDF files (Print to PDF Directory) and exported files (Export directory) and where **Clarity** will look for files to import (Import directory). If the fields are left empty, **Clarity** will use the directory where the exported/printed file is located as default directories for the respective actions. The *Export Directory* can be overridden when the *File Name* field in the [Export Data](#) dialog is specified. In that case, the export location will be changed for a single exported chromatogram (in case the *Export Directory* field in *User Options - Directories* dialog is filled in) or all consecutive chromatograms until **Clarity** [Instrument](#) window is closed (in case the *Export Directory* field in *User Options - Directories* dialog is empty).

2.7 Window


The commands for working with windows of given Instrument.

	Hide All	Hides all open windows of the Instrument.
<p><i>Note:</i> When the <i>Show windows on the taskbar</i> checkbox in the User Options - General (described in the chapter "General tab" on pg. 148.) is left unchecked, the windows will be hidden.</p>		
	Show All	Displays all hidden windows.
	Main <small>✓Full version</small>	Displays the main Clarity window described on pg. 1 .
	Chromatogram	Displays the Chromatogram window described on pg. 162 .
	Calibration	Displays the Calibration window described on pg. 320 .
	Single Analysis	Displays the Single Analysis dialog described on pg. 113 .
	Sequence	Displays the Sequence window described on pg. 385 .
	Station Audit Trail <small>✓Full version</small>	Displays the Audit Trail window described on pg. 417 .
	Data Acquisition	Displays the Data Acquisition window for online monitoring of a signal from detector(s) described on pg. 369 .

2.8 Help

This command invokes Help for the window you are currently using. In this case, it opens Help for Instrument window.

3 Chromatogram

This chapter serves as a crossroad for the *Chromatogram* window which is designed to display, adjust and evaluate chromatograms. It can be displayed using the *Window - Chromatogram* command or using the  icon from the [Instrument](#), [Calibration](#) or [Sequence](#) window. The *Chromatogram* window may also be opened automatically when a new chromatogram is created, see section "Single Analysis - Post Run Settings" on page 120 or alternatively "Sequence" on page 385.

Window division

The window is divided into an upper panel with a graph and two lower panels with the results and the method calculation settings. Preview Graph panel can be displayed above the graph using [Display](#) - Preview Graph.

Tabs

Lower part of the window displays number of tabs with different result tables and other parameters. The tabs enable the user to make adjustments to evaluation or display of the chromatogram.

Some tabs may not be visible following the station start-up, in which case the settings can be checked using the *View - Show Tables* command from the *Chromatogram* window menu.

Tab. 8: List of possible tabs

Type	Name of tab (or alternatives)
Default	the chapter " Result Table " on pg. 296.
Default	the chapter " All Signals Result Table " on pg. 304.
Default	the chapter " Summary Table " on pg. 306.
Default	the chapter " Performance Table " on pg. 310.
Default	the chapter " Integration " on pg. 284.
Default	the chapter " Measurement " on pg. 290.
SST Extension	See SST Manual - M020
<i>Note:</i> Extension appears only with purchased Extension license.	

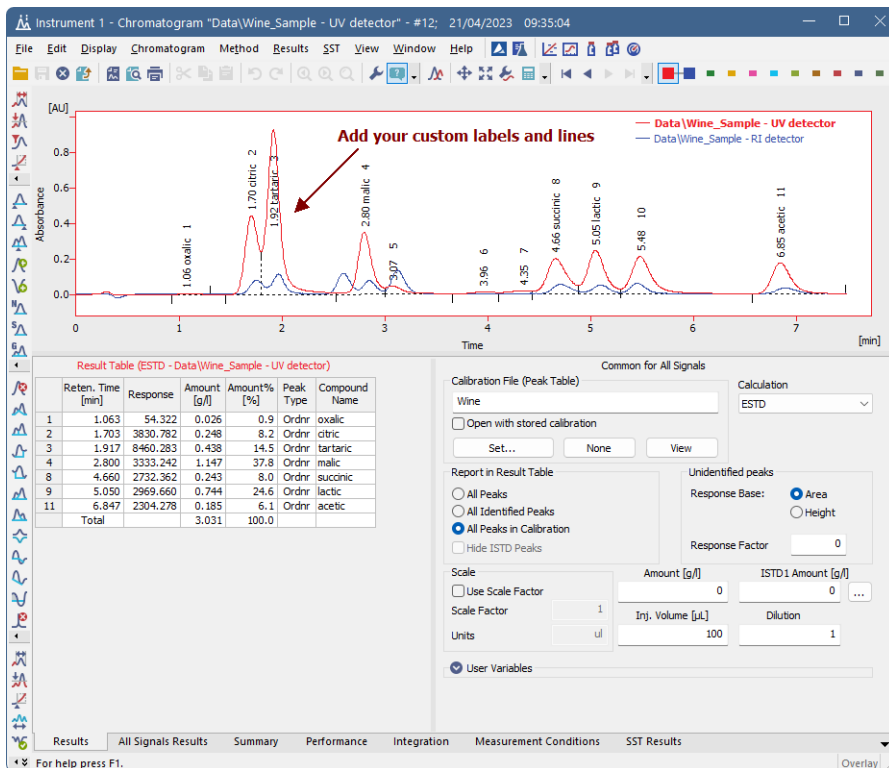







Fig. 107: Chromatogram







Note: The text on the tabs and their number may vary depending on the way they have been set up and the Extensions you have installed.

3.1 File

This is a sub-menu with commands for working with chromatograms and other specific system commands.

	Overlay Mode	Displays a number of chromatograms simultaneously.
	Open Chromatogram...	Selects and displays chromatogram (Ctrl + O).
	Browse Through Chromatograms	Opens and browses chromatograms from the last active folder or from the selection made using Browse Selected Chromatograms in Open Chromatogram dialog. In <i>Overlay</i> mode browses through currently opened chromatograms. For more information see Browse Through Chromatograms .
	Open Chromatogram From Sequence	Displays all chromatograms measured according to the selected sequence.
	Close	Closes the active chromatogram (Ctrl + W). If the chromatogram has been changed and not yet saved, you will be notified accordingly. Modifications not yet saved are always marked by the inscription MODIFIED after the filename.
	Close All	Used to close all displayed chromatograms (Ctrl + Shift + W). If any chromatogram has been changed and not yet saved, you will be notified accordingly. Modifications in not saved chromatograms are always marked by the inscription MODIFIED after the filename.
	Save	The command saves the active chromatogram (Ctrl + S). When a mathematical curve created in the <i>OVERLAY</i> mode by the <i>Chromatogram - Overlay - Mathematics</i> command is to be saved, a chromatogram will be created and saved according to the current method shown in the Instrument window.
	Save As...	Saves active chromatogram under selected name (Ctrl + Shift + S). <i>Note:</i> For existing filenames, message box about file overwriting pops up.



Send Chromatogram by Email	<p>Sends the displayed active chromatogram as an email attachment.</p> <p>In the Overlay mode all displayed chromatograms will be added to the email.</p> <p>The command is analogous to the <i>Send Method by Email</i> command described in the chapter "Send Method by Email" on pg. 70.</p>
Import Chromatogram...	<p>Imports chromatograms in the text, AIA or EZChrom ASCII format.</p>
Export	<p>Initial submenu for the following Export commands:</p>
Export Data...	<p>Exports results and data of the active chromatogram. After selection, the Export Data dialog described on pg. 141. will be displayed.</p> <p>By using the Ctrl + E shortcut it is possible to export the data without opening the Export Data dialog.</p>
<hr/> <p>Caution: User columns are exported only when the <i>In Fixed Format</i> checkbox is not checked.</p> <hr/>	
Export Chromatogram...	<p>Exports chromatographic curve into AIA, text or EZChrom ASCII format.</p>
Export Summary Table...	<p>Exports <i>Summary Table</i> of results into a text file. After selecting the command the <i>Export Summary Table To</i> dialog will be displayed for selecting the name of the file and directory.</p> <p>Individual items of the summary table are divided in the file by a tabulator.</p>
<hr/> <p>Caution: Chromatograms containing unsaved modifications will be saved before exporting. Export is logged in the Audit Trail.</p> <hr/>	
<p>Caution: The <i>Summary Table</i> is exported in "as on screen" format.</p> <hr/>	
Export as Picture to Clipboard	<p>Copies currently displayed chromatogram into clipboard as a vector picture.</p>


Export as Picture to File...	Exports chromatogram as a picture in vector format. All chromatograms from the main graph including all labels are always exported in the format EMF format (Enhanced Metafile). The exported graph is saved into the file. After selecting the command, the <i>Save As</i> dialog will be displayed for selecting the name of the file and directory.
Sign... <small>✓ Full version</small>	Electronically signs the active chromatogram.
Verify... <small>✓ Full version</small>	Displays and verifies electronic signature.
	Report Setup...
Selects print configuration (Ctrl + Alt + P). After selection, the Report Setup dialog described on pg. 432 . will be displayed.	
	Print Preview
Previews selected print configuration before printing (Ctrl + Shift + P). After selection, the Print Preview dialog described on pg. 457 . will be displayed.	
	Print to PDF
Prints report to PDF file.	
	Send Printed PDF by Email
Opens new email message in default email client, prints report to PDF and adds created PDF file as an email attachment.	
	Print...
Command for selecting printer and actual printing (Ctrl + P). After selection, the Print dialog described on pg. 459 . will be displayed. In case the printed chromatogram(s) are modified and some of their results will be included in printing, the chromatograms will be saved in the moment of printing. This includes any non-active chromatograms which add a row to the Summary table (when Summary table is printed) or any chromatograms included in the SST (when <i>Parameters Table</i> on the <i>SST</i> tab is printed).	
	Perform Postrun...
Command for performing the postrun operations from the Chromatogram window. After selection, the PostRun Setting (From Chromatogram Window) dialog described on pg. 187 . will be displayed.	
-----	In this place the <i>File</i> menu contains a list of the last open chromatograms. This list serves for quick access to the currently used chromatograms.

Note: The number of displayed files is set using the *Recent Files* field in the [User Options - General](#) dialog, accessible from the [Instrument](#) window using the *View - Options* command.

Close Window	Closes the Chromatogram window. If any chromatogram has been changed and not yet saved, you will be notified accordingly. Modifications not yet saved are always marked by the inscription MODIFIED after the filename.
---------------------	---

3.1.1 Overlay Mode


The user can work with multiple chromatograms in the *OVERLAY* mode. The activation of this mode is indicated by an activated icon next to the *Overlay Mode* command in the *File* menu, an activated  icon in the *Overlay* toolbar and the highlighted display of the *OVERLAY* inscription in the status bar of the [Chromatogram](#) window (located in the lower right-hand corner of the window). In the *OVERLAY* mode it is possible to display a larger number of chromatograms at the same time by simultaneously or consecutively using the *Open* command or the  icon.


When a fixed range of display has not been set, the main graph will re-plot to display all chromatograms in their entirety even with the selection of variably sized chromatograms. Only the active chromatogram will display the descriptions of peaks and indicate the course of the baseline. The active chromatogram (signal) will have the relevant colored  icon depressed in the *Overlay* toolbar. Its name will be stated in the window header and a bullet will be displayed next to its name in the list of open chromatograms (signals) in the *Chromatogram* menu.

Note: Be careful not to confuse this list of currently open chromatograms with the list of last open chromatograms in the *File* menu.

The active chromatogram is also stated in bold letters in the legend on the right-hand side of the main graph. If no fixed color of the graph axes is selected, these axes always have the color of the active chromatogram.

Another active chromatogram is selected by:

- Clicking on the icon  with the color of the required chromatogram.
- Clicking on its name in the list of open chromatograms (signals) in the *Chromatogram* menu.
- Double-clicking on its name in the graph legend.

When using a multi-detector chromatogram, the icons of signals belonging to one chromatogram will be connected by the  link.

After canceling the *OVERLAY* mode, only the active chromatogram will remain displayed.

3.1.2 Open Chromatogram

Opens the *Open Chromatogram* dialog, where you can select chromatogram(s) to be opened and display their information. You can use shortcut **Ctrl** + **O** to access this dialog.

Note: You can quickly jump between DATA folder **D** and CALIB folder **C** directories within the currently opened project by clicking on the folders icons. More on navigation icons from the right upper corner of this dialog is described in the chapter [Open Dialog](#).

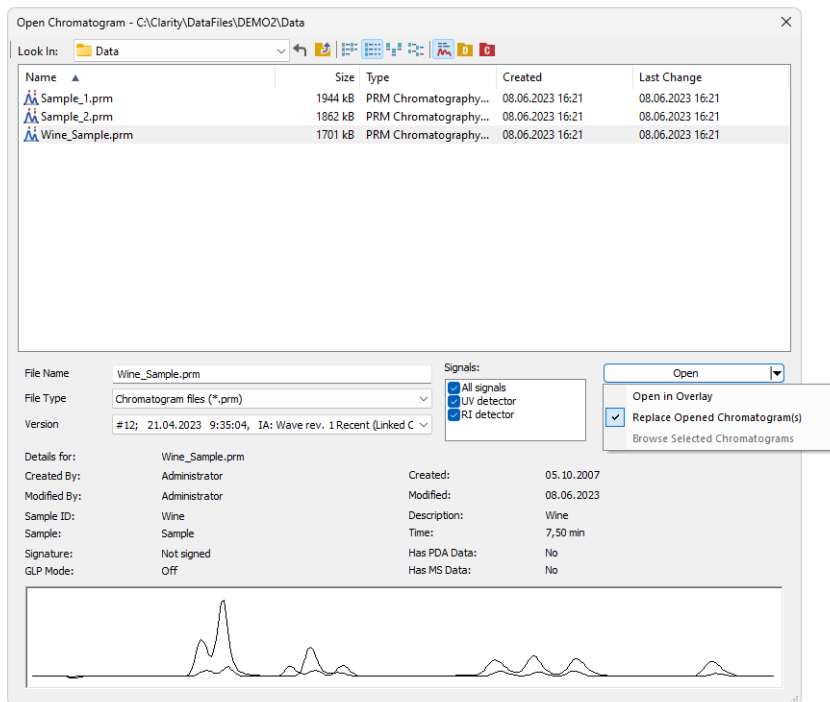


Fig. 108: Open Chromatogram

Chromatograms can be opened in different ways which can be achieved by clicking on the arrow in the *Open* button.

Note: Some commands, like *File - Set Background Chromatogram...* from the *Data Acquisition* window or *MS Method - Subtract MS Spectra - Set...* from the *Method Setup/Chromatogram* windows in the **MS Extension**, invoke similar dialog, which is missing the *Signals* option and the arrow in the *Open* button.

Open in Overlay

This option is preset according to [Overlay Mode](#) option set by the *File - Overlay Mode* command in the [Chromatogram](#) window or in the Toolbar. It is also default option for opening more than one chromatogram at once.

Open in Overlay is not available when opening a chromatogram of a standard in the *Calibration* window.

Note: When *Open in Overlay* is set, it is indicated by the text in the *Open* button. *Open* is changed to *Open in Overlay*.

Note: Continuous selection can be performed by clicking on the first file, pressing and holding down the **Shift** key, and then clicking on the last file in the row. All chromatograms will then be highlighted. Another option is to hold down the left mouse button on the first file in the row, and then drag the pointer over the last file in the row. Click on the *Open* button or hit the **Enter** key to then open these files.

Note: Non-continuous selection can be performed by using the **Ctrl** key. Hold this key down and click on the name of each desired chromatogram to highlight it. Click on the *Open* button or hit the **Enter** key to then open these files.

Caution: When attempting to open a chromatogram that has already been opened and contains unsaved changes, a message will appear asking whether you wish to return to the original version of the chromatogram and thus discard all the unsaved changes. Likewise, if there is an opened chromatogram containing changes and is going to be replaced or another chromatogram is going to be Opened in Overlay a message will appear asking whether you wish to return to the original version of the chromatogram and thus discard all the unsaved changes.

Replace Opened Chromatogram(s)

This option will close all opened chromatograms and will open the one you select. If on, *OVERLAY MODE* will be switched off.

Browse Selected Chromatograms

This option will close all opened chromatograms and will open the first of the selected chromatograms, remaining chromatograms will be set to chromatogram browse list (see more in [Browse Through Chromatograms](#)). If on, *OVERLAY MODE* will be switched off.

Signals

When a multi-detector chromatogram is being used, this command enables to display a selection of certain signals only. All signals are loaded but only selected ones are visible, all signals can be made visible in [Chromatogram Window](#) later on.

Note: At least one signal should be checked to be able to open the chromatogram. This option is not available for opening standards in *Calibration* and for subtraction chromatogram in *Method Setup*.

Version

Shows method version. Also enables to open a previous versions of a chromatogram. The chromatogram file maintains a history of adjustments as a list

of methods. Current version of the method is saved, along with a copy of the currently attached calibration, into this list whenever the chromatogram is saved.

Note: In addition to manually saving a chromatogram using the *Save* and *Save As* commands, the station will automatically save each version when the chromatogram is printed, signed electronically or exported.

The calibrations stored in the chromatogram are stored without their own history and without calibration log. To conform with GLP it is recommended to preserve the linked calibrations containing complete history of the calibration.

A chromatogram opened with a version from history (not the latest one) will be opened as *READ ONLY*. Such chromatogram can still be printed or exported, but in order to perform any other changes in it, it is necessary to store the chromatogram first using the *File - Save As...* command.

Calibration (stored x linked)

Chromatogram is opened by default with *Linked calibration*, i.e. the chromatogram is opened with the current state of the calibration file. Every modification of the calibration file will modify the displayed results in all chromatograms linked to the calibration accordingly.

Opening the chromatogram with *Stored calibration* will open the chromatogram with results according to the method and calibration file at the moment the chromatogram was saved. Each chromatogram can contain more than one version of the method and calibration file depending on the number of chromatogram saves. Only *Recent* stored calibration can be opened and edited, all older versions of chromatogram can be opened as Read-only.

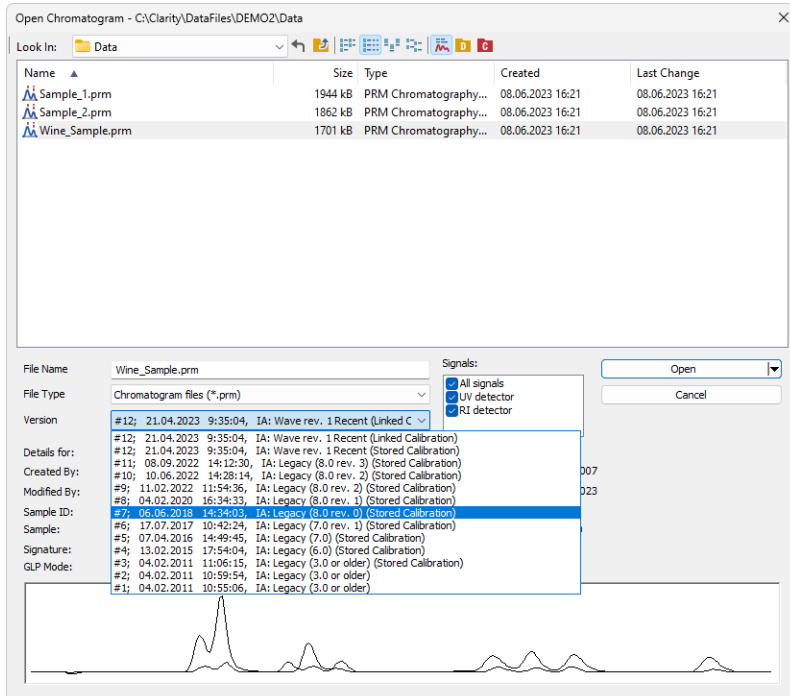



Fig. 109: Open Chromatogram with Stored Calibration

When **Clarity** cannot find the linked calibration while opening the chromatogram, a message offering to use calibration stored in the chromatogram will be invoked.

Note: When opening chromatogram from different location than current project, it is possible to open with stored or none calibration only. However opening files from directories out of current project is not recommended workflow.

Detail Info

The *Detail Info* pane, switched on/off using the  icon, contains detailed description about the chromatogram, i. e. name of the Analyst, Sample name and Sample ID, type of used signature (not signed, signed and not verified or signed and verified), information about GLP Mode, software used for acquisition, range of the detector signal and sampling rate of the detector used (the <varies> inscription is displayed if more detectors were used), duration of the analysis, presence of PDA data, use of comprehensive two-dimensional gas chromatography and preview of the actual chromatogram.

3.1.3 Browse Through Chromatograms

Browse through chromatograms from the last folder opened using *Open Chromatogram* command or browses between selected chromatograms if you

selected the "Browse selected chromatograms" option when opening chromatogram. In *Overlay* mode serves for browsing through currently opened chromatograms in overlay (it enables switching between active chromatograms).

- ◀ **First** Opens the first chromatogram from current folder or currently selected chromatograms or currently overlayed files (**Ctrl** + **F7**)

- ◀ **Previous** Opens the previous chromatogram from current folder or currently selected chromatograms or currently overlayed files (**F7**)

- ▶ **Next** Opens the next chromatogram from current folder or currently selected chromatograms or currently overlayed files (**F8**)

- ▶ **Last** Opens the last chromatogram from current folder or currently selected chromatograms or currently overlayed files (**Ctrl** + **F8**)

Outside of [Overlay Mode Filters](#) and **sorting** can be used to change the order of chromatograms and can limit the list of chromatograms for the browsing in the [Open Chromatogram](#) dialog.

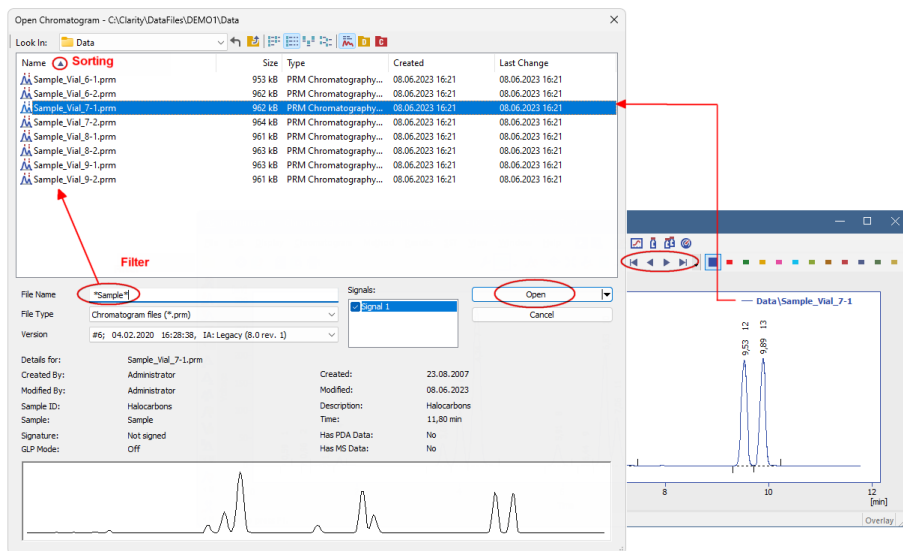



Fig. 110: Browse Through Chromatograms

To apply sorting and filtering do the following:

- Use **File - Open Chromatogram** command and navigate to the folder from which you want to open chromatograms.
- Specify the **filters** by writing partial name in the **File Name** field to limit the set to desired chromatograms only.

Note: It is possible to use the wildcards (*, ?) like in the example displayed in the image *Browse Through Chromatogram*. Asterisk (*) matches zero or more characters, whereas question mark (?) matches exactly one character.

- Click the desired column header to set ascending/descending **sorting** according to that column.
- Select a chromatogram from the defined set and open it using the *Replace Opened Chromatogram(s)* option or select all chromatograms that should be opened and open them using the *Browse Selected Chromatograms* option.
- In the [Chromatogram](#) window use the commands from *File - Browse Through Chromatograms* menu or icons  to browse through the chromatograms from the defined set.

The *Browse Through Chromatograms* function will always open the whole chromatogram (all of its signals).

3.1.4 Open Chromatogram from Sequence

Displays chromatograms measured according to sequence.

Using the command invokes the *Open Sequence* dialog. Once in the dialog, select the sequence file according to which the chromatograms you wish to display were measured. Only the chromatograms that have the checkbox in the *Run* column checked in the appropriate sequence will be opened. All checkboxes in the *Run* column are checked by default, but it might be useful to switch off some lines in the [Sequence](#) window prior to opening the chromatograms from sequence.

Open Sequence dialog (similar in appearance to the [Open Method](#) dialog described on pg. 68.).

Method

Sets whether the opened chromatograms will be opened with the *Linked* calibration (might be changed from the time the chromatogram was opened for the last time) or with the *Stored* calibration.

Signals

Signal X number of opened signals

Only measured chromatograms will be displayed (i.e. chromatograms according to the rows of the sequence table where the *Status* field is colored blue).

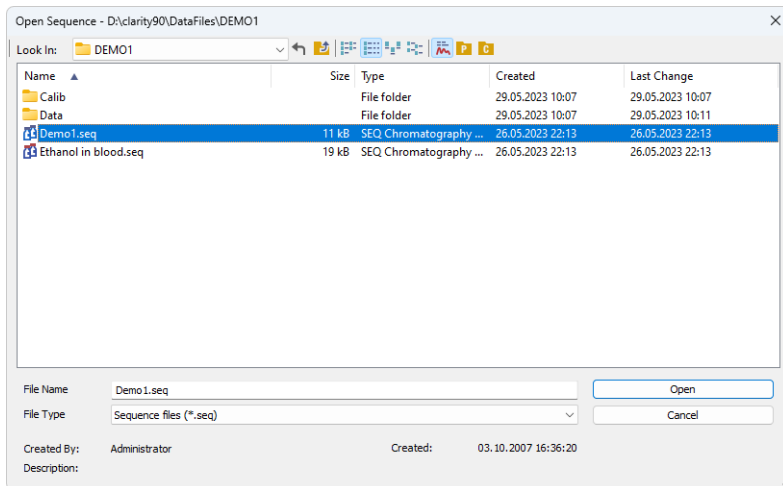


Fig. 111: Open Sequence

If the same sequence was used several times, only the chromatograms from the last run of the sequence table will be remembered.

Note: This command is particularly suitable for a fast evaluation of a series of chromatograms in the summary table.

The sequence file must be saved after completing the measurement! Otherwise it will not be possible to use the *Open Chromatogram from Sequence* command on it, since the current state of the *Status* column has not been saved.

3.1.5 Save As...

Used to save the active chromatogram under a chosen name and/or to another directory (**Ctrl** + **Shift** + **S**). Saving always means that a copy of the active chromatogram is created.

The command opens the [Save As dialog](#), where the new name can be entered or a new directory selected.

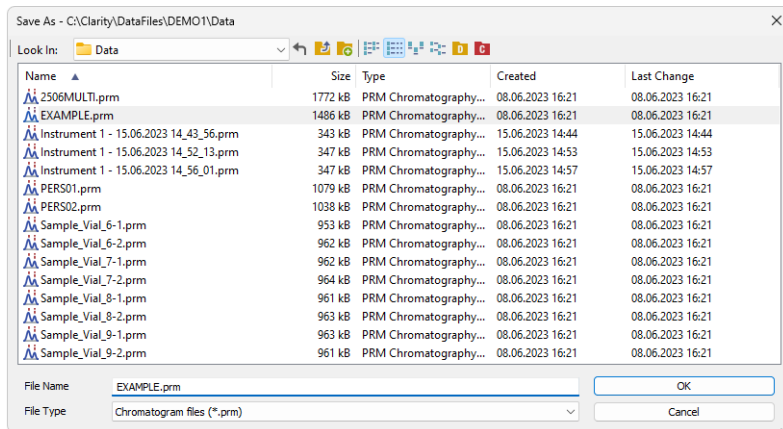


Fig. 112: Save As (Chromatogram)

Note: If a file of that name already exists and has been opened on other Instrument or window, the name cannot be used. Moreover, in the protected mode (full version Full version only), a user may not overwrite a file he/she is not entitled to modify (see the *User Account* command).

3.1.6 Import Chromatogram...

Imports a chromatogram in **AIA**, **Text** or **EZChrom ASCII** format. The Text files are supported with *.TXT, *.CHR and *.CSV suffixes. Select the *Open Files to Import* dialog using the *File - Import Chromatogram...* command. Select the desired directory and one or more files to import. The files displayed may be filtered using the filter in the *File Type* listbox.

Caution: Imported chromatograms are processed using the current method from the [Instrument](#) window and not according to the method of the potentially displayed chromatogram!

Import of several files simultaneously

You may select a number of files simultaneously in the *Open Files to Import* dialog. The [Import Text File](#) or [Import AIA File](#) dialogs will open progressively for each imported file according to the type of imported file. If all the selected files share the same format, it is possible to import them all at once with the same settings.

Import of multi-detector chromatograms

The *Import Chromatogram...* dialog can import multi-detector chromatograms from *.TXT or *.CHR format.

3.1.6.1 AIA

The **AIA** file format has relatively strictly designed form, but not the content. Thus, an **AIA** file may contain various custom items. The dialog for importing files in **AIA**

format is designed as an expandable tree, making it easier to view items contained in the imported file.

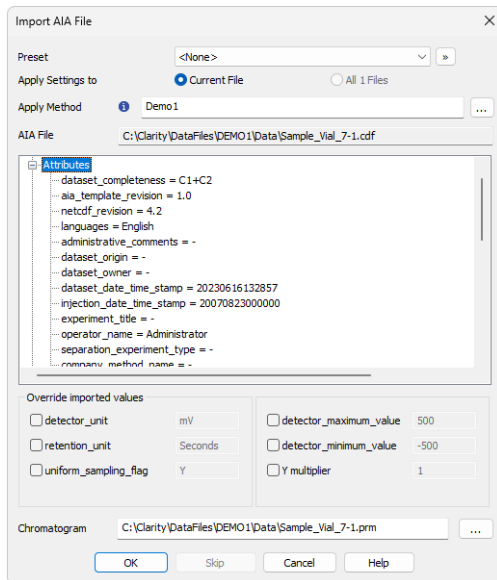



Fig. 113: Import AIA File

Preset

Allows to select a preset from the list of stored import presets. A preset can be created / deleted / managed using the  button.

Apply Setting to

Radio-button deciding whether the settings for the import will be applied just to *Current File* selected (the one as defined by the *AIA File/File* field) or to *All n Files* selected for import (if multiple are selected).

Apply Method

Choose method whose parameters (integration table, attached calibration, etc.) will be applied into the imported chromatogram. By default, displayed method matches method in the [Single Analysis](#) dialog. Leaving this field blank applies default parameters.

AIA File

Name of the imported file including directory path.

Window with parameters

Items found in the current **AIA** file and their parameters. Expand collapsed items by clicking the “+” sign with the left mouse button (similar to working with the **Explorer** application in **Windows**).

Clarity will correctly import only files with following parameters:

uniform_sampling_flag = Y

actual_sampling_interval value set

detector_maximum_value < 10^{12}

detector_minimum_value > -10^{12}

Note: Items and their values cannot be adjusted in the dialog.

Override detected values

Allows to override or fill in the missing value of selected parameters stored in AIA files, thus allowing to import chromatograms exported without required values.

Each parameter values are automatically detected from selected AIA file.

detector_unit (required)

Determines the units in which the signal values are stated.

retention_unit (required)

Determines the units in which time values are stated.

Recognized values are following:

- *milliseconds, millisecond, ms*
- *seconds, second, sec, s*
- *minutes, minute, min, m*

In case of improper values, seconds will be used as time unit.

uniform_sampling_flag (required)

Determines the uniform sampling.

Uniform sampling flag has to be set to Y (=Yes).

Clarity supports only data with equidistant time spacing. Importing AIA file with non-equidistant data time axis will be deformed.

detector_maximum_value & detector_minimum_value


Sets the range of detector signal.

Y multiplier

Sets the multiplier for scaling the data on the signal axis.

Chromatogram

Name and location of the resultant chromatogram created after importing an **AIA** file. By design, the program will store the original name of the imported file along with the *.PRM suffix and the path to the directory of the current project.

To select another name and location of the resultant chromatogram, open the **Save As...** dialog using the  button.

3.1.6.2 Text and EZChrom ASCII

Imports a chromatogram saved in a text file.

A chromatogram in text format may (but need not) contain a heading with a description of the conditions of measurement and must contain data of the chromatographic curve in one or more columns.

The station automatically interprets the headings of text files exported from the **Clarity** station and from the **EZChrom** program.

Note: The **EZChrom ASCII** text format uses the file suffix (*.ASC). It differs from the **text** format exported from **Clarity** station in the naming of individual items in the heading.

After selecting the chromatograms in the *Open Files to Import* dialog and pressing the *Open* button, the *Import Text File* dialog opens.

The conversion program determines the most suitable import setting according to the content of individual imported text files. Individual settings can subsequently be adjusted in the *Import Text File* dialog and saved for further use. Import is performed by the *OK* button.

Note: If a number of files was selected in the *Open Files to Import* dialog, a further *Import Text File* dialog or *Import AIA File* dialog will open (according to the type of the next selected chromatograms) after clicking on the *OK* button.

Preset

When the same type of files are imported frequently, it can be useful and time-saving to save import settings for further use. In drop-down box on the left user can select from previously saved presets, by clicking button right to list the presets management menu will open. The menu contain commands for saving current setting (*Create New...*), *Rename...* or *Remove*presets. Presets are stored as part of **Clarity** Desktop settings.

Apply Settings to

This radio button group indicates whether all the settings below will be applied either to current file only or to all files imported at once. In case multiple files are imported at a time, and this radio buttons are set at *Current File*, the *Import Text File* dialog will be invoked for every file in the sequel. When *Apply Settings to* radio button is switched into the *All n Files* position, subsequent files will be proceeded with the same settings. By checking *Prefer Detected Settings* checkbox you can force Clarity to use setting detected from the imported file (where applicable).

Apply Method

Choose method whose parameters (integration table, attached calibration, etc.) will be applied into the imported chromatogram. By default, displayed method matches method in the [Single Analysis](#) dialog. Leaving this field blank applies default parameters.

Current Text File

The name of imported file including directory path.

Preview

This button will open the current file in simple text viewer. This can help user to identify exact meaning of particular columns when it's not clear from file suffix.

Import From Line

Sets the line of the file on which the data import should start.

Import To Line

Sets the last line of the file that should be imported.

Separator

Selects the sign by which the individual items are separated in the text file. <TAB>, <SPACE>, <COMMA> or <SEMICOLON> are available signs to choose from.

Decimal Separator

Separator of decimal points - <DOT>, <COMMA> or <Windows Locale>. Separator indicated in Windows (as <Windows Locale>) is used as the default.

Note: Parameters entered to *Import From Line*, *Import To Line*, *Separator* and *Decimal Separator* fields will be applied on all simultaneously imported chromatograms.

Import Text File

Preset: <None>

Apply Settings to: Current File All 1 Files Prefer Detected Settings

Apply Method: [Info icon] [Field] [Preview]

Current Text File: C:\Clarity\DataFiles\DEMO1\Data\2506MULTI - RI.txt

Import From Line: [Field] Import To Line: [Field]

Separator: <TAB> Decimal Separator: <Window's Locale>

Analyst: DataApex

Sample ID: SN4616

Sample: 5

Sample Date: 01.08.2003

Amount: 0

Dilution: 1

ISTD Amount: 0

Injection Volume: 0

Imported Data: Time + Signal + Time + Signal...

Number of Detectors: 4

Signal Name	Sample Rate [Hz]	Signal Units	Autoscale	Signal Axis Name	Time Units	Y Multiplier	Data Size
Signal 1	10	mV	<input checked="" type="checkbox"/>	Voltage	min	1	10142
Signal 2	10	mV	<input checked="" type="checkbox"/>		min	1	0
Signal 3	10	mV	<input checked="" type="checkbox"/>		min	1	0
Signal 4	10	mV	<input checked="" type="checkbox"/>		min	1	0

Save as Chromatogram: C:\Clarity\DataFiles\DEMO1\Data\2506MULTI - f ... Load Defaults

OK Skip Cancel Help

Fig. 114: Import Text File

Analyst, Sample ID, Sample, Sample Date, Amount, Dilution, ISTD Amount, Injection Volume

These fields composing the chromatogram heading have the same meaning as described in the chapter "**Single Analysis**" on pg. 113.

Imported Data

Time + Signal + Time + Signal... - Every chromatographic curve is saved in a pair of columns, in which the first one represents a time and the second one a signal.

Signal + Time + Signal + Time... - Every chromatographic curve is saved in a pair of columns, in which the first one represents a signal and the second one a time.

Signal + Signal... - Every chromatographic curve is saved in one column, where the values represent the signal only. The time basis is obtained from the *Sample Rate* field.

Time + Signal + Signal... - Time base is contained in first column, every next column represents a signal of one detector.

Number of detectors

Specifies the number of detectors for the import of multi-detector chromatograms.

Sample Rate

Selects the sampling speed in the number of samples per second (Hz). Select one of the speeds from the list corresponding to the speeds of your A/D converter or enter your own value.

Signal Units

Determines the units in which the signal values are stated.

Note: Imported Data will not be parsed to recognize scaled units.

Autoscale

Sets the possibility to automatically scale the signal units in graphs.

Signal Name

Sets the signal name for further display.

Time Units

Determines the units in which time values are stated.

Possible values are: *ms* - milliseconds, *s* - seconds, *min* - minutes.

Note: Minutes are entered in decimal format (e.g. 1.5 min. = 1 min. 30 seconds).

Y Multiplier

Sets the multiplier for scaling the data on the signal axis.

Data Size

Number of points of a curve.

Note: This field cannot be adjusted. It serves only as referential check whether the import took place correctly.

Save as Chromatogram

Sets the name and location of the resultant chromatogram created after importing a text file. By default, the program will offer to use the original name of the imported file using the suffix *.PRM with a path to the directory of the current project.

To select another name and location for the resultant chromatogram, open the Save As... dialog using the button.

Load Defaults

Selects implicit values of all fields (i.e. returns the dialog into state prior to any changes made after opening).

OK

Confirmation of import.

Skip

Skips current file and proceed to subsequent one while importing multiple files.

Cancel

Cancellation of import.

3.1.6.2.1 Import Preview

This dialog displays the current file in simple text viewer. This preview can help user to identify exact meaning of particular columns when it's not clear from file suffix as it contains information from the chromatogram header, columns and axis description.

By clicking somewhere in the content ① you can get the number of the line selected ②. It is useful if you need to import only part of the data contained in the imported file. Such desired line numbers can be inserted into *Import From Line* and *Import To Line* in the *Import Text File* dialog.

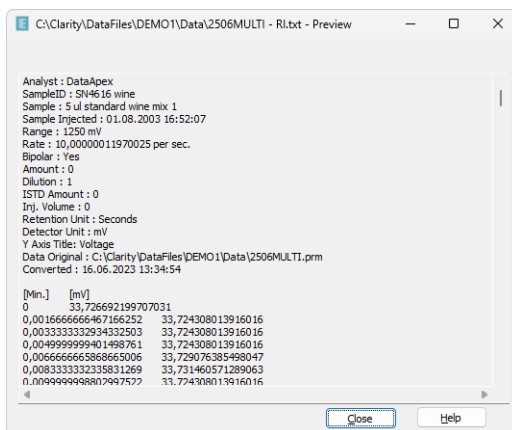


Fig. 115: Import Preview

3.1.6.3 Import RAW...

Transforms raw data (from **CSW17** or the external **PAD** converter) to a chromatogram. Invoking the command opens the *Open RAW Data* dialog (similar in appearance to the [Open Method](#) dialog described on pg. 68.). Here you will be invited to enter the name of the chromatogram to be created.

Caution: Raw data is processed using the current method from the [Instrument](#) window (not by the method of the currently displayed chromatogram, if any!).

3.1.7 Export Chromatogram

Exports chromatographic curve into **AIA** (*.CDF), **text** (*.TXT), **Multidetector text** (*.CHR) or **EZChrom ASCII** (*.ASC) format. Using the command invokes the *Export Chromatogram* dialog.

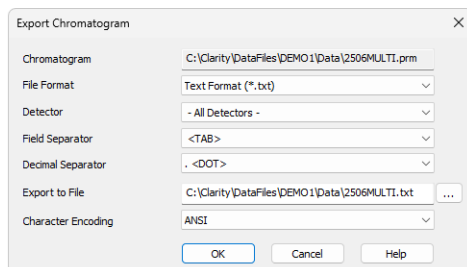


Fig. 116: *Export Chromatogram*

Chromatogram

Name of the exported chromatogram including its full path. This field serves for informational purposes only and cannot be modified.

File Format

Selects one of the available formats for export:

AIA Format (*.CDF) - is one of the standard formats used for exchanging data among various chromatography systems. Multidetector chromatograms will be exported to multiple files, each signal into a separate file distinguished by the name of the detector.

Note: Further information about AIA format can be found for example in following article:
Terrance A. Rooney - "STANDARDS FOR CHROMATOGRAPHY DATA SYSTEMS", Today's Chemist at Work, 1998, 7(5), 15-17.

Clarity only exports raw data and basic chromatogram description, no results, method data, calibration data or GLP data are exported into the *AIA Format*.

Following text formats (*Multidetector Text Format* (*.CHR), *Text Format* (*.TXT), *EZ Chrom ASCII Format* (*.ASC)) will contain a header and exported data in two columns separated by an arbitrary separator (TAB, COMMA, SEMICOLON).

Multidetector Text Format (*.CHR) - will always contain all available signals in a single exported file.

Text Format (*.TXT) - Multi-detector chromatograms will be exported to multiple files, each signal into a separate file distinguished by the name of the detector. Signals generated by the Auxiliary devices can be exported using the .TXT format - Auxiliary Signals will be listed in the combobox.

EZ Chrom ASCII Format (*.ASC) - is a text format used by EZ Chrom software. Comparing to the *Text Format* the data are exported in one column only (voltage), separator can be <TAB> only and the structure of the header is slightly different.

Detector

Selects the signals for export. An individual detector, or all detectors at once can be selected.

Note: Only for *AIA* and *EZChromASCII Format*.

Field Separator

Selects the character to be used as data separator.

Note: Only for *Multidetector Text Format* and *Text Format*.

Decimal Separator

Selects the character to be used as decimal separator.

Note: Only for *Multidetector Text Format* and *Text Format*.

Export File

Invokes the *Save As* dialog in which the name and location of the file into which you wish to export the chromatogram is entered.

Note: If no name is entered, the name of the exported chromatogram is automatically used with the relevant suffix.

Character Encoding

You can chose to export Chromatogram using *ANSI* or *Unicode (UTF 8)* encoding.

Note: Only for *Multidetector Text Format* and *Text Format*.

Caution: Chromatogram containing unsaved modifications will be saved before exporting. Export is logged in the **Audit Trail**.

3.1.8 Sign ✓ full version

Command for electronic signature of current version of chromatogram. After selection, the *Sign* dialog will be displayed.

Caution: Chromatograms cannot be signed unless you have set up a user account in the [User Accounts](#) dialog. It is also impossible to sign a chromatogram which has been opened using one of the methods from the history (*Method* field of the [Open Chromatogram](#) dialog).

Choose User

Selects the user who is to sign the current version. A list of users from the [User Accounts](#) dialog is displayed.

User Description

Content of the *Description* field of selected user from the [User Accounts](#) dialog.

Sign as Current User

The chromatogram will only be signed using the name and password entered within the framework of the **Clarity** station.

Sign Using Certificate

The chromatogram will be signed using the certificate installed in your computer. Select the certificate by using the *Select Certificate* command.

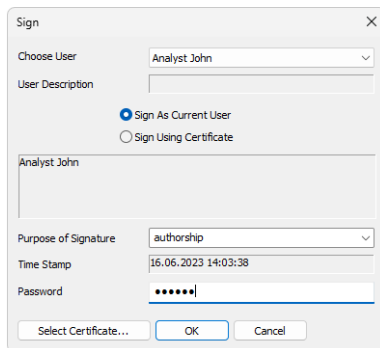


Fig. 117: Sign

Purpose of Signature

Allows to enter the purpose of signature. Select from the preset options or supplement your own.

Time Stamp

Date and time of signature.

Password

Mandatory password of selected user.

Select Certificate

Selects 3rd party certificate when selecting a signature using certificate (*Sign Using Certificate*).

Caution: It is necessary to bear in mind that in case of signing chromatograms with 3rd party certificate it is necessary to have the certificate of each Windows user account installed in the Personal storage of every Windows user account used on the PC where Clarity is operated. If there would be installed more certificates for more Clarity user accounts under single Windows user account it could easily happen that various Clarity users (defined through [User Accounts](#) dialog) could sign chromatograms with someone's else certificate. This situation can occur because it is standard behavior of the certificates in Windows environment to ask currently logged Windows user for password to his/her certificate only for the first usage of the certificate during individual Windows user account login session. Every other request to sign any chromatogram with already used certificate won't invoke any other request for repeated password insertion and the selected chromatogram could be signed using any available certificate for which its correct password was entered during current session of the logged in Windows user. To avoid that, in case of wish or necessity to use 3rd party certificates, it is necessary to have for each Clarity user account its separate Windows user account with unique credentials and 3rd party certificate installed in Private storage of this Windows user account. This condition has to be handled when Clarity should be deployed in regulated environment (such as in organizations working in terms of compliance with GLP guidelines) and there should be used certificates issued by 3rd certification authorities. There is still option to avoid this complication by signing of chromatograms by credentials defined for each Clarity user through option *Sign As Current User*.

Chromatograms cannot be signed unless you have set up a user account in the [User Accounts](#) dialog. It is also impossible to sign a chromatogram which has been opened using one of the methods from the history (*Method* field of the [Open Chromatogram](#) dialog).

3.1.9 Verify

Displays a list of the current chromatogram's electronic signatures. After selection, the *Verify Signatures* dialog will be displayed.

A list of all the signatures of all versions of the chromatogram is displayed in the window. The signatures are arranged according to all the signed versions. Individual versions are displayed in the list by the date that the chromatogram was saved.

Caution: Take note that this is not the date of signature but the date of saving of the signed version of the chromatogram.

Each version may be signed several times.

Each signature is represented in the list by the name of the current user and the purpose of signature. Double-clicking on the signature or clicking on the *Show Details* button will display all details about the currently selected signature:

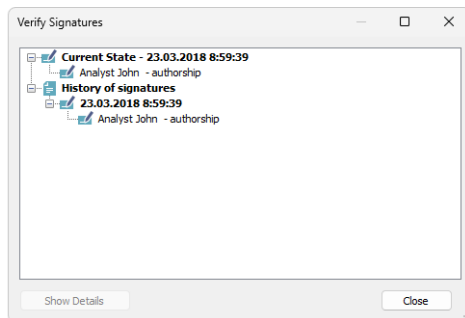


Fig. 118: Verify Signatures

Signature is Valid

Confirms validity of signature (no attempt to forge the signature).

Content was not changed

Confirms validity of content (no attempt to change the signed content).

Purpose of signature



Displays the purpose of signature.

Time Stamp

Displays the date and time of signature.

3.1.10 PostRun Setting (From Chromatogram Window)

Post-processing of an already measured chromatogram. This dialog can be invoked using the *Perform Postrun...* command from the *File* menu of the [Chromatogram](#) window. When prompted, the *PostRun Setting (From Chromatogram Window)* opens, where selected actions can be manually performed on the active chromatogram.

The same function is done by the  icon (hidden by default), as long as the *PostRun Setting (From Chromatogram Window)* dialog is unset. When some actions are selected in the dialog, the  icon only performs the actions set, without opening of the dialog.

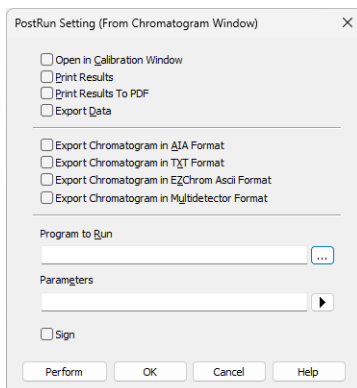



Fig. 119: PostRun Setting (From Chromatogram Window)


Open in Calibration Window

The created chromatogram will be automatically loaded into the [Chromatogram](#) window.

Print Results

A report will be printed according to the print style set in the *Report Setup*  of the [Chromatogram](#) window. The default style is CHROMATOGRAM.STY.

Print Results To PDF

A report will be printed to *.PDF file according to the print style set in the *Report Setup*  of the [Chromatogram](#) window. The default style is CHROMATOGRAM.STY.

Export Data

The created chromatogram will be exported according to settings made in the [Export Data](#) dialog (for more details see also chapter **Export Data** on pg. 141).

Export Chromatogram in AIA Format

Exports a chromatogram in AIA format. This corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window. The exported

chromatogram will be saved under the same name as the source chromatogram (with the *.CDF suffix) and located in the same directory (for more details see also chapter **Export Chromatogram** on pg. 182).

Export Chromatogram in TXT Format

Exports a chromatogram in the TXT format. Corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The exported chromatogram will be saved under the same name as the source chromatogram (with the *.TXT suffix) and located in the same directory.

Export Chromatogram in EZChrom ASCII Format

Exports a chromatogram in the ASC text format, which is used by the EZ CHROM program. This corresponds to *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The exported chromatogram will be saved under the same name as the source chromatogram (with the *.ASC suffix) and located in the same directory.

Export Chromatogram in Multidetector Format

Exports a chromatogram in the TXT format. Multiple signals will be stored in separate columns of the resulting file. Corresponds to the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 182).

The exported chromatogram will be saved under the same name as the source chromatogram (with the *.TXT suffix) and located in the same directory.

Program to Run

Sets the program which will be run after the completion of the measurement.



Searches for the program which should be entered in the *Program to Run* field.

Only with Export

This item has two functions:

- The program specified in the *Program to Run* field will only be run if the *Automatic Export* checkbox has been selected.
- While manually exporting from the [Chromatogram](#) window using **Ctrl** + **E** shortcut this item enables the simultaneous running of the program specified in the *Program to Run* field.


Parameters

Parameters of the run program, which are normally entered in the command line behind the program name (e.g. name of loaded file, macro, etc.).

The following variables can be used in the *Parameters* field:

- Variable %f will be substituted by the name of the chromatogram at the moment of processing.

- Variable %e will be substituted by the name of the file to be exported at the moment of processing. (This does not apply when exporting multidetector chromatograms in TXT or AIA formats.)

Click the  button next to the *Parameters* field to enter the variables automatically. For facilitating of exported chromatogram files copying you can use COPYFILES.EXE utility, located in \Bin\UTILS subfolder. It allows you to copy all the exports from one chromatogram (.TXT, .PDF) at once. An utility is thoroughly described in COPYFILES.TXT file in the same folder.

Sign


Sign the chromatogram in which the changes are performed during the postrun according to the settings done in the [Sign](#) dialog. This function is only available in the Full version.

Caution: Chromatograms cannot be signed unless you have set up a user account in the [User Accounts](#) dialog. It is also impossible to sign a chromatogram which has been opened using one of the methods from the history (*Method* field of the [Open Chromatogram](#) dialog).


Use the *Perform* button to perform the actions set in this dialog, or the *OK* button to save the changes made in the dialog and leave it without performing the actions.


3.2 Edit


Sub-menu of commands for working with clipboard and tables.


 Undo	Cancels adjustments in the integration table. This may be used repeatedly as the station remembers all adjustments made to tables from its initial start-up. The history of commands only applies within the framework of the table and each table maintains its own independent list of operations. The command can also be invoked using the Ctrl + Z shortcut.
---	---

Note: Changes performed interactively in the chromatogram graph are recorded into the **Integration Table** on the [Integration](#) tab. The history of operations for the *Undo* function ceases to be accessible after switching to another table. If you wish to return to the given operation, first place the cursor into the area of the graph or switch to the [Integration](#) tab and then apply the *Undo* function.

 Redo	Countermands the <i>Undo</i> command which can be invoked repeatedly. The station remembers all modifications made in tables during the last session. The history of commands applies within the framework of the table and table of each signal maintains its own independent list of operations. Commands can also be invoked using the Ctrl + Shift + Z shortcut.
---	---



 Cut	Removes selected text and stores it in clipboard. The command can also be selected using the Ctrl + X shortcut.
--	---

 Copy	Copies selected text into clipboard. The command can also be selected using the Ctrl + C shortcut.
--	--

 Paste	Copies the clipboard content to the desired location (Ctrl + V). <i>Paste</i> function automatically inputs the content of the clipboard into the desired fields of tables. If the area is larger than the content, the content will be tiled. You may make use of this characteristic if you wish to insert a larger quantity of identical fields into a table or several periodically repeating fields.
--	--

Paste into the **Integration Table** is prohibited.

Select All	Selects all fields of table. This command can also be selected using the Ctrl + A shortcut.
-------------------	---

Delete All	Deletes all deletable fields of the Integration table .
Delete	Deletes selected deletable fields of the Integration table .
Add User Column... 	<p>Adds column as defined by the user.</p> <p>To access the edition of user columns the user must be authorized to edit methods. See the <i>Edit Method</i> checkbox in the User Accounts dialog.</p>
Delete User Column... 	<p>Deletes all user columns.</p> <p>To delete only some of the user columns use the <i>Setup Columns...</i> command. In the Setup Columns dialog then delete the selected user columns using the <i>Delete</i> button.</p>
<i>Note:</i>	If you wish to remove a user column only temporarily, use the <i>Hide Column(s)</i> command (available from the local menu of the table or from the Setup Columns dialog).
Restore Default Columns...	<p>The command in most tables restores implicit columns, their visibility, order, and width. As no user columns are in default layouts, all user columns are hidden.</p> <p>The behavior is different in the Summary Table, where using the command loads the current layout of the Result Table and mimics it in the right side of the Summary Table (part defined on the <i>Summary</i> tab of the Summary Columns Setup dialog), however the User Columns available in the Result Table are not recreated and displayed in the Summary Table. The left side of the Summary Table (the part defined on the <i>Common</i> tab of the Summary Columns Setup dialog) loads the default set of visible columns.</p>
<i>Note:</i>	By contrast to the <i>Delete User Columns</i> command, user columns are only hidden and not deleted.
User Variables	Sets the user defined analysis and method variables.
Setup Columns...	Sets the appearance of columns. Opens the Summary Columns Setup dialog when in the <i>Summary</i> tab and the Setup Columns dialog when in other tabs.

Hide Column(s)

Hides selected columns.
Select the columns by left clicking the mouse on the column header. Multiple columns can be selected by pressing and holding the **Ctrl** key.

Note: Hidden columns will not be exported from the **Result Table**.

Show Hidden Column(s)

Displays columns that have been hidden using the *Hide column(s)* command or [Setup Columns](#) dialog.

Caution: When the *Show Hidden Columns* command is not active and a column is still not visible, it means that a zero width has been set for the given column. To restore the column, use the *Restore Default Columns* command.

3.2.1 Add User Column Full version

Appends a new column with user-defined calculation and opens the *Add User Column* dialog:

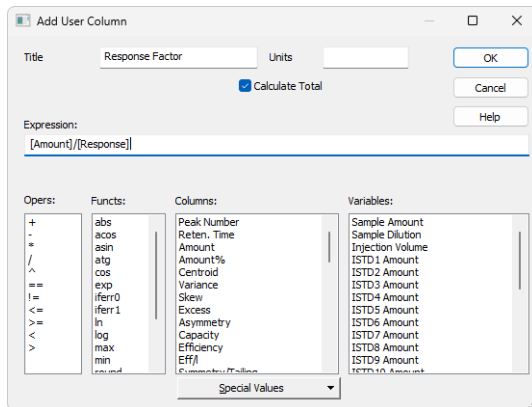
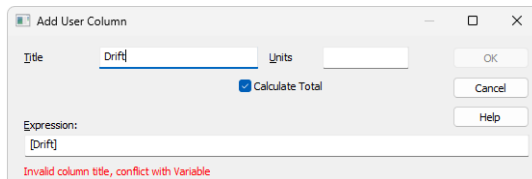


Fig. 120: Add User Column

Note: To access the edit of user columns the user must be authorized to edit methods. See the *Edit Method* checkbox in the [User Accounts](#) dialog.

Title

Enter the name of the new column here. Only one line of text is allowed. *Title* name must be different from default *Columns* and *Variable* names, otherwise conflict of names is triggered.



Units

Enter the units for the user column.

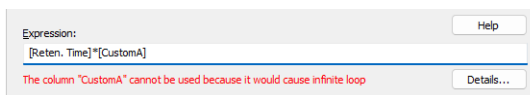
Calculate Total

Determines whether the *Total* row in the corresponding *User Column* should be displayed.

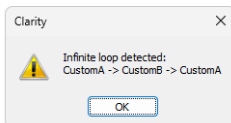
Expression

A calculation formula that can be entered directly or created progressively by double-clicking items in the provided *Columns*, *Ops*, *Functs*, *Special Values* and *Variables* fields.

You will be notified if you have composed an expression that causes a recursion, after clicking the *OK* button.



The *Details* button will appear below the *Expression* field. Click it to display a message box which will identify the columns that have caused the recursion.



Opers

Contains a list of all mathematical operators available. Double-click an operator to insert it in the formula being compiled.

Functs

List of available mathematical functions. Insert a function into an formula by double-clicking the mouse.

Tab. 9: List of available functions

Function	Explanation
abs	- Absolute value
acos	- Arcuscosinus (Result is in radians)
asin	- Arcussinus (Result is in radians)
atg	- Arcustangent (Result is in radians)
cos	- Cosinus (Number used for calculation is in radians)
exp	- Exponential function
iferr0	- Returns 0 when argument is invalid (=value would be displayed as "???"). Does nothing when argument is valid.
iferr1	- Returns 1 when argument is invalid (=value would be displayed as "???"). Does nothing when argument is valid.
ln	- Natural logarithm
log	- Logarithm
max	- Maximum value of parameter of a function. E.g. MAX (1; 5; 3) returns value 5.
min	- Minimum value of parameter of a function. E.g. MIN (1; 5; 3) returns value 1.
round	- Rounding off. Number after semicolon specifies number of decimal places. E.g. ROUND (2,8888;2) returns value 2,89.
sin	- Sinus (Number used for calculation is in radians)
sqrt	- Square root
switch	- SWITCH(n; H ₁ ; H ₂ ; H ₃ ;...) returns the value of the n th item H _n
tg	- Tangent (Number used for calculation is in radians)

Columns

Lists all available columns as variables. Double-click a column to insert it in the formula (by default as a name of the column in square brackets).

Spec. Values

Calculated values related to the current (selected) column.

Tab. 10: List of special values

Value	Description
Sum	- Sum of all values in the column
Average	- Average of the values in the column
Std. Deviation	- Standard Deviation of values in the column
Minimum	- Minimal value in the column
Maximum	- Maximal value in the column
First	- Value from the first peak in chromatogram (peak with the lowest retention time)
Last	- Value from the last peak in chromatogram (peak with the highest retention time)
Previous	- Value from the previous peak in chromatogram (based on peaks' retention order)
Next	- Value from the next peak in chromatogram (based on peaks' retention order)
Compound	- Opens a table, from which is possible to pickup the name of compound (coined in Calibration or Integration table) and use it as a variable. (e.g. its retention time or amount)

Calculations with applied options *First*, *Last*, *Previous* and *Next* are based on retention order of peaks in chromatogram. In case the table is resorted (for example according to increasing *Response*) results for all *User Columns* will be still calculated according to retention order of peaks in chromatogram. In case the table is exported the [Export](#) tool will calculate results for any *User Column* using any of these options according to retention order of peaks. It means there will be mismatch between order of rows displayed in **Clarity** and in exported file (or clipboard). Please refer to image below where [Results Table](#) is sorted differently but the resulting export file is the same.

It can be read on image below how sorting in (for example) in row *Response* influences look of the table but does not influence calculated values for *User Column*. Various sorted table is exported always the same. Different sorting of table does not cause recalculation of any *User Column* which uses any of these four options.

	Reten. Time [min]	Response	Next (Retention Time) [min]	Previous (Retention Time) [min]
2	1,752	0,618	2,302	1,187
1	1,187	0,768	1,752	???
4	2,552	1,590	2,857	2,302
3	2,302	33,048	2,552	1,752
5	2,857	44,529	???	2,552
Total				

	Reten. Time [min]	Response	Next (Retention Time) [min]	Previous (Retention Time) [min]
5	2,857	44,529	???	2,552
3	2,302	33,048	2,552	1,752
4	2,552	1,590	2,857	2,302
1	1,187	0,768	1,752	???
2	1,752	0,618	2,302	1,187
Total				

Peak No.	Reten. Time [min]	Response
1	1,187	0,768
2	1,752	0,618
3	2,302	33,048
4	2,552	1,590
5	2,857	44,529
Total		

Peak No.	Reten. Time [min]	Response
1	1,187	0,768
2	1,752	0,618
3	2,302	33,048
4	2,552	1,590
5	2,857	44,529
Total		

Fig. 121: User Column - Export with Various Sorting of Table

Only peaks displayed in the table are calculated. Due to this, it is possible that the values of these variables may change depending on the setting of the *Report in Result Table* item from the right side of the [Chromatogram - Results](#) tab.

Note: These functions enable the creation of inter-line calculations, e.g. calculation **RRT** - relative retention time. For calculating an individual RRT, one can input expression $[Reten. Time]/[REFER\$Reten. Time]$, where REFER will be the name of selected reference compound.

Note: The missing values ??? from the original column are ignored when using *Special Values*. For example, when using *Special Value - Average* from the column *Next (Retention Time)*, the sum of the 4 valid values would be divided by 4.

Variables

Lists all available **Clarity** internal and user's defined variables. Double-click a variable to insert it in the formula.

Tab. 11: List of Variable

Value	Description
Sample Amount	- Defines sample amount.
Sample Dilution	- Defines dilution of the sample.
Injection Volume	- Defines the volume of injection.
ISTD1-ISTD10	- The amounts of the internal standards for the ISTD method.
Chromatogram Amount	- Sum of the amounts across all signals.
Unretained Peak Time	- Defines the column dead time.
Column Length	- Defines the length of the column.
Noise	- Defines the amount of noise in the specified interval of the chromatogram. The interval is set in the Integration Table .
ASTM Noise	- The noise value calculated as an average from values counted for smaller intervals. The interval is set in the Integration Table and divided into same length parts.
6-Sigma Noise	- The noise value calculated from the whole interval set in the Integration Table .
Drift	- Determines the drift between the beginning and the end point of the specified interval. The interval is set in the Integration Table .
AnalysisUserVar1 - AnalysisUserVar3	- User variables defined for analysis, set in <i>Single Analysis</i> , <i>Sequence</i> or <i>Chromatogram</i> window.
MethodUserVar1 - MethodUserVar3	- User variables defined for method, set in <i>Method Setup</i> window.

3.2.2 Setup Columns

Setup Columns dialog is used to customize the table columns:

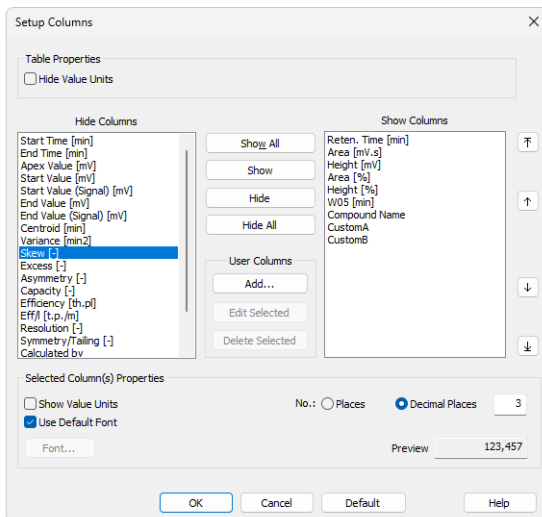


Fig. 122: Setup Columns

Note: To access the edit dialog of user columns the user must be authorized to edit methods. See the *Edit Method* checkbox in the [User Accounts](#) dialog.

Note: *Setup Columns* dialog invoked from *Sequence* window contains additional text field *Custom Name* to set the name of *Analysis User Variables*. For more details about User Variables see the chapter "**Sequence**" on pg. 385.

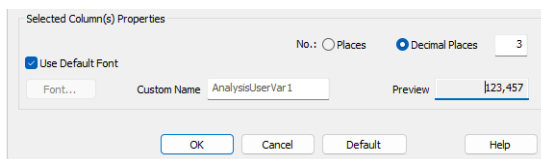


Fig. 123: Setup Columns in Sequence window

Hide Value Units

Hides all value units in the whole table.

Hide Columns

Shows the list of all hidden columns.

Show Columns

Displays a list and specifications of currently displayed columns.

Show All

Displays all existing columns by transferring hidden columns from the left *Hidden Columns* list to the end of the right *Displayed Columns* list.

Show

Transfers the selected hidden column(s) from the left list to the list of displayed columns. The displayed columns are added to the *Show Columns* field in the fixed order they had in the *Hide Column* list, but may be moved forward/backwards via the arrow icons to the right of the *Show Columns* field.

Hide

Hides the selected displayed column(s) by transferring them from the right to the left list.

Hide All

Hides all columns by transferring them from the right to the left list.

User Columns**Add...** ✓ Full version

Opens the [Add User Column](#) dialog (for more details see the chapter **Add User Column** on pg. 193). to add a new column with user-defined calculation.

Edit Selected ✓ Full version

Modifies the selected column containing a user-defined calculation.

Delete Selected ✓ Full version

Deletes the selected column containing a user-defined calculation.

Show Value Units

Shows the values with units for the selected column.

Use Default Font

Applies the default font, specified in the *Table Fonts - Default Fonts* item of the [User Options - General](#) dialog (available from the [Instrument](#) window by using the *View - Options* command), to the columns marked.

Font

Prescribe the font for the column selected. Invoking the command opens the *Font* dialog.

No. of Places

Specifies the number of valid digits to be displayed in the column selected.

No. of Decimal Places

Specifies the number of decimal places to be displayed in the column selected.

Preview

Displays a preview of the results in the selected column.

Default

Restores the default columns and their values and hides the user columns (for more details see the chapter **Edit** on pg. 191).

3.2.3 Summary Columns Setup

Summary Columns Setup dialog is used to customize the *Summary Table* columns in the *Summary* tab in the *Chromatogram Window*:

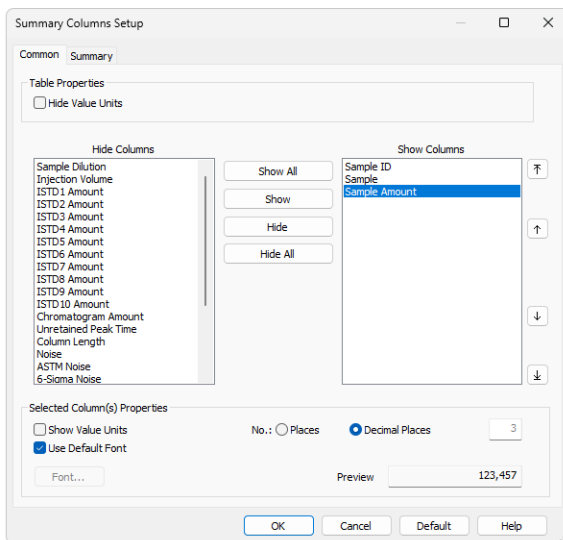


Fig. 124: Summary Columns Setup - Common

The *Common* tab in the *Summary Columns Setup* is used to customize the common columns for the chromatogram or signal.

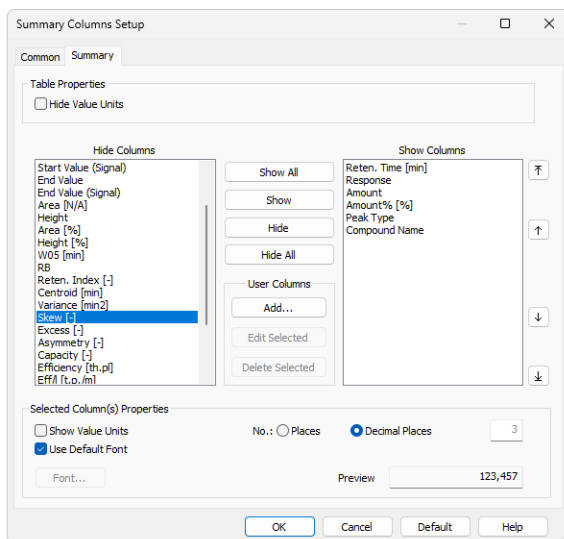


Fig. 125: Summary Columns Setup - Summary

The *Summary* tab in the *Summary Columns Setup* is used to customize the columns for the compounds.

Note: To access the edition of user columns the user must be authorized to edit methods. See the *Edit Method* checkbox in the [User Accounts](#) dialog.

Hide Value Units

Hides all value units in the whole table.

Hide Columns

Shows the list of all hidden columns.

Show Columns

Displays a list and specifications of currently displayed columns.

Show All

Displays all existing columns by transferring hidden columns from the left *Hidden Columns* list to the end of the right *Displayed Columns* list.

Show

Transfers the selected hidden column(s) from the left list to the list of displayed columns. The displayed columns are added to the *Show Columns* field in the fixed order they had in the *Hide Column* list, but may be moved forward/backwards via the arrow icons to the right of the *Show Columns* field.

Hide

Hides the selected displayed column(s) by transferring them from the right to the left list.

Hide All

Hides all columns by transferring them from the right to the left list.

User Columns

Add... ✓ Full version

Opens the [Add User Column](#) dialog (for more details see the chapter **Add User Column** on pg. 193). to add a new column with user-defined calculation.

Edit Selected ✓ Full version

Modifies the selected column containing a user-defined calculation.

Delete Selected ✓ Full version

Deletes the selected column containing a user-defined calculation.

Delete All ✓ Full version

Deletes all previously added user columns.

Show Value Units

Shows the values with units for the selected column.

Use Default Font

Applies the default font, specified in the *Table Fonts - Default Fonts* item of the [User Options - General](#) dialog (available from the [Instrument](#) window by using the *View - Options* command), to the columns marked.

Font

Prescribe the font for the column selected. Invoking the command opens the *Font* dialog.

No. of Places

Specifies the number of valid digits to be displayed in the column selected.

No. of Decimal Places

Specifies the number of decimal places to be displayed in the column selected.

Preview












Displays a preview of the results in the selected column.

Default

Resets the layout of the **Summary Table** columns to the current layout of the **Result Table** (for more details see the chapter **Edit** on pg. 191). The User Columns displayed in the **Result Table** are not created and displayed in the **Summary Table**.

3.3 Display

This is an entry point to a submenu of commands for displaying chromatograms.

	Preview Graph	Displays/hides the orientation graph.
	Zoom Out	Zooms out the current part of chromatogram. Also invoked by pressing - key on numeric keyboard or by turning mouse wheel clockwise with Ctrl pressed.
	Zoom In	Zooms in the current part of chromatogram. Also invoked by pressing + key on numeric keyboard or by turning mouse wheel counter-clockwise with Ctrl pressed.
	Previous Zoom	Using the  icon or Ctrl + ← shortcut on numeric keyboard restores the previously displayed cut. This function can be used repeatedly to go backwards through previous cuts. The station remembers all cuts effected during current session.
	Next Zoom	Restores the original cut abandoned by the <i>Previous Zoom</i> command. (Ctrl + → on numeric keyboard) It can be used repeatedly to go forwards through existing cuts. The station remembers all cuts effected during current session.
	Unzoom	Using the  icon or Ctrl + * shortcut on numeric keyboard cancels all cut-outs and displays the chromatogram in its original size. The original size may not always represent the whole chromatogram. If you have a fixed display range (<i>Range - Fixed</i>) set by the <i>Display - Properties...</i> command on the Time Axis or Signal Axis tabs, the chromatogram will be displayed in this range. Equally, the chromatogram may not be displayed whole if using the <i>Scale Y Mode</i> function from the Signals tab.
	Tables Up	Mutually exchanges the locations of the chromatogram and the tabs with tables so that the tabs with tables are at the top and the graphs are below.
	Show Balloon Help	Displays balloon help next to the cursor lines when user performs interactive modifications of the chromatogram. This feature can also be switched on/off using the  icon on the toolbar in the Chromatogram window.
	Properties	Controls the displayed graph and chromatogram(s).

3.3.1 Preview Graph

Displays/hides an auxiliary graph. The auxiliary graph is designated for displaying the cut-out performed in the main graph. The command can also be found in the local menu invoked by right clicking above the area of the graph. The auxiliary graph is always displayed in its original size.

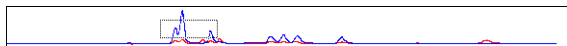


Fig. 126: Auxiliary Graph

Caution: If the size of the graph pane part falls below certain dimensions, the auxiliary graph is no longer displayed, regardless of the activated *Preview Graph* command. In such a case the graph can again be displayed by shifting the splitter separating the graph from the tables or by enlarging the entire [Chromatogram](#) window.

Note: The original size means either the size where the chromatogram fills the entire graph or a fixed size preset by the *Range - Fixed* commands from the [Graph Properties - Signal Axis](#) and [Graph Properties - Time Axis](#) dialog.

Work with cut-outs in auxiliary graph

A cut-out is illustrated in the auxiliary graph by a dotted rectangle. A cut-out can be easily created and shifted and its dimensions changed here.

Tab. 12: Manipulating preview graph using the mouse cursor

Action	Effect
Creation	Place the cursor in one of the corners of the envisaged cut-out. Click and hold the left mouse button, then draw the cursor diagonally to the opposite corner and release the button.
Shifting	Place the cursor inside the illustrated dotted rectangle. The cursor changes to . Click and hold the left mouse button. Shift the cut-out to the required place and release the button.
Change of size	Place the cursor on the edge of the cut-out. The cursor changes to , or . Click and hold the left mouse button. Change the size of the cut-out and release the button.

Tab. 13: Manipulating preview graph using the mouse wheel

Action	Effect
Wheel alone	Shifts cut-out of chromatogram up/down
Shift + wheel	Shifts cut-out of chromatogram left/right
Ctrl + wheel	Enlarges/reduces cut-out of chromatogram
Ctrl + Shift + wheel	Enlarges/reduces the cut-out of the chromatogram in the dimension of the Y-axis only.

Note: Navigation using the mouse wheel will function even when the auxiliary graph is hidden.

3.3.2 Properties

Sets the manner of the graph and chromatogram display. After selection, the [Graph Properties](#) dialog will be opened. The tabs of this dialog are very similar to the tabs of the [User Options](#) dialog described in the chapter "[User Options...](#)" on pg. 148. The difference is found primarily in the validity of set values. Here the set parameters are valid only for the main graph of the [Chromatogram](#) window. By contrast, parameters set in the [User Options](#) dialog are valid for all graphs of the current Instrument where the *Use User Options* checkbox has been checked.

3.3.2.1 Graph Properties - Graph tab

Except for the *Use User Options* and *Show Data Points* parameters, the tab is identical to the [Graph](#) tab of the [User Options](#) dialog described in the chapter "[Graph tab](#)" on pg. 152.

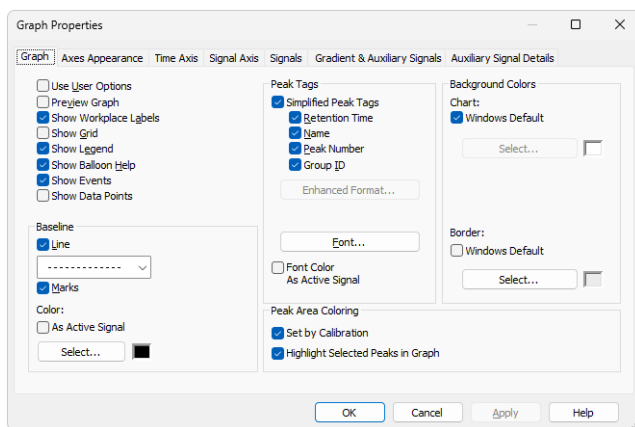


Fig. 127: Graph Properties - Graph

Use User Options

All parameter settings will be taken from the global setting in the [User Options - Graph](#) dialog (accessible from the [Instrument](#) window using the *View - Options...* command).

Show Data Points

When checked, shows the individual data points in the graph. These data points may be inspected using the magnification of the area of the graph.

Note: This parameter setting is not saved in the desktop file and its selection is only valid until the [Instrument](#) window is closed.

3.3.2.2 Graph Properties - Axes Appearance tab

Displays graph axes. Except for the *Use User Options* parameter, the tab is identical to the [Axes Appearance](#) tab of the [User Options](#) dialog described in the chapter "[Axes Appearance tab](#)" on pg. 155.

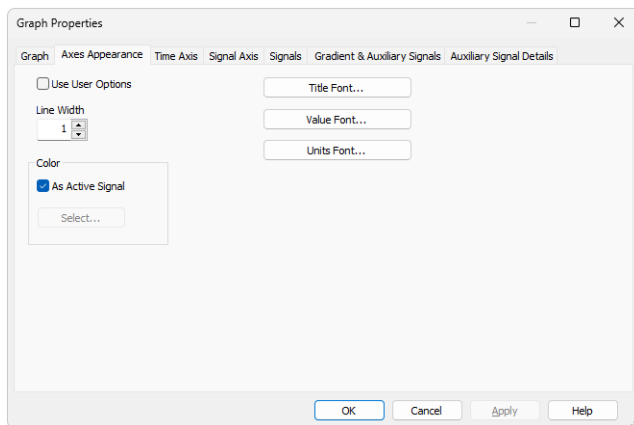


Fig. 128: Graph Properties - Axes Appearance

Use User Options

All parameter settings will be taken from the global setting in the [User Options - Axes Appearance](#) dialog (accessible from the [Instrument](#) window using the *View - Options...* command).

3.3.2.3 Graph Properties - Time Axis tab

Sets the scale of the display and the units for time on the horizontal axis of graph.

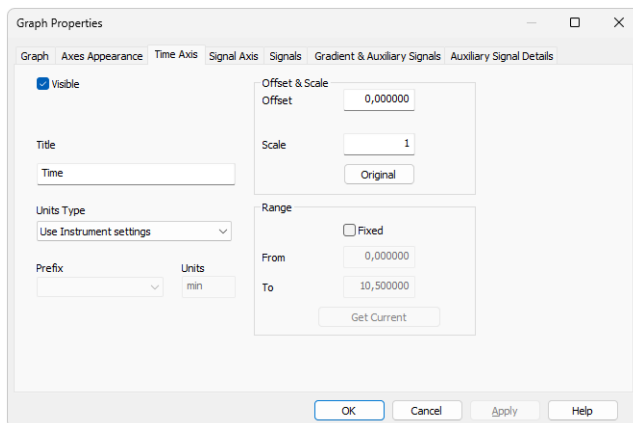


Fig. 129: Graph Properties - Time Axis

Visible

Enables the display of time axis.

Title

Name of the axis.

Units Type

Type of units of the axis, displayed in square brackets. Following unit types are available:

Auto - Numbers will be displayed on the axis by the normalized basic units stated in the *Units* field. The axis is thus automatically normalized. This means that, when necessary, suffixes expressed in multiples of 1000 or fractions of the basic units are added to the basic units.

Fixed - Numbers will always be displayed on the axis in the units stated in the *Units* field without regard to size. Whenever a change of the range of the axis occurs, the numbers are not normalized and thus no prefix is added to the units.

Use Instrument settings - Units will be taken from the *System Configuration - Instrument Units* of the respective instrument.

Time - seconds - The axis will be displayed in seconds.

Time - minutes - The axis will be displayed in minutes and their hundredths.

Time - H:M:S - The axis will be displayed in hours, minutes and seconds.

Time - hours - The axis will be displayed in hours.

Units

By selecting *Auto* or *Fixed* in the *Units Type* field, you can enter the units in which you wish to display the horizontal axis. The conversion between the implicit units (minutes) and your own units is entered with the help of the *Offset* and *Scale* fields.

When the Units Type is switched to *Auto*, only basic units without prefixes can be entered.

Offset & Scale

Offset

Displayed data will be shifted by the value entered here.

Scale

Displayed data will be multiplied by the value entered here.

Original

Sets original values (i.e. *Offset* to 0 and *Scale* to 1).

Note: This settings applies to the graph axis only and not to the results tables. Consequently, only simplified peak tags will be shifted, while enhanced peak tags will keep the original values, as they are derived from result table.

Range

Fixed

Fixes range of horizontal axis of graph. This means that the range is determined by the *From* and *To* parameters and not by the actual size of the chromatogram.

From, To

Values for fixed range on horizontal axis.

Get Current

The *From* and *To* fields are entered by the minimum and maximum time of the active chromatogram (signal) according to the current selection.

3.3.2.4 Graph Properties - Signal Axis tab

Sets scale of display and units for signal (vertical) axis of graph. Both the signal name and signal units are exclusive to the signal displayed and are taken (by default) from the [Device Setup](#) dialog of the detector.

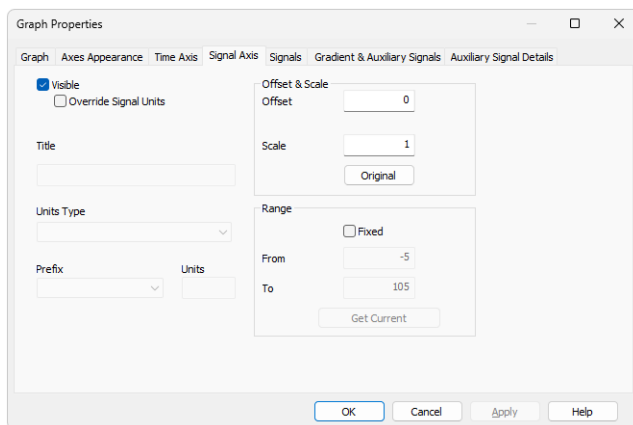


Fig. 130: Graph Properties - Signal Axis

Visible

Enables the display of the vertical axis.

Override Signal Units

Allows to manually enter units which will be displayed on the y-axis of the graph. When unchecked (default), signal units set in the [System Configuration](#) dialog will be used.

Title

Name of the axis.

Units Type

Type of the units of the axis displayed in square brackets.

Fixed

Numbers will always be displayed on the vertical axis in the units stated in the *Units* field without regard to size. When changing the range of the axis the numbers are not normalized and thus no prefix is added to the units.

Auto

Numbers will be displayed on the vertical axis in the normalized basic units stated in the *Units* field. The vertical axis is thus automatically normalized. This means that in the case of necessity, prefixes expressing multiples of 1000 or fractions of the basic units are added to the basic units. For example, instead of the value *0.001 V* the value *1 mV* will be displayed.

Prefix

Sets the prefix for the *Units* if the *Auto* option for *Units Type* is selected.

Units

The type of units entered (e.g. V (Volts), RI (Refractive Index),...). The conversion between the implicit units (volts) and your own units is entered with the help of the fields *Offset* and *Scale* while the *Fixed* option for *Units Type* is selected. When *Auto* option is selected, only the basic units (without prefixes) should be entered.

Offset & Scale**Offset**

Displayed data will be shifted by the value entered here. This applies to the graph signal axis only and not to the result tables.

Scale

Displayed data will be multiplied by the value entered here. This applies to the graph signal axis only and not to the results tables.

Original

Sets original values (i.e. *Offset* to 0 and *Scale* to 1).

Range**Fixed**

Fixed range of the vertical axis of the graph. This means that the range is determined by the *From* and *To* parameters and not by the actual size of the chromatogram.

From and To

Values for fixed range on vertical axis.

Get Current

The *From* and *To* fields are filled in by the minimum and maximum voltage of the active chromatogram (signal) according to the current selection.

3.3.2.5 Graph Properties - Signals tab

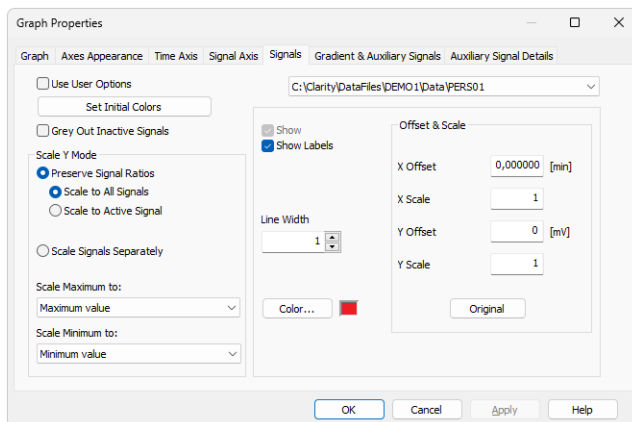


Fig. 131: Graph Properties - Signals tab

Use User Options

Parameter settings (for chromatogram signal colors and line width) will be taken from the global setting in the [User Options - Signals & Curves](#) dialog (accessible from the [Instrument](#) window using the *View - Options...* command).

Set Initial Colors

Sets colors back to those fixed at the initial installation of the station. *Set Initial Colors* button is disabled when option *Use User Options* is checked.

Grey Out Inactive Signals

When checked, all signals available in the [Chromatogram](#) window save the active one will be greyed out.

Scale Y Mode:

Automatically sets a scale on the vertical axis.

Preserve Signal Ratios

Preserves common axis for all displayed chromatograms (signals). Two alternatives may be selected:

Scale to All Signals - The scale will be set so that all the displayed signals fit into the window according to the minimum and maximum value of all displayed signals.

Scale to Active Signal - The scale will be set according to the active signal.

MS Offsetting - Specific display for the **MS Extension** - signal ratios are left untouched, but the individual signals are offset to start at the same height visually. This means the scale on the Y axis is the same for all

signals, but the offset is individual for different signals. This allows to disregard the background noise on some signals (namely on TIC).

Scale Signals Separately

Enlarges or reduces each signal so that they fit, full height, into the graph. Using this method will eliminate the mutual proportions between the various signals and each signal will have its own scale on the vertical axis.

Scale Maximum to

The upper limit for scale for displaying the chromatogram (signal) will be derived from:

Maximum value - maximum value of signal.

Largest peak - highest integrated peak.

2nd largest peak - second highest integrated peak.

3rd largest peak - third highest integrated peak.

Maximum baseline value - maximum value not belonging to any identified peak (useful for negative chromatograms with positive spikes).

Scale Minimum to

The lower limit for scale for displaying the chromatogram (signal) will be derived from:

Minimum value - minimum value of signal.

Largest negative peak - highest negative integrated peak.

2nd largest negative peak - second highest negative integrated peak.

3rd largest negative peak - third highest negative integrated peak.

Minimum baseline value - minimum value not belonging to any identified peak (useful for chromatograms with positive peaks and negative spikes).

List of open chromatograms

Provides a list of all chromatograms (or signals when multi-detector chromatograms are in use) displayed in the right-hand section of the tab. If less than 32 chromatograms are open, the list is supplemented by the *#X unassigned* fields, enabling the color of further chromatograms to be defined without having to open them.

Caution: All fields in the right-hand section are valid only for the chromatogram (signal) selected in this field.

Show

Displays/hides selected chromatogram. This does not close a chromatogram meaning that all the data remain valid (i.e. the results table). It is possible to hide an active chromatogram.

Show Labels

Displays/hides descriptions and lines joined to the chromatogram. Descriptions and lines joined to the working area (Workplace) remain

unchanged (to hide these use the *Show Workplace Labels* command from the [Graph](#) tab).

Line Width

Width of chromatogram curve in points. *Line Width* option is disabled when option *Use User Options* is checked

Color...

Selects the color of a chromatogram.

Color... - Selects user desired color. *Color...* button is disabled when option *Use User Options* is checked

Offset & Scale**X Offset (Y Offset)**

Shifts chromatogram in currently set units.

X Scale (Y Scale)

Enlarges or reduces chromatogram in time or voltage axis. The permitted values range is between *0.01-100*.

Note: The *X Offset* and *Y Offset* fields correspond to the *Move* command, and the *X Scale* and *Y Scale* fields to the *Scale* command. These are performed by right-clicking the mouse within the graph and then using the *Overlay - Move* or *Overlay - Scale* command from the context menu (for more details see the chapter **Overlay & Other** on pg. 267).

Note: The *Offset* and *Scale* operation are not stored in the current chromatogram, after opening the chromatogram again they will be reset to the default values. Only in case the chromatogram window is closed with some chromatogram opened, its offset and scale values will be restored after reopening the window.

Original

Sets original values (i.e. *Offset* to 0 and *Scale* to 1).

3.3.2.6 Graph Properties - Auxiliary Signal Details tab ✔ Full version

This window lets you to adjust the appearance of Auxiliary signals recorded together with the chromatogram. The tab copies part of its functionality from the [Auxiliary Signals](#) tab of the [User Options](#) dialog described in the chapter "[Gradient & Auxiliary Signals tab](#)" on pg. 157.

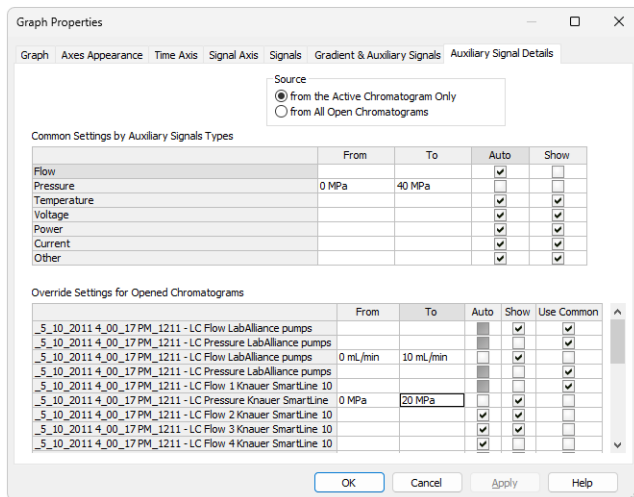


Fig. 132: Graph Properties - Auxiliary Signals

Source

Select for which chromatograms the auxiliary signals will be displayed

Note This option is enabled when *Use User Option* checkbox on the *Gradient & Auxiliary Signals* tab is not checked.

Common Settings by Auxiliary Signals Types

Sets the auxiliary signal axis range for auxiliary detectors. When the *Auto* checkbox is checked, the auxiliary signal axis range starts at a minimal value and enlarges according to the auxiliary signal course. While unchecked, the axis range is fixed with the values entered in the respective *From* and *To* columns. Unchecked checkbox *Show* will not display unchecked auxiliary signals in the chromatogram.

Override Settings for Opened Chromatograms

Override the settings for any particular auxiliary signal from currently opened chromatogram. When the *Auto* checkbox is checked, the auxiliary signal axis range starts at a minimal value and enlarges according to the auxiliary signal course. While unchecked, the axis range is fixed with the values entered in the respective *From* and *To* columns. If checkbox *Use Common* is checked, parameters from the **Common Settings by Auxiliary Signals Types** table will be used in displaying the auxiliary signals.

Note:

It is possible to hide the auxiliary signal directly in the *Chromatogram* window by holding **CTRL** and left mouse double click on the appropriate signal.

3.3.2.7 Graph Properties - Gradient & Auxiliary Signals tab ✓ Full version

Sets the display of gradient graph on directly controlled HPLC configurations. Except for the *Use User Options* parameter, the tab is identical to the [Gradient & Auxiliary Signals](#) tab of the [User Options](#) dialog described in the chapter "[Gradient & Auxiliary Signals tab](#)" on pg. 157.

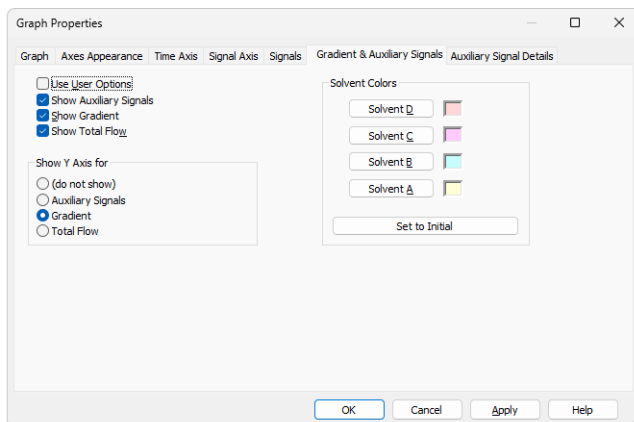










Fig. 133: Graph Properties - Gradient





Use User Options

All parameter settings in the left column will be taken from the global setting in the [User Options - Gradient](#) dialog, accessible from the [Instrument](#) window using the *View - Options...* command.

3.4 Chromatogram


A submenu of commands for working with chromatograms.

 Global Peak Width	Use of this command or <i>Global Peak Width</i>  icon calculates the <i>Peak Width</i> parameter for the whole chromatogram from interactively selected interval. The <i>Global Peak Width</i> can also be set manually in the first row of the Integration Table found on the Chromatogram - Integration tab). Detailed description of the <i>Peak Width</i> parameter can be found in the chapter " Integration " on pg. 253 .
 Global Threshold	Use of this command or <i>Global Threshold</i>  icon calculates the <i>Threshold</i> parameter for the whole chromatogram from interactively selected interval. The <i>Global Threshold</i> can also be set manually in the second row of the Integration Table found on the Chromatogram - Integration tab). Detailed description of the <i>Threshold</i> parameter is in the chapter " Integration " on pg. 252 .
 Global Bunching	Use of this command or <i>Global Bunching</i>  icon calculates the <i>Global Bunching</i> parameter for the whole chromatogram from already entered <i>Global Peak Width</i> value and the frequency of the data acquisition. The calculation sets the <i>Global Bunching</i> parameter so that the peak (as defined in the <i>Global Peak Width</i>) has approximately 30 datapoints. The <i>Global Bunching</i> can also be set manually in the third row of the Integration Table found on the Chromatogram - Integration tab.
 Global Baseline Slope	Use of this command or <i>Global Baseline Slope</i>  icon calculates the <i>Global Baseline Slope</i> parameter for the whole chromatogram from interactively selected graph position. Because of the noise present in the signal the position of peak starts and ends will be just approximate. The <i>Global Baseline Slope</i> can also be set manually in the fourth row of the Integration Table found on the Chromatogram - Integration tab. The command is only available if <i>Wave</i> Integration Algorithm is used.

Baseline	Commands for baseline correction. Detailed description of <i>Baseline</i> parameters can be found in the chapter " Baseline " on pg. 221 .
Peak	Commands for operations with peaks. Detailed description of operations with peaks can be found in the chapter " Peak " on pg. 237 .
Integration	Commands for adjustment of integration parameters. Detailed description of <i>Integration</i> options can be found in the chapter " Integration " on pg. 252 .
Separation	Commands for adjustment of separation parameters. Detailed description of <i>Separation</i> parameters can be found in the chapter " Separation " on pg. 263 .
Noise & Drift	Commands for evaluation of noise and drift. Detailed description of <i>Noise & Drift</i> operations can be found in the chapter " Noise & Drift " on pg. 264 .
 Overlay	Commands for simultaneous work with several chromatograms. Detailed description of <i>Overlay</i> and related options can be found in the chapter " Overlay & Other " on pg. 266 .
Chromatogram list	Contains a chronological list of all currently displayed chromatograms. The active chromatogram is denoted by a point before its name. To set a chromatogram to active status, click on its name. Chromatograms can be displayed using the <i>Chromatograms...</i> command.
Chromatograms...	Displays the Chromatogram List dialog with a list of all chromatograms/signals that are opened in the Chromatogram window.
 Measure Distance	Shows the distance to the relative point in the graph. After invoking the command or clicking on the <i>Measure Distance</i> icon  the cursor changes to  and will prevent you from leaving the Graph pane. Click and drag to see the distance from the location you clicked on and the current cursor position. This distance is shown just out of the upper right corner of the Graph pane. Normally, absolute position of the cursor in the graph is shown.



Show Slope/Level

Shows Slope and Level values of the nearest acquired data point (of the signal line) to a current cursor position. After invoking the command or clicking on the *Show Slope/Level* icon  the cursor changes to a balloon tooltip will prevent you from leaving the **Graph** pane. The balloon tooltip shows values of *Time*, *FC Slope*, *Level* and *IA Slope* related to the current cursor position. The difference between the values of *FC Slope* and *IA Slope* is caused by the signal rate (*FC Slope* does not take frequency into account) and the way of calculation (*FC Slope* is calculated as a non-symmetrical derivative because at the time of measurement the further points are not known yet).

Note: Note that values displayed by *Show Slope/Level* function are influenced by the set *Global Bunching* value in the **Integration Table**. If you need to display *Show Slope/Level* values in order to fill them in **Fraction table** for the fraction collectors, is necessary to have the same values set for the *Global Bunching* in the **Integration Table** and *Filter* in the **Fraction Table**.

Create Label

Adds labels and lines.
Detailed description on how to create labels can be found in the chapter "**Create Label**" on pg. 272.

Remove Label(s)

Deletes labels and lines.
Selected
Deletes the selected label or line.
From Workplace
Deletes all labels and lines attached to the workplace.
From Active Signal
Deletes all labels and lines attached to the active signal.
Remove All
Deletes all labels and lines regardless of whether they are attached to the workplace or to the active chromatogram. Labels of other opened but inactive chromatograms will be retained.

Merge...

Creates multi-detector chromatograms. The command is commonly used when a multi-detector analysis was measured on one of the **CSW** stations which do not allow for the creation of multi-detector chromatograms.

The procedure is following:

1. Open the chromatogram to which you would like to add further signals.
2. Prompt the *Merge* command and the [Open Chromatogram](#) dialog will open where you can select a chromatogram.
3. Select the required chromatogram and click the *OK* button.
4. Repeat the procedure to add more signals.

It is possible to create a chromatogram containing a maximum of 32 signals. Only the whole chromatograms will be merged, regardless of the number of signals selected in [Open Chromatogram](#) dialog. Chromatograms containing PDA data cannot be merged.

Set Signal Names... Edits names of signals.

3.4.1 Baseline

Processes the baseline. Individual commands can also be invoked with the icons in the *Baseline* toolbar.

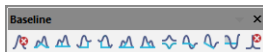














Fig. 134: Baseline Toolbar

All operations involving the use of peaks are performed on an interval, which must include peak beginnings and ends of all participating peaks. Any incomplete peaks are ignored. Another essential condition of the success of an operation is that a new baseline can not intersect the signal.


All interval operation follows the rule that with *Time B* = 0 operation will be applied from *Time A* to the end of the chromatogram. With both *Time A* and *Time B* set to 0, operation is applied over the whole chromatogram.

Note: If done improperly, the process will either be completed without any changes to the actual baseline, effect some peaks only or only some of the beginnings and ends of peaks might be modified.

	Lock	Eliminates peaks within a selected interval from integration.
	Valley	The baseline will pass through all valleys that separate individual peaks.
	Together	An inverse operation to <i>Valley</i> - the baseline will not pass valleys, creating the perpendicular line from the valley.
	Forward Horizontal	The baseline is extrapolated horizontally forwards.
	Backward Horizontal	The baseline is extrapolated horizontally backwards.
	Front Tangent	Rider peaks on the front of the following larger peak are separated by the "tangent skimming method".
	Tail Tangent	Rider peaks on the tail of the preceding larger peak are separated by the "tangent skimming method".
	Clamp Negative	Changes the interpretation of the signal inside given area.
	Cut Negative	Discards negative peaks inside a given interval from integration without baseline modification.

	Reject Negative	Discards negative peaks inside a given interval from integration with baseline modification.
	Allow Crossing	Allows the baseline to cross the signal line.
	Spike Removal	Removes the spike from the chromatogram.

3.4.1.1 Lock

The *Lock* command or  icon excludes all selected peaks from an integration. Only peaks lying entirely within the specified interval are eliminated this way.

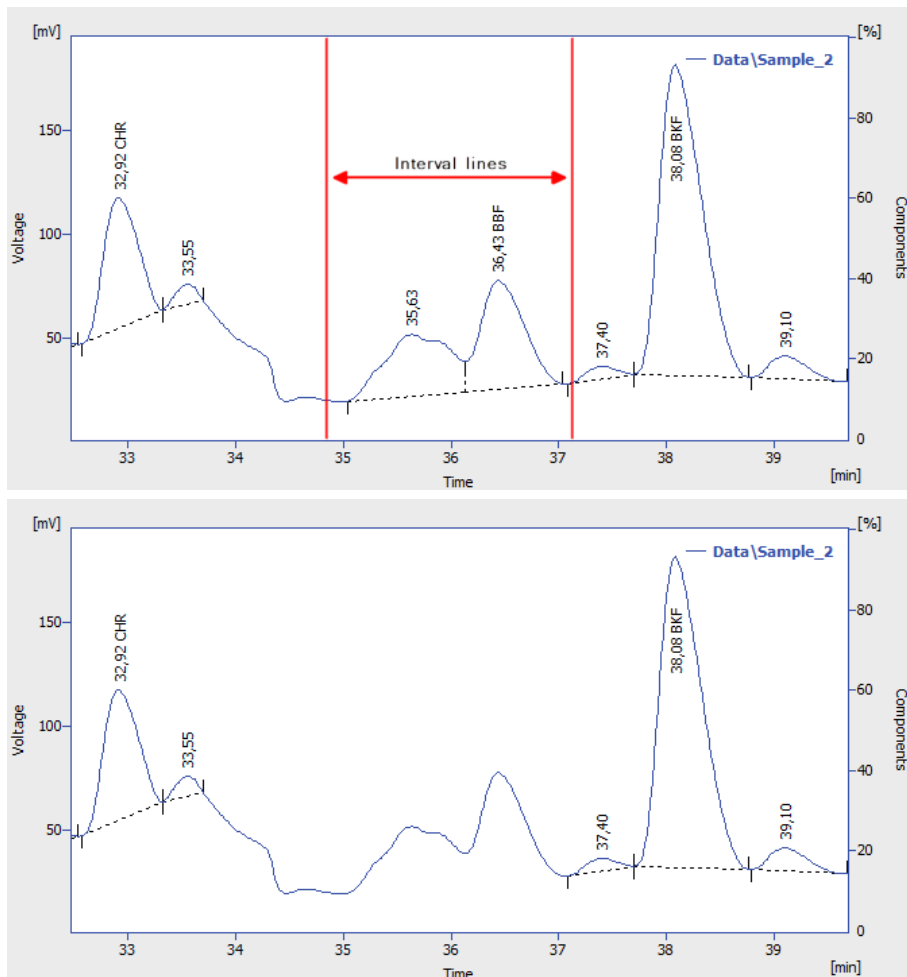



Fig. 135: Peak deletion using Lock

3.4.1.2 Valley

The *Valley* command or  icon forces the baseline into all the valleys situated between the interval lines. In the event this might result in having the baseline intersect with the signal, the station will prevent the intersection by automatically shifting the peak beginning or end. This operation is opposite to the *Together* command.

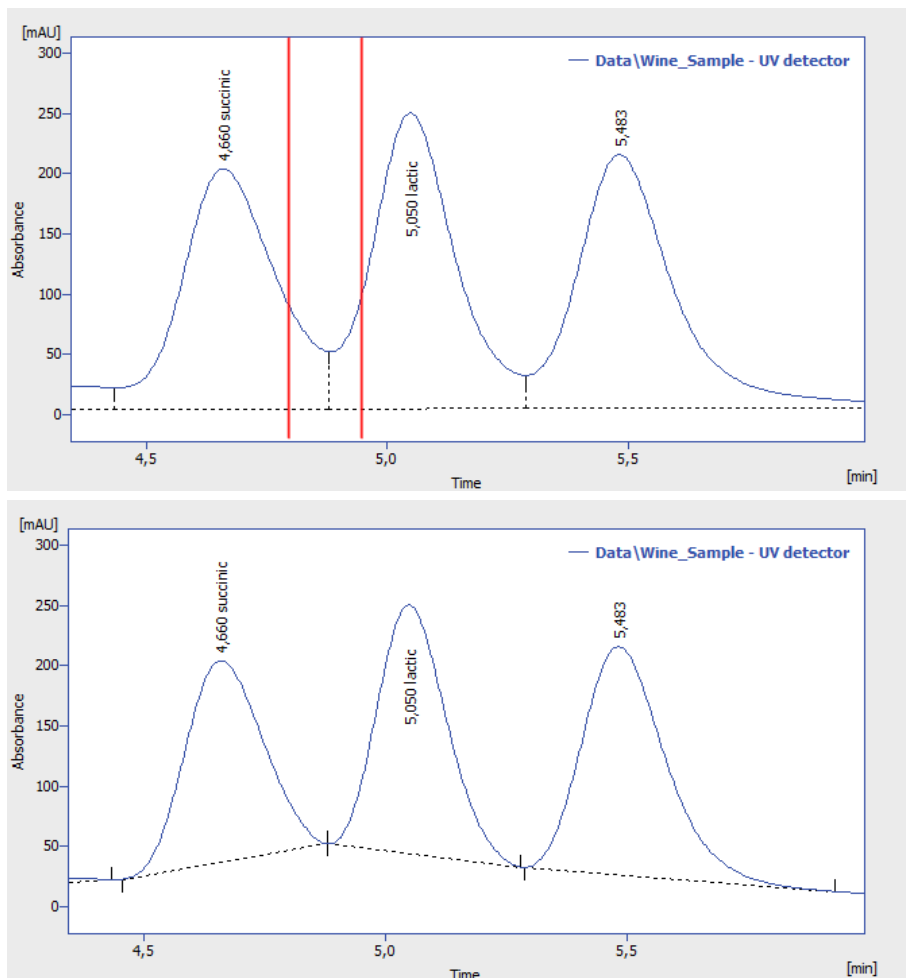



Fig. 136: Baseline into valley

3.4.1.3 Together

The *Together* command or  icon introduces separating verticals to all valleys that are situated between the interval lines. This operation is opposite to the *Valley* command.

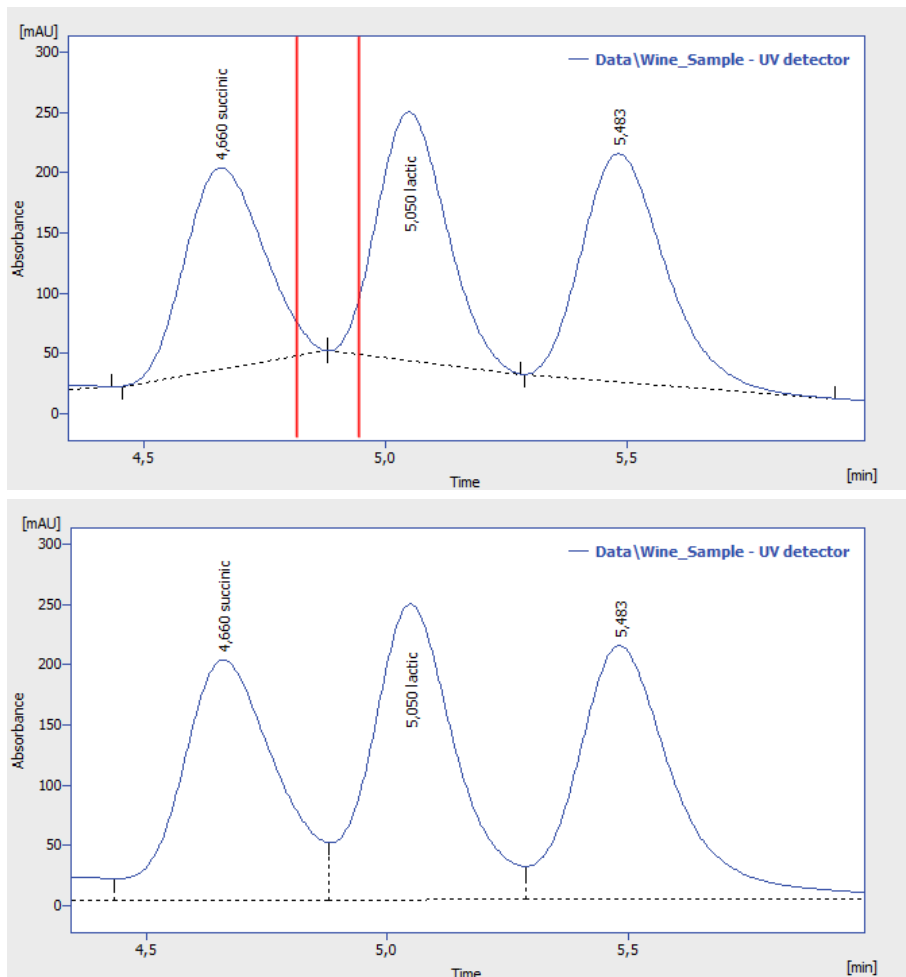



Fig. 137: Vertical separations to all valleys

3.4.1.4 Forward Horizontal

The *Forward Horizontal* command or  icon extrapolates the baseline horizontally forwards. In the selected interval, the baseline will proceed horizontally from the first identified peak beginning and will end in a vertical line at the peak end. Should the baseline intersect the signal prior to the peak end, the forward horizontal method may not be applied. The end of the previous peak is then identified before the point of intersection and the station will again attempt to project a horizontal baseline. In this instance extrapolation is understood to proceed from left to right.

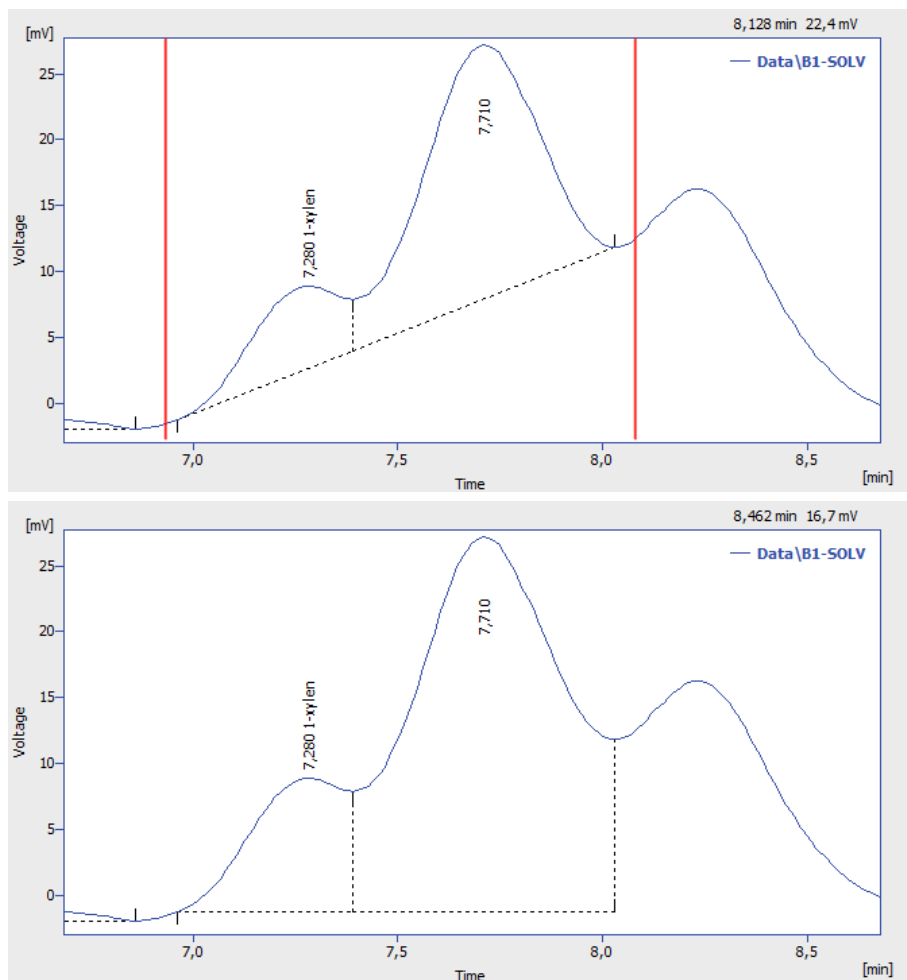



Fig. 138: Forward horizontal baseline

3.4.1.5 Backward Horizontal

The *Backward Horizontal* command or  icon extrapolates the baseline horizontally backwards. The baseline will proceed in the selected interval horizontally from the last identified peak end and will finish in a vertical line at the peak beginning. Should the baseline intersect the signal prior to the peak beginning, the backward horizontal method may not be applied. The end of the previous peak is then identified after the point of intersection and the station will again attempt to project a horizontal baseline. In this instance extrapolation is understood to proceed from right to left.

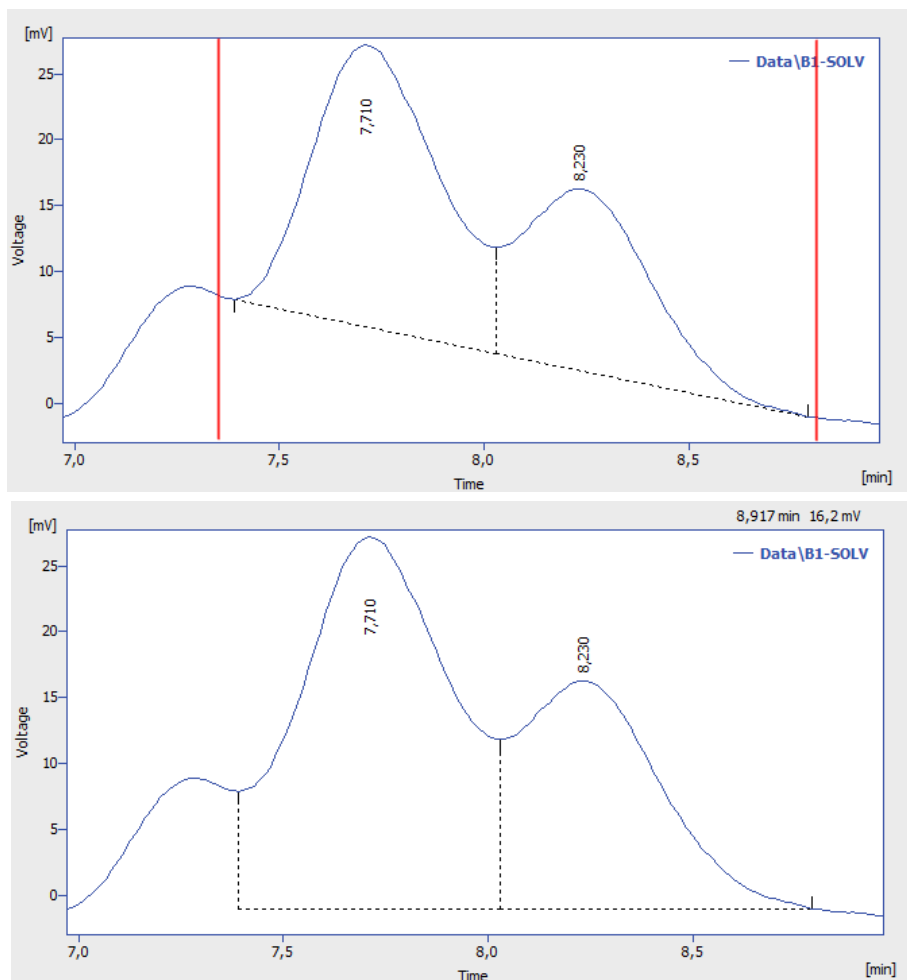



Fig. 139: Backward horizontal baseline

3.4.1.6 Front Tangent

The *Front Tangent* command or  icon separates small peaks on the ascending part of the following larger peak by what is known as the tangent skimming method. Place the left interval borderline before the peak you still wish to separate and place the right interval borderline inside the fronting peak from which you wish to separate the rider.

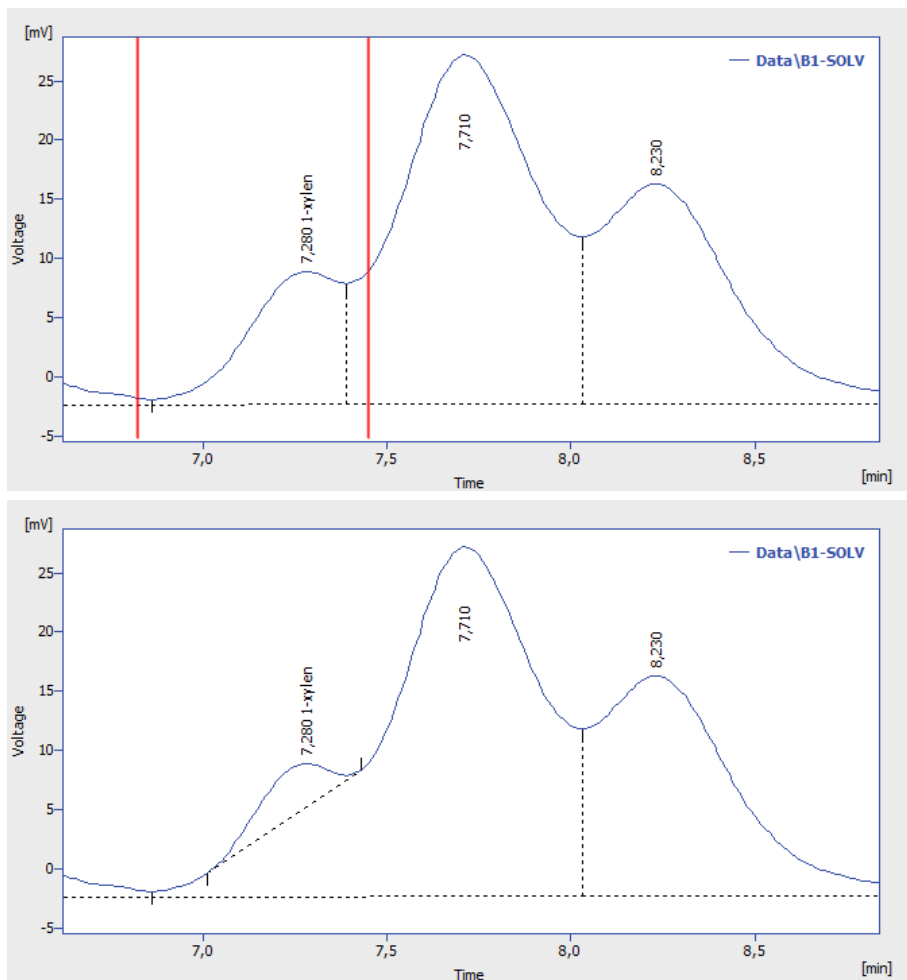



Fig. 140: Front tangent

3.4.1.7 Tail Tangent

The *Tail Tangent* command or  icon separates small peaks on the tail of the preceding larger peak by what is known as the tangent skimming method. Place the left interval borderline inside the peak with the riders you wish to separate. Place the right interval borderline behind the end of last rider to be separated.

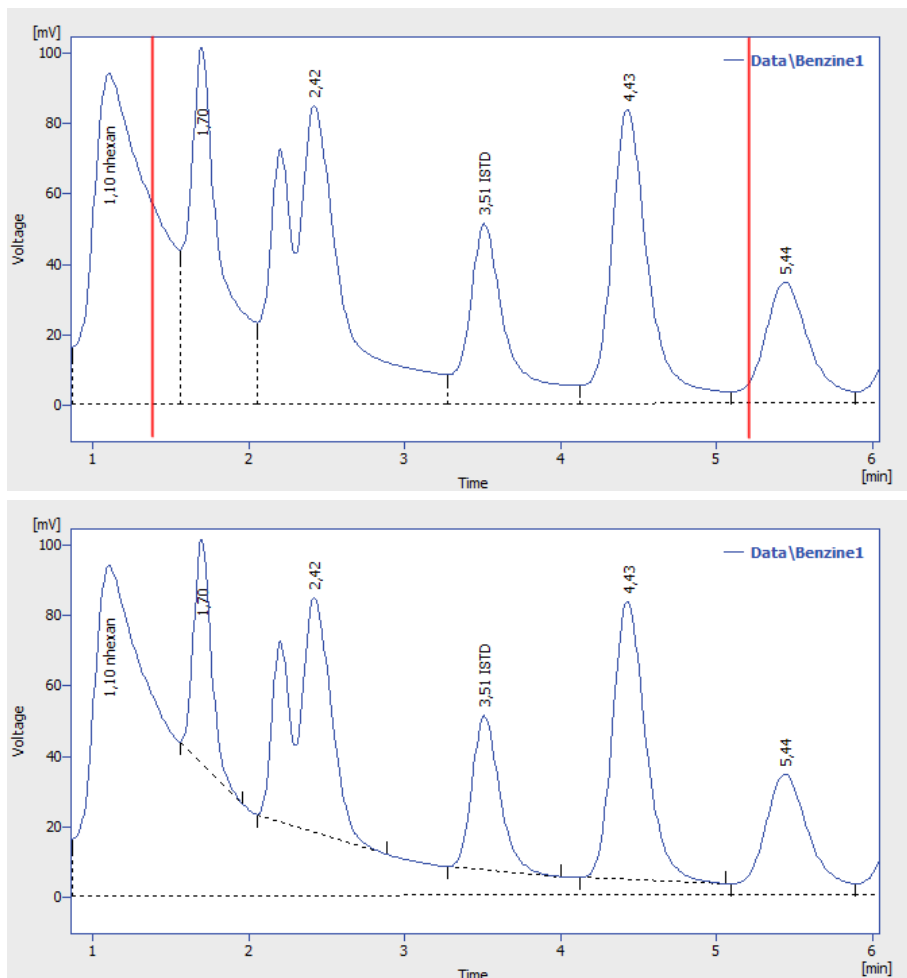



Fig. 141: Tail tangent

3.4.1.8 Clamp Negative

The *Clamp Negative* command or  icon modifies the interpretation of the signal inside the specified interval by creating positive peaks from a group of negative ones inside the region (the original apexes then become valleys and *vice versa*). This works only for at least partially unresolved peaks, totally resolved negative peaks in the interval will just be eliminated (no positive peaks will be created).

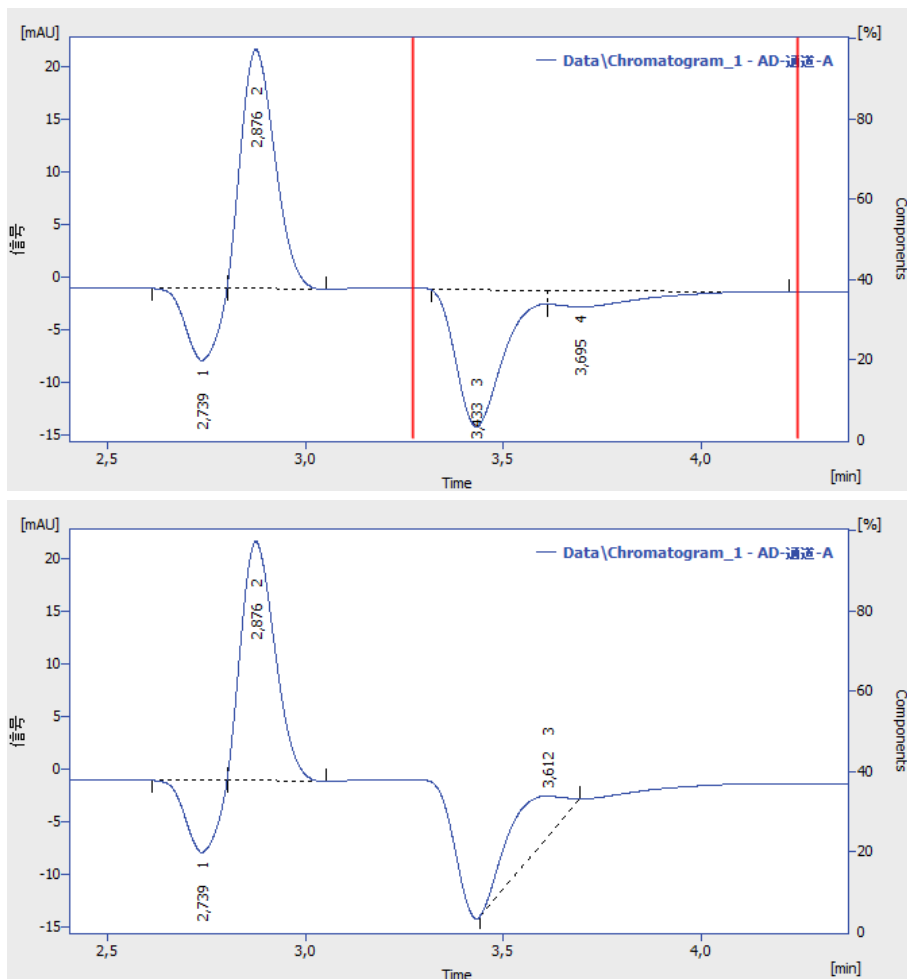



Fig. 142: Clamp negative

3.4.1.9 Cut Negative

The *Cut Negative* command or  icon eliminates negative peaks from the integration. If an eliminated negative peak overlaps the following positive one, neither its beginning nor its end will be shifted. Use this option to eliminate negative baseline disturbances.

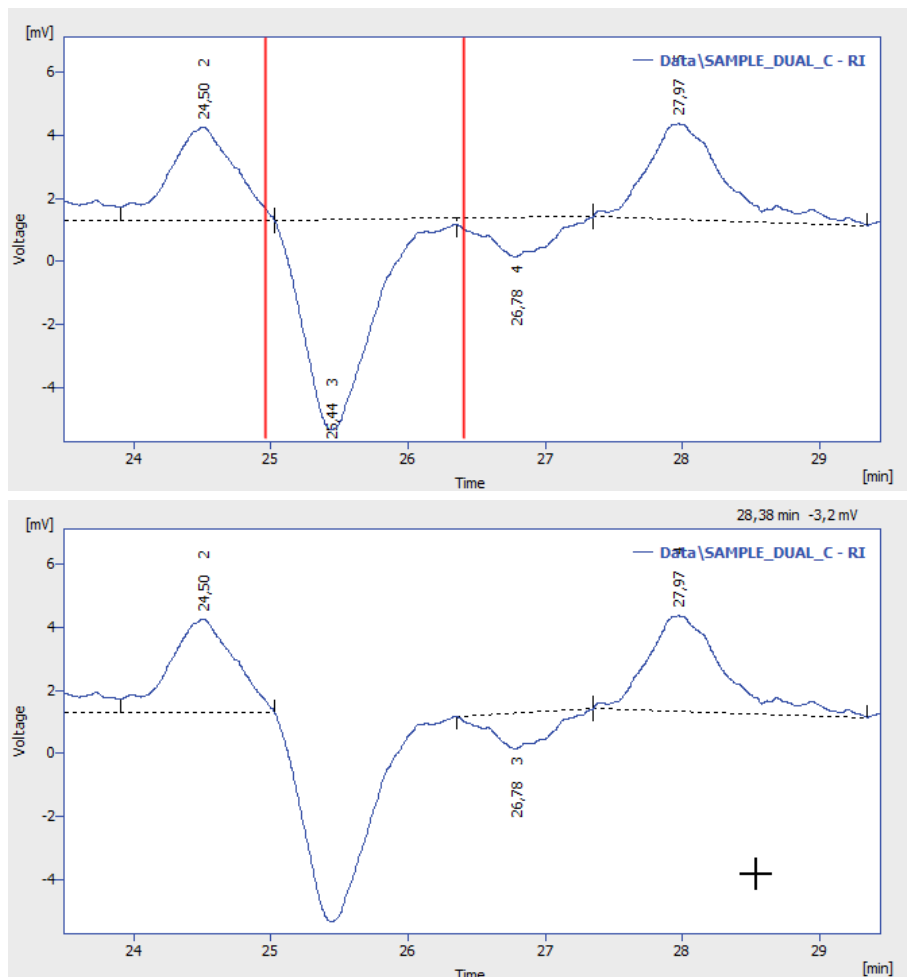



Fig. 143: Cut negative peaks

3.4.1.10 Reject Negative

The *Reject Negative* command or  icon eliminates negative peaks from the specified interval. If an eliminated negative peak is immediately followed by a positive one, the beginning and end of the latter are shifted to the original apex of the eliminated negative peak. Eliminated negative peaks are then considered to be proper part of baseline.

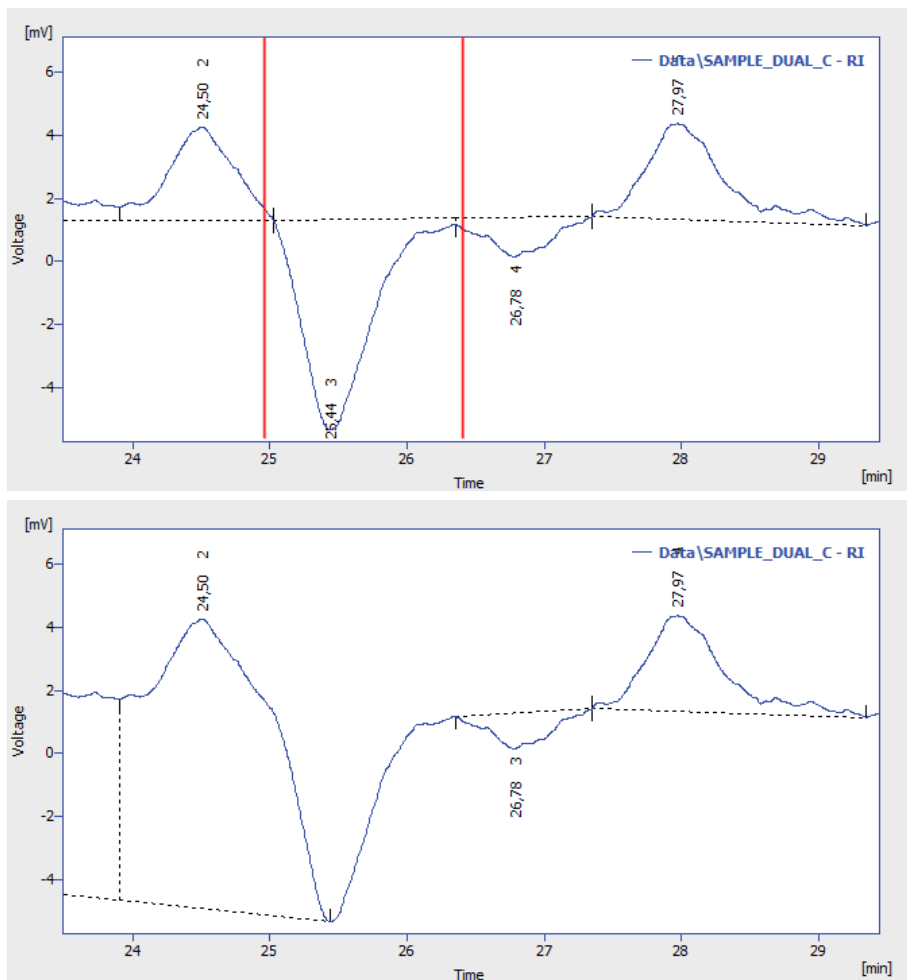




Fig. 144: Cut negative peaks

3.4.1.11 Allow Crossing

This function (icon ) allows the baseline crossing with the signal line inside a specified time interval. In this **Allow Crossing** interval **Clarity** doesn't check if the peak starts and peak ends cross the baseline. If the peak starts and ends were automatically moved by **Clarity** due to not to cross the baseline then with the **Allow Crossing** option set these automatic peak starts and ends moves are discarded further manual moves of peak starts and peak ends will ignore the crossing.

When selected it is possible to set up its application to the current chromatogram through [Integration table](#) where one of three options can be selected by clicking arrow . Note when setting Time A and Time B equally to 0.000 min will result in application of **Allow Crossing** for the whole chromatogram and when setting Time A and Time B with different values it will result in application of **Allow Crossing** only within set time window. Time A value has to be lower than Time B value.


Chromatogram Operation	Grp.	Time A [min]	Time B [min]	Value
Global Peak Width				0,100 min
Global Threshold				0,1000 pA
Global Filter - Bunching				4
Baseline - Allow Crossing		0,000	0,000	No 
				No To First Cross To Start/End

Fig. 145: Allow Crossing Setting

No

Switches **Allow Crossing** option off meaning the integration will take place like there is no **Allow Crossing** selected.

To First Cross

Peak area will be considered only the part of the highest peak, bordered by first intersection of the signal line and the baseline to the right and left next to the highest peak apex. For better understanding see following two images. Pay an attention to different highlighted areas of peaks with respect to different settings of time intervals of individual rows in the [Integration table](#).

This function finds the highest peak apex and locates the crossings of the signal with the baseline to left and right. The resulting area will be considered as the peak area.

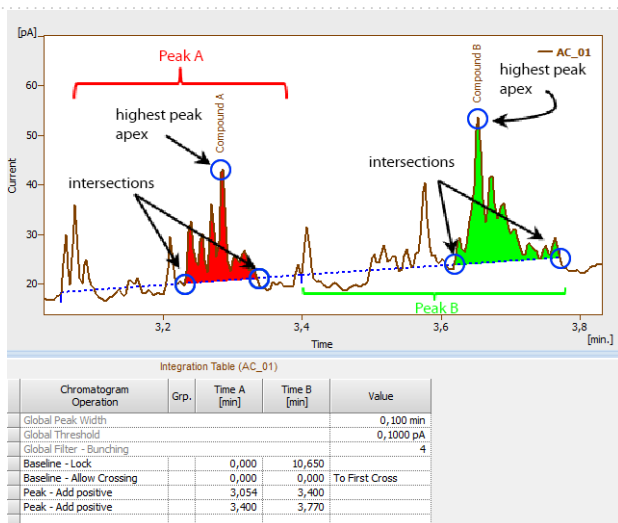


Fig. 146: To First Cross

To Start/End

As a peak area will be considered all parts of signal line above baseline inside the selected time interval for allow crossing operation. For better understanding see following image. Pay an attention to different highlighted areas of peaks compared to peak areas highlighted by **To First Cross** Option.

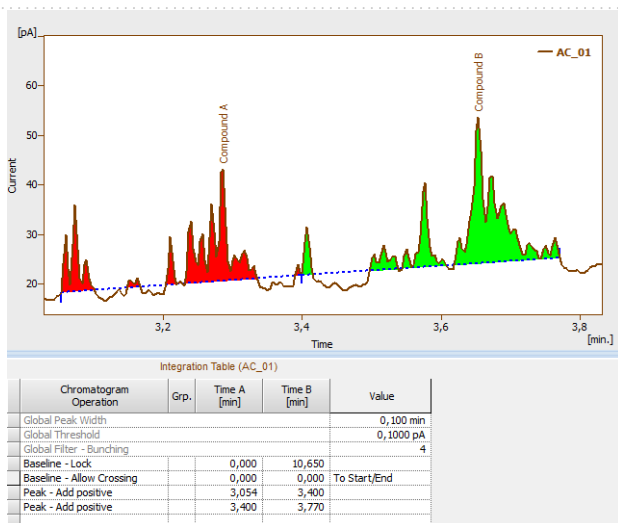


Fig. 147: To Start/End

The **Allow Crossing** operation will be applied only if there is a detected peak apex within the time interval set for the **Allow Crossing**.

On the image you can see that:

- On the left the highest apex of a Compound A peak is detected within **Allow Crossing** time interval.
- On the right the **Allow Crossing** time interval (see ②) does not overlap with the highest apex of the Compound B peak. **Allow Crossing** will not apply to Compound B peak.

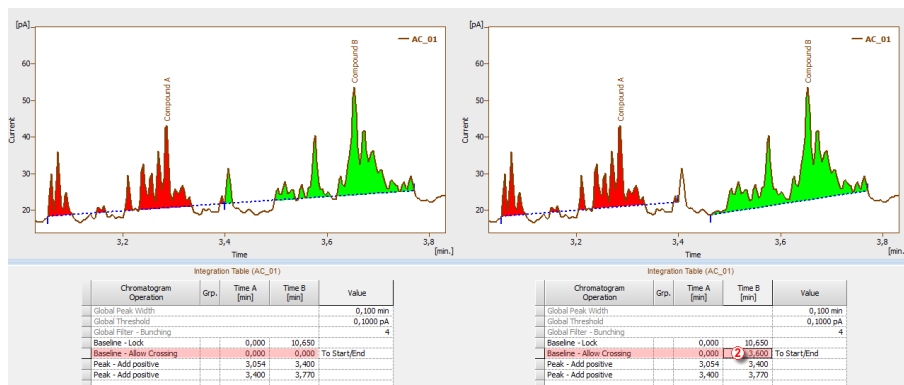



Fig. 148: Comparison of different time intervals set for Allow Crossing

3.4.1.12 Spike Removal

The *Spike Removal* command or  removes spikes in the selected interval and replaces the missing area with a calculated signal line. Usage of this function needs careful placing of the start and end point of the selected interval, as **Clarity** will replace the "missing" data with a polynomial using the same slope at the start point and the end point as the original signal had. The usage of this function only available in **Clarity** version 4.0 and higher may be disabled by the use of the *Disallow Spike Filter and Spike Removal* parameter from the [GLP Options](#) dialog (for more details see the chapter **GLP Options** on pg. 31).

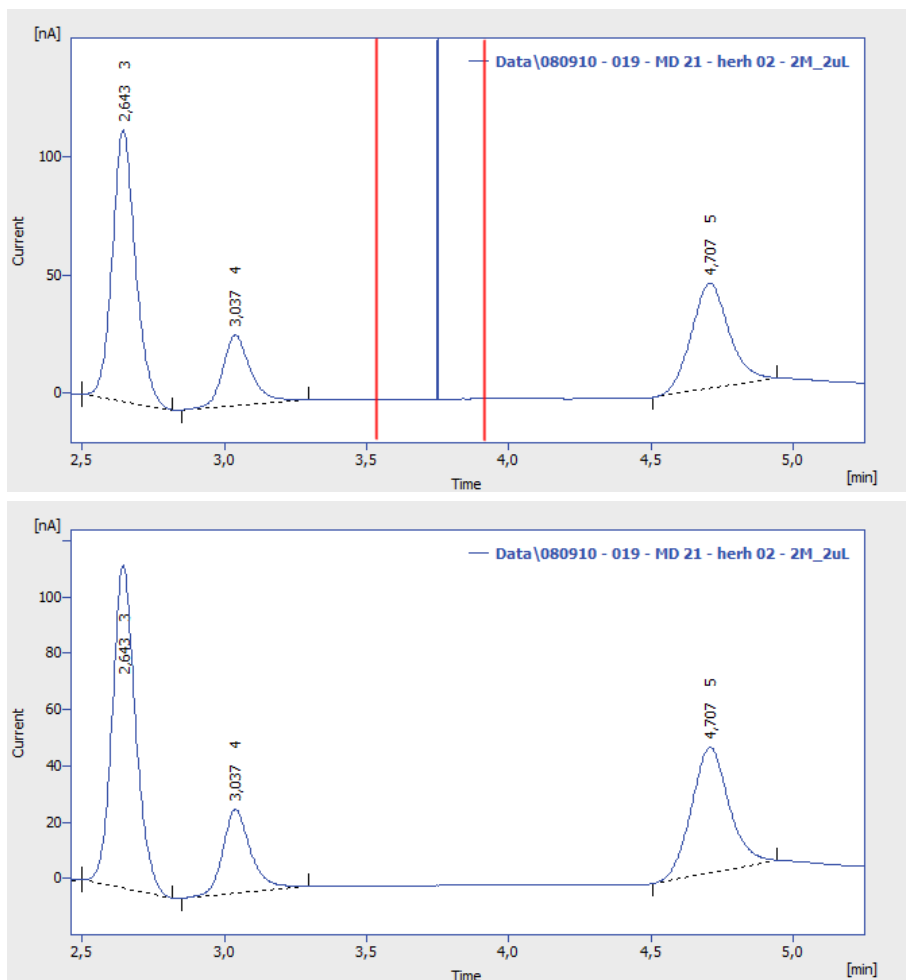


Fig. 149: Spike removal











3.4.2 Peak

Set of commands for operations with peaks. All commands can also be invoked using icons from the *Peak* toolbar.


All interval operation follows the rule that with *Time B* = 0 operation will be applied from *Time A* to the end of the chromatogram. With both *Time A* and *Time B* set to 0, operation is applied over the whole chromatogram.



Fig. 150: Peak Toolbar

	Show	Displays hidden peaks on the selected time interval. Current baseline is applied. Available only if Wave Integration Algorithm is used.
	Hide	Hides all peaks on selected time interval. Baseline remains unchanged. Available only if Wave Integration Algorithm is used.
	Start	Shifts the peak beginning.
	End	Shifts the peak end.
	Both	Shifts the common point of two peaks.
	Add Positive	Creates a new positive peak.
	Add Negative	Creates a new negative peak.
	Force Peak Name	Forces the peak a new name from calibration.
	Solvent Peak	Marks the peak as solvent peak.
	Peak Groups	Invokes a dialog for working with groups of peaks.

3.4.2.1 Start

Invoking this command or the *Start* icon  shifts the beginning of a peak. If this shift would move the peak start ahead of the end of the preceding peak, that end will be shifted to the selected point and both peaks will be separated by a vertical line. If the beginning of the peak before shifting has the same retention time as the end point of the preceding peak and will be shifted closer to the peak apex, the previous peak's end will stay at the original point and both peaks will be separated. The peak beginning may be shifted only within the interval delimited by the apexes of the previous peak and peak being modified.

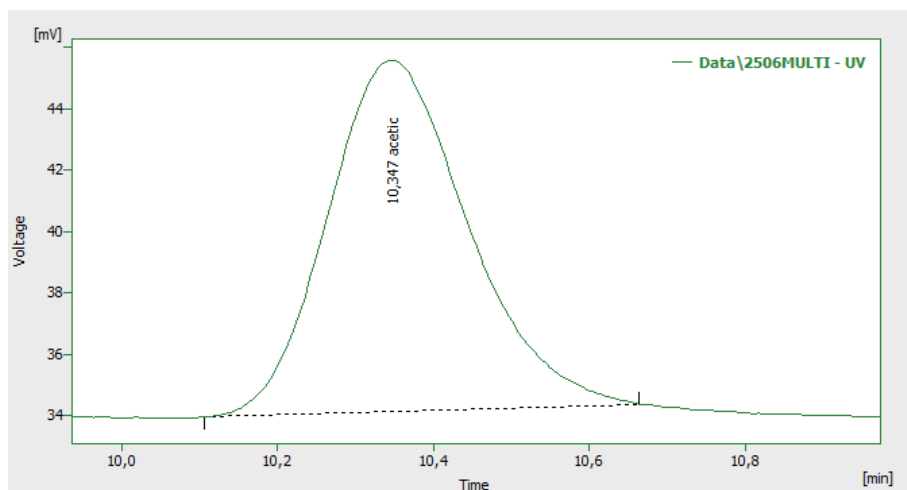
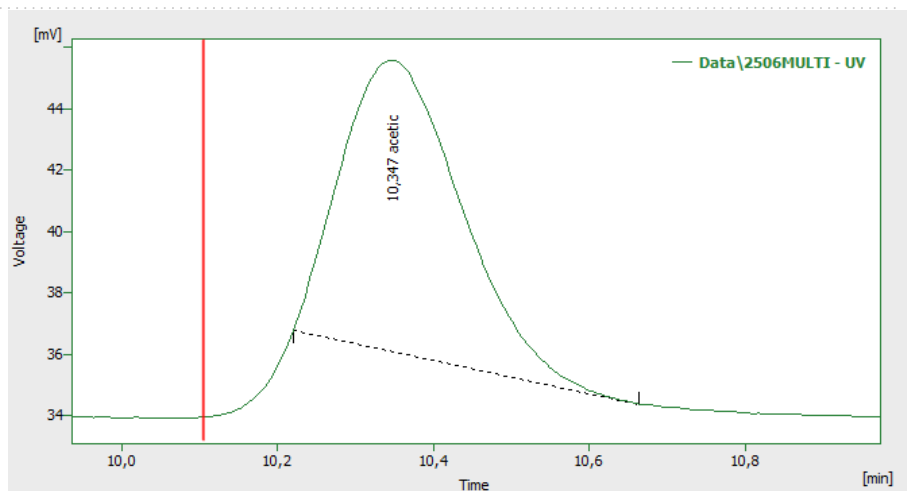



Fig. 151: Shift peak start

3.4.2.2 End

Invoking this command or the *End* icon  shifts the end of a peak. If this shift would move the peak end behind the beginning of the following peak, that beginning will be shifted to the selected point and both peaks will be separated by a vertical line. If the end of the peak before shifting has the same retention time as the start of the following peak and will be shifted closer to the peak apex, the following peak's beginning will remain at the original point and the peaks will be separated. The peak end may be shifted only within the interval delimited by the apexes of the following peak and the peak being modified.

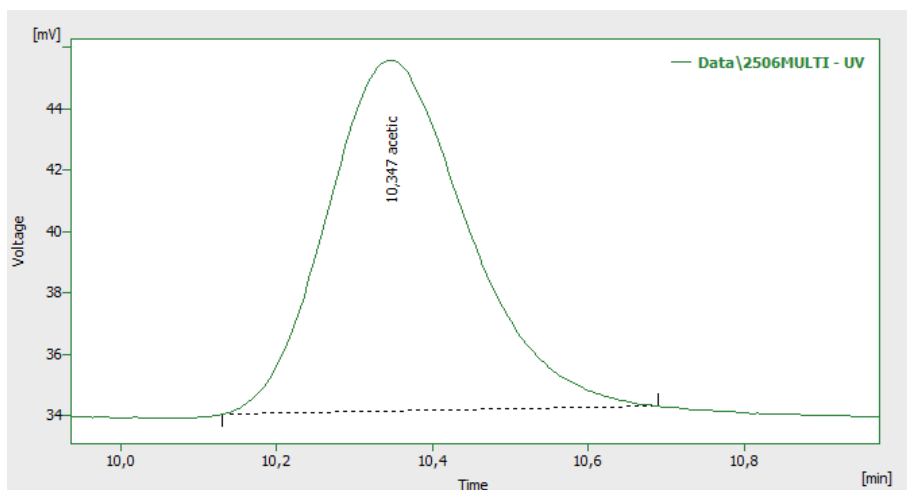
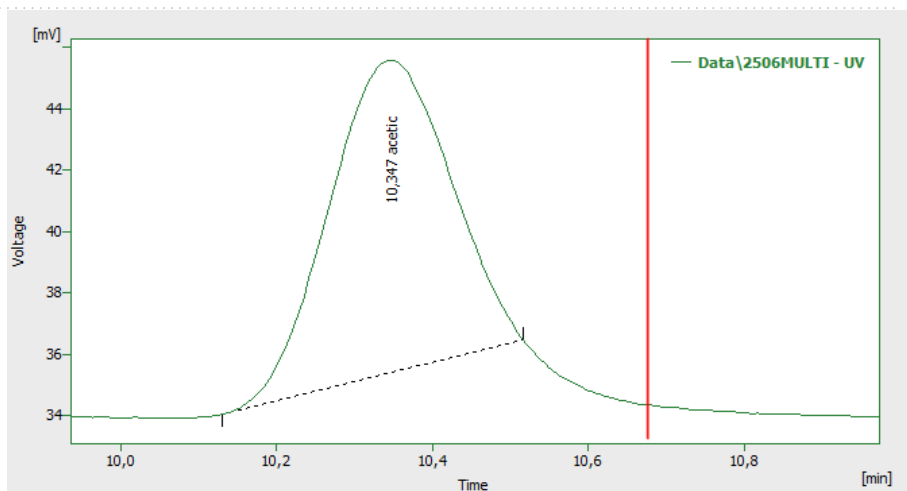



Fig. 152: Shift peak end

3.4.2.3 Both

Invoking this command or using the *Both* icon  shifts the common point of two peaks (a valley or the separating vertical line). The point may be shifted only within the interval delimited by the apexes of the both separated peaks.

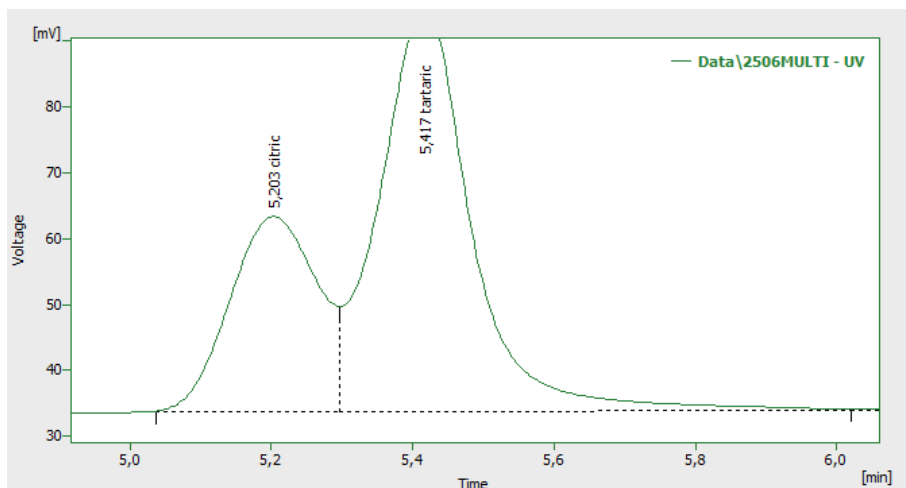
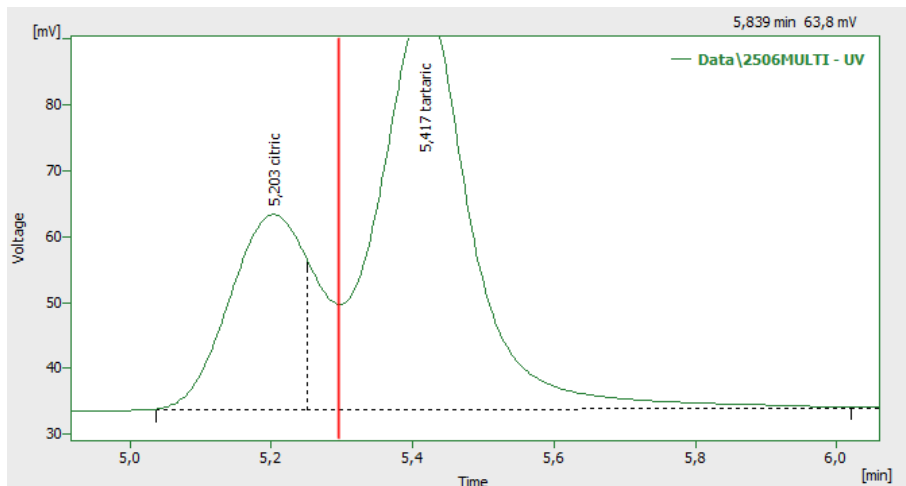



Fig. 153: Shift valley line

3.4.2.4 Add Positive

Invoking this command or using the *Add Positive* icon  creates a new, positive peak. Its beginning and end are defined by the interval borderlines, the apex is identified automatically. If the peak overlaps the neighboring peaks, their respective start and end points will be shifted and the peaks will be separated by vertical lines. New peaks cannot be created inside the interval of tangent skimming, nor close to the apex of an existing peak.

Note: A two-step process must be used to create a peak in the area of a monotonous signal. First, the beginning (end) must be placed at the point where the apex ultimately should be placed and the end (or beginning) placed in its final position. Only then can the peak beginning or end be shifted by the *Start* (or *End*, as the case may be) command to the required position.

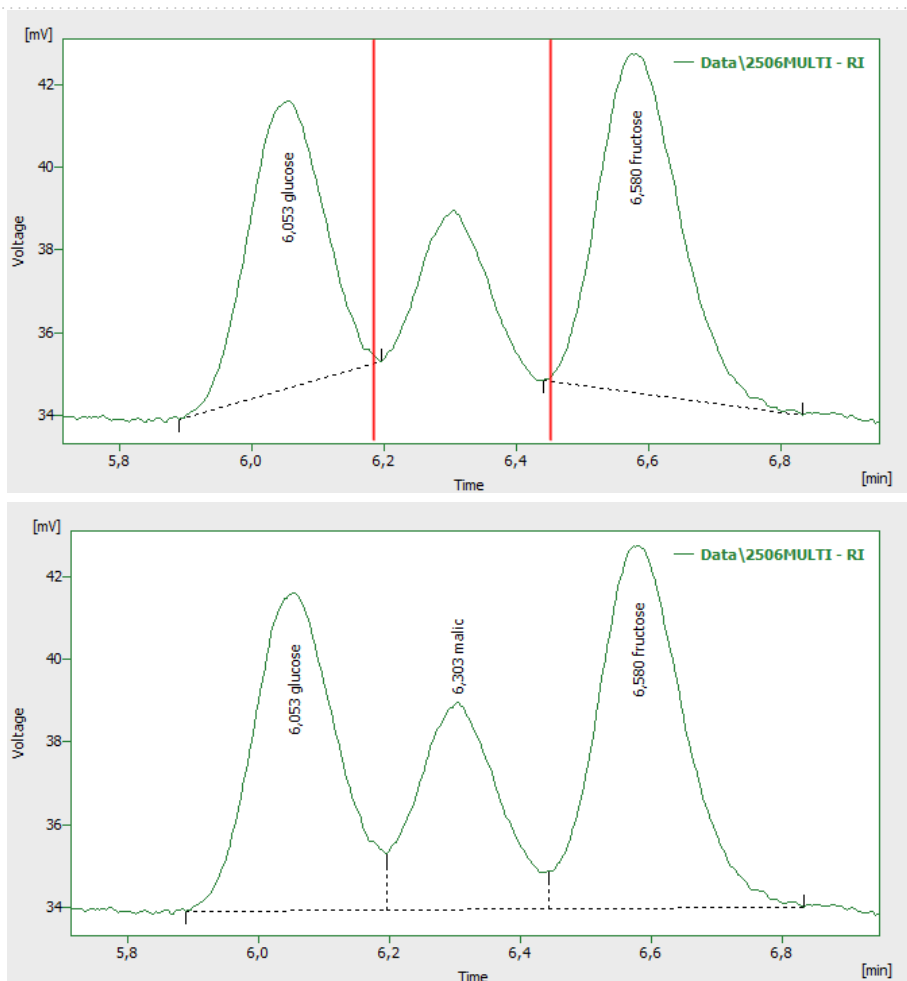



Fig. 154: Add a positive peak

3.4.2.5 Add Negative

Invoking this command or using the *Add Negative* icon  creates a new negative peak. Its beginning and end are defined by the interval borderlines, the apex is identified automatically. If the peak overlaps neighboring peaks, their respective start and end points will be shifted and the peaks will be separated by vertical lines. New peaks cannot be created inside the interval of tangent skimming, nor close to the apex of an existing peak.

Note: A two-step process must be used to create a peak in the area of a monotonous signal. First, the beginning (end) must be placed at the point where the apex should ultimately be placed and the end (or beginning) placed at its final position. Only then can the peak beginning or end be shifted by the *Start* (or *End*, as the case may be) command to the required position.

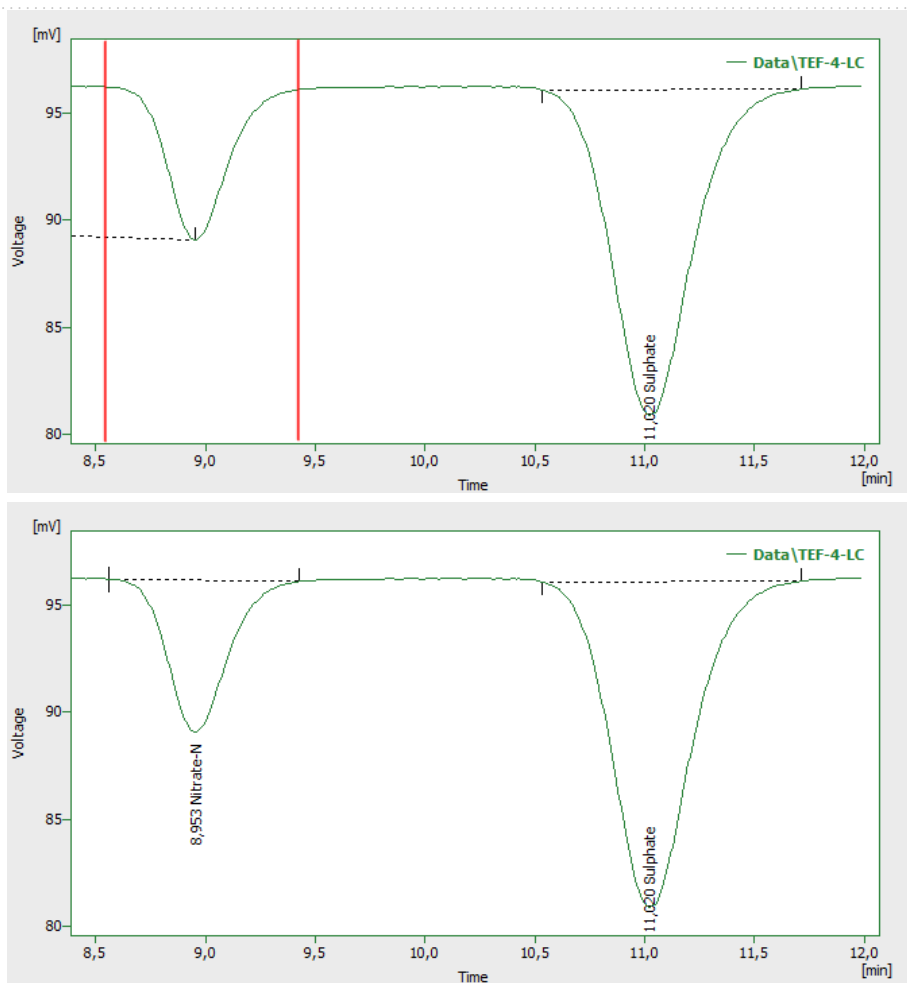



Fig. 155: Add a negative peak

3.4.2.6 Force Peak Name

Invoking this command or using the *Force Peak Name* icon  lets the user to select a peak whose name should be changed and then opens the *Force Peak Name* dialog with a list of all peaks included in the calibration file. Alternatively, user can define its own name in the field on the top of the dialog.

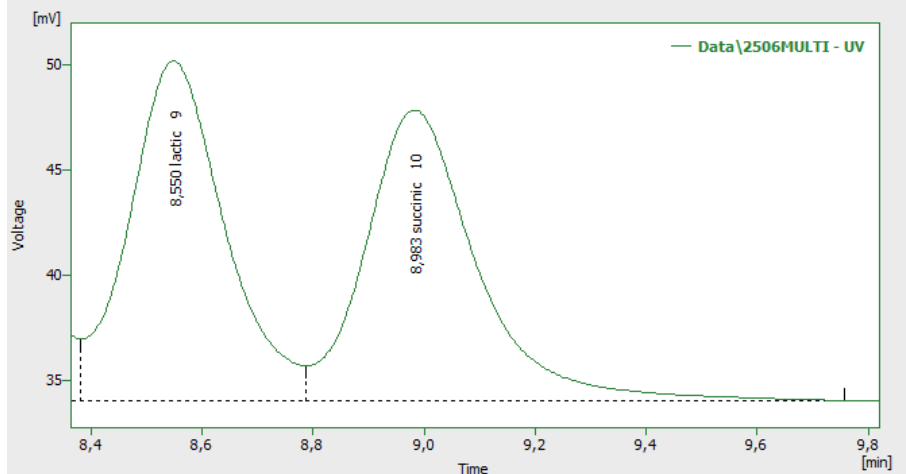
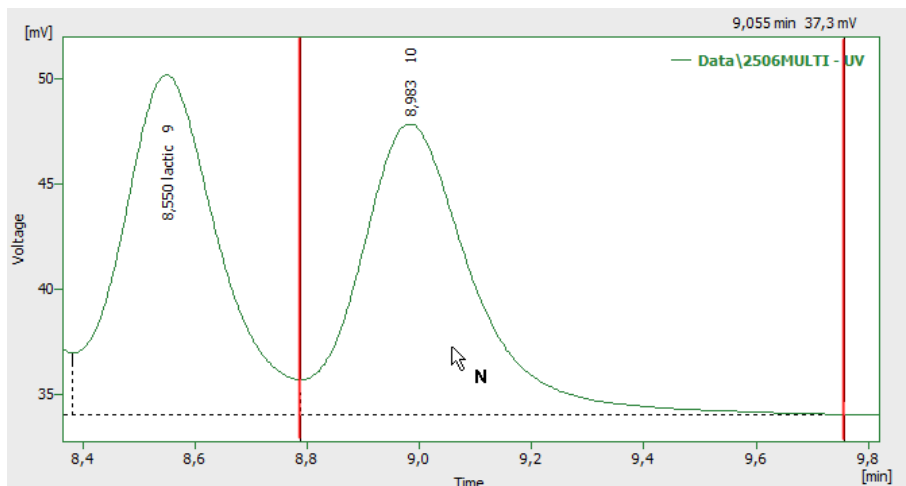


Fig. 156: Override peak name from calibration

Fig. 157:

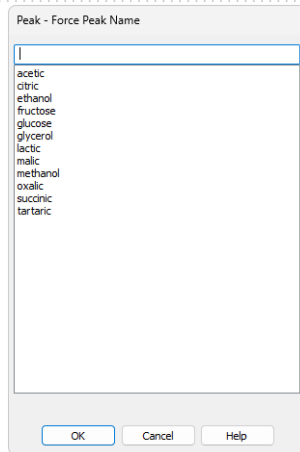



Fig. 158: Force Peak Name

Selected peak name will be set to the given peak.

Note: A peak with the same name cannot appear twice in the **Result Table** - only the peak named so latest will hold it's name, other peaks with the same name will become uncalibrated.

3.4.2.7 Solvent Peak

Invoking this command or the *Solvent Peak* icon  marks the selected peak as solvent peak; several peaks may be marked this way by repeatedly using the command. Solvent peak will be labeled by the letter S before the serial number (if displayed) in the **Result Table** and is excluded from the integration results.

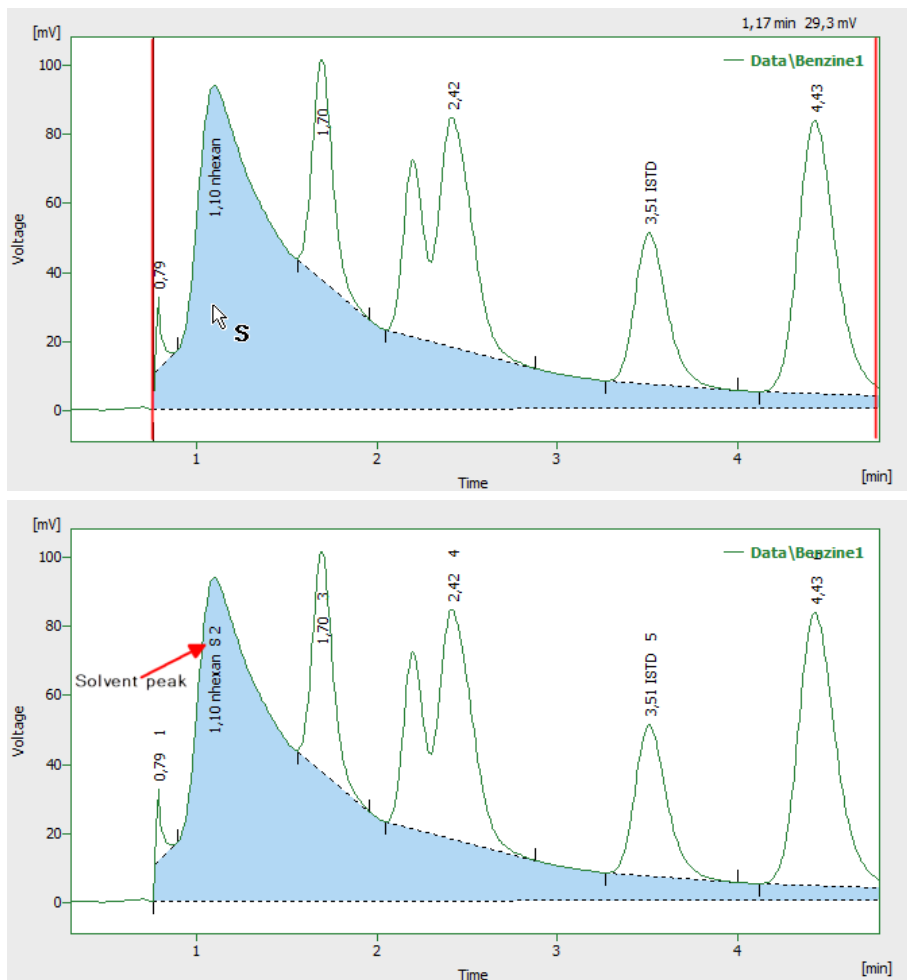


Fig. 159: Set a solvent peak

3.4.2.8 Groups

Invoking this command or the *Group* icon  opens the *Groups* dialog used for the operations with peak groups.

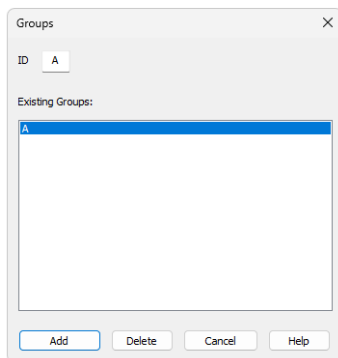


Fig. 160: *Groups*

ID

A group is marked by a single capital letter symbol (26 letters of the English alphabet can be used). If the identifier of a group already containing at least one peak is entered here, the group will be highlighted in the *Existing Groups* list.

Existing Groups

All defined groups containing at least one peak are listed here. When a calibrated calculation is used, the name taken from the calibration file is appended after the group identifier (provided the calibration file contains the relevant group). To transfer the group identified to the *ID* field, click the corresponding line.

Add

Adds peaks to the group selected in the *ID* field or creates a new group, if the one set in the *ID* field does not exist. All peaks with a maximum inside of the selected interval will be added to the group, it is not necessary to include the area to the peak start or end. A peak can only be included in a single group - only the last designation will thus apply.

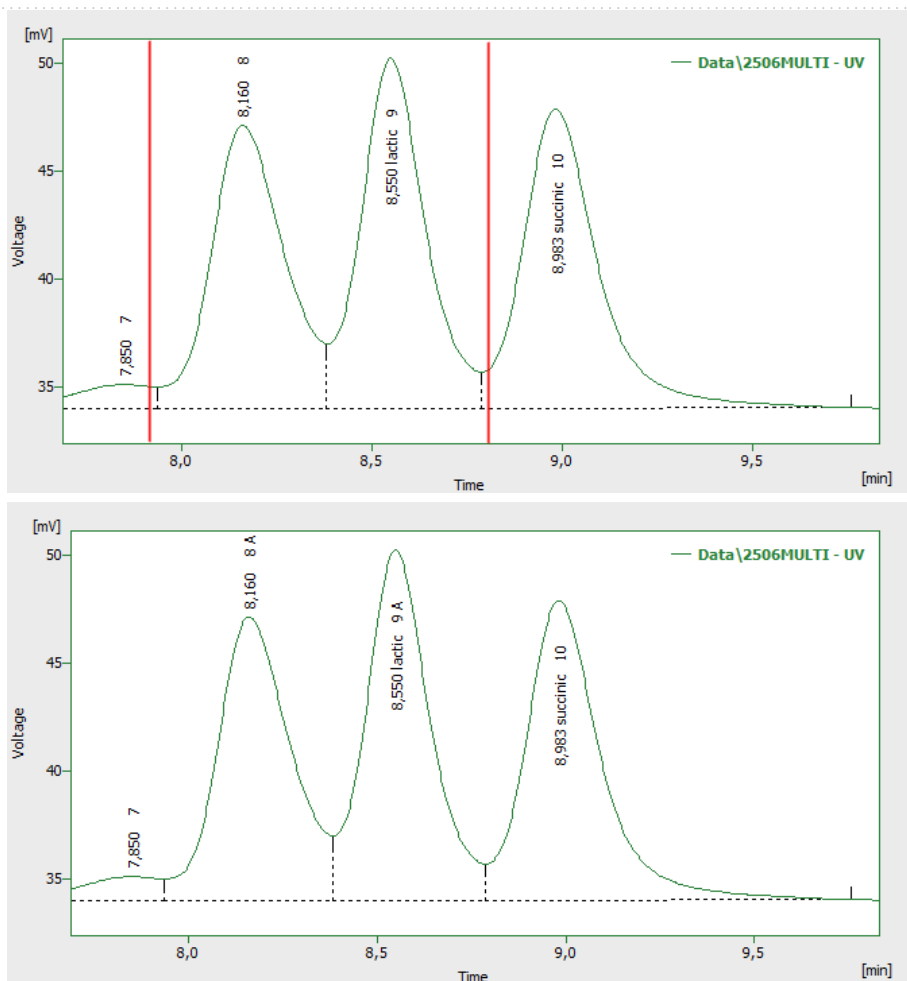


Fig. 161: Add peaks into a group

Delete

Deletes peaks from the group selected in the *ID* field. Only peaks assigned to that group and with maximum within the selected interval will be deleted.

Note: If the *Group ID* field on the [Graph Properties](#) dialog is checked, the capital letter of a group that a peak belongs to will be indicated in the graph at the peak's description.

3.4.3 Integration

Menu for adjustment of integration parameters. All commands can also be invoked using icons from the *Integration* toolbar.

All integration parameters are executed as a part of the **Integration Table** (for more details see the chapter **Integration** on pg. 284). All of these parameters are interval parameters, which means that it is possible to define the time frame of their validity and in particular to select various values for various parts of the chromatogram.

All interval operation follows the rule that with *Time B* = 0 operation will be applied from *Time A* to the end of the chromatogram. With both *Time A* and *Time B* set to 0, operation is applied over the whole chromatogram.




Fig. 162: Integration commands in Baseline bar

	Local Peak Width	Defines minimum width of peak.
	Local Threshold	Describes the threshold of noise.
	Local Baseline Slope	Defines the position of automatically found peak starts and peak ends. The command is only available if <i>Wave Integration Algorithm</i> is used.
	Integration Interval	Sets the interval for the integration algorithm.
	Detect Negative	Detects negative peaks.
	Minimal Area	Sets the minimum peak area.
	Minimal Height	Sets the minimum peak height.
	Minimal Half Width	Sets the minimum peak width in half-height of the peak.
	Detector Delay	Shifts the signal on the time axis.
	FFT Filter	Applies/suspends the FFT Filter (Fast Fourier Transformation) for noise reduction.
	Savitzky-Golay Filter	Applies/suspends the Savitzky-Golay Filter for noise reduction.
	Moving Average Filter	Applies/suspends the Moving Average Filter for noise reduction.

**Spike Filter**

Applies a filter that removes spikes to the selected region of the chromatogram. Only available in **Clarity** version 4.0 or higher.

3.4.3.1 Local Peak Width

Invoking this command or using the *Local Peak Width* icon  opens the *Peak Width* dialog which defines the method of peak integration on a given time interval. **Peak Width** parameter should be set according to the narrowest peak of interest and influences the number of points used in the evaluation. The *Value* must be in the range of 0.001 - 10 minutes.

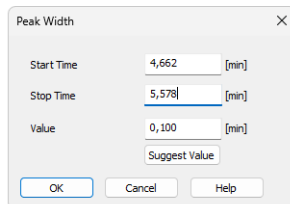


Fig. 163: Peak Width

Caution: Setting an excessively high value will distort the results.

The Local Peak Width command procedure:

- You will be prompted to place the cursor lines to the beginning and the end of the interval and mark each by left-click of the mouse. The *Local Peak Width* parameter will be applied within this interval only.
- Then the *Peak Width* dialog will open in which you may adjust the graphically set interval in the *Start Time* and *Stop Time* fields and enter the required peak width into the *Value* field.
- Click the *Suggest Value* button to user is advised to interactively select the narrowest peak that still has to be integrated (again using the cursor lines). Suggested value will be transferred to the *Value* field.
- Click *OK* to apply the selected value to the specified interval.

Note: The value as well as the interval can be later edited in the **Integration Table**.

Start Time

Enables to edit the interactively set *Start Time* of the interval. The value set in the *Value* field will be applied within this interval only.

Stop Time

Enables to edit the interactively set *Stop Time* of the interval. The value set in the *Value* field will be applied within this interval only.

Value

Enables to edit the suggested value of the *Local Peak Width* parameter. The value can be suggested by **Clarity** using the *Suggest Value* button.


Suggest Value

Clicking the button will display the cursor lines again and the user will be prompted to select the interval containing narrowest peak that still has to be identified. The suggested **Peak Width** value will be transferred to the *Value* field where it can be confirmed or edited.

Note: The *Peak Width* value is not critical, so narrower peaks than the set value are also detected, but this may lead to an imprecise definition of the beginning and end of the peak and incorrect interlining of the baseline.

To adjust the **Peak Width** value for the entire chromatogram, use the *Global Peak Width* command (for more details see the chapter **Chromatogram** on pg. 217).

3.4.3.2 Local Threshold

Invoke this command or press the *Local Threshold* icon  to open the *Threshold* dialog which determines the noise threshold value for the specified interval. The **Threshold** parameter determines the sensitivity of the integration algorithm to distinguish between noise and peaks. The parameter also, unless overridden by **Slope** parameter value, determines the position of the starts and ends of peaks.

The height of all peaks (measured from the baseline to the apex) which you wish to detect should be at least twice this parameter. The *Value* must be in the range of $1 \mu\text{V} - 10 \text{ V}$.

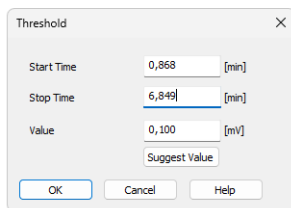


Fig. 164: Threshold

The Local Threshold command procedure:

- You will be prompted to place the cursor lines to the beginning and the end of the interval and mark each by left-click of the mouse. The *Local Threshold* parameter will be applied within this interval only.
- Then the *Threshold* dialog will open in which you may adjust the graphically set interval in the *Start Time* and *Stop Time* fields and enter the required threshold value into the *Value* field.
- Click the *Suggest Value* button to interactively select the area with the "highest peaks" that still should not be integrated (using the cursor lines once more). Suggested value will be transferred to the *Value* field.

Note: Keep in mind that the suggested value will be half of these "highest peaks" because only peaks twice the size of the noise threshold will be detected.

Note: In the *Wave* integration algorithm, peaks that are lower than twice the threshold may still appear in the chromatogram if they are on the same baseline with valid (higher) peaks not to influence the course of the baseline. Such peaks can be hidden using the *Peak - Hide* function or the baseline can be modified to remove them using the *Integration - Minimal Height* operation set to twice the threshold value (baseline changes in the latter case).

- Click *OK* to apply the selected value to the specified interval.

Note: The **Threshold** value as well as the *Local Threshold* interval can be later edited in the **Integration Table**.

Start Time

Enables to edit the interactively set *Start Time* of the interval. The value set in the *Value* field will be applied within this interval only.

Stop Time

Enables to edit the interactively set *Stop Time* of the interval. The value set in the *Value* field will be applied within this interval only.

Value


Enables to edit the suggested value of the *Local Threshold* parameter. The value can be suggested by **Clarity** using the *Suggest Value* button.

Suggest Value

Clicking the button will display the cursor lines again and the user will be prompted to place an interval containing "highest peaks" that still should not be integrated. The suggested **Threshold** value will be transferred to the *Value* field where it can be confirmed or edited.

To adjust the **Threshold** value for the entire chromatogram use the *Global Threshold* command (for more details see the chapter **Chromatogram** on pg. 217).

3.4.3.3 Local Baseline Slope

Invoke this command or press the *Local baseline Slope* icon  to open the *Slope* dialog which determines the expected signal curve slope value to detect peak starts and ends for the specified interval. The **Slope** parameter decides on the position of peak starts and peak ends in the *Wave* integration algorithm. If unused (value left at 0) the **Slope** is derived from the **Threshold** parameter (at $8 * \text{Threshold}$ at given area of chromatogram).

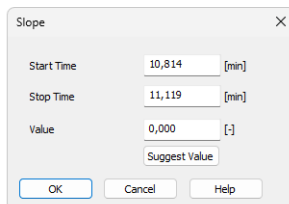


Fig. 165: Slope

The Local Baseline Slope command procedure:

- You will be prompted to place the cursor lines to the beginning and the end of the interval and mark each by left-click of the mouse. The *Local Baseline Slope* parameter will be applied within this interval only.
- Then the *Slope* dialog will open in which you may adjust the graphically set interval in the *Start Time* and *Stop Time* fields and enter the required slope value into the *Value* field.
- Click the *Suggest Value* button to interactively select the position of the expected peak start or peak end. Suggested value will be transferred to the *Value* field.

Note: The suggested value will be exactly as the slope calculated at the position, but the peak start or peak end may be placed slightly differently - the expected slope is checked on the whole signal curve and there may be other areas which fulfill the slope condition closer to the peak apex.

- Click *OK* to apply the selected value to the specified interval.

Note: The **Slope** value as well as the *Local Baseline Slope* interval can be later edited in the **Integration Table**.

Start Time

Enables to edit the interactively set *Start Time* of the interval. The value set in the *Value* field will be applied within this interval only.

Stop Time

Enables to edit the interactively set *Stop Time* of the interval. The value set in the *Value* field will be applied within this interval only.

Value


Enables to edit the suggested value of the *Local Baseline Slope* parameter. The value can be suggested by **Clarity** using the *Suggest Value* button.

Suggest Value

Clicking the button will display the cursor line again and the user is prompted to point to a place where the expected peak start or peak end should be placed automatically by the integration algorithm. The suggested **Slope** value will be transferred to the *Value* field where it can be confirmed or edited.

To adjust the **Slope** value for the entire chromatogram use the *Global Baseline Slope* command (for more details see the chapter **Chromatogram** on pg. 217).


3.4.3.4 Integration Interval

Invoking this command or using the *Integration Interval* icon  allows to define the interval in which the integration algorithm is run. The course of the chromatogram outside of this interval will be ignored.


After using the function you are prompted to select the beginning and end point of the interval in the graph using the mouse. The starting time or ending time of the interval may be adjusted or directly set in the **Integration Table** on the [Integration](#) tab. When the *Integration Interval* command is not used, the integration algorithm is run on the whole chromatogram.

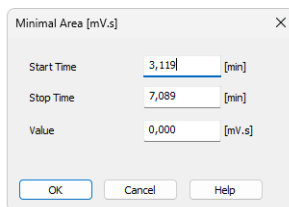
Caution: It is not true that the *Integration Interval* command is an opposite to the *Baseline - Lock* command. Although their logic is opposite (the first command will permit the integration in the interval and in the second will prohibit it) there is a significant difference between using the *Integration Interval* command (which directly defines where the integration algorithm will be used) and using the *Baseline - Lock* command (which only prohibits already integrated peaks). In other words: the *Baseline - Lock* command does not radically change the course of the baseline before and beyond the area with suppressed peaks.

3.4.3.5 Detect Negative

Invoking this command or using the *Detect Negative* icon  enables the detection of negative peaks in the defined interval. When the function is not active on the given part of the chromatogram, all negative peaks present are considered to be the correct course of the baseline (similar to the part of the chromatogram which uses the *Reject Negative* function).

3.4.3.6 Minimal Area

Invoking this command or using the *Minimal Area* icon  allows you to set minimum allowed area of the peak. Peaks with areas smaller than or equal to this value are excluded from the integration.



The dialog box titled "Minimal Area [mV.s]" contains three input fields: "Start Time" with the value "3,119" and unit "[min]", "Stop Time" with the value "7,089" and unit "[min]", and "Value" with the value "0,000" and unit "[mV.s]". At the bottom, there are three buttons: "OK", "Cancel", and "Help".

Fig. 166: Minimal Area

Start Time

Enables to edit the interactively set *Start Time* of the interval. The value set in the *Value* field will be applied within this interval only.


Stop Time

Enables to edit the interactively set *Stop Time* of the interval. The value set in the *Value* field will be applied within this interval only.


Value

Enables to edit the suggested value of the *Minimal Area* parameter.


3.4.3.7 Minimal Height

Invoking this command or using the *Minimal Height* icon  allows to set the minimum height of the peak. Peaks with heights smaller than or equal to this value are excluded from the integration. Parameters and fields in the *Minimal Height* dialog are the same as in the *Minimal Area* dialog.


3.4.3.8 Minimal Half Width

Invoking this command or using the *Minimal Half Width* icon  allows to set the minimum half-width of the peak. Peaks with *W05* parameter smaller than or equal to this value are excluded from the integration. Parameters and fields in the *Minimal Half Width* dialog are the same as in the *Minimal Area* dialog.

3.4.3.9 Detector Delay


Invoking this command or using the *Detector Delay* icon  allows to correct the time delay of a detector. You are advised to point and click the cursor on the desired peak of the active signal and then on a corresponding peak in the reference signal.

3.4.3.10 FFT Filter

Invoking this command or using the *FFT Filter* icon  allows to apply the **FFT Filter** (*Fast Fourier Transformation*) for noise reduction in the selected interval. If more than one type of the filter is set on the same time interval, only the last used filter on that interval is actually used. FFT Filter in **Clarity** is non-parametric and may create artifacts on the signal under certain conditions.


For the description of equations behind *FFT Filter* calculation please check publicly available resources (Wikipedia).

3.4.3.11 Savitzky-Golay Filter

Invoking this command or using the *Savitzky-Golay Filter* icon  allows to apply the **Savitzky-Golay Filter** for noise reduction in the selected interval. If more than one type of the filter is set on the same time interval, only the last used filter on that interval is actually used. Savitzky-Golay Filter in **Clarity** is parametric, ranging the parameter from 1 (no filter applied) to 500 (filter window is 500 points wide). The parameter for the filter may be changed in the **Integration** table for the given signal, found on the [Integration](#) tab in [Chromatogram](#) window. Savitzky-Golay filter may create artifacts on the signal under certain conditions.

For the description of equations behind *Savitzky-Golay Filter* calculation please check publicly available resources (Wikipedia).


3.4.3.12 Moving Average Filter

Invoking this command or using the *Moving Average Filter* icon  allows to apply the **Moving Average Filter** for noise reduction in the selected interval. If more than one type of the filter is set on the same time interval, only the last used filter on that interval is actually used. Moving Average Filter in **Clarity** is parametric, ranging the parameter from 1 (averaging actual point with the previous and next one) to 500 (filter window is 1001 points wide - 500 points to each side). The parameter for the filter may be changed in the **Integration** table for the given signal, found on the [Integration](#) tab in [Chromatogram](#) window. The equation to calculate the moving average filter used in **Clarity** is:

$$E_x = \sum_{i=n-p}^{n+p} \frac{E_i}{(p \cdot 2) + 1}$$

, where E_i is original signal of point i and p is the parameter entered in the **Integration** table.

3.4.3.13 Spike Filter

Invoking this command or using the *Spike Filter* icon  allows to remove the spikes on the chromatogram signal. The parameter of the command (that can be edited from the Integration table) describes how wide spikes will be removed (their missing points replaced by a calculated value). The usage of this function only available in **Clarity** version 4.0 and higher may be disabled by the use of the *Disallow Spike Filter and Spike Removal* parameter from the [GLP Options](#) dialog (for more details see the chapter **GLP Options** on pg. 31).. Spike Filter in **Clarity** is parametric, ranging the parameter from 1 (no filter applied) to 100 (filters out spikes 100 points wide maximum). The parameter for the filter may be changed in the **Integration** table for the given signal, found on the [Integration](#) tab in [Chromatogram](#) window.

3.4.4 Separation

All interval operation follows the rule that with *Time B* = 0 operation will be applied from *Time A* to the end of the chromatogram. With both *Time A* and *Time B* set to 0, operation is applied over the whole chromatogram.

3.4.4.1 Valley To Valley Slope

Specifies the maximum slope of the baseline. If the baseline slope is smaller than the specified value, the separating perpendicular line is canceled and the baseline passes through the valley. The default value of 0 prevents the baseline from passing through the valley.

3.4.4.2 Tangent Area Ratio

Constitutes the first condition imposed on tangential separation. The condition for tangential separation is satisfied if the ratio of areas of the separated and the main peak is lower than specified value. First raider peak not fulfilling the preset conditions ends tangential separation, peaks further from the main peak apex are then integrated to the baseline.

The value of 0 prevents tangential separation. If this operation is selected in the **Integration table**, its value is set to value of 10 and in general increasing value causes higher degree of tangential separation of the raider peaks. If there is no *Tangent Slope Ratio* item defined in the **Integration table** but *Tangent Area Ratio* is defined, the value of the *Tangent Slope Ratio* is considered to be 10.

3.4.4.3 Tangent Slope Ratio

This is the second condition imposed on tangential separation. The condition is satisfied if the angle between the baseline of the raider peak and the baseline of the original cluster peak (connections between starting and final points of the peaks are considered as baselines) exceeds the specified value. The ratio is defined as the tangent to the baseline of the original cluster peak compared to the baseline of the raider. First raider peak not fulfilling the preset conditions ends tangential separation, peaks further from the main peak apex are then integrated to the baseline.

Value of 0 prevents tangential separation. If this operation is selected in the **Integration table**, its value is set to value of 10 and in general increasing value causes lower degree of tangential separation of the raider peaks. The range of possible values is between 0 - 100, value 0 corresponds to angle 0° and value of 100 corresponds to angle 180°. If there is no *Tangent Area Ratio* item defined in the **Integration table** but *Tangent Slope Ratio* is defined, but the value of the *Tangent Area Ratio* is considered to be 10.

3.4.5 Noise & Drift

The *Noise* (all variants) and *Drift* parameters are set as intervals. All values can be utilized in custom calculations in **User Columns**.

All interval operation follows the rule that with *Time B* = 0 operation will be applied from *Time A* to the end of the chromatogram. With both *Time A* and *Time B* set to 0, operation is applied over the whole chromatogram.

Result Table (ESTD - Wine_Sample - UV detector)					
Noise (1,38-4,87 min): 960,6463 [mAU], ASTM Noise (1,90-4,90 min): 237,7274 [mAU], 6-Sigma Noise (1,75-5,90 min): 857,8867 [mAU]					
Reten. Time [min]	Response	Amount [g/l]	Amount% [%]	Peak Type	Compound Name
2	1,063	58,456	0,028	0,9 Ordnr	oxalic
3	1,703	3808,662	0,246	8,1 Ordnr	citric

Fig. 167: Noise & Drift above the Result table

The noise evaluation determines the amount of noise in the specified interval of the chromatogram. The interval for any type of noise evaluation is set in the **Integration Table**.

After invoking the particular *Noise Evaluation* command, select part of the chromatogram that contains noise only (ideally part of the baseline). In case several intervals for the same noise calculation method are set, only the last one is valid. Previous entries can be filtered from the **Integration Table**, so that only the last entry will be displayed. Set the interval to zero to display the noise over the whole length of the chromatogram.

If the interval exceeds the length of the actual chromatogram, only the valid part of the interval will be taken into account.

The noise value will be displayed above the **Result Table** along with appropriate signal units and the interval, from which it was calculated.

Note: It is possible to calculate the noise using all three methods - linear interlining (*Noise Evaluation*), *ASTM Noise Evaluation* and *6-Sigma Noise Evaluation* at the same time.

Current noise during acquisition can also be displayed in the upper left corner of the graph in the [Data Acquisition](#) window.

Note: The **Noise** in the [Data Acquisition](#) window is calculated using the cubic interlining to reduce the influence of the trend to its values.

3.4.5.1 Noise Evaluation

The **Noise** value for the *Noise Evaluation* command is calculated using the linear interlining on the interval defined in the **Integration Table**. If there is a peak in this interval, it will influence the noise values.

3.4.5.2 ASTM Noise Evaluation

The **Noise** value for the *ASTM Noise Evaluation* command is calculated as an average from values counted for smaller intervals. The procedure goes as follows:

- The selected time interval is divided into parts of the same length (30s by default, may be changed in the **Integration Table**, *Value* column). The remaining part is added to the last complete interval or left on its own, if it is the only interval.
- Noise is counted for each of these intervals using the linear interlining and the least squares method.
- The values gained from these intervals are then averaged.

3.4.5.3 6-Sigma Noise Evaluation

The **Noise** value for the *6-Sigma Noise Evaluation* command is calculated from the whole interval set in the **Integration Table**. The value gained is calculated as a six times the square root of least square method for each point in the whole interval divided by the number of points:

$$\text{Noise} = 6 \cdot \sqrt{\left(\frac{\sum_{i=1}^n (E_i - f(E_i))^2}{n-1} \right)}$$

where n is the number of acquisition points, E_i is the signal value of the i -th point and $f(E_i)$ is the value corresponding to the linear regression performed on the selected interval at the i -th point.

3.4.5.4 Drift Evaluation

The drift evaluation determines the drift between the beginning and the end point of the specified interval, which is set in the **Integration Table**.

After invoking the *Drift Evaluation* command, select part of the chromatogram where the **Drift** should be calculated. If more than one interval has been set, the latest one will be applied. Previous entries can be filtered from the **Integration Table**, so that only the last entry will be displayed. Set the interval to zero to get the drift over the whole length of the chromatogram.

If the interval exceeds the length of the actual chromatogram, only the valid part of the interval will be taken into account.

3.4.6 Overlay & Other

Includes commands for working with several chromatograms simultaneously. The maximum number of displayed chromatograms is practically unlimited, the actual limit can be set in the [User Options](#) dialog. Most of the commands identified below can be invoked by the icons found in the *Overlay* and *Other* toolbars.



Fig. 168: *Overlay & Other* Toolbars

	Move	Moves the active chromatogram.
	Scale	Scales the active chromatogram up or down.
	Original	Cancels all shift and scaling operations.
	3D View	Displays chromatograms in a three-dimensional perspective.
	Clear 3D	Restores the original perspective.
	Properties...	Opens the Graph Properties dialog on the Signals tab.
	Mathematics...	Performs mathematical operations with chromatograms.

The *OVERLAY* mode can be activated using the *File - Overlay Mode* command, double-clicking on the **Overlay** inscription in the status bar or clicking on the icon. An active *OVERLAY* mode is indicated by the depressed icon in the *Overlay* toolbar, highlighted **Overlay** inscription in the status bar and by the checkmark by the *Overlay Mode* in the *File* menu.



Note: Too many chromatograms opened at once may (especially on slower computers) notably slow down the response of the computer.

In case there is more than one chromatogram (or a chromatogram with more than one signal), it is possible to hide signal by holding CTRL down and clicking on the respective colour in the toolbar. Hidden signals are represented by empty rectangle in the *Overlay* toolbar (see image below). To once again show the signal, simply hold CTRL down and click on the hidden signal. Alternatively see the "Chromatograms" on page 271 topic.




Fig. 169: *Overlay with hidden signals*



3.4.6.1 Move

Invoking this command or clicking the *Move* icon  enables you to move the active chromatogram. To use the function, left-click the mouse and hold down while dragging the chromatogram to the new location, then release the button. Exact values of the shift or the possibility to return to the original location are found on the [Graph Properties - Signals](#) tab (accessed by using the *Chromatogram - Overlay - Properties...* command or the *Signal Properties* icon ). In the shifted chromatogram (signal) all commands from the *Chromatogram* menu other than those in the *Overlay* group are disabled and **Result Table** and peak labels are not shown.


Caution: The performed moving cannot be stored in the original chromatogram. The only possible way to save such chromatogram is to make a copy of the modified chromatogram by the *Overlay - Mathematics - Copy* command and save the copy. After finished *Move* operation, all the values in the **Result table** will disappear as they are no longer valid.

Note: Hold **Shift** while clicking the menu command or  icon to apply the move to all signals from the current chromatogram. Hold **Ctrl** while moving the chromatogram, to limit the moving direction to vertical or horizontal.

3.4.6.2 Scale

Invoking this command or using the *Scale* icon  allows you to change the scale of the active chromatogram. After invoking the command, left click the mouse and hold it while dragging the chromatogram to the new scale and then release it. The chromatogram will be drawn to the new scale when released. Exact values of the scale operation or the possibility to return to the original state are found on the [Graph Properties - Signals](#) tab (accessed by using the *Chromatogram - Overlay - Properties...* command or the *Signal Properties* icon ). In the scaled chromatogram (signal) all commands from the *Chromatogram* menu other than those in the *Overlay* group are disabled and **Result Table** and peak labels are not shown. The scaled chromatogram is marked by the *MODIFIED* inscription in the title bar.

Caution: The performed scaling operation cannot be stored in the original chromatogram. The only possible way to save such a chromatogram is to make a copy of the modified chromatogram by the *Overlay - Mathematics - Copy* command and save the copy. After finished *Scale* operation, all the values in the **Result table** will disappear as they are no longer valid.

Note: Hold **Shift** while clicking the menu command or  icon to apply the scaling to all signals from the current chromatogram. Hold **Ctrl** while moving the chromatogram, to limit the moving direction to vertical or horizontal.

3.4.6.3 Original

Invoking this command returns the chromatogram to its original location and scale. The initial state is the setting in which the scale is unchanged (**Scale = 1**) and the chromatogram is not shifted from the start (**Offset = 0**).

Note: Hold **Shift** while clicking the menu command to apply the change to all signals from the current chromatogram.


3.4.6.4 3D View

Invoking this command enables to display the chromatogram(s) in three-dimensional perspective. After prompting a pair of lines that serve to set the angle and depth of the 3D rendering is shown. Click the mouse button to uniformly space out all displayed chromatograms along the specified line segment. The actual spacing can be modified by changing the *X (Y) Offset* parameters on the [Graph Properties - Signals](#) tab.

3.4.6.5 Clear 3D


Invoking this command clears the 3D representation mode and restores the original display mode. All chromatograms are restored to their original positions (corresponding to the *0* values of the *X (Y) Offset* parameters). These values can be set for each chromatogram (signal) separately using the *Original* button on the [Graph Properties - Signals](#) tab.

3.4.6.6 Properties...

Invoking this command or using the *Signal Properties* icon  allows you to set the explicit shift and scale parameters for the active chromatogram. Invoking the command opens the [Signals](#) tab of the [Graph Properties](#) dialog (for more details see the chapter **Graph Properties - Signals tab** on pg. 211). All set values refer only to the active chromatogram.

If any parameter from the *Offset & Scale* group differs from the default value, the baseline, all commands from the *Chromatogram* menu other than those in the *Overlay* group are disabled and **Result Table** and peak labels are not shown.

3.4.6.7 Mathematics... (Mathematical Operations dialog)

Invoking this button or using the *Mathematics* icon  enables to perform mathematical operations with chromatograms. After selection, the *Mathematical Operations* dialog will be displayed.

Mathematical operations are only performed with chromatograms (signals) that are currently open in the [Chromatogram](#) window.

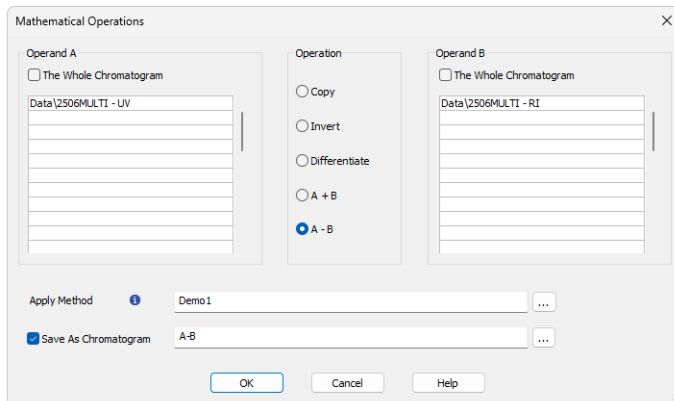



Fig. 170: *Mathematical Operations*

Operand A (Operand B)

Select up to 32 signals in **Operand A** section in the listbox on the left. The whole chromatogram (all of its signals) will be included when the *The whole Chromatogram* checkbox has been checked. When unchecked, you may select individual signals (and change their order) from one chromatogram, or select signals from various chromatograms. This is done by simply clicking the row intended for editing and using the arrow icon  to the right to select the particular chromatogram or signal.

Operand B is selected analogically to the **Operand A**, if appropriate.

Operation

Type of required operation. The following operations are possible:

Tab. 14: *List of available mathematical operations*

Operation	Effect
<i>Copy</i>	- Copies chromatogram (Selection of the Operand A only).
<i>Invert</i>	- Inverts signal or chromatogram (Selection of the Operand A only).
<i>Differentiate</i>	- Calculates first derivation (Selection of the Operand A only).
<i>A+B</i>	- Sum of signals or chromatograms.
	<i>Note:</i> It is necessary to work in <i>Overlay mode</i> to have this option available.

Operation	Effect
A-B	- Difference of signals or chromatograms. <i>Note:</i> It is necessary to work in <i>Overlay mode</i> to have this option available.

Apply Method

Choose method whose parameters (integration table, attached calibration, etc.) will be applied into the created chromatogram. By default, displayed method matches method in the [Single Analysis](#) dialog. Leaving this field blank applies default parameters.

Save As Chromatogram

The name offered is implicitly derived from the performed mathematical operation - e.g. A-B. To create a custom name, it is necessary to check the *Save As Chromatogram* checkbox.

If this checkbox is checked, the mathematical result will automatically be saved as a new chromatogram.

If this field is left unchecked, the mathematical result will only be displayed as a new curve, which you may save using the *Save* or *Save As* command from the *File* menu.

In the full version *full version*, the resultant chromatogram contains information about the manner of its creation in [Chromatogram Audit Trail](#) described on pg. 427.

Time	Group	Severity	User Name	Det	Description
30.11.2023 16:18:29	File		Administrator		Chromatogram saved as Data\A-B.prm
30.11.2023 16:18:29	Chromatogram		Administrator	Signal 1	Mathematical Operations - Self = 'C:\Clarity\DataFiles\DEMO1\Data\2506MULTI.prm - UV' - 'C:\Clarity\DataFiles\DEMO1\Data\2506MULTI.prm - RI'

For help press F1.

Fig. 171: Chromatogram Audit Trail

3.4.7 Chromatograms

Displays the *Chromatogram List* dialog with a chronological list of all opened chromatograms/signals.

Note: Active signal is highlighted in bold letters, hidden signals are displayed in gray color.

The maximum number of signals that can be simultaneously displayed in the [Chromatogram](#) window ranges from 2 to 10 000 (the default setting is 20) is determined by the *Maximum Chromatograms in Overlay* item from the [User Options - General](#) dialog.

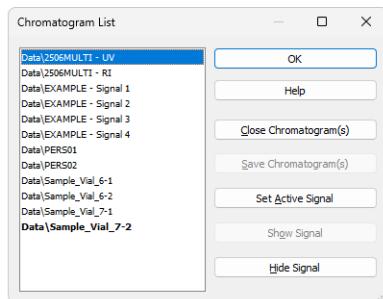


Fig. 172: Chromatogram List

Close Chromatogram(s)

Closes the selected chromatogram(s) and all of its(theirs) signals.

Save Chromatogram(s)

Saves the entire selected chromatogram(s).

Set Active Signal

Sets the selected chromatogram (signal) as active.

Note: You can also double click a signal in the list to make it active.

Show Signal

Displays selected signals.

Note: The command will only be active if the selected signal has previously been hidden.

Hide Signal

Hides selected signals.

3.4.8 Create Label

Adds labels and lines.

Text

Appends a text label. Select the command and click on the desired location to open the *Text Label* dialog. The *Text Label* dialog may also be invoked by double-clicking on the actual text label to modify it.

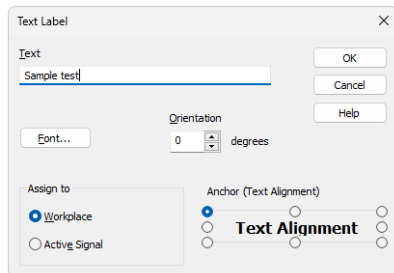


Fig. 173: Text Label

Text

The text of the user's label is entered/edited on this line.

Font...

Selects the font, size and color of characters. Invoking the command opens the standard *Font* dialog.

Orientation

Select the orientation of the label text in degrees counted counterclockwise (e.g. enter 0 for horizontal or 90 for vertical orientation). Allowed values are 0 - 359.

Note: You can use *Orientation* field only when using **TrueType** fonts.

Delete

Deletes the selected label.

Assign to

Workplace

The label will lie, unattached to any specific chromatogram, in the background and will be saved in the current desktop.

Active Signal

The label will be attached and become integral part of the chromatogram. When the signal is scaled up or down, the label will be anchored to the nearest signal point.

Anchor (Text alignment)

Defines the method of label anchoring. One of eight points on the label border or the label center may be selected as the anchor point. The label is then firmly "bound" by that point to the nearest chromatogram point (or to the graph border

when the label is attached to the **Workplace**). This can be of particular use when scaling or shifting a chromatogram where labels supplement peak identification etc. A label can be shifted and/or scaled in the same way as in usual drawing applications. Left clicking on a label displays the controlling frame and handles for sizing it. The font size will change with the frame size. To move the frame containing the label, click inside the frame and drag.

Line

Adds connecting lines. To create a line label, invoke the command and then left click and hold the button on the desired starting point of the line, drag to the desired end point and release. The *Line Label* dialog will open to determine the properties of the line. The dialog can also be called by double-clicking on the actual line label to change its appearance.

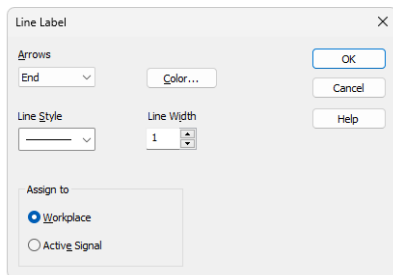


Fig. 174: Line Label

Arrows

Selects optional line end:

None - No arrows will be placed on the line.

Beginning - An arrow will be added to the line beginning.

End - An arrow will be added to the line end.

Both - Both line ends will be provided with arrows.

Color...

Selects the line color.

Line Style

Defines the line style. If the *Line Width* parameter is greater than 1, the line will be solid. Possible variants for the *Line Style* are solid line, broken line, dotted line, dashed and dotted line or dashed and double dotted line.

Line Width

Defines the line width in pixels (1 to 6). Lines with the width greater than 1 have to be solid.

Assign to

Workplace

The label will lie, unattached to any specific chromatogram, in the background and will be saved in the current desktop.

Active Signal

The label will be attached and become integral part of the chromatogram. When the signal is scaled up or down, the label will be sized along with the signal (both ends are anchored to two nearest signal points).

A line can be shifted or sized in the same way as in drawing applications. Left clicking on a line will display the controlling frame and handles the sizing of the line. To shift the line, left click and hold anywhere on the line except the end points, drag to the desired location and release.

3.4.9 Merge

The *Merge* command is used to merge the currently opened chromatogram with signals from another chromatogram. Standard [Open Chromatogram](#) dialog is used for selecting the chromatogram for merging.

3.4.10 Set Signal Names

The *Set Signal Names* command is used to invoke the *Set Signal Names* dialog where existing names of signals can be edited.

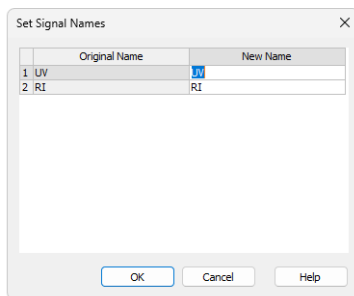


Fig. 175: Set Signal Names

If the signal has no allocated name, the name **Signal n** (where n is the serial number of the signal in the chromatogram) will be displayed in the original name column.

Note: By default, individual signals are named in regards to the name of the detector used or upon import or connection by implicit names (1 .. 32). The default names of the signals can be changed in the [System Configuration](#) dialog by invoking the *Setup* button for the particular detector.

3.4.11 Remove Generated Signal

This command is located in the [Chromatogram](#) window in the menu *Chromatogram*.

The *Remove Generated Signal* command is used to invoke the *Remove Generated Signal* dialog where generated signal can be removed.

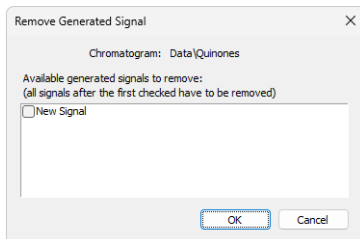



Fig. 176: Remove Generated Signal

Only named signals can be removed. In case there are more generated signals in the chromatogram, with the one selected in this dialogue will be also removed all newer ones.

3.5 Method

An entry point to commands for modifying chromatograms and copying methods.

Calculation	Displays the parameters of chromatographic results calculation.
Integration	Displays integration parameters.
Measurement	Displays the conditions under which the chromatogram was created.
Save as Template...	<p>The command saves the method used for the measurement of active chromatogram as template method, i.e., a method that can be used in the Instrument window for other analyses. Invoking the command displays the <i>Save As</i> dialog, where the name of the new template method should be specified. By default, template methods will be stored to the current project directory, but the path can also be changed.</p> <p>The method is a component of the chromatogram file (files with the *.PRM suffix). The template method will be stored in a separate file with the *.MET suffix.</p>
 Set Model <small>✓ Full version</small>	<p>Marks the method of an active chromatogram as model method. In case the chromatogram is opened in a version which is not the latest one, the given historical method version will be set as model. Any model method can be copied to another chromatogram by the <i>Copy from Model</i> command. The model method selection is valid until the Chromatogram window is closed or another model method is selected by the <i>Set Model</i> command.</p> <p>Integration Table is part of method, therefore contents of the Integration Table will be set as model as well.</p>

**Copy from Model**

✓ Full version

Copies a **Model Method** to another chromatogram. Prior to invoking the command a method must have been marked as model method by the *Set Model Method* command. The model method can then be applied on any chromatogram opened in the [Chromatogram](#) window by using the *Copy from Model* command. Integration Table from the Model method will be copied into the Integration Table of the active chromatogram.

Copy from Template Method...

Copies Template Method into active chromatogram. Use this command to invoke the [Open Method](#) dialog (described in the chapter "**Open Dialog (Sequence, Chromatogram, Calibration, Method)**" on pg. 77., which will display a list of all **Template Methods** from current project.

Copy from Chromatogram...

Copies the method from a selected chromatogram to active chromatogram. Use this command to open the [Open Chromatogram](#) dialog (described in the chapter "**Open Dialog (Sequence, Chromatogram, Calibration, Method)**" on pg. 77., in which you can select the required chromatogram.

3.5.1 Calculation

Selects the method for calculating the results of the chromatogram. Once selected, the *Results* tab will be displayed in the lower part of the [Chromatogram](#) window. In its right-hand section it is possible to define the method of results calculation. Left-hand section displays [Result table](#) with signal related results.

The parameters stated here are common for all signals when a multi-detector chromatogram is being used. The displayed values come from the template method; they are filled in on the [Calculation](#) tab of the [Method Setup](#) dialog as a part of the method according which the chromatogram is measured.

Calibration File (Peak Table)

Name of the calibration file used to obtain calibrated calculations.

Open with stored calibration

When checked, the chromatogram will be opened with calibration stored within the chromatogram file when it is opened next time. 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. Similar behavior may be set directly when the chromatogram is created from [Sequence](#) window or set in the [Single Analysis - Post Run Settings](#) tab.

Note: The differences between *Stored* and *Linked* calibration are explained in the [Open Chromatogram](#) window in the *Method* section.

Set...

Invokes the *Open Calibration* dialog where the calibration file may be selected.

None

Closes the opened calibration file and sets the calculation type in the *Calculation* field to *Uncal* (uncalibrated).

View

Opens the linked calibration file in the [Calibration](#) window. Current chromatogram will be automatically opened in it, ready for adding new levels.

Result Table (ESTD - DataWine_Sample - UV detector)						
Reten. Time [min]	Response	Amount [g/l]	Amount% [%]	Peak Type	Compound Name	
1	1.063	54.322	0.026	0.9	Ordnr	oxalic
2	1.703	3830.782	0.248	8.2	Ordnr	cltric
3	1.917	8460.283	0.438	14.5	Ordnr	tartric
4	2.800	3333.242	1.147	37.8	Ordnr	malic
8	4.660	2732.362	0.243	8.0	Ordnr	sucnic
9	5.050	2969.660	0.744	24.6	Ordnr	lactic
11	6.847	2304.278	0.185	6.1	Ordnr	acetic
Total			3.031	100.0		

Common for All Signals

Calibration File (Peak Table)
Wine

Calculation
ESTD

Open with stored calibration

Set... None View

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 [g/l]: 0
Inj. Volume [µl]: 100
ISTD1 Amount [g/l]: 0
Dilution: 1

User Variables

Analysis Variables		Method Variables	
Name	Value	Name	Value
1 AnalysisUserVar1	0	1 MethodUserVar1	0
2 AnalysisUserVar2	0	2 MethodUserVar2	0
3 AnalysisUserVar3	0	3 MethodUserVar3	0

Results | All Signals Results | Summary | Performance | Integration | Measurement Conditions | SST Results

Fig. 177: Chromatogram - Results tab - Results

Calculation

Selects the type of calculation. Available options are shown **Tab. 15** on pg. **279**.

Tab. 15: List of available calculation types

Calculation type	Way of calculation
<i>Uncal</i>	- Uncalibrated calculation without use of calibration file. The result of the integration is a percentage representation of individual areas and heights of peaks in the chromatogram. When using this option, all other sections on this tab will be inactive and dimmed.
<i>ESTD</i>	- External standard calculation. The result will be both a percentage and absolute representation of individual substances and their names.
<i>ISTD</i>	- Internal standard calculation. The result will be both a percentage and an absolute representation of individual substances and their names.
<i>NORM</i>	- External standard calculation with add-on checks. The result will be both a percentage and an absolute representation of individual substances and their names. In case any peak found in the Result Table is not present in a calibration and/or the <i>Amount</i> parameter differs from zero, the calculation of the <i>Peak Type</i> for all rows in the Result Table will be <i>Error</i> and the <i>Amount [%]</i> values will not be calculated.

Calculation type	Way of calculation
<i>STDADD</i>	- Standard Addition calculation. The result amounts of compounds in an unknown sample are calculated based on standard addition calibration curve by extrapolation of the calibration curve to point with Y coordinate equal to zero. The results are displayed in absolute values.
<i>Note:</i>	If only the <i>Peak Type</i> field for selected rows of the Result Table show the <i>Error</i> code, than the corresponding compounds do not have the <i>Amount</i> value filled in the calibration file.

Report in Result Table

This field determines which peaks will be displayed in the **Result Table** and included in the sum for the **Total** row in the case of calibrated calculations.

All Peaks

All integrated peaks in the chromatogram will be displayed.

All Identified Peaks

Only peaks identified in the calibration file will be displayed.

All Peaks in Calibration

All peaks from the calibration file will be displayed without regard to how many peaks the chromatogram contains and how many were identified. This provides what is known as a fixed table format given by the calculation of peaks in the calibration file.

Hide ISTD Peaks

The peaks identified as the internal standards will not be displayed in the **Result Table**.

Note: The command will be active only when the *ISTD* calculation type has been selected.

Unidentified Peaks

Response Base

Selects a base for calibrated calculation of unidentified substances.

Area - Calculations will be derived from peak areas.

Height - Calculations will be derived from peak heights.

Response Factor

Coefficient used for amount calculation for unidentified substances. Amount is set as area (height) of peak multiplied by this coefficient. This value serves in fact as an artificial single-point calibration for unidentified substances.

Scale

Area for entering the auxiliary calculation parameters.

Use Scale Factor

The whole area is activated by checking this checkbox.

Scale Factor

All values of the *Amount* column in the **Result Table** will be multiplied by the stated value.

Units

Units for application of scale. The original units taken from the calibration file are replaced by the units defined here in the results table.


Amount

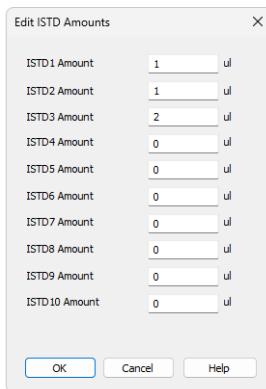
Amount of the sample. This value is used as a basis for the calibrated calculation of the percentage representation of individual substances for *ESTD* and *ISTD* methods.

When the *ISTD* method is used, enter the amount of the sample without the internal standard. State the parameter in units used in the calibration file (*Units - Compound* parameter in the [Calibration Options](#) dialog). The implicit value is 0. In this case the percentage representation is calculated from the *Amount* sum in the *Total* row.

Note: If the *Amount* parameter is set to zero, the percentage representation of individual values will be calculated from the sum of all calibrated amounts (including substances calibrated using the *Uncal. Response* parameter). Otherwise the calculation is based on the *Amount* value entered.

ISTD Amount

Specifies the amount of internal standard (ISTD1) added when the results are calculated using the *ISTD* method. Similar settings are available for the ISTD2 - ISTD10 in the *Edit ISTD Amounts* dialog accessible through the  button.



Label	Value	Unit
ISTD1 Amount	1	ul
ISTD2 Amount	1	ul
ISTD3 Amount	2	ul
ISTD4 Amount	0	ul
ISTD5 Amount	0	ul
ISTD6 Amount	0	ul
ISTD7 Amount	0	ul
ISTD8 Amount	0	ul
ISTD9 Amount	0	ul
ISTD10 Amount	0	ul

Fig. 178: Edit ISTD Amounts

Edit ISTD Amounts dialog allows to set the ISTD Amounts for all internal standards used in particular chromatogram. It is also accessible from the [Single Analysis](#) dialog and amounts can be entered from the [Sequence](#) window (settings in the *ISTD1 Amount - ISTD10 Amount* columns, only *ISTD1 Amount* column is displayed by default). Enter the parameters in units used in the calibration file (*Units - Compound* parameter in the [Calibration Options](#) dialog). The implicit value is 0. If

the same amount of the internal standard is used in all used calibration standards and unknown samples, this amount need not be entered and can be left at 0 in both calibration and chromatograms (sequence).

Caution: When the amount of the internal standard is entered either in the calibration file (**Amount** column) only or in the unknown sample (*ISTD Amount* parameter) only and zero will be left in the other place, the **Result Table** will not display any results and the header will show an inscription stating the cause of the problem. The compound will be also omitted from the **Summary Table**.

The screenshot shows the 'Result Table' on the left and the 'Calculation' settings on the right. The 'Result Table' has the following data:

Reten. Time [min]	Response	Amount [g/kg]	Amount % [%]	Peak Type	Compound Name
1	1,187	0,768			
2	1,752	0,612			
3	2,302	33,096		Ordnr (b) ETHANOL	
4	2,552	1,623			
5	2,857	44,570		ISTD1 T-BUTANOL	
Total					

The 'Calculation' settings on the right include:

- Calibration File (Peak Table): Ethanol
- Calculation: ISTD (circled in red)
- Report in Result Table: All Peaks (selected)
- Response Base: Area (selected)
- Response Factor: 0
- Amount [g/kg]: 4
- ISTD Amount [g/kg]: 0 (circled in red)
- Inj. Volume [µL]: 2
- Dilution: 1

Fig. 179: Chromatogram - Calculation - ISTD settings

Inj. Volume

Specifies the size of the injection. The response of all substances calculated using the calibrated calculation is corrected by the ratio of this value to the value of *Default Injected Volume* field set in the [Calibration Options](#) dialog. *Inj. Volume* parameter will influence the calculation only after the *Default Injected Volume* value is set. The implicit value is 0.

Note: The *Inj. Volume* parameter can be applied for injected amount correction while using autosamplers unable to determine precisely the quantity to be injected, but fully capable to determine (ex-post) the quantity which has been injected.

Dilution

Specifies the dilution of the sample. It is the total number of unit volumes in which the sample was dissolved. In other words, dilution represents the total volume of solute + solvent. Each calibrated amount in the **Amount** column of the **Result Table** is multiplied by this value. The implicit value is 1.

User Variables

Display and enable to edit Name and Value of *User Variables* used in *User Columns* calculations performed in Result Table.

Analysis Variables

Specifies up to three *Analysis User Variables*. *Analysis User Variables* are editable through [Single Analysis dialog](#), [Sequence window](#) or directly in [Chromatogram window](#) at **Results tab** and **All Signals Results tab**.

Method Variables

Specifies up to three *Method User Variables*. *Method User Variables* are editable through [Method Setup dialog](#) at **Advanced tab** or directly in [Chromatogram window](#) at **Results tab** and **All Signals Results tab**.

3.5.2 Integration

Invoking this command switches the results panel of the [Chromatogram](#) window to the *Integration* tab, which contains the selector of the integration algorithm and the **Integration Table**. When using a multi-detector chromatogram, the selection of the integration algorithm is common for all signals in the chromatogram but the **Integration Table** is always displayed for the active signal (the color of the table header corresponds to the color of the signal and signal name is contained within). The displayed operations and values are primarily taken from the *Integration* tab of the template method (i.e., the method according to which the chromatogram has been measured). Integration adjustments are added based on operations performed in the [Chromatogram](#) window (details on these parameters and options can be found in the [Chromatogram](#) submenu).

Integration Algorithm

Selects the integration algorithm for integration of displayed chromatogram. Selected integration algorithm is common to all signals.

Currently **Clarity** offers two different integration algorithm lines - *Wave* and *Legacy*. Both lines differ in the approach to the automated integration and both have their strong sides and drawbacks. Some functions of the integration algorithm may be only present in particular versions of integration algorithm. The default integration algorithm for newly created methods is *Legacy*, the algorithm in newly measured chromatograms is based on algorithm selected in the template method.

Note: In case the selected integration algorithm fails to solve the integration of your chromatograms, we suggest to try the other one to see whether the situation will be better.

In case the chromatogram is opened with the stored method (historical version of the method) and the integration algorithm used by **Reference Guide** changed after it's creation, the *Integration Algorithm* dropdown will contain three integration algorithm versions - newest *Legacy* version, newest *Wave* version and the historical algorithm used in the chromatogram (be it *Legacy* or *Wave*, selected). To distinguish the historical version from the latest in the given line, the descriptions will contain the revision used for both. Upon editing the chromatogram, the algorithm will change to the latest version of the given line and will not be able to be changed back.

Integration table

The integration table records all operations performed on the baseline and peaks. The header of the table contains information on the chromatogram, particular signal and integration algorithm version used. The information is printed along with the integration table when the table is selected for printing.

Chromatogram Operation

Selects the operations to be performed on the chromatogram. Clicking the right border of the field displays a list of all possible operations (identical to the list of

commands from the *Chromatogram - Baseline, Peak, Integration, Separation* and other sub-menus in the [Chromatogram](#) window).

Chromatogram Operation	Time A [min]	Time B [min]	Value
Global Peak Width			0.054 min
Global Threshold			1.1685 mV
Global Filter - Bunching			3
Global Baseline Slope			0.000 mV/min
Integration Interval	5.000	23.000	
Filter - Savitzky-Selay	10.250	14.500	20
Baseline - Allow Crossing	17.700	21.700	To First Cross
Peak - End	19.642	1.050	

Fig. 180: Chromatogram - Integration

Time A

- Indicates the starting time of the operation (for interval commands).
- Indicates the peak retention time (for commands that modify the peak start, peak end, etc.).

Time B

- Indicates the final time of the operation (for interval commands).
- Indicates the position of a new start, end, etc. relative to the peak apex (for commands that modify the start, end, etc.).

Note: Zero entered in the *Time B* for interval operations will set the end of the interval to the end of the chromatogram.

Note: Indicating the relative position (i.e. time) is more suitable than indicating a mere absolute value, since in using the **Integration Table** the peak with the most similar retention time is then found and the peak start/end is shifted to the point calculated from the relative shift on the actual retention time. This substantially diminishes the differences in actual retention time of the same peak in different chromatograms.

Value

Value (if relevant for the operation) with appropriate units.

Description of fields of integration table

Global Peak Width / Local Peak Width [min]

This parameter defines the smallest peak width, which is to be detected. The value range is between 0,001 and 10 minutes.

The value is not critical, so even narrower peaks than the entered value will be detected, but if set incorrectly, the beginning and end of a peak may be inaccurately determined and the baseline could be incorrectly inset.

The *Global Peak Width* parameter is always displayed in the first row of the integration table and is applied to the whole chromatogram.

It is possible to set a different peak width for individual sections by adding the *Local Peak Width* parameters into further rows of the integration table which then override the *Global Peak Width* settings in the given area of chromatogram.

Global Threshold / Local Threshold [mV]

Determines the sensitivity the integration algorithm has to noise. The height of all peaks (measured from the baseline to the top) that should be detected has to be at least double this parameter. The value range must be $1 \mu V - 10 V$.

The *Global Threshold* parameter is always displayed in the second row of the integration table and is applied to the whole chromatogram.

It is possible to set a different noise threshold for individual sections by adding the *Local Threshold* parameters into further rows of the integration table which then override the *Global Threshold* parameter in the given area of the chromatogram.

Global Filter - Bunching

Sets the averaging of data points for the signal displayed (and calculated with) in the chromatogram. *Global Filter - Bunching* serves as a filter and reduces the high frequency noise. The value must be between 1 (no averaging performed) and 250 (for each 250 data points measured, only 1 is displayed). Applying higher *Global Bunching* values will significantly change the signal course.

Global Filter - Bunching parameter is always displayed in the third row of the integration table and is applied to the whole chromatogram.

Global Baseline Slope / Local Baseline Slope

Determines the position of the peak starts and peak ends on peak sides. The value must be between 0 and infinity, the higher the value the higher on the peak slope the starts and ends will be. If the value is set to 0, default peak start and peak end position is used (the value is considered to be $8 * \text{Global Threshold}$). The slope on peak ends is considered as a negative value of the value entered, target slopes for negative peaks are using negative value for starts and positive one for peak ends.

Global Baseline Slope parameter is always displayed in the fourth row of the integration table and is applied to the whole chromatogram. It is only present for *Wave* algorithm.

It is possible to set a different slope for peak starts/ends for individual sections by adding the *Local Baseline Slope* parameters into further rows of the integration table which then override the *Global baseline Slope* parameter in the given area of the chromatogram.

Integration Interval

Limits the time period over which the chromatogram will be integrated. This means that the chromatogram profile will be ignored beyond the set time interval. This is the main difference compared to *Lock* command, which cancels already integrated peaks only in defined sections and does not reintegrate the whole chromatogram. If the parameter is not defined, integration is done on the whole chromatogram.

Detect Negative

Enables the detection of negative peaks. If this function has not been enabled, all negative peaks are considered to be correct course of the baseline (in a similar way

as removing the peak with the use of *Reject Negative* function).

Min. Area [mV.s]

This parameter sets the minimum peak area in mV.s. Peaks whose area is smaller than the specified value are not displayed.

Min. Height [mV]

This parameter gives the minimum peak height in mV. Peaks whose height is smaller than the specified value are not displayed.

Half Width [min]

This parameter gives the minimum peak half-width in minutes. Peaks whose *W05* is smaller or equal to the specified value are not integrated.

ValleyToValley Slope

Specifies the maximum slope of the baseline. If the baseline slope is smaller than the specified value, the separating perpendicular line is canceled and the baseline passes through the valley. The default value of 0 prevents the baseline from passing through the valley.

Tangent Area Ratio

Constitutes the first condition imposed on tangential separation. The condition is satisfied if the ratio of areas of the separated and the main peak exceeds the specified value.

The value of 0 prevents tangential separation. If this operation is selected in the **Integration table**, its value is set to value of 10 and in general increasing value causes higher degree of tangential separation of the raider peaks. If there is no *Tangent Slope Ratio* item defined in the **Integration table** but *Tangent Area Ratio* is defined, the value of the *Tangent Slope Ratio* is considered to be 10.

Tangent Slope Ratio

This is the second condition imposed on tangential separation. The condition is satisfied if the ratio of slopes of the second and the first peak exceeds the specified value. The slope ratio is defined as the tangent to the first peak at its end point divided into the slope of the line connecting the beginning and end of the second peak.

Value of 0 prevents tangential separation. If this operation is selected in the **Integration table**, its value is set to value of 10 and in general increasing value causes lower degree of tangential separation of the raider peaks. If there is no *Tangent Area Ratio* item defined in the **Integration table** but *Tangent Slope Ratio* is defined, but the value of the *Tangent Area Ratio* is considered to be 10.

Filter

Commands from *Chromatogram - Integration* menu:

FFT, Savitzky-Golay, Spike, Moving Average. A detailed description of these functions is provided in the chapter "**Integration**" on pg. 252.

Baseline

Commands from *Chromatogram - Baseline* menu:

Lock, Valley, Together, Forward Horizontal, Backward Horizontal, Front tangent, Tail tangent, Clamp Negative, Cut Negative, Reject Negative, Allow Crossing,

Spike Removal. A detailed description of these functions is provided in the chapter "**Baseline**" on pg. 221.

Peak

Commands from *Chromatogram - Peak* menu:

Start, End, Both, Add Positive, Add Negative, Force Peak Name, Solvent Peak. A detailed description of these functions is provided in the chapter "**Peak**" on pg. 237.

Group

Adds (*Add group*) and removes (*Delete group*) a group of peaks. A detailed description of these functions is provided in the chapter "**Peak**" on pg. 250.

Evaluation

Commands from *Chromatogram - Noise & Drift* menu:

Noise, Drift, ASTM Noise, 6-Sigma Noise. A detailed description of these functions is provided in the chapter "**Noise & Drift**" on pg. 264.

Sequence of evaluation

The evaluation process does not proceed exactly in the same order as the parameters in the integration table are shown. The process is:

- Primarily initiated with the *Global (Local) Peak Width, Global (Local) Threshold, Integration Interval* and *Detect Negative* parameters.
- Secondly the *ValleyToValley Slope* parameter will be applied. After all groups of non-resolved peaks have been tested by this parameter the remaining two parameters *Tangent Area Ratio* and *Tangent Slope Ratio* are applied to all remaining non-resolved groups. Tangential separation is used whenever the relevant criteria are met.
- Only then is the **Integration Table** used, followed by the *Rejections* parameters.

It thus follows that the separation parameters are not applied (e.g. to manually added peaks) and can be suppressed by the *Together* and *Valley* commands included in the **Integration table**.

Paste (CTRL+V) into the Integration Table

Inserting into the **Integration Table** using the *Paste* command or using the keyboard shortcut *CTRL+V* is possible with some limitations - it is only possible to copy non-global lines of the **Integration Table** as a whole. It is not possible to paste global lines, overwrite only particular lines or just selected values. When the *Paste* operation is invoked for the **Integration Table**, **Clarity** evaluates the content of the clipboard on correctness. Incorrect clipboard content is announced by an error message and *Paste* operation fails, while on correct evaluation the focus in the **Integration Table** is moved to the empty edit line and the rows from the clipboard are added to the end of the **Integration Table**.

Note: Typical fails in evaluation of the correctness of the **Integration Table** may be too few columns in the clipboard, global operations in the clipboard or units inside of the value cells of some rows while copying from text file or Excel.

You may consider using one of the alternative approaches of copying the **Integration Table**, as described in the section **Method on pg. 276** - more specifically the *Set Model*, *Copy from Model* and *Copy from Chromatogram* commands.

3.5.3 Measurement

Displays the conditions under which the chromatogram was measured. Once selected, the *Measurement Conditions* tab will be displayed in the lower part of the [Chromatogram](#) window, containing [Instrument](#), [Event Table](#) and possible [Detector](#) sub-tabs; when using a chromatogram that has been measured on an instrument with directly controlled chromatograph, autosampler or any other device having its own tab in the [Method Setup](#) dialog, the *Sampler*, *GC*, *LC Gradient*, *LC* or other sub-tabs are also present. The displayed values are taken from the relevant tabs of the template method describing the way how the chromatogram was measured.

Instrument

This sub-tab is common to all signals in given chromatogram.

The following fields in the **Measurement Conditions** section are designated for the information purposes only and can be filled in or left blank according to your choice.

Description - brief description of method.

Column - description of the column used.

Mobile Phase - description of mobile phase.

Flow Rate - description of flow rate.

Pressure - description of pressure.

Detection - detection method.

Temperature - description of temperature.

Note - any comment primarily connecting to the method.

Common for All Signals		Sample Identification		Chromatogram	
Measurement Conditions		Sample ID	0542	Comments	
Description	Fluorescence Detector PAH1_NDP-PC1A	Sample	DEMO Example - PAH	<input type="text"/>	
Column	Supelcosil LC_PAH, 25cm x 4.6mm, 5µ	Acquired	31.01.2024 11:08	<input type="button" value="Edit..."/>	
Mobile Phase	GRAD ACN/w(2min-50/50, 3min-50/50, 30)	Analyst	DataApex	Audit Trail	
Flow Rate	1.0 ml/min	Acquisition Parameters		No Acquisition Messages	
Pressure	1300 psi at start	AutoStop	50 min, enabled	Range	1250 mV, unipolar
Detection	Fluorescence, prog.	Ext. Start	Down	Sample Rate	2 samples/sec
Temperature	25 degree centigrade	Acquisition Method	N/A	<input type="button" value="Show..."/>	
Note	time Ex Em 00.00 220 324 (RAP) 17.00 270 324 (ANA-FLU)	Processing Method	N/A	GLP Mode	
		Subtraction		Off	
		Chromatogram	<input type="text"/> <input type="button" value="Set..."/> <input type="button" value="None"/>		
		Matching	No Change		
Instrument Event Table GLP info DEMO - 1					
Results All Signals Results Summary Performance Integration Measurement Conditions SST Results					

Fig. 181: Chromatogram - Measurement Conditions

Sample Identification

Fields from the header of the analysis - [Single Analysis](#) dialog or the relevant row of the **Sequence Table** in the [Sequence](#) window.

Sample ID

Sample identifier. This corresponds to the *Sample ID* field from the [Single Analysis](#) dialog or the *Sample ID* column from the [Sequence](#) window.

Sample

Description of the sample. This corresponds to the *Sample* field from the [Single Analysis](#) dialog or the *Sample* column from the [Sequence](#) window.

Acquired

Date and time of the end of the measurement. If the date is not accessible (e.g. in some imports), N/A will be displayed.

Analyst

Name of the user who measured the analysis.

Acquisition Parameters

Parameters of measurement common for all signals. The remaining parameters can be found on the [Method Setup - Measurement](#) tab.

AutoStop

Notifies whether the *Enable Autostop* checkbox was used and what was the *Run Time* value set.

Ext. Start

Notifies whether and by what method the external control of the measurement was defined. This corresponds to the *External Start/Stop* section of the *Method Setup - Measurement* tab (see chapter 2.5.2 on page 59 for more details).

Acq. Method

Name of the template method used for measurement.

Range

Specifies the range of the detector signal used. If more than one detector was used to gather data with different *Ranges* set (including signal units), the *<varies>* inscription will be displayed here.

Sampling Rate

Specifies the sampling rate of the detector used. If more than one detector was used to gather data with different *Sampling Rate* set, the *<varies>* inscription will be displayed here.

Processing Parameters

Parameters of processing method for all signals.

Processing Method

Name, version and date of the method used for processing.

Subtraction 

Sets the automatic subtraction of selected chromatogram. Subtraction of the chromatogram (e.g. solvent) is indicated by the note *Mathematically reprocessed* in the printed report. The use of automatic subtraction is also logged into the chromatogram audit trail.

There are two places in **Clarity** where the subtraction chromatogram can be set - [Method Setup - Advanced](#) dialog accessible from the [Instrument](#) window and *Measurement Conditions - Instrument* tab of the [Chromatogram](#) window.

If you wish to automatically subtract a chromatogram from the newly measured chromatograms, specify it in the template method in the [Method Setup - Advanced](#) dialog.

If you wish to subtract a chromatogram from an already measured chromatogram, specify which on the *Chromatogram - Measurement Conditions* tab (described further in this chapter).

The subtracted chromatogram is saved into the measured chromatogram, it is not simply linked to it. The changes occurring with the subtraction chromatogram thus do not influence the measured chromatogram from which the background is subtracted. The subtraction, however, does not hold its history - only last subtracted chromatogram's data is saved when it is changed, all older subtraction chromatograms are discarded.

Chromatogram

Field specifying the file with subtraction chromatogram.

Set...

Displays the [Open Chromatogram](#) dialog used for selecting the subtracted chromatogram.

None

Cancels subtraction of chromatogram.

Note: If you only wish to display the chromatogram on the background of the acquisition window without automatic subtraction, use the *File - Set Background Chromatogram...* command in the [Data Acquisition](#) window.

Matching

Selects the subtraction method.

No change - The chromatogram is subtracted from the measured chromatogram without any additional adjustments.

Offset Subtraction Chromatogram - Before subtraction, the **Clarity** station attempts to "move" the measured chromatogram with the subtracted chromatogram by shifting along the time axis.

Scale Subtraction Chromatogram - Before subtraction, the **Clarity** station attempts to "align" the measured chromatogram with the subtracted chromatogram by interlining it or shortening the time.

Note: Alignment of chromatograms is achieved using the biggest peaks in the subtraction chromatogram, i.e. either to the highest peak or to the peak with the largest area.

Chromatogram

Section that contains the additional information on the sample or chromatogram.

Edit...

This button serves for adding some information about the chromatogram or additional info on the sample in the [Comments](#) dialog. The button also allows to modify the comment entered prior to the analysis from the [Single Analysis](#) or [Sequence](#) dialog. This field can then be added to the report setup on the [Report Setup - Results](#) tab described on pg. 449.

Audit Trail 

Using the *Show* button allows to display the [Chromatogram Audit Trail](#) dialog containing the log of events happening with the given chromatogram.

Event Table

This tab shows the setting of the **Event Table** defined in the method on the [Method Setup - Event Table](#) tab. It is common for all signals in case of the multi-detector chromatogram. More information on the **Event Table** is in the chapter "**Event Table**" on pg. 85.

GLP Info 

This tab shows the list of control modules (hardware) configured on the instrument and used for the acquisition of the chromatogram, along with the serial numbers of this hardware. The contents of this tab may be added to the printed reports by checking the *GLP Info* checkbox on the [Report Setup - Method](#) tab.

Detector

The tab displaying detailed measurement parameters. In the case of a multi-detector chromatogram there is a tab for every detector in the configuration of the Instrument.

Sampler 

Tab displaying the injection method of the autosampler.

GC/LC/LC Gradient 

Tab displaying instrument method of gas or liquid chromatograph.

3.6 Results

This section contains commands for displaying the result tables.

Result Table	Switches to the Result Table on the Results tab of the Chromatogram window.
All Signals Result Table	Switches to the All Signals Result Table on the All Signals Results tab of the Chromatogram window.
Summary Table	Switches to the Summary Table of all displayed chromatograms on the Summary tab.
Performance Table <small>✓ full version</small>	Switches to the Performance Table characterizing the chromatographic system quality on the Performance tab of the Chromatogram window.
Compound Unique on One Signal	Switches the All Signals Result Table to count only compounds that are present only once among all the signals. See All Signals Results tab for more details.
Summary Options...	Opens the Summary Table Options dialog which sets the layout options for the Summary Table .

All tables are very flexible; the order of particular items and the visibility and size of columns can be adapted and customized, columns appended, fonts defined separately for each column and the number of digits displayed specified for selected columns.

Tables can be modified by commands from the local menu accessible by right clicking the mouse over the table.

3.6.1 Local Table Menu

Local menus contain frequently used commands relevant for the given table. Local menus can thus vary, according to the table you are currently editing. In the following overview commands common for most tables are described:

Select All

Selects all cells in the table. Also available by using the **Ctrl** + **A** shortcut.

Copy

Copies selected cells to the clipboard. Also available by using the **Ctrl** + **C** shortcut.

Paste

Pastes the content of the clipboard into the selected cells of the table. Also available by using the **Ctrl** + **V** shortcut.

Restore Default Columns

Restores the default columns and fonts for a given table. A detailed description of this function is in the chapter "**Edit**" on pg. 191.

Setup Columns...

Invoking the *Setup Columns...* command opens the [Setup Columns](#) dialog, where it is possible to change the appearance and order of table columns. Detailed description of this dialog can be found in the chapter "**Setup Columns**" on pg. 198.

Note: To access the setting of user columns the user must be authorized to edit methods. See the *Edit Method* checkbox in the [User Accounts](#) dialog.

User Columns

Submenu of commands enabling to handle user columns in the full version. The available commands are:

Add...

Use this command to add a customized user column to the table. Invoking this command will open the [Add User Column](#) dialog, whose detailed description can be found in the chapter "**Add User Column**" on pg. 193.

Edit Selected...

Invoking this command will open the *Edit User Column* dialog for the active user column. It is used for modifying of the content of the user columns.

Delete Selected

Invoking this command deletes the active user column or columns.

Delete All

Deletes all previously added user columns. A detailed description is in the chapter "**Edit**" on pg. 190.

Hide Column(s)

Hides the selected columns.

Show Hidden Column(s)

Shows all hidden columns.

3.6.2 Result Table

Invoking this command switches the lower part of the [Chromatogram](#) window to the *Results* tab, displaying the *Result Table* in the left half and the *Common for All Signals* section in the right half (dedicated to [Calculation](#)). When working with a multi-signal chromatogram, the *Result Table* contains only the active signal results.

Note: By default, the *Highlight Selected Peaks in Graph* option in [Graph Properties](#) dialog is selected. This causes that the peak(s) corresponding to the active row(s) in *Result Table* will be colored/highlighted in the *Main Graph*.

The screenshot shows the 'Results' tab of a chromatogram software. On the left is the 'Result Table (ESTD - Data(Wine_Sample - UV detector))' with the following data:

Reten. Time [min]	Response	Amount [g/l]	Amount [%]	Peak Type	Compound Name
1	1.063	54.322	0.026	Ordnr	oxalic
2	1.703	3830.782	0.248	Ordnr	citric
3	1.917	8460.283	0.438	Ordnr	tartaric
4	2.800	3333.242	1.147	Ordnr	malic
8	4.660	2732.362	0.243	Ordnr	succinic
9	5.050	2969.660	0.744	Ordnr	lactic
11	6.847	2304.278	0.185	Ordnr	acetic
Total			3.031	100.0	

On the right is the 'Common for All Signals' panel, which includes a 'Calibration File (Peak Table)' dropdown set to 'Wine', a 'Calculation' dropdown set to 'ESTD', and various options for reporting and scaling results. The 'Report in Result Table' section has 'All Peaks in Calibration' selected. The 'Scale' section has 'Use Scale Factor' checked, with a 'Scale Factor' of 1 and 'Units' set to 'ul'. The 'Unidentified peaks' section has 'Response Base' set to 'Area' and 'Response Factor' set to 0. The 'Units' section has 'Inj. Volume [µL]' set to 100 and 'Dilution' set to 1. The 'User Variables' section is checked.

Fig. 182: Chromatogram - Results tab - Result Table

The *Result Table* consists of the **Heading**, **Header Row**, **Header Column**, and **columns**, which may be predefined or user-defined. The appearance of the *Result Table* of chromatogram with linked calibration differs from the one without it. For chromatograms without calibration, some of the **columns** are unavailable.

Note: The user columns defined in the *Result Table* and in the *Summary Table* are independent.

Columns in the *Result Table* are sorted by *Reten. Time* by default. Double click a column header to change the column for ordering. Displayed results from the *Result Table* are printed in the exact order as seen on the screen (WYSIWYG). Changing the signal or opening a new chromatogram does not reset the order to the default (*Reten. Time*) - this must be done manually.

Note: After modifying primary data (Scale or Move operations) the *Result Table* will disappear as the results are no longer valid.

3.6.2.1 General items

Units in the Result Table

Basic units are set in the [Units Setups](#) dialog and may influence calculations performed with those columns. The y-axis units generally depend on the detector used. Units for user columns can be set via the [Add User Column](#) dialog. The units for the *Amount* column correspond with the units set by the *Compound Units*

parameter of the [Calibration Options](#) dialog. Units are present in the headers of corresponding columns in the *Result Table*.


Heading

Shows the calibration calculation type, name of the active chromatogram, and in the case of multi-detector chromatograms, name of its active signal. [Error messages](#) may appear below the heading providing a description of the cause of the problem (e.g., if it is not possible to use the selected type of calculation).

The heading is always in the color of the active chromatogram (signal) whereas the error is in red. If there are multiple errors, they will be displayed in a list ①.

Header Row

Shows the names of columns. A whole column can be selected by clicking the header cell. By double-clicking the header cell, the table is ordered in an ascending order according to the values in the clicked column. Repeated double-clicking rearranges the table in a descending order.

Each column can be moved by clicking on the selected column header cell and dragging the cursor to the desired position. Columns can be widened or narrowed by pressing the left mouse button above the right edge (when the cursor changes to ) and dragging right or left. By double-clicking above the right edge, the smallest possible width of the column is set, so that the data and column header are entirely visible.

Header Column

Shows the number of a particular peak and the indication of which group the peak belongs to (if applicable) ②. When using the *All peaks in Calibration* option for the *Report in Result Table* selection, the compounds present in the calibration but not found in the active chromatogram are indicated with a red number taken from the calibration beginning with the letter **C** ③.

① Result Table (Uncal - Data(Wine_Sample - UV detector))
!!! No ISTD peak detected !!!
!!! Calibration curve could not be constructed for multiple compounds !!!

	Reten. Time [min]	Response	Amount [g/l]	Amount% [%]	Peak Type	Compound Name
1	1.063	54.322			Error	oxalic
2	1.703	3830.782			Error	citric
3	1.917	8460.283			Error	tartaric
4	2.800	3333.242			Error (Curve Check) - Ordnr	malic
5	3.073	624.116				glycerol
6A	3.957	211.561				
7A	4.350	302.765				
8	4.660	2732.362			Error (Curve Check) - Ordnr	succinic
9	5.050	2969.660			Error (Curve Check) - Ordnr	lactic
10	5.483	3042.300				
11	6.847	2304.278			Error (Curve Check) - Ordnr	acetic
	Group_A	514.326				
	Total					

④ Result Table (ISTD - Data(Wine_Sample - UV detector))

	Reten. Time [min]	Response	Amount [g/l]	Amount% [%]	Peak Type	Compound Name
1	1.063	54.322	ISTD	ISTD	ISTD 1	oxalic
2	1.703	3830.782	0.239	6.9	Refer (by ISTD 1)	citric
3	1.917	8460.283	1.262	36.3	Ordnr (by ISTD 1) (CF = 3.0000)	tartaric
Cd	2.553					glucose
4	2.800	3333.242	0.990	28.5	< LOD Ordnr (by ISTD 1)	malic
5	3.073	624.116	0.683	19.7	Ordnr (by ISTD 1) (Forced)	glycerol
8	4.660	2732.362	0.253	7.3	Ordnr (by ISTD 1)	succinic
9	5.050	2969.660	0.000	0.0	Ordnr (by ISTD 1) Free	lactic
	Group_A	514.326	0.047	1.3	Grp_A	Group A
	Total		3.474	100.0		

Fig. 183: Chromatogram - Results tab - Result Table details

3.6.2.2 Columns

Reten. Time [min] ④

Retention time of peaks in minutes. The peaks in the table are sorted according to their retention time by default.

Response ⑤

Area or height of peaks as selected in the calibrated calculation. Hidden by default if no calibration file is selected. The used response type can be viewed in the *Response Base (RB)* column (hidden by default).

Amount [set units] ⑥

Shows the calculated amounts of compounds in the units set in calibration via the *Compound Units* parameter of the [Calibration Options](#) dialog. These units may be overridden by units entered due to scaling in the *Units* field of the *Scale* section of the [Method Setup - Calculation](#) dialog or on the *Chromatogram - Results* tab. See [Appendix 1](#) below for details on calculations. This column is hidden by default if no calibration file is selected.

Amount% [%] ⑦

Shows the percentage amounts of compounds. The total amount is given by the sum of the calculated amounts of compounds in calibration, or by the *Amount* parameter in the *Common for All Signals* pane, if this is other than zero. See [Appendix 2](#) below for more detailson calculations. This column is hidden by default if no calibration file is selected.

Peak Type ⑧

Shows the type of the identified compound according to the calibration settings. Hidden by default if no calibration file is selected. The type may be a combination of

many different items from the following table:

Tab. 16: List of possible peak types

Peak Type	Description
<i>Ordnr</i>	Peak which is neither a reference peak nor internal standard.
<i>Refer</i>	Reference peak.
<i>ISTD1...10</i>	Peak of an internal standard labeled by the internal standard number.
<i>(by XXX)</i>	Indication that the responses of the peak were calculated using the stated ISTD peak (in ISTD calculations) and/or by the response of a different peak (set via the <i>Calculate By</i> function in the Calibration window). Shown in parentheses after the peak type definition (only if the identification or calculation was not performed in the ordinary way).
<i>(Forced)</i>	If the peak was identified using the <i>Force Peak Name</i> function from the Chromatogram window, the <i>Forced</i> label is shown in the parentheses.
<i>Grp</i>	Indication of a calibrated group.
<i>Named Grp</i>	Indication of a named group, if set in the Calibration window.
<i>(CF = X)</i>	Indication that the peak uses Correction Factor different than 1.
<i>Free</i>	Freely calibrated compound (Free Calibration). The coefficients set in the Calibration window (mainly <i>Manual Response Factor</i>) are used for the calibration calculation instead of the calibration curve.
	Empty cell is an indication that no calculation has been performed for the given compound.
<i>< LOD or < LOQ</i>	The amount is less than limit of detection (LOD) or quantification (LOQ). These limits can be set in the <i>LOD</i> and <i>LOQ</i> columns in the the Calibration .
<i>Error</i>	Indication that calculation for this row could not be performed. This is often caused by the <i>Amount</i> in the calibration being set to 0 or because a part of the calibration curve would result in wrong evaluation (e.g., negative <i>Amount</i> value). Failed result of linearity check (as defined by the <i>Curve Check</i> item in the Calibration Options dialog) is indicated by an <i>Error (Curve Check)</i> (successful checks are not shown). Further description of some of the errors is displayed in the header of the <i>Result table</i> ① .

Area [detector units.s]

Peak area in the detector units × seconds. Hidden by default if calibration is used. Peak Area is determined as a sum of trapezoid areas defined by vertical lines from the individual data points to the baseline drawn between peak start and peak end.

Height [detector units]

Height of a particular peak in detector units. Hidden by default if calibration is used. Peak Height is determined on vertical line from peak apex to the baseline drawn between peak start and peak end.

Area [%], Height [%]

Percentage representation of peak area or height. Hidden by default if calibration is used.

$$Area\%_i = \frac{A_i}{\sum_i A_i} \cdot 100 \quad Height\%_i = \frac{H_i}{\sum_i H_i} \cdot 100$$

W05 [min]

Shows the width of the peak in half of its height. Hidden by default if calibration is used.

Compound Name 

Displays the name of the compound from the calibration file corresponding to the relevant peak based on identification by retention times. If a certain peak is not identified, the *Peak Type* and *Compound Name* columns for that peak are empty, and the *Amount* field value is zero (unless the *Response Factor* parameter in the *Unidentified peaks* section is not equal to zero).

Start Time/End Time [min]

Retention time of particular Peak Start/Peak End. Hidden by default.

Apex Value [detector units]

Shows the y-axis value of the apex of a peak. Hidden by default.

Start Value/End Value [detector units]

Height of the baseline in the Peak Start/Peak End. Hidden by default.

Start Value (Signal)/End Value (Signal) [detector units]

Height of the signal in the Peak Start/Peak End. Hidden by default.

RB

Denotes the response base of the particular peak when calibration is used (*A* stands for area, *H* for height). Unidentified peaks use the response base according to the *Response Base* parameter set in the *Unidentified Peaks* section. Hidden by default.

Reten. Index [-]

Shows the Retention Index (Kovats Index) for the given peak. The calculation of the Retention Index is performed according to the value set in [Calibration](#) in the *Reten. Index* column and the selection of the *Retention Indexes use Log. Interpolation with Unretained Peak* checkbox in the [Calibration Options](#) dialog. The column is hidden by default and it is available only in the *Result Table* for chromatograms with calibration.

Note: The equations used for the calculation of Kovats Indexes are described in the chapter "**Calibration Options**" on pg. 360.

Centroid [min], Variance [min²], Skew [-], Excess [-], Asymmetry [-], Capacity [-], Efficiency [th.pl], Eff/I [t.p./m], Resolution [-], Symmetry/Tailing [-]

These columns belong to functions used in the **Performance Table** on the [Chromatogram - Performance](#) tab. Hidden by default. When displayed in the *Result Table*, the calculation of **Efficiency** and **Eff/I** columns is performed according to the *Column Calculation* selector on the [Performance](#) tab, while the remaining columns are calculated according to the mode under which they appear in the *Performance Table* regardless of the *Column Calculation* selector state. More information can be found in the chapter "**Performance Table**" on pg. 310.

Calculate By

Displays the compound according to which the given peak was calculated. The *Calculate By* option is set in the [Calibration](#) window. Hidden by default.

Response Factor ✓ Full version

This column displays the ratio of **Response** and **Amount**.

$$\text{Response Factor} = \text{Amount} / \text{Response}$$

It is possible to calculate response factor in the inverse form ($RF_{inv} = \text{Response} / \text{Amount}$) by checking the *Response Factor as Response / Amount* checkbox in [Calibration Options](#). Hidden by default.

Correction Factor

Displays the value of the *Correction Factor* as set for the peak in the [Calibration](#) window. Hidden by default.

3.6.2.3 Special rows

Group-X row

This row is visible only in the case that peak groups are used; one for each group. It shows the sum of values of individual peaks belonging to the group in the given column (only for columns when such total makes sense). Setting *Peak Color for Groups* in the [Calibration](#) highlights respective peaks in the chromatogram as well as their background color in the *Result Table* header row cell.

Total

This row shows the total value of a given column (only for columns when such total makes sense). For example, *Total* is not calculated for the *Response* column (the data may have different *Bases*). If a non-zero *Amount* value is given in the *Common for All Signals* section of the window, the *Total* of the *Amount* column is replaced by this value. Values for ISTD peaks are not included in the *Total* values (this applies on the *Area*, *Height*, and *Amount* columns).

Named Group-X row

This row is visible only in the case that named groups are used; one for each group. Named group values appear in the row (rows) below the *Total* row and are not included in the *Total* itself. The sum of amounts of individual peaks belonging to the named group are stated. Setting *Peak Color for Named Groups* in the [Calibration](#) highlights background color in the *Result Table* header row cell but not in the

chromatogram itself, as each peak may belong to more than one *Named Group* unlike for standard groups.

Color, if set in the calibration, will be displayed in the header row cell.

3.6.2.4 Appendix 1

The calculation is determined by the type of calibration:

Tab. 17: Calculation formulas

Calculation	Formula
ESTD, NORM	$Amount_i = CF_i [R_i] \cdot ScaleFactor$
ISTD	<p>If the calibration does not have ISTD amount filled on any level, this equation is used. Same amount of the internal standard is considered to be present both in samples and in calibration standards, ISTD Amount values everywhere in Clarity are set to 0.</p> $Amount_i = CF_i \left[\frac{R_i}{R_{ISTD}} \right] \cdot ScaleFactor$
ISTD	<p>If the calibration contains ISTD Amount filled on at least one calibration level, following equation is used. ISTD Amounts then must be filled in everywhere in Clarity, both in unknown samples and in the calibration file, and these amounts may differ.</p> $Amount_i = RCF_i \left[\frac{R_i}{R_{ISTD}} \right] \cdot Amount_{ISTD} \cdot ScaleFactor$

where:

Tab. 18: Explanation of used symbols

Symbol	Description
$Amount_i$	Amount of component "i" in sample.
R_i	Response of the "i" component (height or peak area).
R_{ISTD}	Response of internal standard (height or peak area).
$CF_i [R_i]$	Amount of "i" th component read out from corresponding calibration curve.
$CF_i \left[\frac{R_i}{R_{ISTD}} \right]$	Amount of "i" th component read out from corresponding calibration curve displaying dependence of response ratio (R_i/R_{ISTD}) of calibration standard on "i" th component amount in that calibration standard for given substance.

Symbol	Description
$RCF_i \left[\frac{R_i}{R_{ISTD}} \right]$	Value read out from corresponding relative calibration curve, displaying dependence of response ratio (R_i/R_{ISTD}) of calibration standard on "i"th component amount ratio ($Amount_i/Amount_{ISTD}$) in that calibration standard for given substance.
$Amount_{ISTD}$	Amount of internal standard added to unknown sample. This value must be entered into both the ISTD Amount field in the chromatogram heading and the Amount column of the calibration, or to none of these places in case all ISTD Amount values are the same (optional, the calculation works the same if the same amounts are included on both places).
$ScaleFactor$	Multiplication factor.

In the case that the corresponding peak is not found in the calibration file, the *Uncal. Response* parameter from the [Method Setup - Calculation](#) dialog is used for the calculation instead of deriving the value from the calibration curve, according to the formulas:

Tab. 19: Calculation formulas for non-calibrated peaks

Calculation	Formula
ESTD	$CF_1[R_i] = Uncal. response \cdot R_i$
ISTD	$RCF_i \left[\frac{R_i}{R_{ISTD}} \right] = Uncal. response \cdot \frac{R_i}{R_{ISTD}}$
NORM	The $CF_1[R_i]$ value is calculated exactly like in the ESTD calculation, but with peaks not found in the calibration, no <i>Amount [%]</i> value may be given in this case and the <i>Peak Type</i> column shows the <i>Error</i> label.

3.6.2.5 Appendix 2

Calculation of percentage representation:

$$Amount\%_i = \frac{\frac{Amount_1}{ScaleFactor}}{\frac{SampleAmount}{Dilution}} \cdot 100$$

3.6.3 All Signals Result Table

Invoking this command switches the lower part of the [Chromatogram](#) window to the *All Signals Results* tab, displaying the *All Signals Result Table* in the left half. When using a multi-detector chromatogram, the *All Signals Result Table* displays all results for all the signals present in the given chromatogram.

Note: The *All Signals Result Table* is not available on instruments with extensions (except PDA and SST).

All Signals Result Table behaves analogically to the [Results Table](#). One of the differences from the *Result Table* is the *Signal Name* column, which defines the name of the signal. For single detector chromatograms, the *Signal Name* remains empty.

Note: User Columns are not supported in the *All Signals Result Table*.

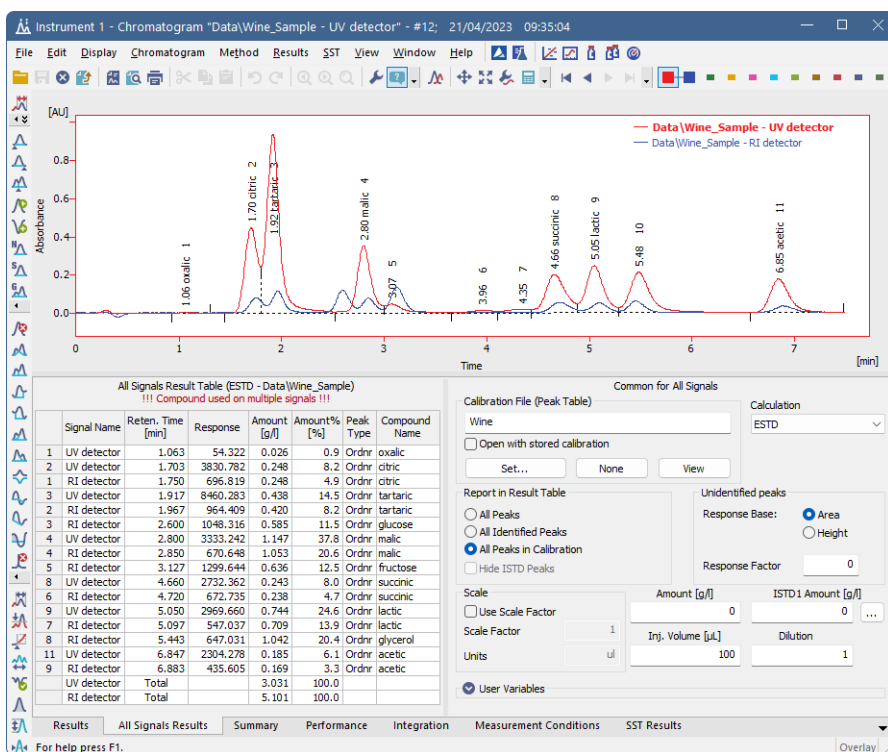


Fig. 184: Chromatogram - All Signals Result Table

Note: The *All Signals Result Table* is visible only when chromatographic data are unchanged. After modifying primary data (Scale or Move operations), *All Signals Result Table* will disappear as the results are no longer valid.

Columns in the *All Signals Result Table* are sorted by *Reten. Time* by default. Double click a column header to change the column for ordering. Displayed results from the *All Signals Result Table* are printed in the exact order as seen on the screen (WYSIWYG).

Note: Changing the signal or opening a new chromatogram does not reset the order to the default (*Reten. Time*) - this must be done manually.

At the bottom of the *All Signals Result Table*, two possible types of total rows can be present: each signal *Total* or *All Signals Total*.

- The *Total* rows display total value of certain columns (e.g., *Amount*, *Area*, and *Height*) separately for each signal.
- *All Signals Total* row is present only under specific circumstances: each compound is calibrated only on one of the multiple signals and the *Compound Unique on One Signal* option (accessible in the *Results* menu) is selected (this is the default).

Caution By default, the *Compound Unique on One Signal* option (accessible in the *Results* menu) is selected. As a result, you will be notified when a compound is used on multiple signals in the header of the table.

Presentation of results

The results table can be added into the print configuration by checking the *All Signals Result Table* checkbox in the [Report Setup - Results](#) dialog described on pg. 449.

3.6.4 Summary Table

Invoking this command switches the lower part of the [Chromatogram](#) window to the *Summary* tab, displaying the **Summary Table** on it. The **Summary Table** serves for easy display and printing of selected parameters from all displayed chromatograms in one table. The table only displays the results of calibrated peaks.

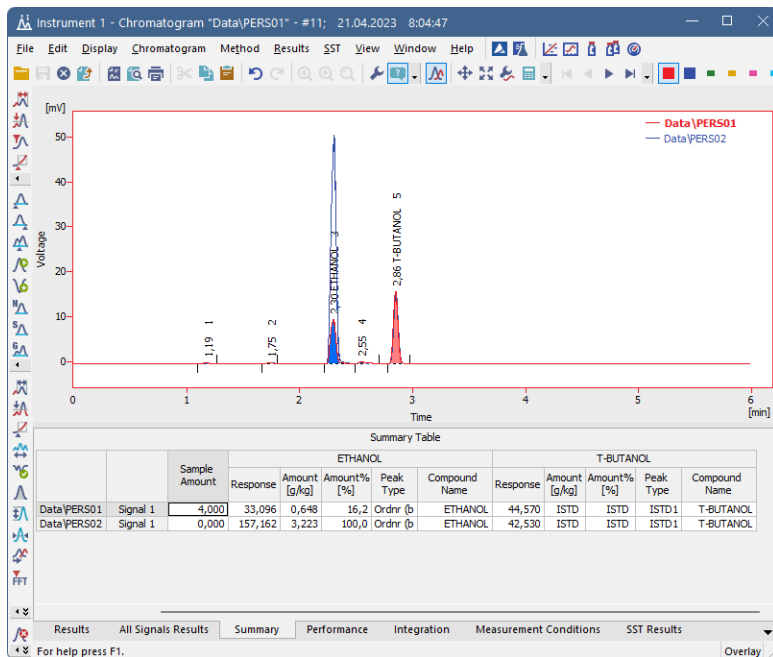


Fig. 185: Chromatogram - Summary

Note: The user columns in **Result Table** and in **Summary Table** are independent. You cannot load the current layout of the **Result Table** into the **Summary Table** by using the *Restore Default Columns* option from the **Summary Table** context menu.

Presentation of results

The results table can be added into the print configuration by checking the *Summary Table* checkbox in the [Report Setup - Results](#) dialog described on pg. 449.

The results table can also be exported using the *File - Export - Export Summary Table* command described in the chapter "File" on pg. 165.

Selection of displayed parameters

Columns display the same parameters for each identified substance as in the [Results](#) tab for all calibrated compounds. The *Amount [x]* and *Amount [%]*

parameters are implicitly offered. The displayed parameters are set using the *Edit - Setup Columns...* command from the main menu or *Setup Columns...* command from the local menu and use the same units as in the **Result Table** described in the chapter "**Result Table**" on pg. 296.

Selection of table layout

In the implicit setting, the rows correspond to individual chromatograms and their signals. The layout best corresponding to your requirements can easily be set using the *Table Inverted* and *Parameter Header* commands from the [Summary Options](#) dialog (see following chapter).

3.6.4.1 Summary Options

By right-clicking on the [Summary](#) tab and selecting the *Summary Options...* command, the *Summary Table Options* dialog with the settings of the **Summary Table** display appears.

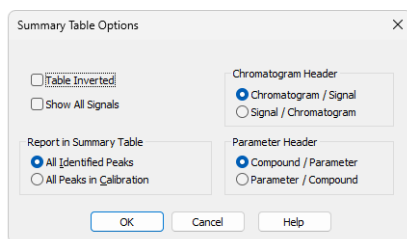


Fig. 186: Summary Table Options

Table Inverted

When checked, chromatograms will be displayed in columns and individual compounds and their parameters will be placed in rows, inverting the table order. This display may be suitable for a smaller number of chromatograms and a large amount of compounds and/or parameters.

Show All Signals

The **Summary Table** implicitly hides signals that do not contain any identified peaks. When checked, all signals from opened chromatograms will be displayed. This can be used to identify problematic signals easily.

Chromatogram Header

Selects the grouping order of rows in the **Summary Table**. This serves for easy comparison of corresponding signals in a set of several multi-detector chromatograms.

Report in Summary Table

This option selects which compounds will be displayed in the **Summary Table**.

All Identified Peaks

Only compounds identified in the corresponding calibration files will be displayed.

All Peaks in Calibration

Summary table will contain all compounds from all used calibration files without regard to whether they were all identified.

Parameter Header

This section determines whether there will be main columns organized by compounds or parameters.

Compound / Parameter(s)

Main columns are organized by compounds. First compound column with all parameters of the first compound is followed by second compound column with all parameters of the second compound and so on.

Parameter / Compound(s)

The columns are organized by parameters. The values of the first parameter will be displayed for all compounds first, followed by the values of second parameter for all compounds and so no.

Available layouts of Summary Table:

Summary Table									
		Chloride		Bromide		Nitrate-N		Sulphate	
		Amount [mg/l]	Amount% [%]	Amount [mg/l]	Amount% [%]	Amount [mg/l]	Amount% [%]	Amount [mg/l]	Amount% [%]
TEF-4LC	Signal 1	0,036	1,3	ISTD	ISTD	0,907	32,9	1,814	65,8
NYL-3LC	Signal 1	0,289	7,7	ISTD	ISTD	2,618	70,0	0,832	22,2

Results All Signals Results Summary Performance Integration Measurement Conditions

Compound / Parameter

Summary Table					
		TEF-4LC		NYL-3LC	
		Amount [mg/l]	Amount% [%]	Amount [mg/l]	Amount% [%]
Chloride	Signal 1	0,036	1,3	0,289	7,7
Bromide	Signal 1	ISTD	ISTD	ISTD	ISTD
Nitrate-N	Signal 1	0,907	32,9	2,618	70,0
Sulphate	Signal 1	1,814	65,8	0,832	22,2

Results All Signals Results Summary Performance Integration

Inverted Compound / Parameter

Summary Table									
		Amount [mg/l]				Amount% [%]			
		Chloride	Bromide	Nitrate-N	Sulphate	Chloride	Bromide	Nitrate-N	Sulphate
TEF-4LC	Signal 1	0,036	ISTD	0,907	1,814	1,3	ISTD	32,9	65,8
NYL-3LC	Signal 1	0,289	ISTD	2,618	0,832	7,7	ISTD	70,0	22,2

Results All Signals Results Summary Performance Integration Measurement Conditions

Parameter / Compound

Summary Table				
		TEF-4-LC	NYL-3-LC	
		Signal 1	Signal 1	Signal 1
Amount [mg/l]	Chloride	0,036		0,289
	Bromide	ISTD		ISTD
	Nitrate-N	0,907		2,618
	Sulphate	1,814		0,832
Amount% [%]	Chloride	1,3		7,7
	Bromide	ISTD		ISTD
	Nitrate-N	32,9		70,0
	Sulphate	65,8		22,2

Results All Signals Results Summary Performance Integration

Inverted Parameter / Compound

3.6.5 Performance Table ✔ Full version

A table containing peak parameters characterizing the quality of the chromatographic system. Invoking the command opens the *Performance* tab.

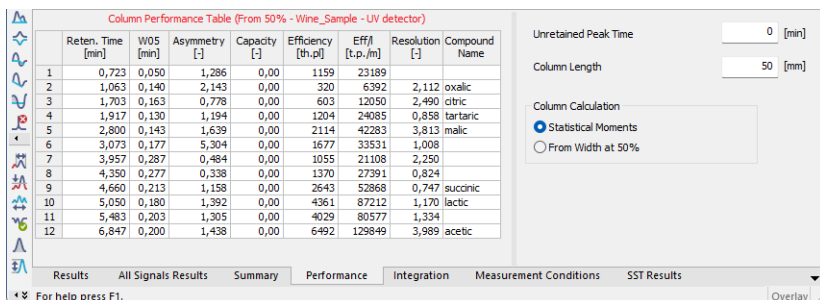


Fig. 187: Chromatogram - Performance

The left-hand part contains the table, while on the right part the calculation type is selected.

Tab. 20: Elements of the Performance Table

Element	Description
Upper Caption	- Shows column names. To display the values of the table in an ascending order, double-click the upper caption; double-click again to change the order to descending. Move the column to some other position by left clicking the mouse twice slowly and dragging the cursor above the desired column. To broaden or narrow a column, click, hold down and then drag the right border. Restore the default column width by double-clicking the right border.
Left caption	- Displays the peak number.
Reten. Time	- Retention time in minutes.
W05 [min]	- Peak half-width (peak width at half-height) in minutes. This column displays only if the Performance table is created using <i>Width at 50%</i> .
Compound Name	- Names of identified compounds.

The following columns vary depending on the type of calculation used:

Statistical Moments

Tab. 21: List of columns in the Performance Table - Statistical Moments

Column	Equation
Centroid [min]	<p>- Peak centroid:</p> $M_1 = \int_{-\infty}^{+\infty} \frac{th(t)dt}{M_0}$ <p>where:</p> $M_0 = \int_{-\infty}^{+\infty} h(t) dt$
Variance [min ²]	<p>- Peak variance:</p> $\overline{M}_2 = \int_{-\infty}^{+\infty} \frac{(t-M_1)^2 h(t)dt}{M_0}$
Skew [-]	<p>- A measure of peak skewness:</p> $Skew = \frac{\overline{M}_3}{\overline{M}_2^{\frac{3}{2}}}$ <p>where:</p> $\overline{M}_n = \int_{-\infty}^{+\infty} \frac{(t-M_1)^n h(t)dt}{M_0}$
Excess [-]	<p>- A measure of Kurtosis:</p> $Excess = \frac{\overline{M}_4}{\overline{M}_2^2} - 3$ <p>where:</p> $\overline{M}_n = \int_{-\infty}^{+\infty} \frac{(t-M_1)^n h(t)dt}{M_0}$
Efficiency	<p>- Column efficiency measured by the plate number:</p> $Efficiency = \frac{M_1^2}{M_2}$
Eff./l	<p>- Relative efficiency:</p> $Eff. / l = Efficiency_i \cdot \frac{100}{Columnlength}$

Column	Equation
Symmetry/Tailing [-]	- Symmetry/Tailing: $Symmetry_i = \frac{A_{05_i} + B_{05_i}}{2 \cdot A_{05_i}}$

From Width at 50%:

Tab. 22: List of columns in the Performance Table - Width at 50%

Column	Equation
Asymmetry[-]	- Peak asymmetry: $Asymmetry_i = \frac{b_i}{a_i}$
Capacity[-]	- The k' factor $Capacity_i = \frac{RT_i - T_0}{T_0}$
Efficiency	- Column efficiency measured by the plate number: $Efficiency_i = 5.54 \cdot \left(\frac{RT_i}{W_{h/2_i}} \right)^2$
Eff./l	- Relative column efficiency in plate numbers per column length: $Eff. / l = Efficiency_i \cdot \frac{100}{Columnlength}$
Resolution[-]	- Represents resolution with regard to the preceding peak: $Resolution_i = \frac{1.18 \cdot (RT_i - RT_{i-1})}{(W_{h/2_{i-1}} + W_{h/2_i})}$

Tab. 23: Description of used symbols

Symbol	Description
RT _i	- is the retention time of the component.
W _{h/2_i}	- is the peak width at half height.
a _i	- is the left half-width at 10 % height.
b _i	- is the right half-width at 10 % height.
T ₀	- is the unretained (dead) time of the column.
Column Length	- in mm.
A _{05_i}	- is the left half-width at 5 % height.
B _{05_i}	- is the right half-width at 5 % height.

Parameters influencing the calculation are stated in the right-hand part of the *Performance* tab:

Unretained Peak Time

The parameter defines the column dead time in minutes. The value is used to determine the capacity factor.

Column Length

The length of the column in millimeters. The value is used to calculate the theoretical column plate height.

Column Calculations

The method used to calculate some parameters in the table is specified here.


Statistical Moments - Calculations are based on statistical moments.

From Width at 50% - The peak width at 50% of the peak height and the corresponding half widths are used in the calculations.

3.6.6 Result Table Error Messages

When it is not possible to use the selected type of Calculation for whatever reason, a red error message in the Result Table header (with exclamation marks) indicates the cause of the problem. Below is a list of possible chromatogram error messages with descriptions and possible reasons.

Tab. 24: List of possible error messages in the Result Table:

Error message	Detailed description
<i>No identified peak(s)</i>	Based on the linked calibration it was not possible to identify any peak. Possible reasons are for example incorrect linked calibration or compounds in calibration are not checked as used.
<i>No ISTD peak detected</i>	The calculation cannot be performed using the internal standard because the calibration does not contain any peak which has been indicated as internal standard (ISTD). Uncalibrated calculation will be used instead. Make sure ISTD Peak with appropriate Retention Time is entered in the calibration or change the chromatogram Calculation type so the ISTD compound is not requested.
<i>No valid level in ISTD%d compound</i>	ISTD peak is identified in the calibration but does not have a valid level. View the linked Calibration, switch to the ISTD compound tab and make sure there is valid level and it is checked as used.
<i>Missing ISTD Amount in Sample</i>	When ISTD calculation is selected, it is necessary to enter the ISTD Amount used in the sample. It can be entered in the Common for All Signals part of Results (<i>Chromatogram</i> window). For the ISTD2 - ISTD10 click the  button.
<i>No ISTD Amount given in Calibration</i>	When ISTD calculation is selected, it is necessary to enter the Calibration ISTD Amount. It can be entered in the Amount column in the <i>Calibration</i> window.
<i>Calibration curve could not be constructed</i>	<p>If calibration curve could not be constructed for one compound in calibration, no results are calculated for all compounds. The problematic compound can be detected in the Peak Type column as "Error". To construct the calibration curve View the linked Calibration and check the Amounts and Responses for given compound are set correctly.</p> <p>If compounds do not need to be quantified (e.g. Calibration is used only to identify peaks) Free Calibration can be used (On the given compound tab in the Calibration set the Curve Fit Type to <i>FREE CALIBRATION</i> for the compound)</p>

Error message	Detailed description
<i>Calibration curve could not be constructed for multiple compounds</i>	Same as the error message above, only calibration curve could not be constructed for more than one compound. Curves for all compounds have to be constructed to get calculated results.
<i>Signal is moved/scaled</i>	It is not possible to quantify results as the signal has been moved or scaled. To get the signal into the original position go to the menu Display - Properties - Signals tab, use the Original button in the Offset & Scale part.
<i>Not all sample peaks are identified</i>	This message appears when the Calculation is set to NORM and it is not possible to identify all peaks. It is possible that some required compounds in the calibration have incorrect retention time, are not checked as used or are not entered in the calibration.
<i>Sample Amount must be zero.</i>	When the Calculation is set to NORM the Amount must be zero. Both Calculation and Amount can be modified in the Common for All Signals pane in <i>Chromatogram</i> window.

Tab. 25: List of possible error messages in the Result Table when using MS extension:

Error message	Detailed Description
<i>Failed to load the NIST library. Please check whether the location of NIST libraries is correctly set.</i>	Please check the library specified on the MS Method tab in the Library Compound - ID column exists or is set correctly
<i>Failed to load the library spectrum. Please check if the compound is present within the library.</i>	Please check the spectrum specified on the MS Method tab in the Library Compound - ID column exists in the library

Tab. 26: List of possible error messages in the All Signals Result Table:

Error message	Detailed description
<i>Compound used on multiple signals</i>	By default Clarity controls whether one compound is used on one signal only. It can be turned off using menu <i>Results - Compound Unique on One Signal</i> .
<i>Some signals are hidden or moved/scaled</i>	All Signals Results cannot be quantified because of hidden/moved or scaled signal. <ul style="list-style-type: none"> - Hidden signal can be noticed/viewed in the <i>Chromatogram List</i> which is invoked from menu <i>Chromatogram - Chromatograms...</i> - To get the moved or scaled signal into the original position go to the menu Display - Properties - Signals tab, use the Original button in the Offset & Scale part.

Error message	Detailed description
<i>Note:</i> In the All Signals Result table are also messages mentioned in the Result Table tab.	

Tab. 27: List of possible error messages in the Column Performance Table:

Error message	Detailed description
<i>Signal is moved/scaled</i>	It is not possible to quantify results as the signal has been moved or scaled. To get the signal into the original position go to the menu Display - Properties - Signals tab, use the Original button in the Offset & Scale part.

List of possible error messages in the DHA Results table and in the DHA Group Results table can be found in DHA Manual (M150)




3.7 SST ✓ Full version

SST stands for the **System Suitability Test** characterizing the measurement quality. Invoking the command opens the **SST Results** tab.

A detailed description of this **Clarity Extension** can be found in a separate **SST Extension** manual.




3.8 View

This section contains commands used to set up the appearance of the [Chromatogram](#) window.

Toolbars	<p>Displays commands for toolbars. The command is similar to the <i>Toolbars</i> command in the main Clarity window.</p> <ul style="list-style-type: none"> • Standard, Other, Sequential Open, etc.: Hides/shows the respective toolbar. • Customize: Customization of items in the toolbars. • Reset All: Returns all menus and default toolbars in the Chromatogram window into their initial state.
<p><i>Note:</i> <i>Reset All</i> does not display hidden toolbars. To show them invoke <i>Customize... - Toolbars</i> menu.</p>	
Maximize Graph	<p>The command maximizes the graph to cover the entire window (hides the bottom tabs). Double click near the splitter (the cursor will change to ) to achieve the same effect.</p>
Maximize Spectrum	<p>The command maximizes the spectrum to cover the entire window (hides the bottom tabs). Double click near the splitter (the cursor will change to ) to achieve the same effect.</p>
<p><i>Note:</i> Only available in MS extension.</p>	
Show All	<p>The command restores default view showing chromatogram, spectrum and the bottom tabs.</p>
<p><i>Note:</i> Only available in MS extension.</p>	
Show Both	<p>Used to display both parts of the window (the chromatogram and the tabs).</p>
Maximize Tables	<p>The command maximizes the bottom tabs to cover the entire window (hides the chromatogram). Double click near the splitter (the cursor will change to ) to achieve the same effect.</p>
Show Tables	<p>The submenu for displaying/hiding of the tabs of Chromatogram window. Checked tabs are displayed. The Results tab cannot be hidden this way.</p>

3.9 Window

This is an entry point to a submenu of commands for displaying other main windows.

Main 	Displays the Clarity main station window described on pg. 1 .
Instrument	Displays the Instrument window described on pg. 60 .
Calibration	Displays the Calibration window described on pg. 320 .
Single Analysis	Displays the Single Analysis window described on pg. 113 .
Sequence	Displays the Sequence window described on pg. 385 .
Data Acquisition	Displays the Data Acquisition window described on pg. 369 .
Device Monitor	Displays the Device Monitor window described on pg. 135 .
Station Audit Trail 	Displays the Audit Trail window described on pg. 413 .
Chromatogram Audit Trail 	Displays the Chromatogram Audit Trail window described on pg. 427 .

4 Calibration

The name of the current calibration file is displayed in the window header of the *Calibration* window. When displaying calibration curves saved in the chromatogram, the header contains the name of the chromatogram and the date the displayed calibration curves were saved. The window contains the main *Compounds* tab as well as tabs of every compound which is defined in the displayed calibration file. The *Compounds* tab contains the main calibration table and, eventually, the current calibration standard. The *Individual Compound* tabs contain a table for the displayed compound, several parameters and its calibration curve.

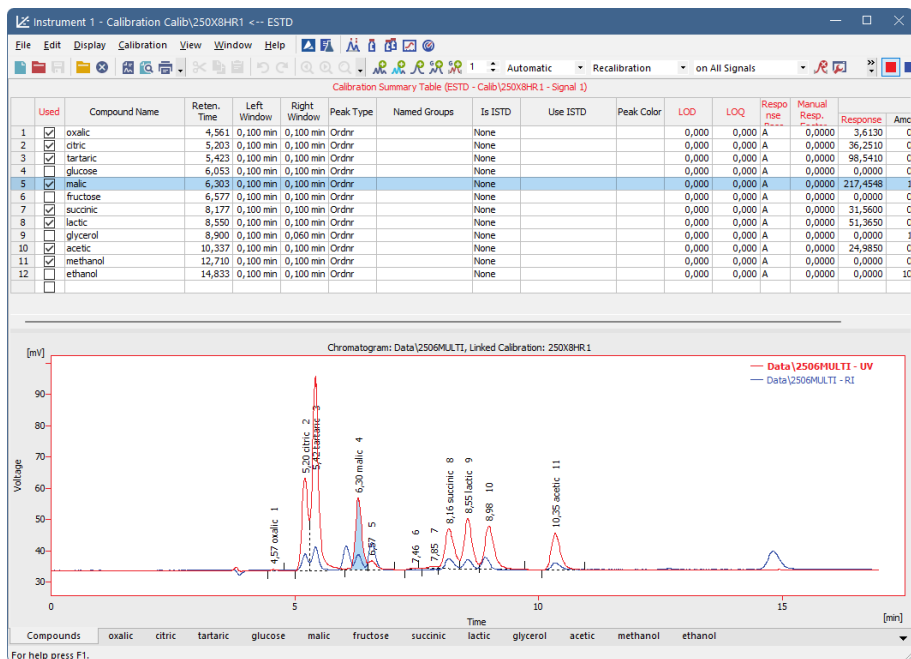


Fig. 188: Calibration - Compounds

The window contains the main *Compounds* tab as well as tabs of every compound which is defined in the displayed calibration file. The *Compounds* tab contains the main calibration table (*Calibration Summary Table*) and, eventually, the chromatogram of the current calibration standard. The *Individual Compound* tabs contain a table for the displayed compound, several parameters and its calibration curve.

Compounds tab

Calibration Summary Table

When using a multi-detector measurement, the main calibration table in the header contains the name of the current signal (detector) for which the data is being displayed.

Certain columns (e.g. *Compound Name*, *Reten. Time*, *Amount*) are **common for all signals** and are displayed in **black**, other columns which are **dependent on the corresponding signal** are displayed in the **color of the active signal**.

Serial number of compound according to retention time. This column is common for all signals.

Used

The *Used* column has the following functionality:

- It allows to prohibit the use of a selected compound - meaning that unchecked compound will not be used for quantification.
- It serves as a check that two compounds do not have the same retention time on one signal - if this situation occurs, user is notified via a message box.
- Only compounds with checked *Used* checkbox will be (re)calibrated.

This column is individual for each signal.

Note: This column is particularly useful in multi-detector chromatograms where each compound is assessed on one signal and can be removed from the results table on the remaining signals using this selector.

Compound Name

Name of the compound. This column is common for all signals. When a new compound is manually created there is no pre-filled any default name.

Reten. Time

Retention time of the compound. This column is common for all signals. When a new compound is created there is pre-filled default value 0.

Search Window

Defines whether the *Left Window* and *Right Window* content will be inserted in *Abs* (absolute - set in minutes) or *Rel* (relative - set in percents of the *Reten. Time*) values. When a new compound is created there is pre-filled value currently set by item *Search Window* in [Calibration Options - Defaults](#) tab.

Left (Right) Window	Defines the width of the left (right) window for identification of compounds (the value is set in minutes). Maximum width is 50 minutes. This column is common for all signals. When a new compound is created there are pre-filled values currently set by items <i>Left Window</i> and <i>Right Window</i> in Calibration Options - Defaults tab.
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Peak Selection	Defines the way the correct peak is matched with the Retention time when several peaks are present in the same identification window. The options available are <i>Nearest</i> (closest possible to the selected retention time - default for standard peaks), <i>First</i> , <i>Last</i> and <i>Biggest</i> (default for Reference peaks).
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Note: The *Peak Selection* choice is overridden whenever a peak is forced-linked to a compound in the calibration by the *Set Peak Name* function in the [Chromatogram](#) window. For more details see the chapter **Peak** on pg. 237.

Peak Type	Type of the calibrated compound. This column is common for all signals. The possible options are: <i>Ordnr</i> - Peak which is not a reference peak. <i>Refer</i> - Reference peak. <i>Grp_</i> - Group consists of peaks from the chromatogram standard. <i>Named Grp</i> - Named group consists of peaks already present in the Calibration Summary Table. When a new compound is created, the default value is <i>Ordnr</i> . Such compound can be changed to <i>Refer</i> but not to <i>Grp</i> nor <i>Named Grp</i> . When a new group is created, the default value is <i>Grp_</i> + a letter (A-Z) where the letter originates from the chromatogram of standard. When a new named group is created, the default value is <i>Named Grp</i> . Once created, <i>Grp_</i> nor <i>Named Grp</i> cannot be changed to any other type - the cell is disabled.
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Is ISTD	Defines whether the given compound is ISTD peak for the purposes of ISTD calculation and assigns the ISTD peak number to ISTD peaks. Up to 10 compounds in the calibration file may be indicated as internal standards from Clarity version 5.0 - before that only one ISTD peak was possible. When a new compound is created there is pre-filled default value <i>None</i> .
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Use ISTD	Sets which ISTD peak will be used for the calculations of the given compound. When first ISTD peak is selected in the <i>Is ISTD</i> column of the calibration file, the <i>Use ISTD</i> column of all other compounds is automatically pre-filled with that peak name. ISTD peaks themselves have the <i>Use ISTD</i> column empty.
<i>Note:</i>	A group of peaks can be neither an internal standard nor reference peak.
Peak Color	Sets the coloration of the peak area to the desired color. Whenever the given peak will be identified in the chromatogram using this calibration, it will be colored accordingly. When a new compound is created there is pre-filled default color corresponding to RGB color code 255,255,255.
Reten. Index	Retention (Kovats) indexes. When a new compound is created there is pre-filled default value 0.
<i>Note:</i>	This column is hidden in the default layout. For more details see the chapter Setup Columns on pg. 198.
LOD	Limit of Detection (LOD) - the exceeding of the limits can be displayed in the result table. This column is individual for each signal. When a new compound is created there is pre-filled default value 0.
LOQ	Limit of Quantification (LOQ) - the exceeding of the limits can be displayed in the result table. This column is individual for each signal. When a new compound is created there is pre-filled default value 0.
Response Base	Response Base - Calculations are displayed for height - <i>H (Height)</i> , area - <i>A (Area)</i> or area % - <i>P (Area Percent)</i> . This column is individual for each signal. When a new compound is created there is pre-filled value currently set by item <i>Response Base</i> in Calibration Options - Defaults tab.
Resp. Factor	Global response coefficient for free calibration. The value must be entered manually (not automatically calculated) and is used upon a calibrated calculation for compounds which have the flag filed <i>Curve Fit Type</i> set to <i>Free Calibration</i> . This column is individual for each signal. When a new compound is created there is pre-filled default value 0.

Correction Factor	Allows for the correction of amount due to the lower recovery etc. The <i>Amount</i> value is multiplied by the <i>Correction Factor</i> to calculate the final <i>Amount</i> . When a new compound is created there is pre-filled default value 1.
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Calculate By	<p>Allows to set a compound whose <i>Calibration curve</i> will be used for <i>Amount</i> calculation for a given compound. Only peaks already added to the calibration are valid for selection. By default this column is empty.</p> <p>In case of ISTD calculation type, the ISTD compound may be used for calculation of the amounts for different peak, in which case the ISTD Amounts must be filled in both in the calibration file and in the unknown sample. <i>Calculate By</i> option for an ISTD peak will not calculate Amount and for ISTD calculation the setting will not be used.</p>
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Note: *Named Group* cannot be selected as *Calculate By* parameter.


Curve Fit Type	Determines the type of the curve used to fit the data - the available options are described in the section Curve Fit Type on pg. 331 When a new compound is created there is pre-filled value currently set by item <i>Curve Fit Type</i> in Calibration Options - Defaults tab.
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Origin	Specifies the method for including origin zero point into the calibration curve. This value is individual for each signal and is described in the section Origin on pg. 332 When a new compound is created there is pre-filled value currently set by item <i>Origin</i> in Calibration Options - Defaults tab.
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Ending Point	Specifies the maximum interpolation of <i>Sigmoid</i> and <i>Half Sigmoid Curve Fit Type</i> . The column is only editable when either of these <i>Curve Fit Type</i> options is selected and is described in the section Ending Point on pg. 333 When a new compound with these two <i>Curve Fit Types</i> is created default value is <i>Last Point</i> .
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Weighting Method	Determines the value of the weight of individual points when calculating the interposing curve. The function and its possible options are described in the section Weighting Method on pg. 333 described on pg. 333. When a new compound is created there is pre-filled value currently set by item <i>Weighting Method</i> in Calibration Options - Defaults tab.
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Linearization X	Sets the X-axis linearization for the calibration curve calculation. The function and its possible options are described in the section Linearization X on pg. 333 described on pg. 333. When a new compound is created there is pre-filled value currently set by item <i>Linearization X</i> in Calibration Options - Defaults tab.
Linearization Y	Sets the Y-axis linearization for the calibration curve calculation. The function and its possible options are described in the section Linearization Y on pg. 334 described on pg. 334. When a new compound is created there is pre-filled value currently set by item <i>Linearization Y</i> in Calibration Options - Defaults tab.
Level X	Number of the calibration level to which the following columns relate. This column is common for all signals.
<i>Note:</i>	Calibration table can contain up to 21 calibration levels including the blank.
Response	Area or height of peak as a response. Type is determined by the <i>RB</i> column. This column is individual for each signal. When a new compound is created there is pre-filled default value 0.
Amount	Amount of compound on the level displayed. Units are determined by the <i>Units - Compound</i> field from the Calibration Options dialog and are common for the entire calibration file. This column is common for all signals.
<i>Note:</i>	On any level other than 21 (blank), zero in the response or amount columns excludes the level from the calculation. Default Amount for blank level is <i>Blank</i> , default value for all other levels is 0. In case of combination Standard Addition Display Mode and <i>Unknown</i> level there is pre-filled default value <i>Unknown</i> . Standard Addition Display Mode is described in the STDADD section the chapter " Calibration Options " on pg. 360.
Resp. Fact.	Response coefficient for each level. A more detailed description is provided below with the description of the compound table. This column is individual for each signal. When a new compound is created there is pre-filled default value 0.

Rec No. Shows number of used recalibrations to number of total recalibrations on the level displayed. After the recalibration with *Replace* type, the number is set to 1/1. This column is individual for each signal. Clicking  invokes the [Details of Calibration Point](#) dialog with a detailed log of the selected level of the calibration point. When a new compound is created there is pre-filled default value 0/0.

Note: A double-click on the row header with the number of compound (gray field to the left next to the name of the compound) displays the tab of the corresponding compound.

Lin Response Displays calculated value of *Response*; the calculation is based on the option selected in *Linearization Y*. When a new compound is created there is pre-filled default value 0.

Note: This column is hidden in the default layout. For more details see the chapter **Setup Columns** on pg. 198.

Lin Amount Displays calculated value of *Amount*; the calculation is based on the option selected in *Linearization X*. When a new compound is created there is pre-filled default value 0.

Note: This column is hidden in the default layout. For more details see the chapter **Setup Columns** on pg. 198.

Local menu of the Calibration Summary Table

In addition to the common commands for the majority of tables, the local menu contains the following items:

Delete Compound

Removes the actual substance from the calibration.

Delete All Compounds

Removes all compounds from the calibration (from all calibration levels).

Filter Not Used Compounds

Hides/shows rows (and related tabs of individual compounds) of Calibration Summary Table with disabled *Used* checkbox.

Note: Warning is displayed above the Calibration Summary Table when rows are hidden. Clicking *Show all* disables filtering.

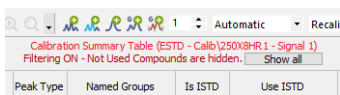


Fig. 189: Filtering ON warning

Graph of the calibration standard

The graph refers to the calibration standard loaded by the *File - Open Standard* command. Its name is shown at the bottom right of the **Status Bar** and in the upper right corner of the graph. The graph facilitates the transfer of retention times and responses from the calibration standard to the calibration table, and is the same as the chromatogram graph in the [Chromatogram](#) window, including the characteristics set up by the *Properties...* command from the *Display* menu or the local menu. The only difference is the **Peak Area Coloring** area referring to the **Calibration Table**.

Note: To see the colored peaks in the *Calibration* window, the calibration standard must have the current calibration linked to it (this can be done in the [Chromatogram - Results](#) tab).

Tabs of individual compounds:

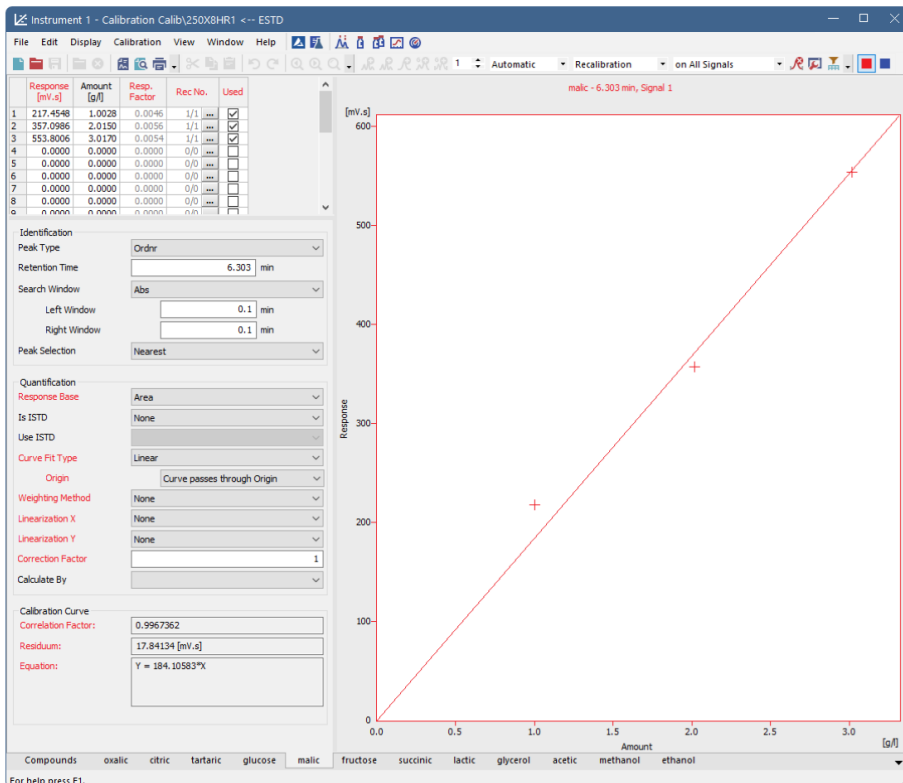


Fig. 190: Calibration - Individual Compound (malic)

Compound Table

The table can be found in the top left corner of the individual compound tab.

First column

Contains the level number of each displayed line.

Note: Calibration table can contain up to 21 calibration levels, including blank.

Response

Represents the response at a given level. Whether it will be area or height is defined in the *Response Base* field.

Amount

The amount of the compound at a given level.

Response Factor

The response factor at a given level is equal to the reciprocal value of the slope of a straight line passing through the origin and the calibration point

at the given level. It is calculated as the amount of the compound divided by the response at the relevant level. The value serves for information only.

$$LRF_i = \frac{A_i}{R_i}$$

where:

A_i - is the amount of the compound at level i.

R_i - is the response (height or area) at level i.

It is possible to calculate response factor in inverse form (RF = Response / Amount) by checking *Response Factor as Response / Amount* checkbox in [Calibration Options](#)

Rec No.

Shows the number of recalibration points that have *Used* checkbox in the [Details of Calibration Point](#) checked to number of total recalibrations.

Used

Sets validity/invalidity of a calibration level for the purpose of the calibration curve. Cleared checkbox means that the calibration level will not be used in the calibration curve. It will be illustrated by a circle in the graph.

Note: To omit calibration of a level from a *Sequence*, clear the *Used* checkbox on the corresponding calibration level.

Deviation [%]

Deviation of the *Amount* of the calibration point from the calculated *Amount* given by the calibration curve. The column is hidden by default.

$$Deviation[\%] = ((Amount - Amount_C) / Amount_C) * 100$$

where:

Amount - The actual Amount on the concentration level.

Amount_C- The calculated Amount corresponding to the concentration level (calculated from the calibration curve).

RSTD [%]

Displays the relative standard deviation of averaged points used during the recalibration of the respective concentration level. The column is hidden by default.

Lin Response

Displays calculated value of *Response*; the calculation is based on the option selected in *Linearization Y*. The column is hidden by default.

Lin Amount

Displays calculated value of *Amount*; the calculation is based on the option selected in *Linearization X*. The column is hidden by default.

Local menu of the Compound Table

In addition to common commands available for the majority of tables, the local menu contains the

Clear All Levels	Erases all entered values on all levels of the given substance.
Clear Selected Level	Erases all values on the given level.
Clear Selected Value	Erases the value in the current field of the table.
Delete Compound	Removes the current substance from the calibration.
Show Details	Invokes the Details of Calibration Point dialog with a detailed log of the selected level of the calibration point. Dialog window provides following details: used, peak retention time, area, height, date of a (re)calibration and the name of the calibration standard.

Resettable parameters

The section with resettable parameters is positioned in the bottom left part of each compound tab, below the **Compound Table**, and is divided into three logical groups: *Identification*, *Quantification* and *Calibration Curve*.

Identification

Resettable parameters which state how will be the compound identified.

Peak Type

This setting is individual for each compound, but common for all signals.

Ordnr - Designates a peak or group that is neither a reference peak nor an internal standard.

Refer - Designates a reference peak.

Retention Time

Retention time of the compound.

Search Window

Defines whether the *Left Window* and *Right Window* content will be inserted in *Abs* (absolute - set in minutes) or *Rel* (relative - set in percents of the *Reten. Time*) values.

Peak Selection

Defines the way the correct peak is matched with the Retention time when several peaks are present in the same identification window.

Quantification

Resettable parameters which state how will be the compound quantified.

Response Base

Sets whether the response will be used as the base for calculation of the calibration curve, calibration dependency equation and two response

factors and specifies the base to be displayed in the *Response* column. This setting is individual for each signal. Please note that the height is calculated as the distance from the peak maximum vertically to the peak baseline, so for the small peaks on very steep baselines, the peak height may be imprecise.

Area - Peak area constitutes the base.

Height - Peak height is the base.

Area Percent - Calibration based of area percentage of peaks. Only peaks used in calibration are summed into the whole (100%), thus it is required to add them all into calibration, even when user don't need to calculate their results. Recommended type of calculation is ESTD.

Note: Other fields from the tabs of individual compounds are dependent on the *Response Base* selected - switching the *Response Base* will thus switch the content of all editable fields to the set of saved parameters connected to the other *Response Base* option, the graph display will change accordingly and the content of the *Response* column in the **Compound Table** will change too.

Is ISTD

Defines whether the given compound is ISTD peak for the purposes of ISTD calculation.

Use ISTD

Sets which ISTD peak will be used for the calculations of the given compound. When first ISTD peak is selected in the *Is ISTD* column of the calibration file, the *Use ISTD* column of all other compounds is automatically pre-filled with that peak name. ISTD peaks themselves have the *Use ISTD* column empty.

Curve Fit Type

Determines the type of the curve used to fit the data:

Free Calibration - No calibration curve is construed and calibration equation is in the form of $Y = \text{Manual Response Factor} * \text{Correction Factor} * X$. Instead of a value read off the calibration curve the calculations use the corresponding global *Response Factor* from the global calibration table.

Point to Point - The calibration points are connected by a broken line. No common calibration equation is calculated, the equation of the relevant line segment is used instead in the calibration calculations.

Linear - A straight line is passed through the points.

Quadratic - The calibration curve will be interlined by a quadratic polynomial.

Cubic - The calibration curve will be interlined by a cubic polynomial.

Sigmoid - The calibration curve will be interlined by a sigmoid.

$$z = 2 \cdot \sqrt[b]{\frac{\text{Response}}{d}} - 1$$

$$\text{Amount} = c \cdot \sqrt{\frac{a}{2} - \frac{1}{2k} \cdot \text{sign}(z) \cdot \ln(1 - \text{abs}(z) \cdot (1 - e^{-k}))}$$

c - Maximum Amount

d - Maximum Response

The **c** and **d** parameters can be increased up to 125% using the *Ending Point* field (both parameters are changed at once).

b = 1

a, **k** - are coefficients that are calculated using iteration from the interval $\langle 0, 1 - 100 \rangle$ so that the curve will best fit the given calibration points.

ln - The calibration curve will be interlined by a logarithm function.

log10 - The calibration curve will be interlined by a decimal logarithm function.

exp - The calibration curve will be interlined by an exponent line.

pow10 - The calibration curve will be interlined by a decimal exponent line.

Hyperbola - The calibration curve will be interlined by a hyperbola.

Half Sigmoid - The calibration curve will be interlined by a half-sigmoid.

If the number of available points does not suffice for the required curve type, the curve will automatically be changed to the next lower type. The *Curve Fit Type* selection remains unchanged.

Note: The *Curve Fit Type* selection is disabled in the Standard Addition display mode - only *Linear* curve fit is available in this mode.

Origin

Specifies the method for including origin zero point into the calibration curve. This value is individual for each signal.

Ignore Origin - Origin will not be included.

Compute with Origin - Considers the Origin to be one of the calibration points.

Curve passes through Origin - Always passes the Curve through the origin.

Note: The *Ignore Origin* option is recommended for the *Origin* field when the blank response is included in the calibration curve calculation.

When interposing using the sigmoid, the *Origin* field will be replaced by the *Ending Point* field. In the Standard Addition display mode, the Origin Field is replaced with the Unknown field.

Ending Point

Enables the calculation of sigmoid interposing outside of the end points. The end calibration points are taken as limit values, increased by the relevant percentage according to the *Ending Point* field. Best used when the possibility to measure the calibration points within the sufficient range is limited.

Manual Response Factor

Serves as a manual amendment of a response for a whole compound and directly affects the constructed equation of the calibration curve. *Manual Response Factor* can only be changed when *Curve Fit Type* is set to *Free Calibration*.

Unknown

Specifies the method for including the unknown sample into the calibration curve calculation in the Standard Addition mode (for more details see the chapter **Calibration Options** on pg. 360).. This value is individual for each signal.

Without Unknown Sample - Unknown sample will not be included in the calculation.

Compute with Unknown - Considers the Unknown sample to be one of the calibration points.

Curve passes through Unknown - Always passes the calibration curve through the origin.

Weighting Method

Determines the value of the weight of individual points when calculating the interposing curve. When weighting is not applied, points of higher concentrations (larger quantity and response) have a greater influence over the calibration curve than points with a lower concentration.

Weighting enables to apply the same relative influence to each point ($1/x$ weighting method) or assign greater influence to points of lower levels ($1/x^2$ weighting method).

Weighting may be related to either the amount of the compound in the given point of the calibration curve ($1/Amount$ or $1/Amount^2$) or to the response of the compound in the given point of the calibration curve ($1/Response$ or $1/Response^2$).

Linearization X

Linearizes the values of the X-axis using the selected formula, and uses these linearized values to calculate the calibration curve equation. The X-axis and all calibration points are still displayed for the non-linearized values, so the interleaved curve will usually not match the calibration points.

Note: To display the curve as a linear line, it is also necessary to check the *Show Linearized Values* checkbox in the [Graph Properties](#) dialog. For more details see the chapter **Graph Properties** on pg. 345.

Possible linearization formulas are *None* (no linearization), $1/Amount$, $\ln(Amount)$, \sqrt{Amount} , $1/\sqrt{Amount}$, $Amount^2$, $1/(Amount^2)$ and $\log(Amount)$.

Linearization Y

Linearizes the values of the Y-axis using the selected formula, and uses these linearized values to calculate the calibration curve equation. The Y-axis and all calibration points are still displayed for the non-linearized values, so the interleaved curve will usually not match the calibration points.

Note: To display the curve as a linear line, it is also necessary to check the *Show Linearized Values* checkbox in the [Graph Properties](#) dialog. For more details see the chapter **Graph Properties** on pg. 345.

Possible linearization formulas are *None* (no linearization), $1/Response$, $\ln(Response)$, $\sqrt{Response}$, $1/\sqrt{Response}$, $Response^2$, $1/(Response^2)$ and $\log(Response)$.

Correction Factor

Allows for the correction of amount due to the lower recovery etc. For more details see described in the section **Correction Factor** on pg. 324.

Calculate By

Allows to set a compound whose *Response* will be used for *Amount* calculation for a given compound. For more details see described in the section **Calculate By** on pg. 324.

Calibration Curve - parameters

Parameters of calibration curve which are read only and cannot be modified directly here.

Correlation Factor

A number from the interval $<0, 1>$ that characterizes the closeness-of-fit of the calibration curve. The closer is the number to 1, the better is fit of particular points to the calibration curve. The calculated value is individual for each signal.

$$Cor. Coeff = \sqrt{\frac{\left(\sum(x_i - \bar{x}) \cdot (y_i - \bar{y})\right)^2}{\sum(x_i - \bar{x})^2 \cdot \sum(y_i - \bar{y})^2}}$$

where:

x_i - the actual response at level i

y_i - the calculated response at level i
 x - the mean value of all actual responses (in case of *Compute with Origin* and *Curve passes through Origin* settings including zero point)
 y - the mean value of all calculated responses (in case of *Compute with Origin* and *Curve passes through Origin* settings including zero point)

Residuum

The calculated value displays the calibration curve fit residuum calculated according to the following equation:

$$\text{Residuum} = \sqrt{\frac{1}{n} \cdot \sum (x_i - y_i)^2}$$

where:

x_i - the actual response at level i
 y_i - the calculated response at level i
 n - number of calibration points (in case of *Compute with Origin* and *Curve passes through Origin* settings including zero point)

Equation

Contains the equation of the calibration curve, which determines the relationship between the response and the actual amount of the compound according to the curve type fit selected.

Curve Check

The calculated value displays the result of the linearity check for the calibration curve. The item is only displayed when the *Curve Check* option is set in the [Calibration Options](#) dialog. The result may be either *OK* (if all performed *Curve Check* tests are passed) or *ERROR* (if any of the performed tests is failed).

Calibration curve - graph

The calibration curve of any particular compound is located in the right-hand section of each compound tab.

Name of compound and retention time.

Shows the data which identify the displayed compound. These data come from the main calibration table and include *Compound Name*, *Reten. Time* and the name of the active signal.

Graph

Displays the calibration points of the current compound along with the calibration curve. The graph has identical properties to the other graphs, including cut-outs, auxiliary lines and optional setting using the *Properties* command from the local menu.

A calibrated point is indicated with a cross, a recalibrated point indicated with a star. In the *STDADD* calibration type, *Blank* sample is displayed as a vertical line along with multiplication cross sign to signal that the amount of the sample is not calculated from the intersection of the calibration curve with the X-axis on zero response, but from the intersection of the calibration curve with the blank horizontal line.

When using the *ISTD* method, a relative calibration curve will be displayed, depending on whether the same or a different amount of the internal standard has been used:

Same amount of internal standard

Relative calibration curve as dependence of response ratio of compound and internal standard on amount of injection of compound.

$$\frac{R_i}{R_{ISTD}} = f(A_i)$$

R_i - response of i-th compound

R_{ISTD} - response of internal standard

A_i - amount of i-th compound

Different amount of internal standard

Relative calibration curve as dependence of response ratio of compound and internal standard on ratio of amount of compound and internal standard.

$$\frac{R_i}{R_{ISTD}} = f\left(\frac{A_i}{A_{ISTD}}\right)$$

R_i - response of i-th compound

R_{ISTD} - response of internal standard

A_i - amount of i-th compound

A_{ISTD} - amount of internal standard

4.1 File

This is an entry point to a submenu of commands for working with calibration files:



New

Creates a new calibration file and at the same time closes the currently opened file (user is notified if there are any unsaved changes). May also be invoked by pressing the **Ctrl** + **N** shortcut.

New sequence will be based on the template calibration file (TEMPLATE.CAL) from the common directory (C:\CLARITY\DATAFILES\COMMON\ by default).

If the template calibration file does not exist in the project, the new calibration will be based on values internally preset in **Clarity**.



Open

Selects and opens a calibration file. Invoking the command or using the **Ctrl** + **O** shortcut opens the *Open Calibration* dialog.



Save

This command or the **Ctrl** + **S** shortcut saves the current calibration file. If a new file is to be saved, the *Save As* dialog will open where the name of the new file has to be filled in. The default name NONAME.CAL is reserved only for files that have not been saved yet.





Save As

Saves the calibration file under a chosen name (**Ctrl** + **Shift** + **S**).

Note: For existing filenames, message box about file overwriting pops up.

Send Calibration by email

Sends the displayed calibration file as an email attachment. It is analogous to the *Send Method by Email* command (for more details see the chapter **Send Method by Email** on pg. 70).

	Open Standard	Selects and opens a chromatogram that will be used as a calibration standard. Invoking the command opens the Open Chromatogram dialog, which offers (by default) the content of the calibration subdirectory. The selected chromatogram is subsequently loaded and its name shown in the upper right corner of the chromatogram graph and in the middle the above chromatogram as well.
	Close Standard	Closes the displayed calibration standard.
Open Standard as Chromatogram	Opens the Standard in the Chromatogram window. Available only if the Standard is opened.	
Link Calibration To Standard	Links currently opened chromatogram of standard to calibration file in which this standard is used. This will enable showing the names of peaks, as they were coined in the calibration file.	

Export

Displays the following Export commands:

- **Export Calibration Curve as Picture to Clipboard** : This command will copy the calibration curve picture into the Windows Clipboard, from which it can be instantly copied by using standard *Paste* command (Ctrl+V). This allows user to quickly utilize picture in another software, e.g. spreadsheet or word processor. This command is also available from the context menu invoked by right mouse-click in the calibration curve area.
- **Export Calibration Curve as Picture...** : This command will open Save As dialog, which will save the picture of current calibration curve into Enhanced Metafile Format (.EMF). This format is extensively supported by Microsoft Windows and Microsoft Office.

This command is also available from the context menu invoked by right mouse-click in the calibration curve area.

**Report Setup**

Selects a report style (**Ctrl** + **Alt** + **P**). The command opens the [Report Setup](#) dialog described on pg. **432**.

**Print Preview**

Displays a preview of the printout prior to actual printing (**Ctrl** + **Shift** + **P**). The command opens the [Print Preview](#) dialog described on pg. **457**.

**Print to PDF**

Prints the report to *.PDF file.

**Send Printed PDF by Email**

Opens new email message in default email client, prints the report to *.PDF and adds created *.PDF file as an email attachment.

**Print**

Selects a printer and starts actual printing (**Ctrl** + **P**). Invoking the command opens the [Print](#) dialog described on pg. **459**.

List of recently opened files so that you can easily get to the method files you are currently working with. The number of files in the list is determined by the *Recent Files* parameter in the [User Options - General](#) tab available from the [Instrument](#) window by *View - Options...* command.

Close Window

Ends the work with the calibration standard and closes the [Calibration](#) window. A message will be displayed if the current calibration file has been changed and not saved yet. Modifications that are not saved are always marked by the inscription MODIFIED after the filename.

4.1.1 Save As...

This command (or the **Ctrl** + **Shift** + **S** shortcut) saves the opened calibration file under a newly desired name. The command opens the *Save As* dialog, similar to the [Open Method](#) dialog described on pg. 68., where the new name can be entered or a new directory selected.

If a file of that name already exists and has been opened in some other Instrument or window, the name cannot be used. Moreover, in the protected mode (in full version Full version only) a user may not overwrite a file he/she is not entitled to modify (for more details see the chapter **User Accounts** on pg. 4).

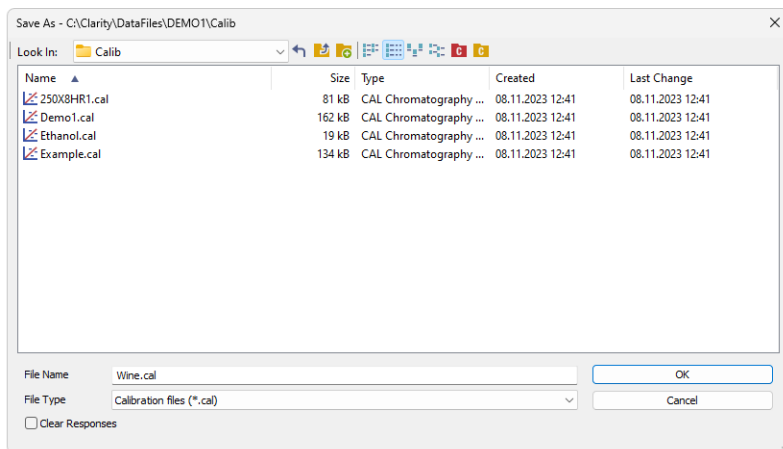







Fig. 191: Save As (Calibration)

Clear Responses

The *Clear Responses* checkbox enables to clear all responses in the new calibration file.

4.2 Edit












Commands for working with the clipboard and individual tables.

 Undo	Cancels the modifications effected in tables (Ctrl + Z).
 Redo	Countermands the <i>Undo</i> command (Ctrl + Shift + Z).
 Cut	Moves the selected text to the clipboard (Ctrl + X).
 Copy	Copies the selected text to the clipboard (Ctrl + C).
 Paste	Copies the clipboard content to the indicated place (Ctrl + V).
Fill Down	Copies the content of current cell to all cells bellow it or to selected range (Ctrl + F). <i>Fill Down</i> is disabled when multiple cells in the same row are selected or when the whole Calibration Summary Table is selected.
Fill Series...	Displays the Fill Series... dialog for filling up incremental values to all cells below it or to selected range. <i>Fill Series</i> is disabled on these columns: <i>Search Window, Peak Selection, Peak Type, Is ISTD, Use ISTD, Peak Color, Response Base, Calculate By, Curve Fit Type, Origin, Weighting Method, Linearisation on X, Linearisation on Y</i> or when the whole Calibration Summary Table is selected.
Select All	Selects all cells of the table (Ctrl + A).
Restore Default columns	Restores the default view of columns.
Setup Columns...	Using this command invokes the Setup Columns dialog, where you can set the display of columns.
Hide Column(s)	Hides selected columns. You can select columns by left-clicking the mouse over the column header, more columns can be selected while holding the Ctrl key.
Show Hidden Column(s)	Shows columns hidden by <i>Hide Column(s)</i> command or Setup Columns dialog.

Detailed description of the commands from the *Edit* menu can be found in the chapter "**Edit**" on pg. **190**.

4.3 Display

This is an entry point to a submenu of commands for displaying chromatograms.

	Preview Graph	Displays/hides the orientation graph.
	Zoom Out	Zooms out the current part of chromatogram. Also invoked by pressing  key.
	Zoom In	Zooms in the current part of chromatogram. Also invoked by pressing  key.
	Previous Zoom	Restores the previous chromatogram cut. (Ctrl + )
	Next Zoom	Restores the original cut abandoned by the <i>Previous Zoom</i> command. (Ctrl + )
	Unzoom	Cancels all cuts. (Ctrl + )
	Tables Up	Swaps the placement of the graph with tables.
	Properties	<p>Controls the displayed graph and chromatogram(s). If you are on the Compounds tab, this command will invoke the Graph Properties - Graph dialog described on pg. 205. If you are on the Individual Compound tab, the Graph Properties dialog will be opened.</p> <p>This command is also available from the context menu invoked by right mouse-click in the calibration curve area.</p>

Detailed description of the *Preview Graph*, *Previous Zoom*, *Next Zoom*, *Unzoom* and *Tables Up* commands is in the chapter "**Display**" on pg. **203**.

4.3.1 Graph Properties

Sets the characteristics for displaying the graph of the calibration curve on the tabs of individual compounds.

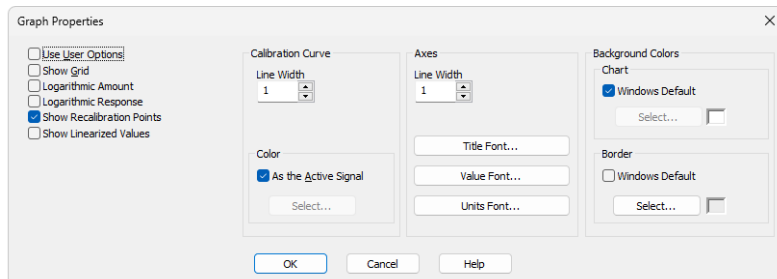


Fig. 192: Graph Properties

Use User Options

All parameter settings will be taken from the global setting in the [User Options](#) dialog - [Graph](#), [Axes Appearance](#) and [Signals & Curves](#) tabs. These tabs are accessible from the [Instrument](#) window by using the *View - Options...* command.

This option is also available directly from the context menu invoked by right mouse-click in the calibration curve area.

Show Grid

Displays/conceals an auxiliary grid to help reading the values from a graph.

Logarithmic Amount

Sets the logarithmic axis for Amount.

Logarithmic Response

Sets the logarithmic axis for Response.

Show Recalibration Points

Displays calibration points along with all of their older versions.

Show Linearized Values

Displays the axes (both X and Y axis) in a linearized form of particular values of calibration points instead in the non-linearized form. Only effective when any linearization (*Linearization X* or *Linearization Y*) is set on the tab of a particular compound.

Calibration Curve

Line Width - Defines the width of calibration curve in points.

Color - Selects the color of the calibration curve.

As the Active Signal - Uses the color of the current signal.

Select... - Selects any desired color.

Axes

Line Width - Sets the width of a line in points.

Title Font... - Selects the font for the graph axes title.

Value Font... - Selects the font for the numerical figures on the axes.

Units Font... - Selects the font for the displayed units of the axes.

Background Colors

Chart - Sets the graph background color (the surface between axes).

Windows Default - Sets the Windows system initial color.

Select... - Selects the desired color.





Border - Sets the window background color (the surface of the outside axes).




Windows Default - Sets the Windows system initial color.

Select... - Selects the desired color.

4.4 Calibration

Commands for creation of calibration and setting parameters.

Set Level	<p>Sets the level to be displayed in the Calibration Summary Table. This serves the identical purpose to the one for level setting in the <i>Calibration</i> toolbar.</p> <p>The selected level is indicated by the heading above the last four columns of the Calibration Summary Table. While the global Calibration Summary Table displays all substances on one of the selected levels, the tabs of individual substances will display all levels of that one particular substance.</p>
Set Signal	<p>Selects the active signal (when using multi-detector calibration). The sub-menu contains a list of available signals in the form of names taken from the signal names used for calibration in the first calibration standard. You can also select the active signal by clicking on the square with the color of the required signal in the <i>Calibration</i> toolbar.</p> <p>The name of the active signal is displayed in the header of the calibration table and in the header of the calibration curve next to the name and retention time of the active compound.</p>
 Add All	<p>Adds or updates all peaks and groups in the calibration standard into the calibration.</p>
 Add Existing	<p>Updates all peaks and groups of peaks that are already in the calibration with the data in the calibration standard.</p>
 Add Peak	<p>Adds or updates the peak selected in the calibration standard into the calibration.</p>
 Add Group	<p>Adds or updates a group of peaks selected in the calibration standard into the calibration.</p>

	Add Named Group	Opens the Edit Named Group dialog to create a new named group to the Calibration Table . Named groups are used for summing the amounts of already calibrated peaks for the purposes of reporting grouped results.
	Delete Compound	Deletes a selected compound from the calibration file. After invoking the <i>Calibration - Delete Compound</i> command or the  icon, use the cursor to select the peak of the compound to be deleted. The command can be aborted anytime by using the Esc key. Compounds may also be deleted from a calibration by deleting the corresponding line from the global table of compounds by using the Delete key or the <i>Delete Compound</i> command from the local menu.
Delete All Compounds	Deletes all compounds from the calibration file. Use of the commands in the Compounds tab cannot be undone using the <i>Undo</i> command. Before using the command a warning message will appear informing you of this condition.	
Clear All Responses	Clears responses on all levels. Use of the commands in the Compounds tab cannot be undone using the <i>Undo</i> command. Before using the command a warning message will appear informing you of this condition.	
Clear All Levels	Clears all responses and amounts on all levels. Use of the commands in the Compounds tab cannot be undone using the <i>Undo</i> command. Before using the command a warning message will appear informing you of this condition.	
Clear Selected Level	Clears all responses and amounts on the selected level. Use of the <i>Clear All Responses</i> , <i>Clear All Levels</i> or <i>Clear Selected Level</i> command on the Compounds tab cannot be undone using the <i>Undo</i> command. Before using the command a warning message will appear informing you of this condition.	

Show Details

Invokes the *Details of Calibration Point* dialog with a detailed log of the selected level of the calibration point. Dialog window provides following details: used, peak retention time, area, height, date of a (re)calibration and the name of the calibration standard.

Note: Changing the response of a compound manually on any level that includes at least one recalibration completely clears the history of a given calibration point. You will be warned by a warning message before doing so.

**Filter Not Used
Compounds**

Hides/shows rows (and related tabs of individual compounds) of **Calibration Summary Table** with disabled *Used* checkbox. Warning is displayed above the table when rows are hidden. Clicking *Show all* disables filtering.

**Options...**

Sets the calibration or recalibration method and implicit values.

4.4.1 Add All

Adds or updates all peaks and groups from the calibration standard into the calibration. Updating refers to recalibration or calibration on further levels. Unlike the *Add Existing* command, the *Add All* command will also add new compounds to the calibration during an update.

When using a multi-signal standard, the command is governed by the *On All Signals / On Active Signal* option.

In the **Calibration Summary Table**, peaks are searched for according to retention time and identification windows. Groups are identified by a letter.

Dependence on type and method of calibration:

- When using Automatic Calibration, all compounds will be brought into the first available calibration file without regard to the current level.
- When using Automatic Recalibration, compounds are recalibrated on the current level. Further adjustments and supplements to the data can be performed later at any time.
- When using Manual Calibration or Recalibration, the (Re)Calibrate Peak or (Re)Calibrate Group dialog will be displayed for direct checking and amendment of data for each compound.
- When using On All Signals or On Active Signal, all peaks are either added on all signals or only on the active signal into the **Calibration Summary Table**.

Note: If you hide the part of the Calibration window with the calibration standard, for example by reducing the Calibration window or enlarging the **Compound Summary Table**, the *Add All*  command will not be active.

4.4.2 Add Existing

Adds or updates existing peaks and existing groups from the calibration standard into the calibration. The behavior of the command depends on whether or not the calibration file already contains compounds:


- When using calibration of a further level or recalibration, only data from already calibrated peaks and groups will be transferred. If you wish to add new compounds to the calibration file, you must use the *Add All*, *Add Peak* or *Add Group* commands.

When using a multi-signal standard, the command is governed by the *On All Signals / On Active Signal* option.


In the **Calibration Summary Table**, peaks will be searched for according to retention time and identification windows. Groups are identified by a letter.

Dependence on type and method of calibration:

- When using Automatic Calibration, all compounds are brought into the first completely free level in the calibration file without regard to the current level.
- When using automatic Recalibration, compounds are recalibrated at the current level. Further adjustments and supplements to the data can later be performed at any time.
- When using Manual Calibration or Recalibration the (Re)Calibrate Peak or (Re)Calibrate Group dialog for the direct inspection and amendment of data will be displayed for each compound.
- When using On All Signals or On Active Signal, existing peaks are either added on all signals or only on the active signal into the **Calibration Summary Table**.

Note: If you hide the part of the Calibration window with the calibration standard, for example by reducing the Calibration window or enlarging the **Compound Summary Table**, the *Add Existing*  command will not be active.

4.4.3 Add Peak


Adds the selected peak from the calibration standard into the calibration. Invoking the *Calibration - Add Peak* command or  icon moves the cursor to the graph of the calibration standard, where the desired peak should be selected. Use the **Esc** key to exit the command at anytime.

When using a multi-signal standard, the command is governed by the *On All Signals / On Active Signal* option.



Dependence on type and method of calibration:

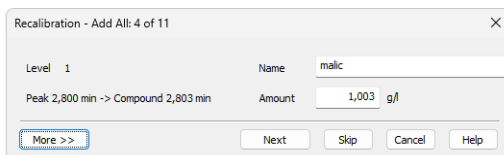
- When using Automatic Calibration, the first available level of the calibration file will be calibrated regardless of the current level.
- When using Automatic Recalibration, the current level is always recalibrated. Data can be modified and supplemented at any later time.
- When using Manual Calibration or Recalibration, the [\(Re\)Calibrate Peak](#) dialog will open once a peak has been selected to enable immediate control and editing of the data.
- When using On All Signals or On Active Signal, the selected peak is either added on all signals or only on the active signal into the **Calibration Summary Table**.

In the **Calibration Summary Table** peaks are identified by their retention times and identification windows. If a peak is not identified in automatic (re)calibration, it is inserted as a new compound at the first level.

Note: If you hide the part of the [Calibration](#) window with the calibration standard, for example by reducing the [Calibration](#) window or enlarging the **Compound Summary Table**, the *Add Peak*  command will not be active.

4.4.3.1 Manual Calibration and Recalibration

This dialog is opened by using the *Add All* () or *Add Peak* () commands when Manual option is selected (default is Automatic). It serves for editing/supplementing data transferred from the chromatogram to the calibration.



Recalibration - Add All: 4 of 11	
Level 1	Name malic
Peak 2,800 min -> Compound 2,803 min	Amount 1,003 g/l
More >>	Next Skip Cancel Help

Fig. 193: Calibrate Peak

Click the *More >>* button to display a more detailed dialog.

When using *Add All* command, information about the currently (re)calibrated peak out of the total number of peaks, is displayed in the title bar (e.g. Recalibration - Add All: 4 of 14).

Fig. 194: Calibrate Peak - More options

Next/OK

Goes to next compound. When last compound is calibrated OK button appears.

Skip

Skips the current compound when calibrating using the *Calibration - Add All* (📌) icon) command.

Cancel

Cancels calibration of the current compound and any remaining (if there are any).

4.4.3.1.1 Level

First Free Level

Indicates the first free level in the calibration.

Current Level

After invoking *Add All* or *Add Peak* command in the *Calibration* mode, *Current Level* is set to the entirely **First Free Level**. In *Recalibrate* mode, *Current Level* displays the level as it has been set in the *Calibration* window.

Caution: Changing current level may result in situation when *Calibration* was selected but *Recalibration* will be performed because current level is already calibrated. User is notified about such situation by blue information icon ⓘ.

4.4.3.1.2 Compound

Name

Refers to the calibrated peak (compound).

Type

Defines the function of the peak in the calibration. The compound *Type* may be:

Ordinary - Designates a peak that is neither a reference peak nor an internal standard. Changing to *Ordinary* sets *Peak Selection* as it is set in the [Calibration Options - Defaults](#).

Reference - Designates a reference peak.

Is ISTD

Defines whether the peak is an internal standard (ISTD) or not (for more details see the chapter **Calculation** on pg. 278)..

Note: Up to 5 compounds in the calibration file may be marked as an internal standard. A group of peaks can neither be an internal standard nor a reference peak.

4.4.3.1.3 Identification

Identification Windows

Search Window

Set *Absolute* if the search window will be set absolutely or *Relative* if it will be set by a percentage value.

Left (Right) Window

Refers to the width of the left/right identification window and is common to all levels of the given peak. For an identified peak the value is taken from the global calibration table, otherwise the default value set by the *Identification Window* fields of the [Calibration Options - Defaults](#) dialog will be displayed. The value set there is used for identification purposes in automated or manual (re)calibrations and in all calibration calculations.

Peak Selection

Defines how the correct peak is matched with the Retention time when several peaks are present in the same identification window. The options available are *Nearest* (closest possible to the selected retention time - default for standard peaks), *First*, *Last* and *Biggest* (default for Reference peaks).

Retention Time

Peak From Standard

Displays retention time of the peak from the standard.

Compound Current

Displays current retention time of the compound that is being calibrated.

Update

Two states are possible:

- *On* will replace the retention time of the **Current Compound** by the value from the **Peak From Standard**.
- *Off* will keep the current retention time.

Note: This option is set in the [Calibration Options](#) dialog - *Update Retention Time* check box and is common to the entire calibration file.

4.4.3.1.4 Quantification

Amount

Indicates the amount of the calibration compound. The units are taken over from the *Quantity Units - Compound* field in the [Calibration Options](#) dialog and are common to the entire calibration file.

Caution: In multi-detector calibration, the *Amount* column is common to all detectors. The amount can be modified on any level, it will always apply to all signals.

Response Base

Area

Peak area in mV.s as the response.

Height

Peak height in mV as the response.

Area Percent

Displays area in mV.s. Percentage is calculated and displayed in the *Calibration Summary Table* once the compound has been calibrated.

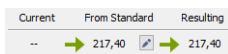



Fig. 195: Cut of Calibrate Peak dialog

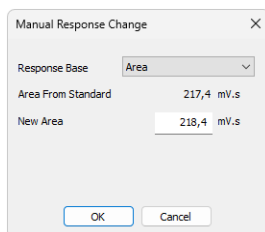
When performing calibration on a new level, the field *Current* will be empty. Field *From Standard* displays response for the given compound from the standard. *Resulting* field displays the new response which will be calibrated when the *OK* button is pressed.

Departure

Departure is displayed only in the *Recalibration* mode. It calculates the deviation between *Current* and *From Standard* fields - indicated by absolute and relative value.

Clicking on the Pencil  button invokes the *Manual Response Change* dialog. *Response Base* can be set to: *Area*, *Height* and *Area Percent*. Text fields change dynamically depending on the selected *Response Base*.


Caution: Manual changes to responses are not recommended, for that reason they are recorded in [Audit Trail](#).



4.4.4 Add Group

To be able to use this command, it is necessary to have the groups already added in the calibration standard, otherwise this command will not work, [see "Add Group"](#).

Adds the selected peak group from the calibration standard to the calibration.


Invoking the *Calibration - Add Group* command or  icon moves the cursor to the graph of the calibration standard, where the desired group should be selected. Use the **Esc** key to exit the command at anytime.

When using a multi-signal standard, the command is governed by the *On All Signals / On Active Signal* option.



Dependence on type and method of calibration:

- When using [Automatic Calibration](#), all data items will be assigned to the first free level of the group regardless of the currently set level.
- When using [Automatic Recalibration](#), the current level is always recalibrated using pre-set values. Data can be modified and supplemented at any time in the calibration table.
- When using [Manual Calibration or Recalibration](#), the [\(Re\)calibrate Group](#) dialog will open once the group has been selected and enable modification of previously entered data.
- When using [On All Signals or On Active Signal](#), the selected group is either added on all signals or only on the active signal into the **Calibration Summary Table**.



Groups are identified by the corresponding letter.

Note: If you hide the part of the [Calibration](#) window with the calibration standard, for example by reducing the [Calibration](#) window or enlarging the **Compound Summary Table**, the *Add Group*  command will not be active.


4.4.4.1 Calibrate Group

Adds data from the calibration standard to the calibration file. This dialog is either opened by the *Calibration - Add All*  icon) or *Add Group*  icon) commands in manual calibration mode. The identifier of the selected group will be displayed in the identification section. The dialog contains items analogous to those displayed in the [Calibrate Peak](#) dialog

4.4.4.2 Recalibrate Group

Adds data from the calibration standard to the calibration file. This dialog is either opened by the *Calibration - Add All*  icon) or *Add Group*  icon) commands in manual recalibration mode. The identifier of the selected group will be displayed in the identification section. The dialog contains items analogous to those shown in the [Recalibrate Peak](#) dialog

4.4.5 Add Named Group

Use the *Calibration - Add Named Group* command (or  icon) to create a new named group in the **Calibration Table**. Named groups are used for summing the amounts of already calibrated peaks for the purposes of reporting grouped results. Invoking the command or icon opens the *Edit Named Group* dialog:

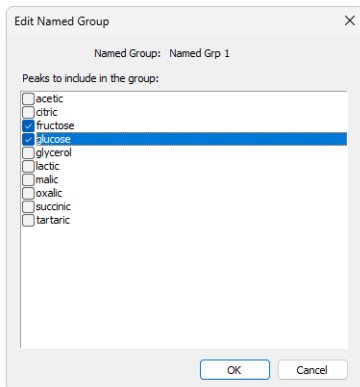


Fig. 196: *Edit Named Group*


Select any number of peaks in **Calibration Table** to be included in the particular **Named Group**. Unlike for standard groups, a peak may be present in several **Named Groups**. All compounds from the **Calibration Table** are listed in the *Edit Named Group* in alphabetical order. To change the compounds included in the given **Named Group**, press the *Edit...* button in the *Named Groups* column of the **Calibration Table** on the appropriate row.

Named groups are identified by the compound name, which can be changed in the **Calibration Table**. Named groups also do not have any particular compound tab in the [Calibration](#) window as their purpose is only to sum the amounts of other calibrated peaks.

In the **Result Table** in the [Chromatogram](#) window, named groups are listed below the *Total* row (to emphasize their amounts are not calculated into the total).

4.4.6 Details of Calibration Point

The *Details of Calibration Point* dialog lists the recalibrations of the given level for the specific compound. Based on the checked recalibrations, the final calibration point for the given level is calculated.

Use the *Calibration - Show Details* command or click  on the row of the level, to invoke the *Details of Calibration Point* dialog.

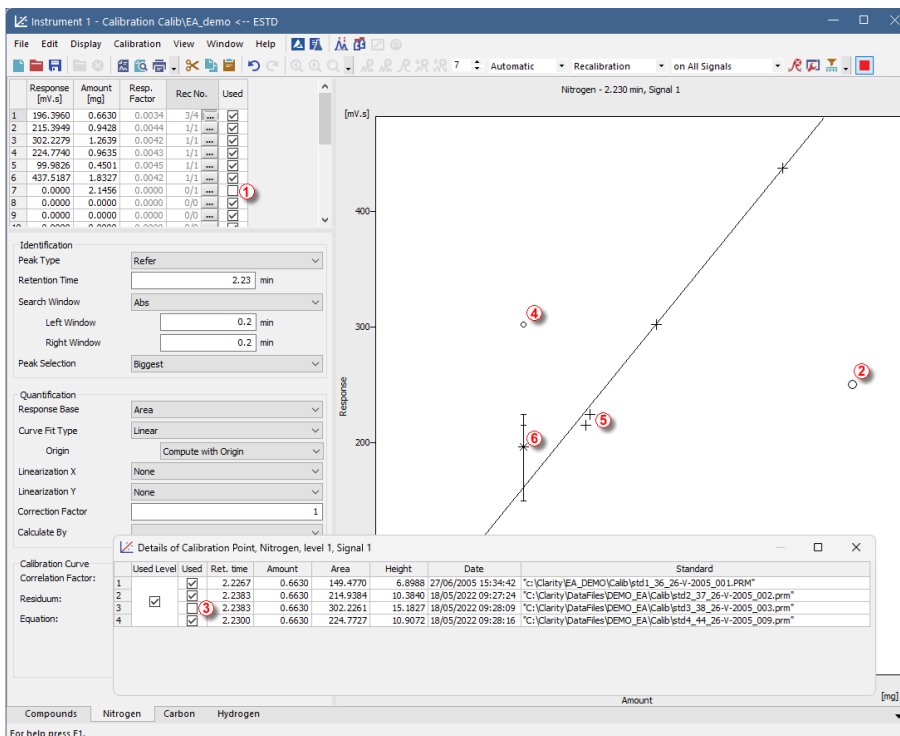







Fig. 197: Details of Calibration Point

The graph displays the calibration curve for the selected compound - *Nitrogen* in this case. If the *Used* check box , in the Levels Table, is not checked, the calibration curve will not use the calibration level in the construction of the calibration curve. Such calibration point is indicated by a big circle  (normally if checked, the point is presented by + sign ).

To omit individual recalibration response from the calculation of calibration curve, deselect the *Used* check box  in the *Details of Calibration* dialog invoked by  in the *Rec No.* column on the respective level.

The calibration point at level 1 consists of overall 4 recalibrations. Only 3 recalibrations were used to compute the calibration point of level 1. Unchecked

recalibrations of a level are indicated in the graph as small circles (4). The resulting point for a level with recalibrations is indicated by an asterisk (6).

Note: If a recalibration is disabled then this recalibration is not used to compute the calibration curve. Moreover the recalibration at (4) is an outer recalibration and hence the line of scattering does not go through that point.

Caution: Once a new recalibration is performed the oldest recalibration will be permanently deleted. Meaning that if **No. of Points** is for example set to 3 and the total number of recalibration is equal to 3, new recalibration (number 4) will delete the oldest one.

4.4.7 Filter Not Used Compounds

Filter Not Used Compounds function can be turned on/off from toolbar (a), **Calibration** menu (b) and local menu of **Calibration Summary Table**.

When active, all rows of **Calibration Summary Table** with disabled **Used** checkbox are hidden. Related individual compound tabs are hidden as well.

When some rows are hidden, warning "**Filtering ON - Not Used Compounds are hidden.**" (c) is displayed above the **Calibration Summary Table**. Clicking **Show all** disables **Filter Not Used Compounds** function. Same warning is also displayed in reports.

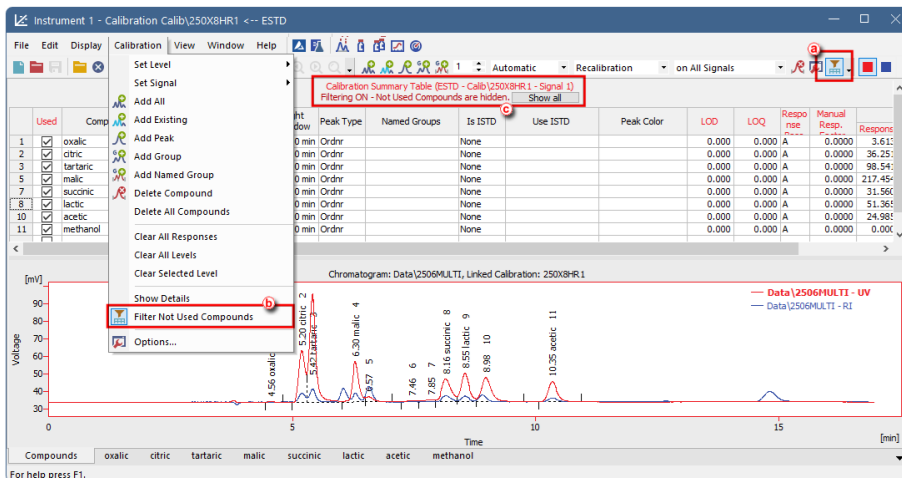



Fig. 198: Filter Not Used Compounds

4.4.8 Calibration Options

This section contains commands for selecting the (re)calibration mode. Invoking the command or using the  icon opens the *Calibration Options* dialog. Settings performed here are then stored in the calibration file. When a new calibration file is created, default values for all of its options are loaded from here.

Calibration Options - Calibration Options

Fig. 199: Calibration Options - Calibration Options

Calibration Description

Contains a brief description of the calibration file. When a calibration file is loaded, this text is displayed in the *Description* field of the [Open Method](#) dialog; it is also shown in the *Description* field of the [Method Setup - Calculation](#) dialog when a calibration is loaded there.

Display Mode

Sets the method of the calibration curve display (suitable for different types of calibration curve use):

ESTD

Displays the dependence of a compound's response to its quantity.

ISTD

Relative calibration curve:

- If the amount of the internal standard has not been entered, displays the dependence of compound/internal standard response ratio to amount of compound.

- If the amount of the internal standard has been entered, displays the dependence of compound/internal standard response ratio to the compound/internal standard amount ratio.

NORM

Displays the dependence of a compound's response to its quantity, just like for the *ESTD* type, but with added checks on calibration and chromatogram validity. Namely, the chromatogram must have empty *Amount* value and all peaks found in the chromatogram must have *Amounts* calculated, either through the calibration or through *Unidentified Peak Response* parameter.

STDADD

Displays the dependence of a compound's response to its quantity, but the graph is shifted so that the calibration curve crosses the x-axis.

Caution: This parameter only indicates the display method. The actual type of calculation upon evaluation of unknown compounds can be selected in the [Chromatogram](#) window in the [Result](#) tab using the *Calculation* parameter.

Number of Signals

Selects the number of displayed signals when a multi-detector calibration is used. The implicit value is *1*. The change is manifested in the number of commands in the *Calibration - Set Signal* menu and in the number of colored squares on the [Overlay](#) toolbar. If a calibration standard chromatogram is opened, the *Number of Signals* matches the number of signals from the calibration standard chromatogram and cannot be changed, i.e. the field is disabled.

Note: You do not risk deleting the calibration values when you reduce the number of signals, since the file always remembers the values for all 32 possible signals.

Calibration

Sets the calibration or recalibration method for the *Add All*, *Add Peak* and *Add Group* commands. Possible options are:

Automatic

Automatically transfers all data related to compounds from a chromatogram to the calibration file. The data can be modified and supplemented later on.

Manual

Enables to enter the amount of the component or to modify or add the remaining data for each compound by opening one of the [Manual Calibration and Recalibration](#) or [\(Re\)Calibrate Group](#) dialogs.

Mode

Sets the mode of the calibration process, unless in the Standard Addition calibrations, where it is disabled.

Calibrate

Calibration mode. Data from the calibration standard will be transferred into the first empty calibration level. Changing the opened standard or closing and reopening the [Calibration](#) window starts checking for a new empty calibration level again. After all 20 calibration levels have been filled in, **Clarity** will rewrite the responses in the last (20th) calibration level.

Recalibrate

Recalibration mode. Unlocks the *Recalibration* section for setting up recalibration conditions.

Caution: The *Calibrate* mode applies only while manually working from the [Calibration](#) window. In the [Single Analysis](#) or [Sequence](#) with calibration level filled in the calibration always recalibrates applying the setting from *Recalibration* options.

Curve Check

Enables to check the linearity of the calibration curve based on the two following parameters. The result of the linearity check is displayed on the tabs of each individual compound in the [Calibration](#) window and in case the *Curve Check* test is failed also in the *Peak Type* column of the **Result Table** in the [Chromatogram](#) window. Fail in any *Curve Check* test part that is switched on fails the whole *Curve Check*.

Deviation

Sets the value for the maximal allowed standard deviation of each point in the calibration curve of the given compound.

Correlation

Sets the value for the minimal allowed correlation factor as calculated on the tab of the individual compounds of the [Calibration](#) window.

Apply On

Specifies where the (re)calibration will be performed. It can be also changed in the toolbar of the [Calibration](#) window.

On All Signals

Calibration or recalibration is performed on all signals. With this option selected, clicking the *Add All* icon adds all peaks from the currently active signal into the **Calibration Summary Table**, existing peaks are then added from all the subsequent signals. This option is default when creating a new calibration.

All added peaks have the *Used* checkbox on all the signals checked.

On Active Signal

Calibration or recalibration is performed on the currently active signal. With this option selected, clicking the *Add All* icon adds all peaks from the currently active signal into the **Calibration Summary Table**.

All added peaks have the *Used* checkbox checked only on the active signal, rest of the signals have it cleared.

Recalibration

Specifies the recalibration mode conditions:

Replace

The original response is replaced by the new one and the number of recalibrations is set to one.

Average

The resulting value is calculated as the arithmetic mean of the new value and all previous values (their number is taken over from the *Rec. No.* column of the *Compound Summary Table*).

No. of Points

Sets the number of recalibrations used for the Averaging. When the number of recalibrations exceeds this number, averaging calculates floating average.

Available range is 0 - 100, default value is 10.

Note: Change in the number of recalibrations will not immediately affect the calculation of Average. Changes will affect future recalibrations.

Compound Units

Specifies the units for compound quantities. Units are stated for all displayed amounts in calibration tables and graphs as well as in the table of integration results in the [Results](#) tab, unless other units are specified by *Scale Factor* and *Units after Scaling* fields.

Recalibration Search Criteria

The maximum percent deviation (departure) of the new values for the recalibration to be effected. In the event it has been exceeded in manual recalibration the inscription *Over* replacing the numerical value of the deviation will notify you. When using automatic recalibration components whose deviation in height or area exceeds the pre-set value are not recalibrated. The allowed range is 1 to 50 %.

Enable Manual Response Value Change

Enables the manual modification of responses (in the *Response* or *Area* and *Height* fields).

Update Retention Time

Enables the automatic update of retention time after each calibration or recalibration. The retention time is replaced using the value from the last used standard, regardless of its level.

Default Injected Volume

The value is used to perform automatic correction for differences in injected volume. In calibration, recalibration and calibration calculations the value of *Inj. Volume* from the chromatogram header is compared with *Default Injected Volume* and a new response is calculated from their ratio.

This correction method is only applicable to small deviations since it assumes that the amount is proportional to the response.

If the checkbox is left unchecked, the last recalculated values remain in effect regardless of potential changes effected in *Injected Volume* and *Default Injected Volume* fields. In this instance the last two parameters serve only for information.

Checking the checkbox and filling a value for *Default Injected Volume* will be recorded in [Calibration Audit Trail](#) and [Details of Calibration Point](#) - detail of the changes are recorded in the following format: *Corrected by Injection Volume (Default X mL, Actual X mL)*.

Retention Indexes use Log. Interpolation with Unretained Peak

Use *Unretained Time* value (set on the [Method Setup - Advanced](#) tab) for retention index calculation (for more details see the chapter **Calculation** on pg. 101).

Caution: When this option is unchecked, then the retention indexes are calculated using the **linear interpolation** and when it is checked, then the **logarithmic interpolation with unretained peak time** is used.

Equation used for the linear calculation of the Retention Indexes:

$$I = 100 \cdot \left[n + (N - n) \frac{t'_{r(\text{unknown})} - t'_{r(n)}}{t'_{r(N)} - t'_{r(n)}} \right]$$

Where:

- I = Kovats retention index,
- n = the number of carbon atoms in the smaller n-alkane,
- N = the number of carbon atoms in the larger n-alkane,
- z = the difference of the number of carbon atoms in the smaller and larger alkane,
- t_r = the retention time.

Equation used for the logarithmic calculation of the Retention Indexes:

$$I = 100 \cdot \left[n + (N - n) \frac{\log(t'_{r(\text{unknown})}) - \log(t'_{r(n)})}{\log(t'_{r(N)}) - \log(t'_{r(n)})} \right]$$

Where:

- I = Kovats retention index,
- n = the number of carbon atoms in the smaller n-alkane,
- N = the number of carbon atoms in the larger n-alkane,
- t_r' = the adjusted retention time ($t_r' = t_r - t_0'$).

Response Factor as Response / Amount

Enables calculating Response Factor as $RF = \text{Response} / \text{Amount}$ (on default : $RF = \text{Amount} / \text{Response}$). This setting changes the format of RF in [Calibration](#) window

as well as on [Results](#) tab of the [Chromatogram](#) window.

4.4.8.1 Defaults

Calibration Options - Defaults

Defines parameters that will be used for new compounds.

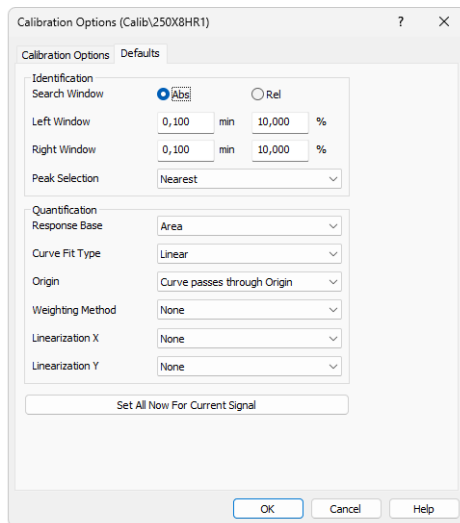


Fig. 200: Calibration Options - Defaults

Identification

This section handles the defaults for the identification, such as parameters of *Search Window* or *Peak Selection*. These conditions are more closely described in the chapter "**Calibration**" on pg. 321.

Search Window

Defines the default calculation type of both Left and Right identification window boundaries. Defines whether the Left Window and Right Window content will be inserted in *Abs* (absolute - set in minutes) or *Rel* (relative - set in percents of the Reten. Time) values.

Left (Right) Identification Window

Defines the width of the left (right) identification window (in minutes or percents).

Peak Selection

Defines how the target peak will be selected in a given identification window. The available options are the peak *Nearest* to the exact retention time set in the calibration, *First* peak in the identification window, *Last* peak in the identification window and the *Biggest* peak in the identification window.

Note: The peaks that are identified must still follow the trend of rising retention times, so when two identification windows are selected so that they overlap each other, the first compound must define a peak with lower retention time than the second compound. Moreover, each peak in the calibration must be defined using a unique retention time.

Quantification

This section handles the defaults for the quantification, or in other words how it will be quantified. These conditions are more closely described in the chapter "**Calibration**" on pg. 321.

Response Base

Indicates the type of response used: *Area*, *Height* or *Area Percent*.

Curve Fit Type

Indicates the type of curve fitted to the data (for more details see the chapter **Calibration** on pg. 331).

Origin (Ending Point)

Defines the treatment of the origin point in the calibration graph (for more details see the chapter **Calibration** on pg. 332).

Weighting Method

Defines the weighting method of calibration points upon interlining of the curve (for more details see the chapter **Calibration** on pg. 333).

Linearization X

Defines the default X-axis display on the tabs of individual compounds. Possible values are *None*, *1/Amount*, *ln(Amount)*, *sqrt(Amount)*, *1/sqrt(Amount)*, *Amount^2*, *1/Amount^2* and *log(Amount)*.

Linearization Y

Defines the default Y-axis display on the tabs of individual compounds. Possible values are *None*, *1/Response*, *ln(Response)*, *sqrt(Response)*, *1/sqrt(Response)*, *Response^2*, *1/Response^2* and *log(Response)*.



Set All Now For Current Signal

Sets the selected parameters for all compounds in current calibration and current signal.

Caution: Pressing the *Set All Now For Current Signal* button is different from pressing the OK button, which will cause the use of set parameters for future signals and compounds.




4.5 View

This section contains commands that govern the appearance of the [Calibration](#) window.


Toolbars	<p>Displays commands for toolbars. The command is similar to the <i>Toolbars</i> command in the main Clarity window.</p> <ul style="list-style-type: none">• Standard, Edit, Calibration, Signals: Hides/shows the respective toolbar.• Customize...: Customization of items in the toolbars.• Reset All: Returns all menus and default toolbars in the Chromatogram window into their initial state. <p><i>Note:</i> <i>Reset All</i> does not display hidden toolbars. To show them invoke <i>Customize... - Toolbars</i> menu.</p>
Maximize Graph	<p>Enlarges the chromatogram over the whole window or conceals the Compound Summary Table underneath. This may also be performed by double-clicking on the edge of the graph close to the splitter where the cursor arrow changes to . This command is only valid for the Compounds tab.</p>
Show Both	<p>Displays both parts of the window (chromatogram and tabs). This command is only valid for the Compounds tab.</p>
Maximize Table	<p>Enlarges the part of the window with the Compound Summary Table over the whole window or conceals chromatogram. This action may also be performed by double-clicking on the edge of the table section close to the splitter where the cursor arrow changes to . This command is only valid for the Compounds tab.</p>

4.6 Window

This is an entry point to a submenu of commands for displaying other main windows.

Main 	Displays the Clarity main station window described on pg. 1 .
Instrument	Displays the Instrument window described on pg. 60 .
Chromatogram	Displays the Chromatogram window described on pg. 162 .
Single Analysis	Displays the Single Analysis window described on pg. 113 .
Sequence	Displays the Sequence window described on pg. 385 .
Data Acquisition	Displays the Data Acquisition window described on pg. 369 .
Device Monitor	Displays the Device Monitor window described on pg. 135 .
Station Audit Trail 	Displays the Audit Trail window described on pg. 413 .
Calibration Audit Trail 	Displays the Calibration Audit Trail window described on pg. 427 .

5 Data Acquisition

Displays the signal from detectors configured on the given Instrument. The *Data Acquisition* window can be opened using the *Monitor - Data Acquisition* command or using the  icon in the [Instrument](#) window. During the measurement the name of the measured chromatogram is displayed in the window header.

Note: It is possible to switch between signals and hide/display them in the same way as in the [Chromatogram](#) window.

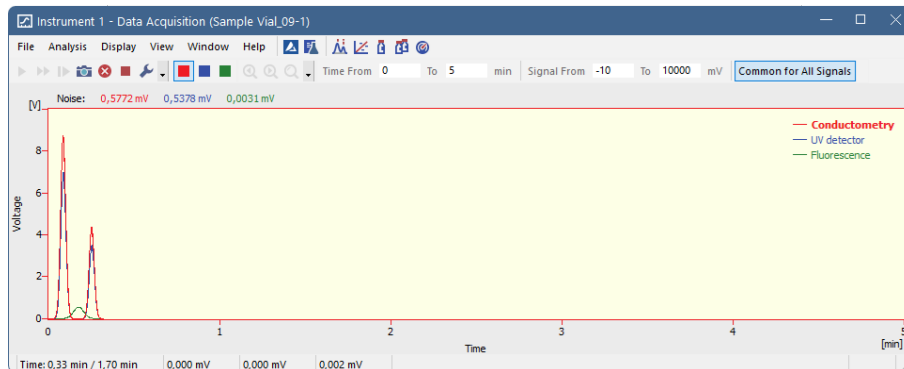


Fig. 201: Data Acquisition

Note: When the analysis is started, it takes some time to initialize the detector (200 ms for **DataApex** Converters). In this time, the data is not valid.

The window contains two fundamental parameters, **Time** and **Signal**. In the default setting (if you have the *Context Axes* item set in the *View* menu) the function of these two parameters will be dependent on whether an analysis is currently taking place:

a) Analysis not running (state *STOP*, *WAITING* or *IDLE*):

The axes are set as *Floating Axes*.

Time Range

Sets the width of display window in minutes (e.g. 0 - 20 min). Should the signal exceed the set time, the window will be reset and the signal will once again be displayed from the start. Maximum value is 300 min.

Signal Range

Sets the height of display window in units set for the given active signal. (in range 0.01 - 1000000000 mV or equivalent units). The window dynamically monitors the course of the signal and is automatically redrawn after reaching the upper or lower edge for the given signal.

b) Analysis running (state *RUNNING*):

The axes are set as *Fixed Axes*. This means that if the current time or the level of the signal exceeds any of values set, the window is not redrawn and the signal is not displayed.

Time: from... to...

Sets the fixed range of displayed time in minutes.

Signal: from... to...

Sets the fixed range of the signal in units selected for the given active signal.

Note: Automatic switching between the fixed and floating range of axes, depending on whether analysis is taking place or not, may be canceled by switching the axes display in the *View* menu from *Context Axes* to *Fixed Axes* or *Floating Axes* (for more details see the chapter *View* on pg. 380).

Common for All Signals

If selected (highlighted in orange) the Y axis is common for all signals as is the range selected either in the *Signal Range* (when Analysis is not running) or in the *Signal: from... to...* (when Analysis is running). All signals are shown proportionally, so their Y value can be approximately read from the Y axis.

Note: If the *Common for All Signals* is not selected, the Y axis is scaled to the active (i.e. selected) signal only. The remaining signals are not shown adequately to the Y axis of the selected signal.

Status Bar

Fig. 202: Data Acquisition - Status Bar

The *Data Acquisition* window contains the following items in the status bar:

Time [min]

Displays the current time of an analysis in minutes (only during the measurement).

Current Signals

Displays the immediate value of all signals connected to the Instrument, along with appropriate signal units.

Note: If the detector range exceeds the tolerance limit by $\pm 1.285\%$, the *OVER* string in red lettering will be displayed in the part of the status bar corresponding to the detector.

Background Chromatogram ✓ Full version

If it has been defined, using the *File - Set Background Chromatogram* command, the name of the background chromatogram will appear in the

status bar. If the workstation is in the *WAITING* state, the chromatogram will not be displayed and its title in the status bar will be shaded gray.

Subtraction Chromatogram

If it has been defined in the [Method Setup - Advanced](#) dialog and the display has been set using the *File - Show Subtraction Chromatogram* command, the name of the subtraction chromatogram will appear in the status bar.

5.1 File

A submenu of commands used for displaying chromatograms in the background.

Set Background

Chromatogram

Displays the background chromatogram on the background of the [Data Acquisition](#) window. Invokes the [Open Chromatogram](#) dialog, in which you may select which of the measured chromatograms you would like to display on the background of the running analysis.

The background chromatogram is colored gray in order to prevent it from being mistaken with the measured signal. It will only be displayed after the measurement has been started.

Close Background

Chromatogram

Switches the display of the background chromatogram off.

Show Subtraction

Chromatogram



Determines whether the subtracted chromatogram defined in the *Subtraction* section of the method file ([Method Setup - Advanced](#)) will be displayed in the background of the [Data Acquisition](#) window. The checkmark will appear before the command if the display is activated.





Close Window

Closes the [Data Acquisition](#) window.

5.2 Analysis

Submenu with commands for controlling the running of the analysis.

 Send Method	It sends the method to all connected control modules/hardware. This button is not available during data acquisition.
 Run Single	Starts individual measurement. A change of color in the background of the graph in the Data Acquisition window and the commencement of time counting in the status bar will indicate a running measurement. This command can be selected during the measurement only when <i>External Start</i> setting in the Method Setup - Measurement dialog is set to <i>Start-Restart</i> . Invoking the command terminates measurement and at the same time starts another one. This feature is often called "Continuous Measurement". Invoking the command during analysis is possible only when there are analog detectors (INT7, Net-PAD, ...) on instrument. If there is one or more digital detectors on instrument, invoking the command during analysis is not possible. This command is inactive during sequence measurement.
 Run Sequence	Starts the sequence measurement. Measurement will be performed according to the current sequence file in the Sequence window. A change of color in the background of the graph in the Data Acquisition window and the commencement of time counting in the status bar will indicate a running measurement. This command is inactive during analysis.
 Resume Sequence	Resumes the operation of a suspended sequence. This function may also be invoked by pressing the Ctrl + Space bar shortcut (for more details see the chapter Sequence on pg. 402).

	Snapshot	<p>Saves the data from the running analysis to a chromatogram without terminating the measurement. The snapshot chromatogram will be automatically replaced by the final chromatogram after the analysis is finished.</p> <p>If the modifications of a snapshot chromatogram have to be preserved, it is necessary to save the snapshot chromatogram under a different name (using the <i>Save As</i> command) before the end of the analysis.</p>
	Stop	<p>Immediately terminates an individual measurement and processes it. The Instrument will return to the <i>STOP</i> or <i>WAITING</i> state. If the control program for HPLC pumps or other devices is still running, the <i>CONTROL</i> state will be displayed.</p> <p>When running a sequence measurement, it will be terminated after the length of analysis set in the <i>Enable Autostop - Run Time</i> field of the Method Setup - Measurement dialog has elapsed.</p>
	Abort	<p>Terminates the measurement without storing and processing any data. The Instrument will return to the <i>STOP</i> or <i>WAITING</i> state. Any control program for HPLC pumps will be stopped. Running gradient will be also stopped immediately and the device should be properly conditioned by the user before next analysis.</p> <p>The sequence will be terminated without processing the current analysis. The sequence run can be continued from the actual point using the <i>Resume</i> command.</p>
Set Autostop		<p>Opens the Method Setup - Measurement dialog where the <i>Enable Autostop and Run Time</i> parameters can be set.</p>
	Set Zero	<p>Sets the active signal value as offset. That means that the current value of the signal will be subtracted from the signal from now on. The offset value can be reset using <i>Reset Zero</i> command. The <i>Set Zero</i> function is only active when the measurement is not running.</p>

**Reset Zero**















Resets the subtracted offset value set using the *Set Zero* command to 0.

The offset value is automatically reset when an Instrument is closed.

Note: The above commands are similar to the commands in the [Single Analysis](#) dialog described on pg. 113.

5.3 Display

A submenu of commands for setting up the graph display.

	Zoom Out	Zooms out the current part of chromatogram. Also invoked by pressing  key on numeric keyboard.
	Zoom In	Zooms in the current part of chromatogram. Also invoked by pressing  key on numeric keyboard.
	Previous Zoom	Invoking the command, using the  icon or the Ctrl +  shortcut on numeric keyboard displays the previous cut-out. Use the command repeatedly to browse backwards through the history of the cut-outs - the workstation remembers cut-outs which have been performed since the Data Acquisition window was opened.
	Next Zoom	Invoking the command, using the  icon or the Ctrl +  shortcut on numeric keyboard progressively returns to original cut-outs, which had been abandoned using the <i>Previous Zoom</i> command. Use the command repeatedly to browse forwards through the history of the cut-outs. The workstation remembers cut-outs which have been performed since the Data Acquisition window was opened.
	Unzoom	Invoking this command, using the  icon or Ctrl +  shortcut on numeric keyboard cancels all cut-outs and displays chromatogram in its original size.
	Properties...	Opens the Graph Properties dialog for displaying the graph display settings.

5.3.1 Properties...

Sets the characteristics of the [Data Acquisition](#) window display. Invoking the command opens the *Graph Properties* dialog.

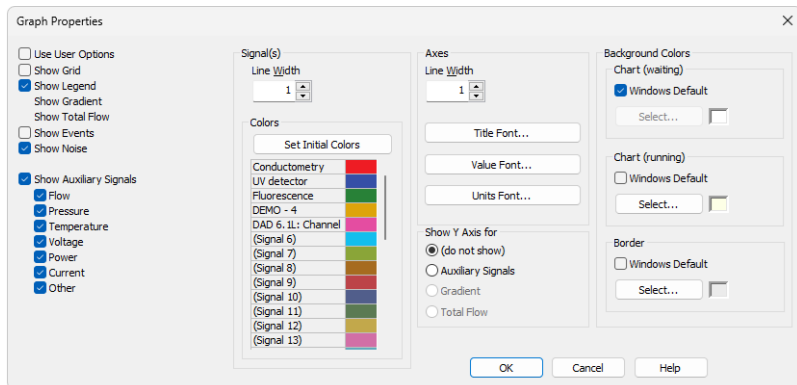


Fig. 203: *Graph Properties*

Use User Options

All parameter settings will be taken from the global settings of the [Graph](#), [Axes Appearance](#) and [Signals & Curves](#) tabs of the [User Options](#) dialog, accessible from the [Instrument](#) window by using the *View - Options...* command.

Show Grid

Displays/conceals auxiliary grid for easier reading of values in graph.

Show Legend

Displays/conceals names of the individual signals including the eventual subtraction chromatogram and background chromatogram.

Show Gradient

Permits the display of gradient when using direct control of LC pumps.

Show Total Flow

Permits the display of total flow when using direct control of LC pumps.

Show Events

Permits the display of events from the **Event Table** in the [Data Acquisition](#) window.

Show Noise

Permits the display of **Noise** (along with appropriate units) in the upper left corner of the graph. Noise in the [Data Acquisition](#) window is calculated using the cubic interlining to reduce the influence of the trend to its values.

In the [Chromatogram](#) window and [Results](#) tab the **Noise** values are calculated using the linear interlining on the interval defined in the **Integration** table. If there is a peak in this interval, it will influence the noise values. If there are multiple intervals defined in the **Integration** table the last one will be applied.

Show Auxiliary Signals

This section determines which auxiliary signals will be displayed in the graph of the [Data Acquisition](#) window. Each auxiliary signal is included in one of the following categories: *Flow*, *Pressure*, *Temperature*, *Voltage*, *Power*, *Current* and *Other*. The display of all signals in each category is allowed together. Note those options are only available if they are configured on the instrument.

Signal(s)

Line Width

Selects the curve width in points.

Colors

Selection of color of the signal

Set Initial Colors - Sets the display colors to the default state. It will be overridden by **Use User Options** if checked.

Select... - Click the particular color to change it.

Axes

Line Width

Selects the axes width in points.

Title Font...

Selects the font for graph axes title.

Value Font...

Selects the font for numerical figures on axes.

Units Font...

Selects the font for displayed units of axes.

Show Y Axis for

Determines whether the second (right) Y axis will be displayed and for which signal. The axis may be displayed for the **Gradient** (the percentage rate of individual compounds), **Total Flow** or **Auxiliary Signals**. The *Show Gradient* and *Show Total Flow* options must first be checked in order to display the Y axis for this particular signal. Applies only to the directly controlled devices with auxiliary signals.

Background Colors

Chart (waiting)

Sets the color of the graph background (surface of the graph between axes).

Windows Default - Sets the initial color of Windows system.

Select... - Serves for selecting of the desired color.

Chart (running)

Sets the graph background color (surface between axes) when the analysis is running. Setting a different colored background to the graph enables you to quickly differentiate as to whether an analysis is actually

running or if the detector signal is merely being monitored in the [Data Acquisition](#) window.

Windows Default - Sets the initial color of Windows system.

Select... - Serves for selecting of the desired color.

Border

Sets the color of the window background (surface outside axes).

Windows Default - Sets the initial color of Windows system.

Select... - Serves for selecting of the desired color.

5.4 View

Toolbars	<p>Displays commands for toolbars. The command is similar to the <i>Toolbars</i> command in the main Clarity window.</p> <ul style="list-style-type: none"> • Analysis, Signals, Zoom, Axis Range: Hides/shows the respective toolbar. • Customize...: Customization of items in the toolbars. • Reset All: Resets the menu and toolbars back to their initial state as they were from the initial installation of the Clarity. <p><i>Note:</i> <i>Reset All</i> does not display hidden toolbars. To show them invoke <i>Customize... - Toolbars</i> menu.</p>
Grid Lines	<p>Displays/conceals auxiliary grid for easier reading of values in the graph.</p>
Fixed Axes	<p>Sets the fixed range axes display. The range of signal axis is determined by entering the lower and upper limit (e.g. 15 - 30mV) both in the analysis and outside of it, the range of the time axis is determined by entering the time range (outside of the analysis) or lower and upper limit (during the analysis - e.g. 0 - 20min).</p>
Floating Axes	<p>The range is defined by its size (e.g. $\pm 20\text{ mV}$; 5 min) While being displayed, the display will "float" so that the signal always stays in the displayed part of the graph. If the signal exceeds the y-axis range, the graph is moved vertically so the actual signal value will be in the center of the left axis. If the signal reaches end of the time range, the graph is redrawn from beginning.</p>
Context Axes	<p>Automatically switches between <i>Fixed Axes</i> and <i>Floating Axes</i> setting according to whether the workstation is measuring the analysis (in the <i>RUNNING</i> state) or is merely monitoring the signal (<i>WAITING</i> state). When measuring, the <i>Fixed Axes</i> display will automatically be used, while when in the <i>WAITING</i> state, the <i>Floating Axes</i> will be used.</p>

Auto Axes	<p>For the time axis, automatically switches between <i>Fixed Axes</i> and <i>Floating Axes</i> setting according to whether the workstation is measuring the analysis (in the <i>RUNNING</i> state) or is merely monitoring the signal (<i>WAITING</i> state). When measuring, the <i>Fixed Axes</i> display will automatically be used, while when in the <i>WAITING</i> state, the <i>Floating Axes</i> will be used.</p> <p>The signal axis behaves the same as when set to <i>Floating Axes</i> while the analysis is not <i>RUNNING</i>. While it is <i>RUNNING</i>, the range of the signal axis starts at a minimal value and enlarges according to the signal course; thus, the signal is always displayed in the graph and the view is not overly large at any moment of the analysis - the signal always fits in it.</p>
Reset Axes Ranges	Sets the default values into all fields of the Axes Ranges dialog.
Set Axes Ranges...	Opens the Axes Ranges dialog used for defining the ranges of all signals in the Data Acquisition window, both in the run and outside of the analysis run, including ranges used for auxiliary signals.
Show Spectrum	Toggle command displaying the current spectrum during running acquisition. Only available on the PDA or MS instrument types (requires PDA Extension or MS Extension).

5.4.1 Axes Ranges

The *Axes Ranges* dialog, serving for setting the axes ranges both during the acquisition run and outside of it, can be invoked using the *Set Axes Ranges...* command from the *View* menu of the [Data Acquisition](#) window.

Common Settings			
	From	Fixed To	Floating Range
Time Axis	0 min	5 min	1 min
Signal Axis	-10 mAU	1000 mAU	5 mAU

Individual Settings			
	From	Fixed To	Floating Range
Detector 1	-10 mAU	1000 mAU	10 mAU
Detector 2	-10 mAU	1000 mAU	10 mAU
Detector 3	-10 mAU	1000 mAU	10 mAU

Auxiliary Signals			
	From	To	Auto
Oven Temp			<input checked="" type="checkbox"/>
Inj. Temperature			<input checked="" type="checkbox"/>
Det. Temperature			<input checked="" type="checkbox"/>
Pressure			<input checked="" type="checkbox"/>
Det. Pressure			<input checked="" type="checkbox"/>
Lamp. Pressure			<input checked="" type="checkbox"/>

Fig. 204: Axes Ranges

The settings performed in the *Axes Ranges* dialog are applied to all of the display possibilities in the [Data Acquisition](#) window - *Fixed Axes*, *Floating Axes*, *Context Axes* and *Auto Axes*. Only some of the settings are usually valid for each axes display type. Default values in the *Axes Ranges* dialog may be set by using the *Reset Axes Ranges* command from the *View* menu of the [Data Acquisition](#) window.

Common Settings

Sets the ranges for time axis and for the signal axes in case when *Common for All Signals* button in the [Data Acquisition](#) window is selected. The values are set in appropriate value units for the given detector.

Time Axis

Sets the range of the time axis both in the mode where start display time (*From*) and end display time (*To*) are set and where the total range (*Range*) of the time axis is set. The time values are set in minutes.

Signal Axis

Sets the range for the signal axes, both for the regular and auxiliary signals.

Individual Settings



Sets the signal axis ranges for individual detectors.

Auxiliary Signals


Sets the auxiliary signal axis range for auxiliary detectors. When the *Auto* checkbox is checked, the auxiliary signal axis range starts at a minimal value and enlarges according to the auxiliary signal course. While unchecked, the axis range is fixed with the values entered.

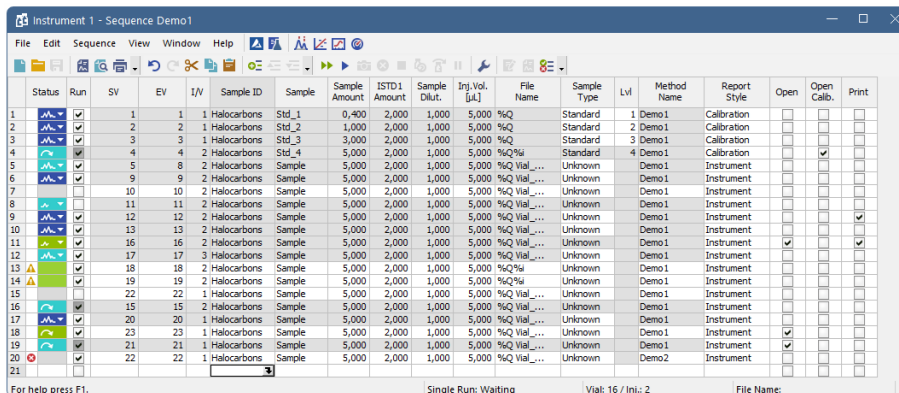
5.5 Window

This is an entry point to a submenu of commands for displaying other main windows.

Main 	Displays the Clarity main window described on pg. 1 .
Instrument	Displays the Instrument window described on pg. 60 .
Chromatogram	Displays the Chromatogram window described on pg. 162 .
Calibration	Displays the Calibration window described on pg. 320 .
Single Analysis	Displays the Single Analysis window described on pg. 113 .
Sequence	Displays the Sequence window described on pg. 385 .
Device Monitor	Displays the Device Monitor window described on pg. 135 .
Station Audit Trail 	Displays the Audit Trail window described on pg. 413 .

6 Sequence

This Chapter describes window which is used for consecutive measurement of multiple samples. Open the window using the  icon or the *Analysis - Sequence* command from the [Instrument](#) window.



Status	Run	SV	EV	I/V	Sample ID	Sample	Sample Amount	ISTD1 Amount	Sample Dilut.	Inj. Vol. [µL]	File Name	Sample Type	Lvl	Method Name	Report Style	Open	Open Calib.	Print
1	1	1	1		Halocarbons Std_1	0,400	2,000	1,000	5,000	%Q	Standard	1	Demo.1	Calibration				
2	2	1	1		Halocarbons Std_2	1,000	2,000	1,000	5,000	%Q	Standard	2	Demo.1	Calibration				
3	3	3	3		Halocarbons Std_3	3,000	2,000	1,000	5,000	%Q	Standard	3	Demo.1	Calibration				
4	4	4	4		Halocarbons Std_4	5,000	2,000	1,000	5,000	%Q	Standard	4	Demo.1	Calibration				
5	5	8	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
6	9	9	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
7	10	10	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
8	11	11	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
9	12	12	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
10	13	13	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
11	16	16	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
12	17	17	3		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
13	18	18	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
14	19	19	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
15	22	22	1		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
16	15	15	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
17	20	20	1		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
18	23	23	1		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
19	21	21	1		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.1	Instrument				
20	22	22	2		Halocarbons Sample	5,000	2,000	1,000	5,000	%Q	Via_...	Unknown	Demo.2	Instrument				
21																		

Fig. 205: Sequence


The window includes a [toolbar](#), sequence table and status bar.

Table description

Each line defines the settings for one or more injections. To process several vials from a single line enter a different value for the initial = start (SV) and last = end (EV) vial. The I/V parameter indicates that there will be multiple injections taken from a single vial.

Status

Status of the row in the sequence.

 Indicates a row with one or more errors, such row is disabled from running.





 Indicates a row with one or more warnings, measurement will still be carried out.

Note: Warning *Calibration already exists* is caused by non-unique name of cloned calibration. Adjusting the name for cloned calibration in *Method Setup - Calculation* resolves the problem.


Point mouse cursor over the icon in the *Status* column to display a tooltip with detailed description about the injections - it displays how many were measured, skipped, aborted and how many are remaining on the specific row.

Note: Analysis will be marked as finished after the analysis time elapsed. Note that the instrument method may be still running.

Tab. 28: List of possible states of sequence rows

Status	State	Description
	Ready	No analysis has been carried out from this row. Measurement will be carried out.
	Ready	No analysis has been carried out from this row. At least one vial has been skipped. Rest of the vials will be measured.
	Ready	Analysis has been stopped during acquisition. At least one chromatogram has been measured. Rest of the vials will be measured.
	Running	Analysis from this row is being carried out.
	Completed	All analyses on this row have been measured.
	Partially completed	Apart from the vial(s) where the <i>Skip Vial</i> command has been used, all analyses on this row have been measured.
	Partially completed	Command <i>Skip Vial</i> has been used on all vials. No more measurement will be carried out from this row. If icon changes color to green and back to original when (un)checking <i>Run</i> checkbox then there are vial(s) that still can be measured.
	Partially completed	Analysis has been stopped during acquisition. At least one chromatogram has been measured. <i>Run</i> checkbox is unchecked and measurement will not continue unless checking the <i>Run</i> checkbox.
	Disabled	Row that has been omitted from the sequence. Caused either by an error on the row or by unchecked <i>Run</i> checkbox.

Already measured rows will be blocked against changes (dimmed) in all columns except for *Run*, *Sample Type*, *Lvl*, *Report Style* and *Postrun functions*, columns which can be changed for reprocessing.

If there is a chromatogram resulting from this row, small triangle will appear in the icon - e.g.  (currently measured row with at least one already measured chromatogram). Left mouse click on the triangle will reveal option to open the chromatogram(s). See **Fig. 206** on pg. 387..

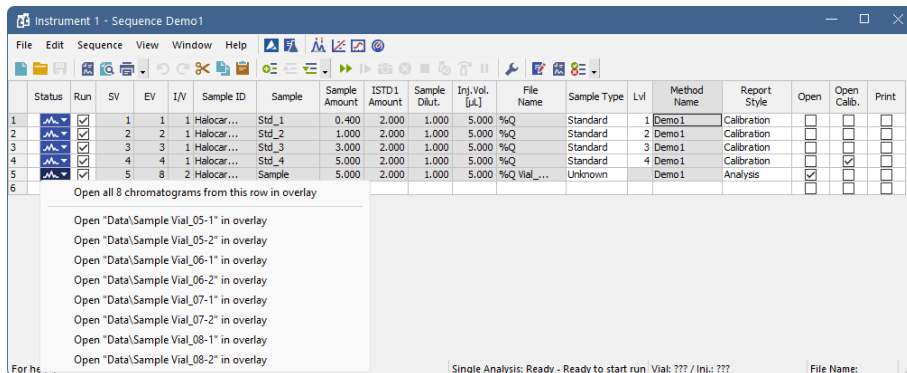


Fig. 206: Open chromatograms in overlay

It is possible to open one specific chromatogram or open all measured chromatograms in overlay.

Selected row(s) will return to their initial *Status* (all fields green) in the following cases:

- Running of the sequence (by *Run* command, the icon or **F5** or **Ctrl + Q** shortcut) and clicking *Reset* button in the displayed dialog.
- Using the *Edit - Reset Status* command (**Ctrl + E**).

Note: A text description will be printed in the printouts instead of colored tags in the *Status* column.

Run

Selects whether the particular line in the **Sequence Table** will be measured. The column corresponds to the *Run Lines* field in [Sequence Options](#) dialog. Working with *Run* column is more suitable for discontinuous selection of lines or for exclusion of individual lines from measurement.

SV

Number of the first vial used in the processing of the given row.

EV

Number of the last vial used in the processing of the given row. Its number must be the same or higher than the number entered in the *SV* field. The difference between the end and start vial defines how many vials will be processed by selected line.

If *Options - Format - Automatically* setting has been applied, then for more than one vial or injection, the *File Name* pattern will automatically be verified and corrected to ensure that it is in the correct format. In other words, *%v* and *%i* variables will be added to the pattern.

If automatic formatting has been applied, the variables in the filename will be supplemented with zeros from the left in order to correspond with defined number of injected samples (e.g. names will be supplemented by numbers ranging from 001 to 100 for *SV 1* and *EV 100*).

Note: Some autosamplers may support alphanumerical or graphical setting of the SV or EV parameter. In such case, an arrow will appear in the right side of the given field, and clicking it will open particular *Select Vial* dialog.


I/V

Indicates how many injections will be processed from each vial based on this line in the **Sequence Table**.

If the *Format - Automatically* item from [Sequence Options](#) dialog has been activated, then, for multiple vials or injections, the *File Name* pattern will automatically be verified and corrected to ensure that it is in the correct format. In other words, the %v and %i variables will be added to the template.


Sample ID

The sample identification field will be transferred to the headers of all created chromatograms. Maximum number of characters in this field is limited to 64. The parameter corresponds to the *Sample ID* field from the [Single Analysis](#) dialog.


This field serves for information only. After clicking on the cell in this column the  icon will appear. Using it invokes the list where you can pick from the available variables for composing the name. Variables that can be used are described in the **Chromatogram File Name** section of the [Single Analysis](#) dialog described on pg. 113.

Sample

Sample description - will be transferred to the headers of all created chromatograms. Maximum number of characters in this field is limited to 64. The parameter corresponds to *Sample* field from the [Single Analysis](#) dialog.

This field serves for information only. After clicking on the cell in this column the  icon will appear. Using it invokes the list where you can pick from the available variables for composing the name. Variables that can be used are described in the **Chromatogram File Name** section of the [Single Analysis](#) dialog.

Comments

Enable to add user comments. Text is editable directly in the cell or after clicking on dropdown arrow of the  icon in [Comments](#) dialog. Comments column is hidden and empty by default. Sample comments are saved with the chromatogram and can be displayed on *Measurement Conditions* tab and in *Print Preview*.

Note: Comments in the already measured chromatogram are also editable from *Measurement Conditions* tab.

Sample Amount

The value is used in calibration calculations of individual components percentage in the *ESTD* and *ISTD* methods. In *ISTD* enter the sample amount without the addition. Enter values using the same units that were used in the calibration file (*Units - Compound* parameter in [Calibration Options](#) window). The default value is 0. The parameter corresponds to the *Amount* field of the [Single Analysis](#) dialog and the value will be transferred to the chromatogram header.

ISTD1 Amount

The amounts of the internal standards for the *ISTD* method. Other columns for entering amounts of ISTD2 - ISTD10 are hidden by default. This value has to be entered in the same units as those used in the calibration file (as defined in the *Units - Compound* field of the [Calibration Options](#) dialog). The default value is 0. The parameter corresponds to the homonymous field from the [Single Analysis](#) dialog and the value will be transferred to the chromatogram header.

Sample Dilut.

This field holds the sample dilution factor - its value is used to multiply each calibrated amount in the *Amount* column of the **Result Table**. The default value is 1. The parameter corresponds to *Dilution* field in the [Single Analysis](#) dialog and the value will be transferred to the chromatogram header.

Inj. Vol.

Defines the volume of injection. The response of all compounds in a calibration or when using calibrated calculations is modified by the ratio of this value and *Default Injected Volume* value from the calibration file. This parameter corresponds to the analogous field from [Single Analysis](#) dialog and its value will be transferred to the chromatogram header. The units are set in the [Instrument Units](#) dialog (described in the chapter "**Right section of System Configuration dialog**" on pg. 19.).

Caution: When using a directly controlled autosampler this value will define the injection volume! The station then automatically verifies whether the entered volume corresponds to the current autosampler setting.

When the value set in this column is 0, no correction to the *Default Injection Volume* value will be made. However, when *Inj. Vol.* of 0 is entered into the sequence when using a directly controlled autosampler, a warning will be given.

AnalysisUserVar1 - AnalysisUserVar3


Sets numerical value of *User Variables* (up to 3 per row). *User Variables* can be used for User Column calculations. Columns *AnalysisUserVar1 - AnalysisUserVar3* are hidden and set to value 0 by default. Name of the columns can be changed in *Setup Columns...* through *Custom Name* line. If the field is left empty, default name *AnalysisUserVar1-AnalysisUserVar3* would remain filled in.

Note: User Variables columns can be edited after sequence end and reprocess in the next batch.

Caution: Users who do not have the right to *Edit Method* in the "User Accounts" on page 4 dialog cannot edit *AnalysisUserVar1 - AnalysisUserVar3*; fields will be grayed out.

File Name

Defines the chromatogram name pattern. The pattern may use a combination of fixed text and variables (usually entered in the form of % and a character). The same variables may be used as in the [Single Analysis](#) dialog, plus %v and %i variables for automatic calculations of vials and injections when measuring multiple analysis from one line.

After clicking on the cell in this column the  icon will appear. Using it invokes the list where you can pick from the available variables for composing the file name. You can also enter a subfolder in the chromatogram name. Variables and how to enter the subfolder name are described in the **Chromatogram File Name** section of the [Single Analysis](#) dialog described on pg. 113.

It is possible to include also the name of a subfolder in the name to store chromatograms into subfolders of the [Data Subdirectory](#). E.g. the *MySubProjectMyFileName* in the DEMO1 project will result in the MYFILENAME.PRM stored in the C:\CLARITY\DATAFILES\DEMO1\DATA\MYSUBPROJECT folder. If the subfolder doesn't exist, then it will be created when the chromatogram will be stored.

Note: If variable %n is being used, it will be independent from the variable using the same name in the [Single Analysis](#) dialog.

Sample Type

Sets the type of the sample being measured. The possible options are:

Unknown - denotes an unknown sample.

Standard - specifies the calibration standard. Samples marked as *Standard* must have the calibration level filled in the *Lvl* column. Chromatograms created on the sequence rows marked as calibration standards will be stored in the CALIB subdirectory instead of the DATA subdirectory.

Bypass - this *Sample Type* type allows for performing an analysis in the *ACTIVE* sequence with controlled autosampler without actually injecting a sample. This may be useful for system clean-up etc..

Blank - in fact a calibration standard with no amount of added sample. The *Blank* is thus one point of a calibration curve (with the *Amount* of 0).

Caution: When measurement of recalibration standard is finished, the calibration file being recalibrated is updated by the sample responses and saved. In case there are any unsaved changes within the calibration file at that moment, those changes are discarded.

Lvl


Indicates the number of the calibration level when the resulting chromatogram is to be used for automatic recalibration when the *Sample Type* column of the sample is set to *Standard*. The file has to be set as the calibration standard in the *Sample Type* column and a proper calibration file has to be set in the current method as a prerequisite for automatic recalibration.

Method Name

Indicates the name of the method governing all analyses set on a given line. The active template method name from the [Instrument](#) window will automatically be inserted in the first line of the new sequence table.

Note: If you point the mouse cursor to the title of the method, a tooltip will open, in which the title of the method including the entire path will be displayed.

Report Style

Sets the report style to be used for printing. If no name has been entered, no printing on a given row of the **Sequence Table** will be performed. After clicking on the cell in this column the  icon will appear. Using it opens the *Insert File Name* dialog for specifying the print method.

Caution: Print style cannot be selected while a sequence is running.

If you point the mouse cursor to the title of the print style, the yellow tooltip will open, in which the title of the print style including the entire path will be displayed.

Postrun functions

The commands *Open*, *Open Calib.*, *Print*, *Print to PDF*, *Export Data*, *Export AIA*, *Export TXT*, *Export EZChrom*, *Export Multidetector*, *Run Program*, *Program to Run* and *Parameters* generally correspond to analogous items in the [Single Analysis - Post Run Settings](#) tab. All of these columns contain checkboxes, with the exception of the *Program to Run* column (corresponding to the *Program to Run* field of the *Single Analysis - Post Run Settings* tab) and the *Parameters* column.

Note: When there is *Print*, *Print to PDF* or *Export Data* set in the *Postrun functions*, the *Open chromatogram Postrun function* has to be selected too. Only chromatograms opened in the [Chromatogram](#) window can be reported. In sequence with either of the above functions set on a row without *Open* set as well, sequence row validation fails.

Include in SST


This checkbox allows user to set whether the particular chromatogram will be included in the SST calculations or not.

Stored Calib.

This checkbox causes the created chromatogram to be opened with the recent stored version of the calibration file, as opposed to the linked calibration when not checked. The checkbox corresponds to the *Open with stored calibration* checkbox in the right part of the *Chromatogram - Results* tab.

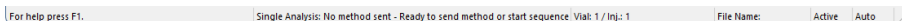
Close All

This checkbox allows to close all chromatograms currently opened in *Chromatogram window* after the analysis is finished. If the checkbox *Open* is checked at the same time, the already measured chromatogram will be opened in *Chromatogram window*. If *Open* checkbox is not checked, *Chromatogram window* will remain empty. For multiple injections it works in the same manner. Postrun operations always follow after *Close all* command.

Note: To resize a column, point mouse cursor on the edge of the column to display , left mouse click and drag to a desired width. All columns, apart from *Status*, can be resized.

Status Bar

The status bar provides the following information:



State

If the sequence is running, the runtime of the actual sample is displayed. If the sequence is not running, status from the [Instrument](#) window in the form of <short status> - <long status> is displayed.

Vial No.

The vial number / injection number from a given vial.

File Name

The name of the chromatogram currently being measured.

Active (Passive)

Active/passive sequence flag.

Auto (Manual)

Chromatogram name control flag showing the settings of the *Format* section in the [Sequence Options](#) dialog described on pg. **405**.

6.1 File

This is an entry point to a submenu of commands for working with sequence files.




New

Creates a new sequence and at the same time closes currently opened sequence (user is notified if there are any unsaved changes). An empty sequence table will be created with default parameter values based on the template sequence file (TEMPLATE.SEQ) saved in the common directory (C:\CLARITY\DATAFILES\COMMON\ in the default projects). New sequence is *ACTIVE* by default (or set according to the setting in TEMPLATE.SEQ). If the template sequence file does not exist in the project, the new sequence will be based on internal preset values in Clarity. The first row in a new sequence takes its settings from the Method and Report setup currently loaded to the Instrument, the **PostRun** information is loaded from the actual setting of the [Single Analysis - Post Run Settings](#) tab. By checking the *Run* checkbox for further rows, the settings are copied from the previous line.



Open

Selects and opens a sequence file. Invoking the command or using the **Ctrl + O** shortcut opens the *Open Sequence* dialog.

In the full version , the same particular sequence cannot be opened on multiple Instruments at once.




Save

Saves changes in the currently opened sequence.



Save As






The command invokes the *Save As* dialog similar to [Open Method](#) dialog where you can set a new name or select a different directory to save the sequence.

When another file of the same name already exists, you will not be able to use this name. Also, in the protected mode (full version ) only, you are not allowed to change a file without the appropriate access rights (see *System - User Accounts...* command).

Note: For existing filenames, message box about file overwriting pops up.

Send Sequence by Email

Sends the displayed sequence as an email attachment. It is analogous to the *Send Method by Email* command (for more details see the chapter **Send Method by Email** on pg. 70). The sequence will automatically be saved prior to sending.

Import...	Imports the sequence table from a text file (for more details see the chapter Import... on pg. 395).
Export...	Exports a Sequence Table to a text file. Values are exported in tab delimited format, first row contains column headers. <i>Status</i> and hidden columns are not exported.
 Report Setup	Selects and configures the report style. The command opens the Report Setup dialog described on pg. 432 .
 Print Preview	Displays a preview of the printout prior to actual printing. The command opens the Print Preview dialog described on pg. 457 .
 Print to PDF	Prints the Sequence Table to *.PDF file.
 Send Printed PDF by Email	Opens a new email message in default email client, prints the Sequence Table to *.PDF and adds created file as an email attachment.
 Print...	Selects a printer and starts actual printing. Invoking the command opens the Print dialog described on pg. 459 .
-----	Displays the list of recently opened sequence files so it is easily possible to get to the files you are currently working with. The number of files in the list is determined by the <i>Recent Files</i> parameter in the User Options - General dialog available from the Instrument window by <i>View - Options</i> command.
Close Window	Closes the Sequence window.

6.1.1 Import...

Imports a **Sequence Table** that has been stored in a text file. Values have to be in delimited format and separated by an arbitrary delimiter.

Import of the sequence is one of the functions that enables an interconnection between the **Clarity** and **LIMS** systems. It can be performed in three steps:

Select text file and set import settings

Invoking the command will open the *Import Sequence Step 1* dialog, that is used to select which text file will be imported, set the delimiters and preview the values.

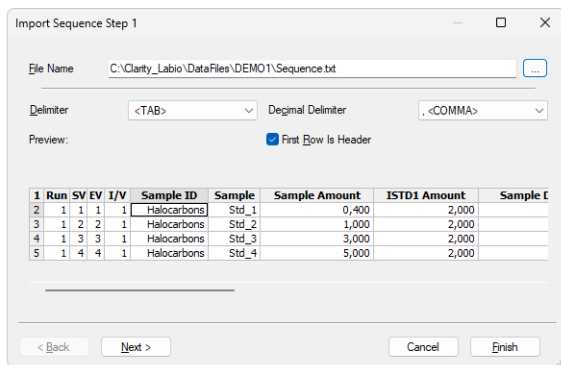


Fig. 207: Import Sequence Step 1

File Name

Serves for setting the filename and directory path of the imported file. Use the button to invoke the *Open Files To Import* dialog and locate the desired file. Press *OK* to confirm the selection of the file.

Delimiter

Selects the character used as field delimiter. Possible options are *<TAB>*, *<SPACE>*, *<COMMA>* or *<SEMICOLON>*.

Decimal Delimiter

Defines the character used as decimal delimiter. Options for the decimal delimiter are *<Window's Locale>* (the station will use the setting specified in the local settings of MS Windows), *<COMMA>*, *<DOT>* or *<SEMICOLON>*.

First Row is Header

If the text file to be imported contains column descriptions in the first row, use this checkbox to immediately transfer it to the column headers of the *Preview* section and also use this row for mapping in the *Import Sequence Step 2* dialog.

Preview

Preview of the first five rows of the imported sequence table.

Column mapping

After clicking the *Next >* button the dialog changes to the *Import Sequence Step 2*. This section is used to map the columns of the imported file with the corresponding columns in the **Sequence Table**.

Import can only be finished after the required columns (SV, File Name, Method Name - all marked in bold) have been mapped.

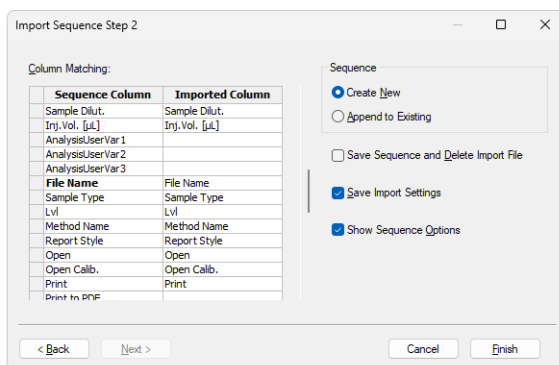


Fig. 208: Import Sequence Step 2

Column Matching

Set the mapping so that the columns used in **Clarity** (*Sequence Column*) will correspond to the columns from the imported file (*Imported Column*). Columns that are highlighted in bold letters are required.

When the imported table contains column headers (the *First Row is Header* checkbox from the *Import Sequence Step 1* dialog has been checked), **Clarity** will attempt to automatically map the columns according to their names. Manual mapping will override the default name mapping. **Clarity** will store these names for future imports.

Sequence

Determines whether the imported table will be appended to the end of the currently opened sequence table in the [Sequence](#) window (*Append to Existing*) or whether a new sequence table will be created (*Create New*).

Save Sequence and Delete Import File

When checked, automatically saves the imported sequence file and deletes the source text file. When the *Create New* checkbox has been checked, the *Save As* dialog for selecting the filename and path of the new **Sequence Table** will open automatically after import.

Save Import Settings

Saves the current import settings for future imports. The setting will be stored in the station configuration and is thus shared by all users and Instruments.

Show Sequence Options

Automatically opens the [Sequence Options](#) dialog after the import.

Note: When importing into a running sequence, this checkbox will be disabled.

Adjust the Sequence Options

If you checked the *Show Sequence Options* checkbox, the [Sequence Options](#) dialog will automatically open after the import. This is where the sequence settings can be adjusted. A detailed description of the [Sequence Options](#) dialog can be found in the chapter "**Sequence Options**" on pg. **405**.









6.2 Edit


Submenu containing commands for work with clipboard and tables.

Note: Commands may also be found in the local tables menu, accessed by right clicking the mouse on the table.

Note: The procedure for selecting lines is detailed in the **User Manual**.

Note: It is possible to change the move direction of the focus after pressing the Enter in [User Options](#).

	Insert New Line	Inserts a new line ahead of a currently selected one. The inserted line will be filled with the same values as the selected line.
	Line Up	Moves selected rows one position up. Moving can be also easily done using the mouse - left click and hold the mouse on the first column of the Sequence Table (with line numbers), drag the line up to the desired position and release. Selected lines do not have to form a continuous block.
	Line Down	Moves selected rows one position down. Moving can be also easily done using the mouse - left click and hold the mouse on the first column of the Sequence Table (with line numbers), drag the line down to the desired position and release.
	Undo	Cancels the modifications effected in tables (Ctrl + Z).
	Redo	Countermands the <i>Undo</i> command (Ctrl + Shift + Z).
	Cut	Moves the selected text to the clipboard (Ctrl + X).
	Copy	Copies the selected text to the clipboard (Ctrl + C).
	Paste	Copies the clipboard content to the indicated place (Ctrl + V). If you are pasting to an area that is larger than the clipboard content, the content will be tiled (<i>Fill</i> function). This is useful if you want to insert a large number of the same fields or several periodically repeating fields into the table.

Paste Insert	<p>Pastes clipboard content to automatically inserted new lines (Ctrl + I). Unlike the <i>Paste</i> command, the original table content is not replaced, but new lines are instead inserted.</p> <p>New lines will be inserted above (ahead of) the currently selected line.</p>
Fill Down	<p>Copies the content of current cell to all cells below it or to selected range (Ctrl + F). <i>Fill Down</i> is disabled for the <i>End Vial (EV)</i> column or when multiple cells in the same row are selected.</p>
Fill Series...	<p>Displays the Fill Series... dialog for filling up incremental values to all cells below it or to selected range. <i>Fill Series</i> is disabled for the <i>End Vial (EV)</i> column, when multiple cells in the same row are selected or when the whole Sequence Table is selected.</p>
Delete	<p>Deletes the selected table fields. Deleted fields will be reset to their default values. If you have selected entire lines, the lines will be removed.</p>
Mark for Run	<p>Checks the checkbox in the <i>Run</i> column for selected lines. These rows will be processed when the sequence will be run.</p>
Clear Run Marks	<p>Unchecks the checkbox in the <i>Run</i> column for selected lines. These rows will not be processed when the sequence will be run.</p>
Invert Run Marks	<p>Inverts the marks in the <i>Run</i> column of the Sequence Table. All selected rows with the <i>Run</i> column not checked will be checked (marked for run) and all rows currently checked will be excluded from the run (unchecked).</p>
	Reset Status
<p>Invoking this command (or using the Ctrl + E shortcut) resets the measured line flags on the selected lines. The command will change the color of <i>Status</i> column fields of all selected rows to green (not measured yet). The status of all lines will be automatically reset while running a sequence using the <i>Run</i> command. During running analysis the <i>Reset Status</i> command is disabled for all rows.</p>	

Restore Default Columns	Restores the default columns setting (for more details see the chapter Edit on pg. 191).
Setup Columns...	Opens the Setup Columns dialog for the Sequence Table .
Select All	Invoking the command (or using the Ctrl + A shortcut) selects the whole Sequence Table .
Remove All	Deletes the entire Sequence Table , only the empty first row will remain.
Hide Column(s)	Hides all selected columns.
Show Hidden Column(s)	Shows all hidden columns.

6.2.1 Fill Series

Dialog for filling up a series in selected cells of the sequence or other table. When selected one cell or multiple cells in one row, the changes will apply from the first top selected line to the last. To apply changes in selected cells only, select multiple cells (rows and columns) as you are used to do in your favorite spreadsheet.

This dialog is also available using the popup menu in the [Gradient Table](#).

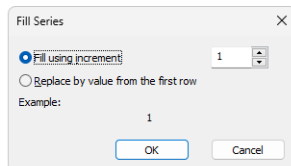


Fig. 209: Fill Series dialog

Fill using increment

Sets this option if you want to fill up the series incrementally using the entered step in the box on the right. Starting value will be taken from the first top cell of the each selected column. The number is also detected at the end of the string in the cell.

Replace by value from the first row

Replaces all selected cells with the value from the top selected cells.

Example

Contains preview how the first and second cell in the first selected column will look like.

6.3 Sequence

Summarizes commands for the control of the running sequence. The majority of these commands is also placed on the toolbar by default.

Note: If icons representing these commands are disabled, the tooltip may help in discovering the reason of the disablement.

▶▶ Run

Invoking this command or using the ▶▶ icon or **Ctrl** + **Q** shortcut runs the sequence. The command is only active when the sequence is not in the *RUNNING* state. Before the sequence is run, the validity check is performed. All methods used in *ACTIVE* sequence must:

- have *External Start/Stop* option in the [Method _ Setup _ - _ Measurement](#) dialog checked.
- have *Enable Autostop* checkbox in the [Method _ Setup _ - _ Measurement](#) dialog selected and *Run Time* field filled.

The *Run* command invokes dialog with options to: *Reset*, *Resume* or *Cancel*. *Reset* command, resets the status of all lines in the **Sequence Table** (all fields in the *Status* column will turn green).

Running a partially measured sequence using the *Resume* command starts the measurement from the first non-measured line, while running it using the *Run* command the entire sequence will be measured again. The station automatically checks the entire sequence upon its start. During the measurement only the currently used line is checked in this way, which means that the sequence can be modified during the run. User has to have *Start Acquisition* right to be able to perform this option.

|| Pause

Using the *Pause* command, **||** icon or **Ctrl** + **Space bar** shortcut suspends the active sequence. A suspended sequence does not allow injections and does not react to an external start signal issued.

The status of the sequence after the use of the *Pause* command depends on the status of the sequence before invoking the command:

WAITING, *IDLE* sequence is turned to *PAUSED* status.

RUNNING sequence is turned to the *PAUSED* status only after the data acquisition of the current analysis is completed (the intermediate status is *RUNNING/PAUSE*).

▶ Resume

Using this command, **▶** icon or the **Ctrl** + **Space bar** shortcut resumes the operation of a suspended sequence. The sequence status becomes *IDLE* or *WAITING* and, accordingly, the signal that allows the injection defined on the next row will either be sent immediately or after the **Idle time** has passed.

When returning to the *IDLE* state, the sequence counts the time from the moment it was set to the *PAUSED* state.







When the *Resume* command is used while in the *RUNNING/PAUSE* state, the planned pause of the sequence will be canceled.


If you run a partially measured sequence using the *Resume* command, measurement continues from the first line that wasn't measured yet. If you run it using *Run*, the entire sequence will be measured again.

User has to have *Start Acquisition* right to be able to perform this option.

✘ Abort Sequence or Acquisition

Invoking this command or using the **✘** icon or **Ctrl** + **B** shortcut immediately aborts the running sequence. Any data acquisition in progress will be interrupted, the results will not be processed, and the sequence will be terminated.

 Stop Sequence or Acquisition	<p>Using the command,  icon or Ctrl + T shortcut halts the running sequence. Currently running analysis will be completed (the actual state will change to <i>RUNNING/STOP</i>).</p> <p>If the <i>Stop</i> command is used for the second time, it will stop the running analysis.</p>
 Repeat Injection	<p>Invoking this command or using the  icon or Ctrl + ← shortcut interrupts the actual measurement and repeats the injection (runs the analysis according to the row in the Sequence Table). If the sequence is in the <i>PAUSED</i> state before using the <i>Repeat Injection</i>, triggering the command will repeat the measurement of last completed injection.</p> <p>User has to have <i>Start Acquisition</i> right to be able to perform this option.</p>
 Skip Vial	<p>Using this command,  icon or Ctrl + ↓ shortcut terminates the analysis of active vial and also omits all remaining injections using the current vial defined on the same row of the Sequence Table. This command works principally in the same way as the <i>Abort</i> command does, but only for the currently measured sample. The sequence continues with the measurement of the next vial.</p> <p>The line containing skipped injections will be indicated in the <i>Status</i> column by light blue color.</p> <p>Potential re-measurement of skipped vials has to be done manually (e.g. by creating a new line in the Sequence Table).</p> <p>User has to have <i>Start Acquisition</i> right to be able to perform this option.</p>

	Check Sequence	<p>This command performs a check of every row in the Sequence Table for potential errors. These may be attempt to use a non-existent method or print style, incorrectly set control parameters, prohibited chromatogram name entered etc. The check same as the one invoked by the <i>Check Sequence</i> command is automatically performed on the start of the sequence measurement.</p> <p>During a measurement, only the line currently being measured is checked. Manual use of the <i>Check Sequence</i> command allows the user to test the whole sequence, for example after modifying the sequence while it is running to verify that all changes are correct.</p>
	Snapshot	<p>Invoking the command,  icon or Ctrl+H shortcut processes and shows the data from currently measured sample without terminating the measurement. This command is identical to the <i>Snapshot</i> command from the Single Analysis dialog described on pg. 113. The snapshot chromatogram will be automatically replaced by another snapshot or the final chromatogram after the analysis is finished.</p> <p>Sample counter %n, if used, will be incremented (only once) in the chromatogram name, even though more <i>Snapshots</i> are used and the resulting chromatogram is either created or not.</p>
	Options...	<p>When invoked, opens the Sequence Options dialog used for defining the sequence parameters (for more details see also chapter Sequence Options on pg. 405).</p>
	Edit Current Method...	<p>Displays and modifies the method defined on the row of the Sequence Table with currently active field. The command opens the Method Setup - Measurement dialog described on pg. 92. The operation may also be performed by the <i>Edit Method...</i> command from the local menu for the given row of the Sequence Table.</p>
	Edit Current Report...	<p>Displays and modifies the report style set on the row of the Sequence Table with currently active field. The command opens the Report Setup dialog described on pg. 432. The operation may also be performed by the <i>Edit Report...</i> command from the local menu for the given row of the Sequence Table.</p>

6.3.1 Resume/Reset Sequence

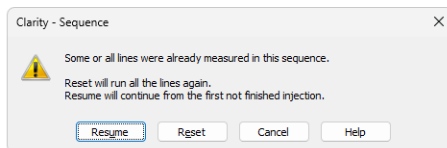



Fig. 210: Dialog to Resume or Reset Sequence

In case the user wants to run a sequence which contains already measured lines, it is necessary to *Resume* the sequence to continue measuring first unfinished injections or *Reset* to start measuring the sequence from first injection in the first line. By clicking the *Cancel* the status of the sequence will be not changed.

6.3.2 Sequence Options

The *Sequence Options* dialog serves for defining the sequence parameters. It can be opened using the  icon or the *Sequence - Sequence* command of the [Sequence](#) window.

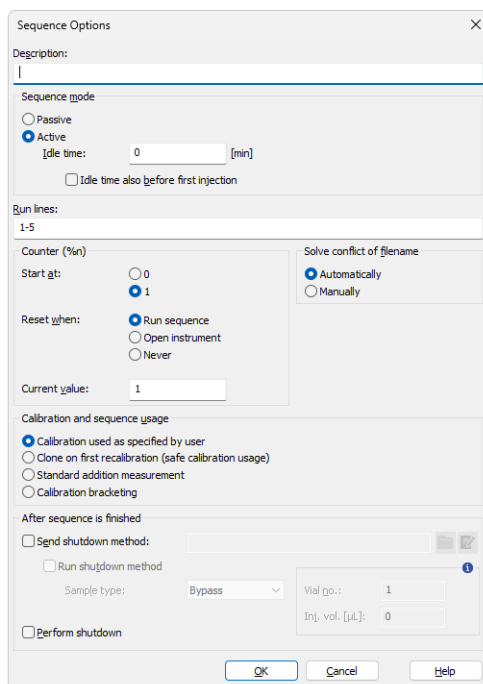


Fig. 211: Sequence Options

Description

The description of the displayed sequence.

Sequence mode

Serves for setting the operation mode of the sequence.

Active

In an *ACTIVE* sequence, the sequence start is controlled by the station.

Clarity sends the permission signal to the autosampler and waits until the sampler acknowledges the injection. Data acquisition will be started after the confirmation signal has been sent back to **Clarity** and the permission for another injection is disabled.

Caution: When the *ACTIVE* sequence is used, *Enable Autostop* and *External Start/Stop* must be set in the [Method Setup - Measurement](#) dialog and the *Start-Restart* option of the *External Start/Stop* behaves as *Start Only*.

Passive

In a *PASSIVE* sequence, the start is controlled by the autosampler.


Clarity only waits for external start signal from the autosampler and then starts the sequence and data acquisition.

Caution: When the *PASSIVE* sequence is used, *External Start/Stop* must be set in the [Method Setup - Measurement](#) dialog.

Once the analysis time of the method in question has elapsed (as set in the *Run Time* field of the [Method Setup - Measurement](#) dialog), the analysis will be completed and injection will be permitted once again.

Note: Only the **Start In** and **Ready Out** synchronization cables are needed for the *ACTIVE* sequence to function. The *ACTIVE* sequence can thus be used even with an autosampler not governed by a specialized control module.

Note: The confirmation signal is represented by a change against the initial value of the selected digital output (e.g., change from High to Low, or vice versa). The default assignment of outputs is described in the corresponding hardware manual.

The assignment of digital inputs and outputs used for the synchronization in the full version  can be changed on the tab of the appropriate Instrument in the [System Configuration](#) dialog, in the *Ext. Start Dig. Input* and *Ready Dig. Output* fields. For more detailed information, see *chapter 6* in the *Getting Started* manual.

Idle time

Delays the sending of the permission to inject. The next injection after the end of an analysis will always be permitted only after the defined *Idle time* has elapsed. Possible values are within the *0.01-100* min range. This field can only be edited when the sequence is set to *ACTIVE*.

Idle time also before first Injection

Determines whether the *Idle time* parameter will be used even before the first injection in the *ACTIVE* sequence. This field can only be edited when the sequence is set to *ACTIVE*.

Run lines

Sets the line numbers of the *Sequence Table* to be run in the measurement. Particular line numbers should be separated by a comma (e.g. 1,3,5), ranges should be entered using a dash (e.g. 1-8).

A list of lines to be run can be defined interactively using the checkboxes in the *Run* column of the *Sequence Table* (the selected lines will be automatically filled in the *Run lines* field).

Counter (%n)

Sets the value and properties of the %n variable (analysis counter) used in the *Sequence Table*.

Value of the counter increases every time an analysis (injection) is performed and a chromatogram is created.

When taking *Snapshots*, the value of the *Counter* is incremented only once, even if more than one snapshot is taken. Old snapshots are thus overwritten by new snapshots and eventually by the resulting chromatogram.

Start at:

Defines if the %n variable will be reset to 0 or 1 at the moment defined in the following **Reset when** field.

Reset when:

Sets the condition when the counter (%n variable) is reset. Available options are:

Run Sequence - The counter is reset every time the sequence is run.

Open Instrument - The counter is reset every time the [Instrument](#) window is opened.

Never - The counter is never reset.

Current value

This field shows (and allows to modify) the current value of the sequence counter (%n variable). Each time a chromatogram is measured the value of counter increases by 1.

Caution: The station keeps two separate counters: one for the sequence and another one for the single analysis. This means that two %n variables with possibly different values exist simultaneously.

Solve conflict of filename

Sets the method for resolving the conflict of chromatogram names when a chromatogram with a name identical to an existing chromatogram is to be created (according to the set *File Name*). This may happen when measuring more than one chromatogram from a particular line or after restarting a measurement.

Automatically

The pattern will be automatically modified to correspond to the number of measured chromatograms and to avoid possible loss (overwriting) of chromatograms.

Note: When using the automatic format, variables will be complemented by additional three-digit counter corresponding with the defined number of samples (e.g., in a sequence where SV = 1 and EV = 100, the file names will be automatically numbered from 001 to 100).

Manually

The pattern will not be modified. Once the sequence has been run, you will be notified of a possible overwriting of chromatograms.

Calibration and sequence usage

Selects the mode of the calibration and sequence usage.

Calibration used as specified by user

Sets the sequence and calibration to the standard **Clarity** use (the only way available since version 3.0). The calibration set in the [Method Setup - Calculation](#) dialog is used for calibration and recalibration, no calibration cloning is performed.

Clone on first recalibration (safe calibration usage)

Sets the sequence and calibration to the safe calibration usage mode. This option will create a clone (copy) of the 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. The option is not available on EA Instruments.

Standard addition measurement

Sets the sequence to the standard addition mode (it is necessary to set the *Display* and *Calculations* mode to *STDADD* in the calibration and method). As each unknown sample will use one calibration file, the calibration will be cloned from the original calibration file whenever an unknown sample or blank follows the calibration standard. All responses are cleared from a newly cloned calibration. The option is not available on EA Instruments.

Calibration bracketing

Bracketing is a simplified direct calibration method used to compensate for variations in the instrument response with time.

This option sets the sequence and calibration to the calibration bracketing mode. In this mode, every unknown sample series is enclosed between calibration standards and uses a single calibration file. The calibration is cloned from the previous calibration clone whenever an unknown sample or blank follows a calibration standard in a sequence. The newly cloned calibration file has all the previous responses cleared except for the last series of calibration standards (standards that immediately precede the current unknown sample).

Calibration bracketing will work correctly only if the used calibration has the *Recalibration* option selected and set to *Average* (at least 2 points) in the *Calibration Options*.



In the EA mode, the name of the cloned calibration file is hard-set as the original name incremented by the sequence line number (%L parameter).

Note: At each calibration cloning, the original calibration and thus the results of the chromatograms measured earlier are preserved, under the name as set in the [Method Setup - Calculation](#) dialog, *Calibration Cloning In Sequence* option (conflicting names will be complemented by a three-digit counter to avoid overwriting).

After sequence is finished

Allows to set actions to be performed when the sequence is finished

Send shutdown method

Specifies a method to be sent to the instrument when the sequence is finished. The method can be selected using the  button. The  button allows to edit the currently selected method.

If no other options are checked, **Clarity** will send the parameters of the specified method to the instrument and no acquisition will be performed.

Run shutdown method


An analysis according to the specified method will be performed. The resulting chromatogram will be saved to the current project as <SEQUENCENAME> - SHUTDOWN - <METHODNAME> - %R.PRM

Sample type

Sets the type of the sample being measured by the shutdown method. The possible options are:

- *Unknown* - a controlled autosampler will perform an injection
- *Bypass* - no injection will be performed

Vial no.:

The vial number / injection number of the given vial. If the configured autosampler supports graphical interface for inserting vial number, the  button is present - clicking this button invokes the *Select Vial* dialog for selecting a vial.

Inj. vol. [units]:



Defines the volume of injection. The present units are as set in the *Instrument Units* dialog available in *System Configuration*.

Note: Several autosamplers require specific values for the *Vial no.* or *Inj. vol.* although no injection is performed. If these values are missing, the user is informed during the validity check.

Perform shutdown

When the sequence is finished, all connected **controlled** devices will be shut down. The shutdown command is sent after sending (and possibly completing) the run of the shutdown method. When the shutdown method is just sent and no shutdown method run is performed, invoking

the shutdown does not wait for the controlled instruments to become ready.

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

6.4 View

Commands for setting up the [Sequence](#) window.

Toolbars

Displays/hides all toolbars. The command is similar to the *Toolbars* command in the main [Clarity](#) window.

- **File, Edit, Sequence:** Hides/shows the respective toolbar.
- **Customize...:** Customization of items in the toolbars.
- **Reset All:** Restores all menus and toolbars in the [Sequence](#) window to their default state.

Note: *Reset All* does not display hidden toolbars. To show them invoke *Customize... - Toolbars* menu.

6.5 Window

This section contains commands allowing to open other base windows.

Main <small>✓ Full version</small>	Displays the Clarity main station window described on pg. 1 .
Instrument	Displays the Instrument window described on pg. 60 .
Chromatogram	Displays the Chromatogram window described on pg. 162 .
Calibration	Displays the Calibration window described on pg. 320 .
Single Analysis	Displays the Single Analysis window described on pg. 113 .
Data Acquisition	Displays the Data Acquisition window described on pg. 369 .
Device Monitor	Displays the Device Monitor window described on pg. 135 .
Station Audit Trail <small>✓ Full version</small>	Displays the Audit Trail window described on pg. 413 .
Sequence Audit Trail... <small>✓ Full version</small>	Displays the Sequence Audit Trail window described on pg. 427 .

7 Audit Trail Full version

Audit Trail window is used for logging of individual operations of the station. By allowing backward control of all performed operations, including information about who and when it was performed, the logging of operations supports higher reliability and repeatability of results in the means of Good Laboratory Practice (GLP) rules.

Time	Group	Severity	User Name	Instrument	Area	Description	Info
17.07.2020 13:42:29	Start/Close		Administrator	Instrument 1	Instrument	Close Instrument	Clarity 8.4.0.26 FULL; SN: 088-000898
17.07.2020 13:42:28	File		Administrator	Instrument 1	Files	Save File C:\Clarity-08-04-00-026\DataFiles\Projects\DEMO1.p...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:28	Acquisition		Administrator	Instrument 1	Acquisition and Se...	Ready - Ready to start run: Instrument was aborted by user	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:24	File		Administrator	Instrument 1	Files	Close Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:24	Acquisition		Administrator	Instrument 1	Acquisition	Control - Performing remaining time program: Control time elap...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:23	File		Administrator	Instrument 1	Files	Close Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:22	File		Administrator	Instrument 1	Files	Open Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:22	File		Administrator	Instrument 1	Files	Open File C:\Clarity-08-04-00-026\DataFiles\DEMO1\Calib\Exa...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:22	File		Administrator	Instrument 1	Files	Open File C:\Clarity-08-04-00-026\DataFiles\Common\Chromat...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:21	Acquisition		Administrator	Instrument 1	Acquisition	Control - Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:21	Acquisition		Administrator	Instrument 1	Chromatogram	C:\Clarity-08-04-00-026\DataFiles\DEMO1\Data\Instrument 1...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:21	File		Administrator	Instrument 1	Files	Open File C:\Clarity-08-04-00-026\DataFiles\DEMO1\Calib\Exa...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:21	Stop		Administrator	Instrument 1	Acquisition	Acquisition was stopped by detection of stop of all detectors	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:18	Stop		Administrator	Instrument 1	Acquisition and Se...	Running - Acquisition running: Acquisition was stopped by user	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:19	Start		Administrator	Instrument 1	Acquisition	Ready - Ready to start run: Acquisition was started by user	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:42:19	File		Administrator	Instrument 1	Files	Open File C:\Clarity-08-04-00-026\DataFiles\DEMO1\Calib\Exa...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:57	Calibration		Administrator	Instrument 1	Calibration	Noname: cal - Calibration has been discarded.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:56	File		Administrator	Instrument 1	Files	Open Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:46	File		Administrator	Instrument 1	Files	Open Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:40	File		Administrator	Instrument 1	Files	Open Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:36	File		Administrator	Instrument 1	Files	Open File C:\Clarity-08-04-00-026\DataFiles\Common\Calibrat...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:36	File		Administrator	Instrument 1	Files	Open Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:36	Calibration		Administrator	Instrument 1	Calibration	Noname: cal - Calibration has been created.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:21	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 4 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:21	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 3 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:21	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 2 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:21	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 1 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:21	Acquisition		Administrator	Instrument 1	Acquisition	Method C:\Clarity-08-04-00-026\DataFiles\DEMO1\Demo1.m...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:41:20	File		Administrator	Instrument 1	Files	Open File C:\Clarity-08-04-00-026\DataFiles\DEMO1\Calib\Exa...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:51	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 4 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:51	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 3 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:51	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 2 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:51	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 1 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:51	Acquisition		Administrator	Instrument 1	Acquisition	Method C:\Clarity-08-04-00-026\DataFiles\DEMO1\Demo1.m...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:51	File		Administrator	Instrument 1	Files	Save File C:\Clarity-08-04-00-026\DataFiles\DEMO1\Demo1.m...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:51	Method		Administrator	Instrument 1	Method Change	C:\Clarity-08-04-00-026\DataFiles\DEMO1\Demo1.Lm.t...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:47	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 4 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:47	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 3 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:47	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 2 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:47	Acquisition		Administrator	Instrument 1	Detector	Colbrick - 1 (SN 1808): Method sent to sub-device.	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:47	Acquisition		Administrator	Instrument 1	Acquisition	Method C:\Clarity-08-04-00-026\DataFiles\DEMO1\Demo1.m...	Clarity 8.4.0.26 FULL; SN: 088-000888
17.07.2020 13:40:47	File		Administrator	Instrument 1	Files	Save File C:\Clarity-08-04-00-026\DataFiles\DEMO1\Demo1.m...	Clarity 8.4.0.26 FULL; SN: 088-000888

Fig. 212: Audit Trail - Session

Audit Trail window is accessible from the main [Clarity](#) window via *System - Audit Trail* command or from all other station windows using *Window - Station Audit Trail* command. Other windows, such as [Calibration](#) or [Chromatogram](#), have their own [Local Audit Trails](#).

Clarity station keeps three tables with logs of operations. Each of them corresponds to one tab in *Audit Trail* window - these are *Session* audit trail, *Daily Audit Trail* and *Global*.

Session Audit Trail

The audit trail logs changes from the time the station was started until the station is turned off.

Daily Audit Trail

The audit trail logs changes for each day the station was turned on.

Global Audit Trail

This audit trail is mainly for regulated environment as it keeps track about each station start, users logging to instruments, creating of daily audit trails and other important settings and file changes. Logging to this audit trail can't be turned off.

Audit Trail files for Session and Daily Audit Trail are stored in YYYY-MM-DD.AUDIT file in the C:\CLARITY\CFG\AUDIT_TRAILS directory, the files for Global audit trail are stored YYYY-MM-DD_GLOBAL.AUDIT file in the C:\CLARITY\CFG\AUDIT_TRAILS\GLOBAL directory.

By default, all operations are logged in the language Clarity is currently switched to.

Note: To display column *Description* in English, right mouse click in the *Audit Trail*, choose *Setup Columns* and show *Description EN* column. To show column *Area* in English, perform similar steps as before but show the *Area EN* column.

Tab. 29: Audit Trail Columns

Column Name	Description
Time	Displays time-stamp of the logged operation.
Group	Displays icon and group which is associated with the logged operation. <i>Note:</i> Icon and Group will not be displayed for Audit Trails created by Clarity prior to 8.3.
Type ID	This column is hidden by default. It displays a numeric value of the logged operation. This columns serves primarily for compatibility purposes.
Severity	Displays the severity of the logged operation - only when logged operation is considered as a warning (🚧) or an error (❌).
User Name	Displays the name of the Clarity user who performed the operation.
Instrument	Displays the name of the <i>Instrument</i> where the operation appeared.
Area	Displays the area (domain) of the logged operation - brief information about the location of the logged operation.
Area EN	This column is hidden by default. Displays <i>Area</i> but the logged text is always in English (EN).
Description	Displays a detailed description of what has happened. Logs previous value and new value, if applicable.

Column Name	Description
Description EN	This column is hidden by default. Displays <i>Description</i> but the logged text is always in English (EN).
Windows User	This column is hidden by default. Displays the name of the logged-in Windows user.
Computer	This column is hidden by default. Displays the name of the computer.
Info	<p>Displays general information about the station.</p> <p>Text in the <i>Info</i> column of the Audit Trail such as <i>Clarity 8.3.0.38 FULL, SN: 11-12345</i> can be more easily understood using guidance given below.</p> <p>Clarity 8.3.0.38 stands for Clarity version number.</p> <p>FULL stands for type of version, other possible texts are <i>OFFLINE</i> in case of offline version and <i>DEMO</i> in case of demo version.</p> <p>SN: 11-12345 stands for serial number of the station.</p>
Checksum	<p>Describes the validity of the row. If <i>Fail</i>, the row is not valid and further details are in the Description column.</p> <p><i>Note:</i> Column is hidden by default and in Clarity prior to 8.4 is called OK. Invalid row is also indicated by yellow background color.</p>

Note: In versions of Clarity prior version 8.0 the *Info* column used different formatting. The description of this column for previous versions of Clarity follows.

Text in the *Info* column of the Audit Trail such as *Ver: 7.3.0.56, Demo: 0, SN: 11-12345* can be more easily understood using guidance given below.

Ver - version of Clarity

Demo - possible values are 0, 1 and 2

0 - Full mode (Clarity)

1 - Evaluation mode (Clarity OFFLINE)

2 - Demo mode (Clarity DEMO)

SN: - serial number of the station

In Clarity versions prior to 6.0, additional possible values of 3-10 indicated Forced DEMO mode. Since version 6.0, Clarity will not start instead.

7.1 Station Audit Trail

Session

Log of all operations performed since the last station startup can be found in the *Station Audit Trail* on *Session* tab. Once the **Clarity** station is closed, the **Session** table will be reset and upon next station start the logging will start from the beginning.

Daily Audit Trail

Logs all operations performed during a single day (24 hours). It will form something of a daily sum of all the **Session** logs. Daily logs can be found in the AUDIT_TRAILS subdirectory CLARITY installation group (C:\CLARITY\CFG\AUDIT_TRAILS by default).

Global Audit Trail

This audit trail is mainly for regulated environment as it keeps track about each station start, users logging to instruments, creating of daily audit trails and other important settings and file changes.

7.1.1 File

Open Audit Trail (Append)	Opens audit trail file. An opened file will be appended to the end of current listing.
Clear Session Audit Trail	Temporarily clears the Session audit trail tab. Only actions done after this command are shown here, unless Audit Trail window is closed. When this window is closed and re-opened, the Session tab again shows log of all operations performed since the last station startup.
Export	Exports data from the audit trail to the text, database file or excel.
Print Preview...	Prints a preview of the audit trail (Ctrl + Shift + P).
Print...	Prints the audit trail (Ctrl + P) from a specified printer.
Close Window	Exit from Audit Trail window.

Note: The print format of the audit trail is in the WYSIWYG (What You See Is What You Get) format - all columns displayed on the screen will be displayed accordingly in the report.

7.1.2 Open Audit Trail (Append)

When invoked, displays the selection of all previously saved **Daily Audit Trail** files. Newly opened files will be displayed together within the current **Daily Audit Trail** table, appended to its upper part. Opening previous day's tables will not threaten the process of logging data into the current audit trail file.

Other than current **Daily Audit Trails**, that have been opened, will be indicated on the **Daily Audit Trail** tab by their date separated by the “+” sign.

26	20.12.2023 16:45:07	Start/Close	Administrator
27	20.12.2023 16:45:07	File	Administrator
28	20.12.2023 16:45:07	Acquisition	Administrator

Session: Daily Audit Trail: 2023_12_20 Global

For help press F1.

Fig. 213: Daily Audit Trail tab - several audit trails open

7.1.3 Export

Exports a record of logged operations of the station into the text, database, or excel file. The submenu contains two fields:

Text...

Exports data into a text file with the *.TXT or *.CVS extension. Individual items in the export will be separated by semicolons. When invoked, the *Export As* dialog will appear where you must enter the name of the new file or select some existing file.

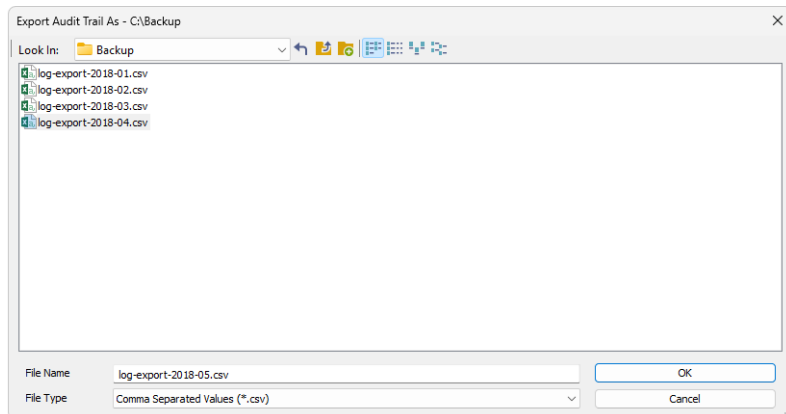


Fig. 214: Audit Trail - Export - Save As dialog

When trying to use an existing file a dialog will appear where you need to select whether exported data will be appended to the end of file (*Append*), or if the data will overwrite any existing content of the file (*Overwrite*).

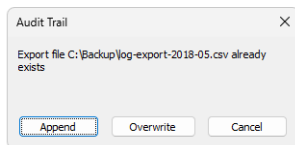


Fig. 215: Audit Trail System Message

Note: You need to select the extension to be used to filter the list of available files or the extension of a newly saved file in the *Export Audit Trail As* field.

DBF...

Exports the logged data in database format. The procedure is similar to the export into text file (it is necessary to select whether to append the exported data to the end of the existing file or overwrite the file).

Note: MS Access supports import of DBF files with **DOS** filename (eight characters max) format only.

Excel Workbook (*.xlsx)...

Exports the logged data with *.XLSX extension. Unlike export to text or to database format, excel file cannot be appended. It can only be overwritten.

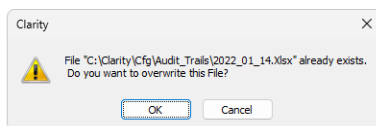


Fig. 216: Overwriting existing excel file.

Excel 97-2003 Workbook (*.xls)...

Exports the logged data with *.XLS extension. Same as *.XLSX files exported *.XLS files cannot be appended. They can only be overwritten.

Caution: Excel must be installed for exporting to excel files. Excel 2016 or newer is required for exporting to *.XLSX format.

7.1.4 Edit

Submenu of commands for working with the clipboard and tables.

Copy	Invoking the command or using the Ctrl + C shortcut copies the selected text into clipboard.
Select All	Invoking the command or using the Ctrl + A shortcut selects all fields of the table.
Restore Default Columns	Invoking the command returns the display of the given table to default settings (for more details see the chapter Edit on pg. 191).
Setup Columns...	Using this command opens the Setup Columns dialog which allows to set the visibility and order of appearance of columns in the given table (for more details see the chapter Setup Columns on pg. 198).
Hide Column(s)	Invoking the command hides all selected column(s) from display (for more details see the chapter Edit on pg. 192).
Show Hidden Column(s)	Using this command displays columns hidden by the <i>Hide Column(s)</i> command (for more details see the chapter Edit on pg. 192).

7.1.5 Filter

This menu helps to define which operations will be displayed in the table on the [Session](#) and [Daily Audit Trail](#) tabs. Using this setting will not impact the logging of items into file, just their display. To set the items to be logged, use the [Audit Trail Settings](#) dialog (accessible by using the *View - Properties* command).

Individual menu items will work like checkboxes. If the item is checked, the corresponding logs will be displayed.

Show All	Displays all items of the <i>Filter</i> menu.
Show Instrument X	Displays items from individual instruments.
Show System	Displays system logs and items from the main Clarity window.

7.1.6 View

Displays the setting for the [Audit Trail](#) window.

Toolbar

Displays commands for toolbars. The command is similar to the *Toolbars* command in the main [Clarity](#) window.

- **Default:** Hides/shows the default toolbars.
- **Customize...:** Customization of items in the toolbars.
- **Reset All:** Returns all menus and toolbars in the [Audit Trail](#) window into their initial state.

Note: *Reset All* does not display hidden toolbars. To show them invoke *Customize... - Toolbars* menu.

Properties...

Invokes the [Audit Trail Settings](#) dialog where the user can specify the operations to be logged.

7.1.7 Properties...

The *Audit Trail Settings* dialog is used to specify which operations will be automatically logged by **Clarity** station. The operations are classified into six categories: *System Messages*, *Chromatogram*, *Calibration*, *Sequence* and *Method* operations and *Other*. This corresponds to six tabs.

Note: Optional Extensions, like the GPC Extension, may use and display additional tabs. For its description see the manual of the particular Extension.

You can always select whether the events should be logged to *Daily Audit Trail* or to current audit trail (*Session*) table and, in case of the events concerning the [Chromatogram](#), [Calibration](#) or [Sequence](#) windows, to their local audit trails: *Chromatogram*, *Calibration* and *Sequence*.

Local audit trails are displayed from the respective window through the *Window - Audit Trail* command and their description is in the chapter "**Local Audit Trails**" on pg. 427.

The default setting will log all operations into all relevant files.

You can easily disable the access to the *Audit Trail Settings* dialog for selected users in the *Open Audit Trail Setting* field of the [User Accounts](#) dialog.

Messages

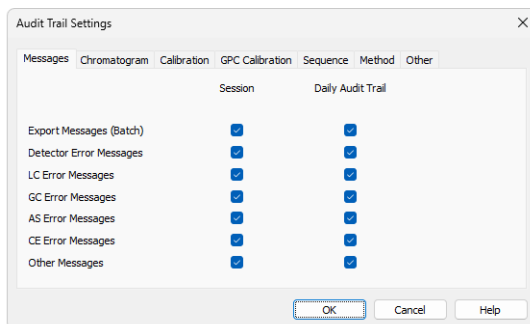


Fig. 217: Audit Trail Settings - Messages

Export Messages (Batch)

Sets whether to log messages concerning export of files and batch operations into the *Session* audit trail and/or *Daily Audit Trail*.

Detector Error Messages

Defines whether to log messages concerning problems with acquisition into the *Session* audit trail and/or *Daily Audit Trail*.

LC Error Messages

Defines the logging of messages concerning communication problems with a directly controlled LC chromatograph into the *Session* audit trail and/or *Daily Audit Trail*.

GC Error Messages

Defines the logging of messages concerning communication problems with a directly controlled GC chromatograph into the *Session* audit trail and/or *Daily Audit Trail*.

AS Error Messages

Defines the logging of messages concerning communication problems with a directly controlled autosampler into the *Session* audit trail and/or *Daily Audit Trail*.

CE Error Messages

Defines the logging of messages concerning problems with CE module into the *Session* audit trail and/or *Daily Audit Trail*.

Other Messages

Sets whether to log any other system messages into the *Session* audit trail and/or *Daily Audit Trail*.

Chromatogram

Selects which chromatogram operations will be logged (for more details see the chapter **Properties...** on pg. 429).

Calibration

Selects which calibration file operations will be logged (for more details see the chapter **Properties...** on pg. 430).

Sequence

Selects which sequence operations will be logged (for more details see the chapter **Properties...** on pg. 431).

Method

Selects which method operations will be logged (for more details see the chapter **Properties...** on pg. 431).

Other

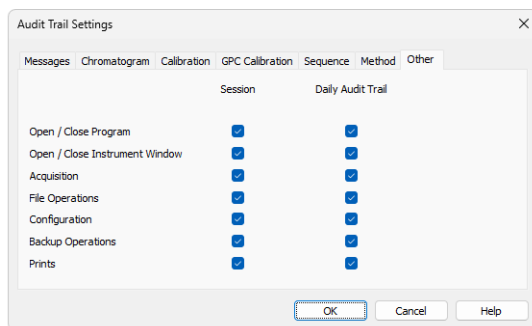


Fig. 218: Audit Trail Settings - Other

Open / Close program

Defines whether the data concerning the running and shutdown of **Clarity** station will be logged into the *Session* audit trail and/or *Daily Audit Trail*.

Open / Close Instrument Window

Defines whether the data concerning the running and shutdown of the [Instrument](#) window will be logged into the *Session* audit trail and/or *Daily Audit Trail*.

Acquisition

Defines whether the data concerning the running and shutdown of data acquisition will be logged into the *Session* audit trail and/or *Daily Audit Trail*.

File Operations

Defines whether the operations with files (opening, closing, deleting) will be logged into the *Session* audit trail and/or *Daily Audit Trail*.

Configuration

Defines whether the changes of the station's configuration will be logged into the *Session* audit trail and/or *Daily Audit Trail*.

Backup Operations

Defines whether the use of the *Backup* command from the [Instrument](#) window will be logged into the *Session* audit trail and/or *Daily Audit Trail*.

Prints

Defines whether print operations will be logged into the current Global audit trail (*Session*) or Daily audit trail (*Daily Audit Trail*).

7.1.8 Window

A submenu of commands for working with the station windows.

Main	Displays the main Clarity window of the station described on pg. 1.
Instrument 1 ... 4	Displays the relevant Instrument window described on pg. 60.

7.2 Local Audit Trails

Besides the events logged in the global audit trail, the **Clarity** station may also log all operations with chromatograms, calibrations and sequences. The audit trail always forms the integral part of a given file. A list of logged operations is selectable using the *View - Properties* command either from the global [Audit Trail](#) window on the relevant tab or by using the same command directly in window of corresponding local audit trail.

Chromatogram Audit Trail

The audit trail of the active chromatogram can be displayed using the *Window - Chromatogram Audit Trail* command from [Chromatogram](#) window.

Chromatogram Audit Trail also keeps log of errors that occurred during its acquisition (Pump Errors, missing spectra, etc.)

Calibration Audit Trail

An opened calibration log can be displayed using *Window - Calibration Audit Trail* command from [Calibration](#) window.

Sequence Audit Trail

An opened sequence log can be displayed using the *Window - Sequence Audit Trail* command from [Sequence](#) window. The sequence audit trail is reset when the sequence itself is reset.

Method Audit Trail

An opened method log can be displayed using the *Audit Trail* button from the [Method Setup](#) dialog.

7.2.1 File

Export	Invoking this command exports logged operations into a text, database file or excel (for more details see the chapter Export on pg. 418).
Report Setup...	Invoking the command opens the Report Setup dialog which allows you to set the print style and the content of the printed report.
Print Preview...	Displays a preview of the print output. The printing format of the audit trail table is WYSIWYG (What You See Is What You Get) and thus depends on the current display of the table.
Print...	Opens the Print dialog used for specifying the printer and starting the actual printing.
Close Window	Exits the Audit Trail window.

7.2.2 Edit

Submenu of commands for working with the clipboard and tables.

Copy	Invoking the command or using the Ctrl + C shortcut copies the selected text into clipboard.
Select All	Invoking the command or using the Ctrl + A shortcut selects all fields of the table.
Restore Default Columns	Invoking the command returns the display of the given table to default settings (for more details see the chapter Edit on pg. 191).
Setup Columns...	Using this command opens the Setup Columns dialog which allows to set the visibility and order of appearance of columns in the given table (for more details see the chapter Setup Columns on pg. 198).
Hide Column(s)	Invoking the command hides all selected column(s) from display (for more details see the chapter Edit on pg. 192).
Show Hidden Column(s)	Using this command displays columns hidden by the <i>Hide Column(s)</i> command (for more details see the chapter Edit on pg. 192).

7.2.3 View


Submenu of commands for displaying and modifying of the [Local Audit Trail](#) window settings.

Toolbar

Displays commands for toolbars. The command is similar to the *Toolbars* command in the main [Clarity](#) window.

- **Default** : Hides/shows the default toolbars.
- **Customize...** : Customization of items in the toolbars.
- **Reset All** : Invoking this command returns all menus and toolbars in the [Local Audit Trail](#) window into their initial state.

Properties...

Invoking this command or using the  icon opens the [Audit Trail Settings](#) dialog where you can specify operations to be logged.

7.2.4 Properties...

The *Audit Trail Settings* dialog specifies the operations that will be logged automatically by the **Clarity** station. When invoked from any [Local Audit Trail](#) window, only the tab for changing the settings for the given local audit trail is displayed.

Note: Default setting will log all operations.

Note: The option to change the settings for specified users can easily be disabled using the [User Accounts](#) dialog in the *Open Audit Trail Setting* field.

According to the window from which the local audit trail was opened, one of the tabs described below will appear:

Chromatogram

Sets the logging of chromatogram operations into particular audit trails.

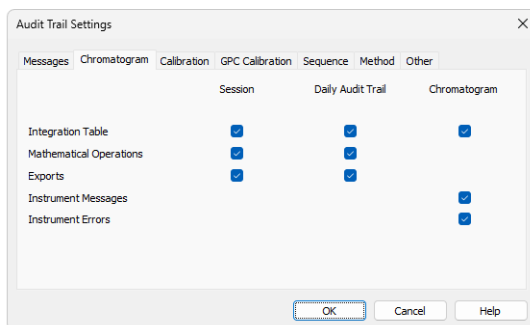


Fig. 219: Audit Trail Settings - Chromatogram

Integration Table

Defines whether the changes in the integration table will be logged into the current Global audit trail (*Session*), Daily audit trail (*Daily Audit Trail*) or Chromatogram audit trail (*Chromatogram*).

Mathematical Operations

Defines whether a performed mathematical operations will be logged into the current Global audit trail (*Session*) or Daily audit trail (*Daily Audit Trail*).

Note: Logging of mathematical operations into the chromatogram audit trail is not performed because they create a new chromatogram instead of modifying the current one.

Exports

Defines whether the exporting operations will be logged into the current Global audit trail (*Session*) or Daily audit trail (*Daily Audit Trail*).

Instrument Messages

Defines whether the communication messages sent by and to the controlled instrument will be logged into the current Chromatogram audit trail (*Chromatogram*).

Instrument Errors

Defines whether the errors sent from the controlled instruments will be logged into the current Chromatogram audit trail (*Chromatogram*).

Calibration

Sets the logging of calibration operations into particular audit trails.

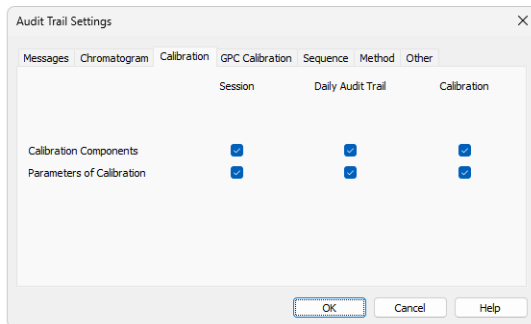


Fig. 220: Audit Trail Settings - Calibration

Calibration Components

Defines whether the changes in calibrated compounds will be logged into current Global audit trail (*Session*), Daily audit trail (*Daily Audit Trail*) or Calibration audit trail (*Calibration*).

Parameters of Calibration

Defines whether the changes to calibration parameters will be logged into the current Global audit trail (*Session*), Daily audit trail (*Daily Audit Trail*) or Calibration

audit trail (*Calibration*).

Sequence

Sets the logging of sequence states into particular audit trails.

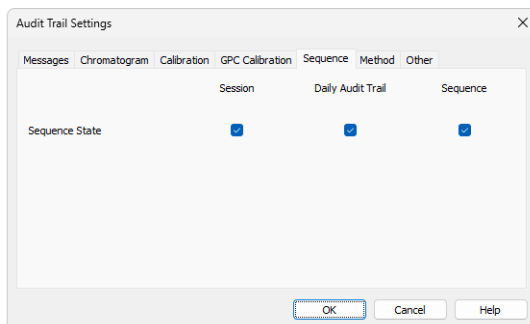


Fig. 221: Audit Trail Settings - Sequence

Sequence State

Defines whether the changes of the sequence status will be logged into the current Global audit trail (*Session*), Daily audit trail (*Daily Audit Trail*) or Sequence audit trail (*Sequence*).

Method

Sets the logging of method changes into particular audit trails.

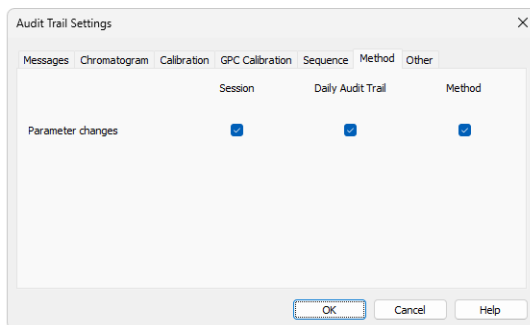





Fig. 222: Audit Trail Settings - Method

Parameter Changes

Defines whether the changes in the method will be logged into the current Global audit trail (*Session*), Daily audit trail (*Daily Audit Trail*) or Method audit trail (*Method*).

8 Report Setup

This dialog serves for selecting and adjusting the report style, setting of a printer and initiating of the print itself. The dialog opens either by using the *Report Setup* command or  icon from any major window. The displayed report style depends on the window from which the *Report Setup* window was opened - report styles set may differ between different windows.

Note: When the mouse cursor is placed over the  icon (*Report Setup*) and left still for a moment, the tooltip will appear with the name of the current report style. When placed over the  icon (*Print*) the tooltip will display the current report style and currently selected printer.

The station is supplied with pre-set report styles that are set to be used from all windows that contain printing report commands. These styles may be modified, copied, relocated or replaced by user specified styles. Report styles are located in C:\CLARITY\DATAFILES\COMMON. Default report style is dependent from which location it has been opened, e.g. while in *Chromatogram* window, after invoking *Report Setup* command, the CHROMATOGRAM.STY report style is used for printing. Analogous behavior applies for other windows.

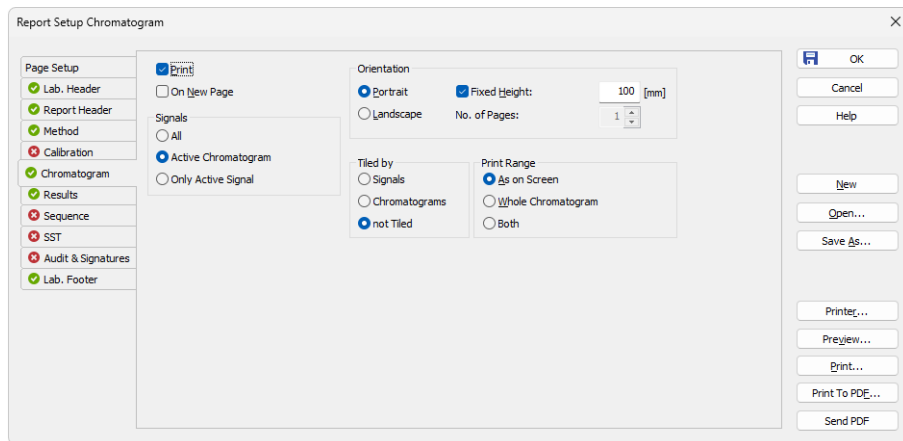


Fig. 223: Report Setup

The report is printed in order respective to tabs order on the left. By right click on the tab you can move the tab up or down. The order of *Page Setup* and *Audit & Signatures* can't be changed since they don't represent the print section.

All tabs of the *Report Setup* dialog use the same set of buttons aligned to the right side. These buttons perform following actions:

OK

Saves any changes made in the *Report Setup* dialog and exits it.

Cancel

Exits the *Report Setup* dialog. If there were any changes made to some parameter, the user is asked if he wants to save the new values.

New

Creates a new, empty report style. The values of all variable items of the report style will be erased or reset to default values. If the previously opened report style contains unsaved changes, *Save As* dialog is invoked.

Open...

Selects and opens a report style. Invoking the command will open the *Open Report Style* dialog similar to the [Open Method](#) dialog described on pg. 68. If the previously opened report style contains unsaved changes, *Save As* dialog is invoked.

Save As...

Saves the print style under a newly specified name. When invoked, the *Save As* dialog will be displayed with the name of the original file. Change the file name to save the file as a new report style, or leave the name as it is to save the changes to the same report style. When the file name selected is already used, you will be notified.

Note: For existing filenames, message box about file overwriting pops up.

Printer...

Selects the printer to be used. When invoked, the standard [Print Setup](#) dialog for selecting and setting up the printer will open.

Preview

Displays a preview of the printout (for more details see the chapter **Print Preview** on pg. 457).

Print

Initiates the printing of the report. When invoked, the command will open the standard [Print](#) dialog. The date and time of the report will be printed on each page. For tabs where the *OVERLAY* mode is possible only information about the active chromatogram will be printed.

Print To PDF

Prints the report to *.PDF file. Using the button invokes the *Print to PDF* dialog where the user can select filename and location of the resulting *.PDF file.

Note: *.PDF files can be read by freely available Adobe Acrobat Reader.

Send PDF

Sends the *.PDF file as an email attachment. The command will automatically print the report to *.PDF file, create new message in your default email client and enclose the created *.PDF file as an attachment.

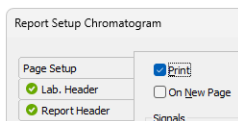
Then you can fill in the remaining information (recipient, text of the message, etc.) into the email message and send it.

8.1 List of tabs:


- [Page Setup](#) - Sets up the printed page.
- [Lab. Header](#) - Sets up the page header.
- [Report Header](#) - Reported data about the analysis.
- [Method](#) - Sets up the method printout.
- [Calibration](#) - Sets up the calibration printout.
- [Chromatogram](#) - Sets up the chromatogram printout.
- [Results](#) - Sets up the results printout.
- [Sequence](#) - Sets up the sequence printout.
- [SST](#) ✓ Full version - Sets up the system suitability report.
- [PDA](#) ✓ Full version - Sets the printout for the **PDA** method.
- [NGA](#) ✓ Full version - Sets the printout for the **NGA** method.
- [Audit & Signatures](#) ✓ Full version - Sets up the audit trail and electronic signatures report.
- [Lab. Footer](#) - Sets up the page footer.

The report itself is ordered in the order of the tabs shown - to change the order of the item groups in the resulting reports, re-order the tabs in the *Report Setup* dialog by using the *Move to the Top/Move Up/Move Down/Move to the Bottom* commands from the local menu on each tab. The [Page Setup](#) tab cannot be moved down, same as the [Audit & Signatures](#) tab cannot be moved up.

Most of the tabs contain the following two checkboxes:



Print

Allows/disallows the printing of the relevant part. If checked, the symbol  will be shown before the tab name and other fields on the tab will become editable.

On New Page

If checked, the relevant part will be printed on a new page.

8.2 Page Setup

Specifies the setup of the printed page.

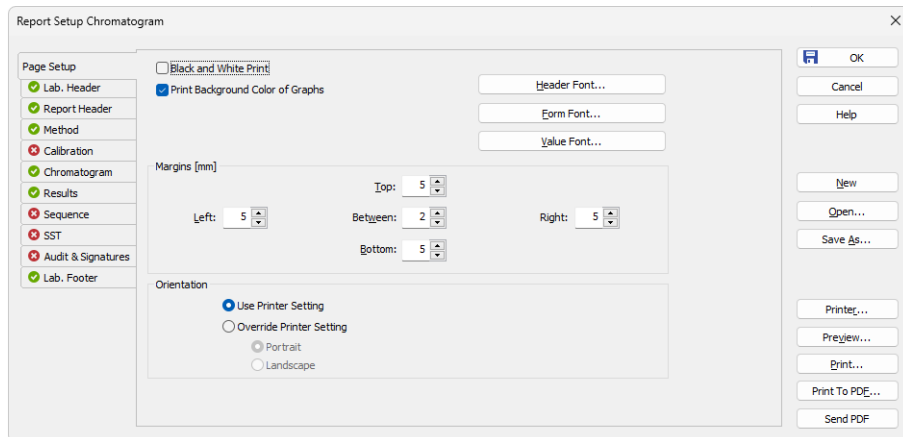


Fig. 224: Report Setup - Page Setup

Black and White Print

Prints the report in black and white color (even on color printers).

Note: Some black&white printers in MS Windows are identified as color printers. In such case it is necessary to use the *Black and White Print* checkbox to ensure that the B&W optimization will be applied. These printers would otherwise, for example, not print background colors of the graph.

Print Background Color of Graphs

Prints the background color of the graphs. If not checked, the graph background will be white.

Header Font...

Selects the font for the report header. Invoking the command will open the standard *Font* dialog.

Note: There is always the method name, date and time of the printing and the page number displayed in the header. To hide this header, use white color for the *Header Font*.

Form Font...

Selects the font for item names and table headers. Invoking the command will open the standard *Font* dialog.

Value Font...

Selects the font for values. Invoking the command will open the standard *Font* dialog.

Caution: In case you want to print PDF Reports in Chinese:

- You have to install True Type font supporting Chinese signs on your system.
- You have to set this font to use in **Clarity** reports.

Margins [mm]

Sets the margins. The allowed range is 0 to 50 mm.

Left, Right, Top, Bottom

Specifies the corresponding margin.

Between

Indicates the space left blank between individual parts of the printed report.

Orientation

Sets the orientation of the printed page. This may be either left on the selected printer setting or overridden by custom page orientation, which is advantageous when using two report styles with different page orientation on the same printer.

Use Printer Setting

Uses the printer page orientation selection for the given report style.

Override Printer Setting

Overrides the printer page orientation selection by one of the available options - *Portrait* or *Landscape*. During the selection and preparation of the report style, you might be prompted to select the printer that will be used for the print.

The size and print quality of the printed page are set in the [Print Setup](#) dialog of the selected printer (opened by the *Printer* command in the [Report Setup](#) dialog).

8.3 Lab. Header

Specifies the page header.

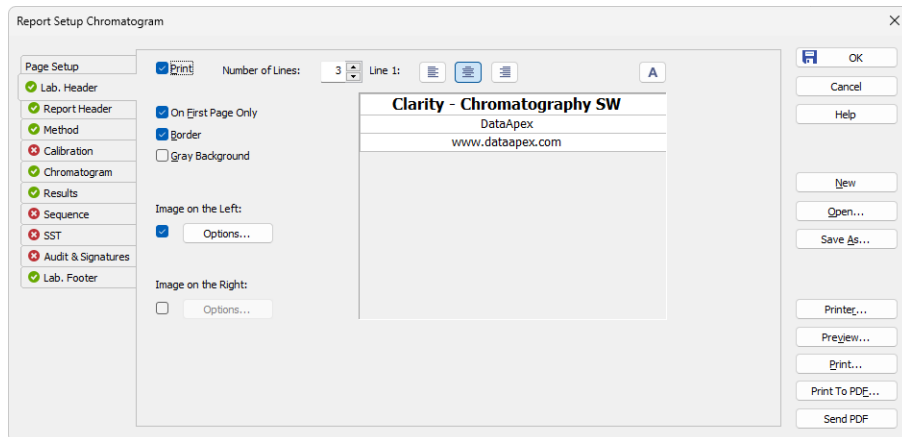


Fig. 225: Report Setup - Lab. Header

On First Page Only

Sets the print of the header on the first page only.


Border

When checked, places the header in a frame made of thin lines.

Gray Background

When checked, prints the header with a gray background (blue when using a color printer).

Number of Lines

Defines the number of lines in the header. New lines will be appended/removed to/from the end of the current list. Maximum number is 9. After clicking on any row, icon for selecting  appears in the right corner of the row. Upon clicking it, a list where you can pick available variables for additional details to be placed in the header is invoked. Variables that can be used:

Tab. 30: Variables to display on the Report Setup - Lab. Header tab





Name	Variable	Description
<i>Analyst</i>	%g	Inserts name of the <i>Analyst</i> who acquired the chromatogram.
<i>Sample</i>	%Q	Inserts name of the <i>Sample</i> .

Name	Variable	Description
<i>SampleID</i>	%q	Inserts value of the <i>SampleID</i> .
<i>Method</i>	%J	Inserts name of the method that was used to acquire the chromatogram.
<i>Chromatogram</i>	%C	Inserts name of the chromatogram and path to the chromatogram.
<i>Instrument Name</i>	%e	Inserts value of the <i>Instrument Name</i> .
<i>The per cent sign %</i>	%%	Inserts per cent sign.

Line 1(...9)

Indicates the current line for the purpose of formatting. Use arrows or click a line to make it current, then use one of the icons to change the alignment or format of the text:

Tab. 31: Description of icons on the Report Setup - Lab. Header tab

Icon	Description
	Left-aligns the text on the current line.
	Centers the text on the current line.
	Right-aligns the text on the current line.
	Selects the font for the current header line. Invoking the command will open the standard <i>Font</i> dialog.

The changes in the header are then shown in the preview. Click the corresponding line and enter the required text, or click the existing text to edit it.

Image on the Left (Right)

Mark the checkbox to print an image on the left (right) side of the page header. Use the *Option...* button to define the picture.

Options...

Invoking this button opens the *Set Image Options* dialog where the desired image and its dimensions can be set.

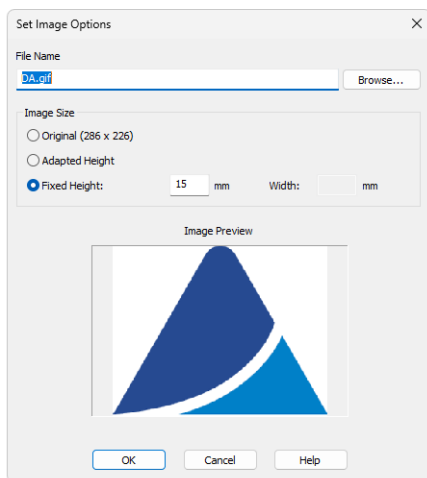


Fig. 226: Set Image Options

File Name

Displays the filename of the image including its path (relative to the **Clarity** root directory). **Clarity** supports various image files formats. It is recommended to use preferably *.PNG, *.JPG or *.JPEG image files.

Image Size

The image size can either correspond to the specifications in the file (*Original*) or can be resized to the height of the header (*Adapted Height*) or to explicitly specified dimensions (*Fixed Height*).

If the image and text do not fit to the page width, **Clarity** will provide a warning when opening the [Print Preview](#) dialog, divide the header in thirds (halves when only one image is selected) and print its contents without respect to the actual dimensions.

Caution: Check the page header using the *Preview* button to see whether the image and text fits on the page.

Caution: The size of the page depends on the selected printer. Re-check the page when you switch to another printer.

8.4 Report Header

Selects the information that will be used in the report header. Everything but some parameters from Printed Version Info (and its GLP Information) is printed from chromatogram. These information may include the origin of the chromatogram, date and time of analysis, user account used, calibration file name, name of the report style, data from the chromatogram header or directory where the chromatogram is stored.

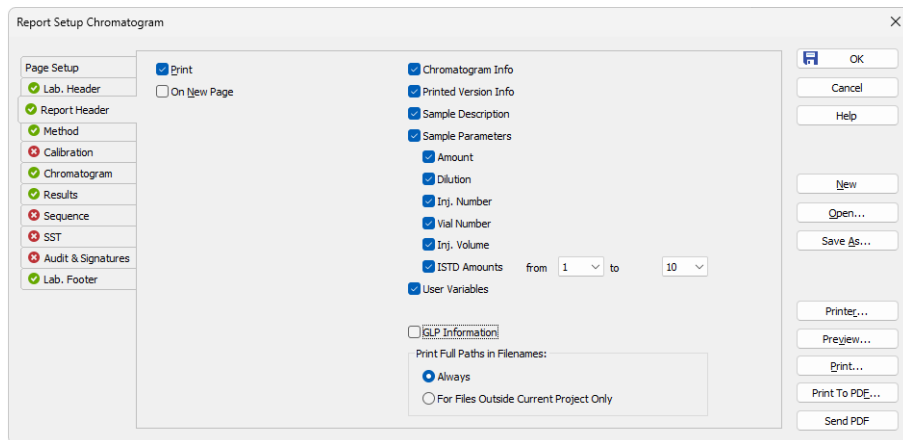


Fig. 227: Report Setup - Report Header

Chromatogram Info

Adds the detailed info about the origin of the chromatogram to the printed report. Following parameters are added:

Filename - shows the filename of the chromatogram.

Origin - defines whether the chromatogram was *Acquired*, *Imported* or *Self* created by mathematical operations.

File Created - shows the date and time when the chromatogram file was created (according to the Windows file system).

Acquired Date - shows the date and time when the chromatogram was acquired (the end of acquisition as stored in the chromatogram).

By - displays the name of the user account used to acquire the chromatogram.

Original Project - shows the name of the original project used to acquire the chromatogram, such information is stored within chromatograms since version 8.3.

Printed Version Info

Adds the detailed info about the print to the printed report:

Printed Version - shows the date and time in which the chromatogram version being printed was saved, thus enabling to trace the given chromatogram version.

Report Style - shows the report style used to print the report.

Calibration File - shows the name of the calibration file used.

Printed Date - shows the date and time when the report was printed.

By - displays the name of the user account used to print the report.

Project - shows the name of the [Project](#) currently opened on the [Instrument](#) when printing of respective chromatogram took place.

Sample Description

Adds the detailed info about the sample to the printed report. This info comes from the chromatogram header and is defined in the [Sequence](#) or [Single Analysis](#) dialog. The fields reported are **Sample ID** and **Sample**.

Sample Parameters

Adds the detailed info about sample parameters of the respective chromatogram to the printed report:

Amount - shows the Amount value as on right side pane of the [Chromatogram - Results](#) and [Chromatogram - All Signals Results](#) tabs.

Dilution - shows the Dilution value as on right side pane of the [Chromatogram - Results](#) and [Chromatogram - All Signals Results](#) tabs.

Inj. Number - shows the serial number of the injection as in respective [Sequence](#) if chromatogram was measured using sequence.

Vial Number - shows the vial number in ordinary format from [Sequence](#) or [Single Analysis](#) relevant to printed chromatogram.

Inj. Volume - shows the vial injection volume value as on right side pane of the [Chromatogram - Results](#) and [Chromatogram - All Signals Results](#) tabs.

ISTD Amounts - shows ISTD1 ... ISTD10 (internal standards) values. Two dropdown menus to the right of the **ISTD Amounts** allows to set a range which ISTD values should be included in the printed report. For example, if there are selected values 3 and 5, there will be printed values for ISTD3, ISTD4 and ISTD5.

Note: In GPC Extension, there is an extra section GPC Parameters that adds the detailed info about GPC parameters to the printed report. This info comes from the chromatogram header and is defined in the [Sequence](#) or [Single Analysis](#) dialog. The fields reported are **K** and **Alpha**.

User Variables

Adds the detailed info about Analysis and Method user variables to the printed report. This info comes from the chromatogram header and is defined in the [Sequence](#), [Single Analysis](#), [Method Setup](#) or [Chromatogram](#) window. The fields reported are **Name** and **Value**.

Note: To print *Method user variables* from Method Setup window, use the *Calculation Parameters* checkbox on Method tab. The *Analysis user variables* set in Sequence window can be printed in the table from sequence tab.

Print Full Paths in Filenames

Determines the format of filenames by switching on and off the full path in the name of the files in the given project directory. For files outside of the project directory the full path is always printed.

Always

The full path will be printed for all files.

For Files Outside Current Project Only

- The files that are in the appropriate directory specified by the project will be printed without path.
- Files that are in any other directory or subdirectory will be printed with full path.

GLP Information

Adds the information about the computer, **Clarity** version and methods used for obtaining the printed information to the *Chromatogram Info* and *Printed Version Info* sections. If none of these sections is selected for display, the *GLP Information* checkbox will be disabled.

8.5 Method

Determines the elements of the method that will be printed.

Note: Parts of the method report dedicated to a particular device are printed only when this device is configured on the instrument in the moment of printing.

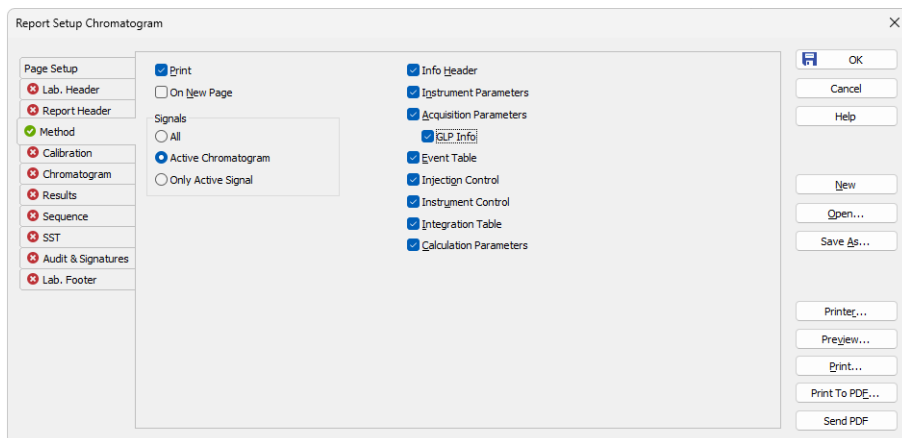


Fig. 228: Report Setup - Method

Signals

Determines which signals (detector) information will be printed when using a multi-detector configuration. You can choose to include either method parameters from all signals of all chromatograms (*All*), all signals from active chromatogram (*Active Chromatogram*) or only the parameters from the active signal (*Only Active Signal*).

Info Header

Adds the section containing method **Name**, method **Description**, the name of the **User Account** used to create the method and the time of the **Creation** and **Last Modification** parameters to the report.

Instrument Parameters

Adds the content of the text fields (**Column**, **Mobile Phase**, **Flow Rate**, **Pressure**, **Detection**, **Temperature** and **Note**) from the [Method Setup - Measurement](#) dialog to the report.

Acquisition Parameters

Adds *Autostop* and *External Start/Stop* sections from the [Method Setup - Measurement](#) tab, measurement scale from the [Method Setup - Acquisition](#) tab and the *Subtraction* section from the [Method Setup - Advanced](#) dialog to the report.

GLP Info

Adds the content of the *GLP Info* sub-tab of the [Measurement Conditions](#) tab in the [Chromatogram](#) window.

Event Table

Adds the **Event Table** from the [Method Setup - Event Table](#) dialog to the report.

Injection Control

Adds the injection control parameters from the [Method Setup - AS](#) tab to the report. This checkbox adds no parameters to the report if there is no directly controlled autosampler used.

Instrument Control

Adds any parameters set on the tabs of individual directly- controlled chromatographs ([Method Setup - LC](#) tab, [Method Setup - GC](#) tab) and other directly controlled instruments to the report in case these instruments are used. This section also includes settings of the signals from A/D converters used on the given Instrument when analog acquisition is used.

Integration Table

Adds the **Integration Table** from the [Method Setup - Integration](#) dialog to the report.

Calculation parameters

Adds the parameters from the [Method Setup - Calculation](#) tab and from the **Column Calculations** section of the [Method Setup - Advanced](#) tab to the report.

PDA Method

Adds the parameters from the *Method Setup - PDA Method* tab to the report. This section is only active when the method has **PDA** part. Detailed description is provided in a separate **PDA** manual.

MS Method

Adds the parameters from the *Method Setup - MS Method* tab to the report. This section is only active when the method has **MS** part. Detailed description is provided in a separate **MS** manual.

8.6 Calibration

Determines the contents and layout of the calibration printout.

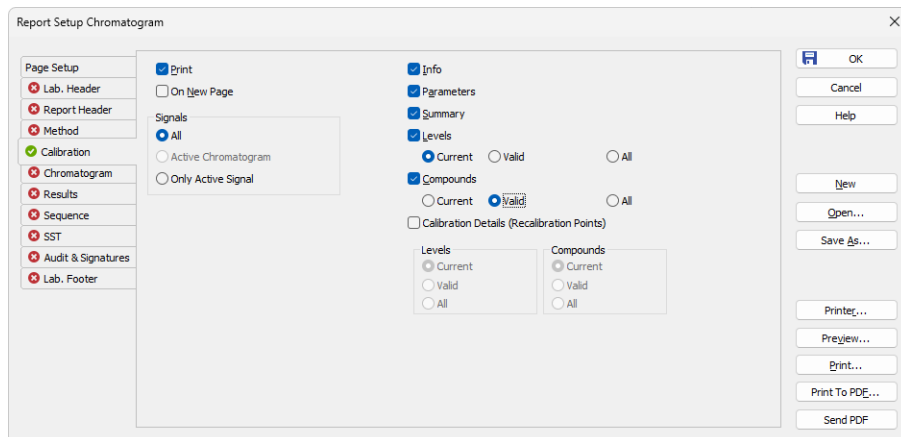


Fig. 229: Report Setup - Calibration

Signals

Determines which signals (detectors) will be printed when using a multi-detector configuration. Include either calibration parameters from all signals (*All*) or only the parameters from the active signal (*Only Active Signal*).

Info

Prints the name and description of the calibration.

Parameters

Prints the parameters from the [Calibration Options](#) dialog.

Summary

Prints the **Calibration Summary Table** from the [Compounds](#) tab of the [Calibration](#) window.

Levels

Prints Calibration Summary Table(s) for specified levels including the section related to the active level and signal only.

Current

Prints only the table which refers to the current level.

Valid

Prints only tables of levels which contain at least one valid compound. A compound will be valid when the *Response* and *Amount* columns differ from zero and the *Used* checkbox in the **Calibration Summary Table** has been checked.

All

Prints the table for all calibration levels (including blank) irrespective of the fact if the level has any valid data.

Compounds

Prints calibration tables from tabs of individual compounds including the calibration graphs. Information concerning individual compounds is printed on separate pages.

Current

Prints only the table and graph of the current compound.

Valid

Only tables and curves of compounds having at least one valid level will be printed. A level is valid when columns *Response* and *Amount* in the calibration table of compound differ from zero and on the same level the parameter *Used* has been checked.

All

Prints calibration tables and graphs for all compounds.

Calibration Details

Allows to print the details of calibration points for the selected combination of calibration levels compounds.

Levels

Defines which levels will be used for the display of calibration point history. Options are *Current*, *Valid* and *All*.

Compounds

Defines which compounds will be used for the display of calibration point history. Options are *Current*, *Valid* and *All*.

8.7 Chromatogram

Sets the sections and layout of printed chromatograms.

All tags, descriptions and labels in the graphs are WYSIWYG (*What You See Is What You Get*). That means that the printed report will correspond to the display set on the screen.

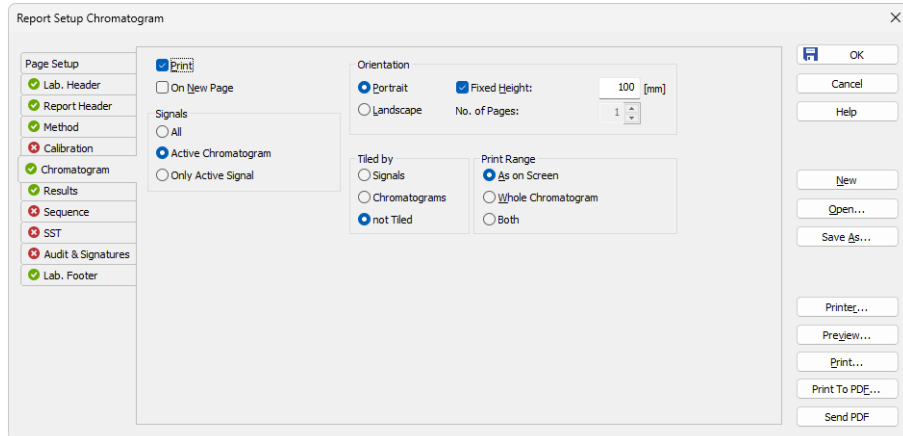


Fig. 230: Report Setup - Chromatogram

Signals

Determines which signals (detector) information will be printed when using a multi-detector configuration. You can choose to include either method parameters from all signals of all chromatograms (*All*), all signals from active chromatogram (*Active Chromatogram*) or only the parameters from the active signal (*Only Active Signal*).

Orientation

Sets the type of the chromatogram orientation:

Portrait

Prints the chromatogram crosswise (the time axis is parallel to the printed lines). The width will always be given by page width and pre-set borders. Unless *Fixed Height* has been selected, the chromatogram will be printed with a fixed ratio of sides (approximately 2:3) on a single page.

Landscape

Prints the chromatogram on a separate page with the time axis perpendicular to the printed lines. The size will be given by page size and pre-set borders.

Fixed Height

If the graph orientation is set to *Portrait*, the chromatogram will be printed with a fixed height instead of the fixed ratio 2:3. The permitted lower

height range is *30 mm*, the upper height range is not set - the graph will be scaled to the page height if larger than the page itself.

No. of pages

If the graph orientation is set to *Landscape*, this field determines the chromatogram length display by number of pages. The permitted range is from 1 to 9.

Tiled by**Signals**

Prints multiple curves in separate graphs tiled by signals (each signal will have its own graph in the report).

Chromatograms

Prints multiple curves in separate graphs tiled by chromatograms (each chromatogram will have its own graph in the report, possibly consisting of more than one signal in case of multi-detector chromatograms).

not Tiled

Prints all curves overlaid in one graph.

Print Range**As on Screen**

Prints only the portion of the chromatogram which is visible on screen.

Whole Chromatogram

Prints the entire chromatogram(s) regardless of the size of the cut displayed in the [Chromatogram](#) window.

Both

Prints both the whole chromatogram and the active cut-out zoomed, in this order.

8.8 Results

Determines the content and layout of the printed analysis results.

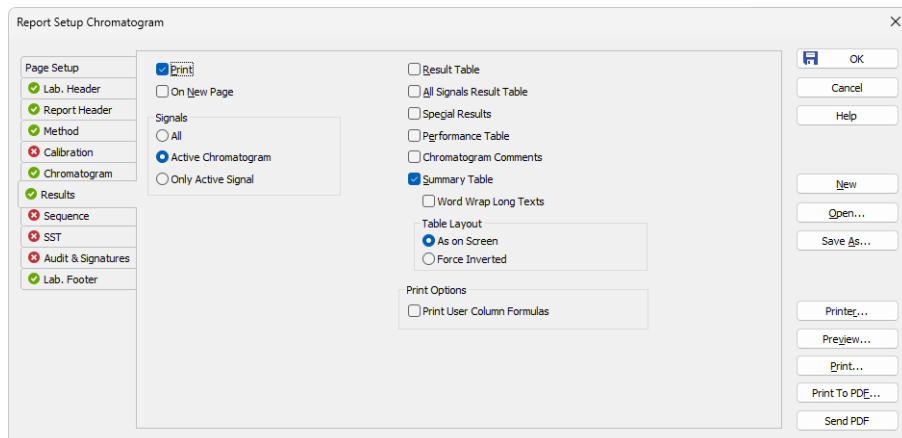


Fig. 231: Report Setup - Results

Signals

Determines which signals (detector) information will be printed when using a multi-detector configuration. You can choose to include either method parameters from all signals of all chromatograms (*All*), all signals from active chromatogram (*Active Chromatogram*) or only the parameters from the active signal (*Only Active Signal*).

Result Table

Prints the **Result Table** from the [Chromatogram - Results](#) tab.

All Signals Result Table

Prints the **All Signals Result Table** from the [Chromatogram - All Signals Results](#) tab.

Special Results

Prints special **Result Tables** generated by some control modules such as Virtual FC module.

Performance Table

Prints the **Performance Table** from the [Chromatogram - Performance](#) tab.

Chromatogram Comments

Adds the chromatogram comments entered into the [Comments](#) dialog from the [Single Analysis](#) or [Sequence](#) dialog or from the [Measurement Conditions](#) tab of the [Chromatogram](#) window to the report.

Summary Table

Prints the **Summary Table** from the [Chromatogram - Summary](#) tab.

Word Wrap Long Texts

Enables long texts to be broken so the text may continue on the next line.

Table Layout

The option *As on Screen* will print the Summary Table exactly as seen on the screen whereas the *Force Inverted* option will invert the Summary Table (rows will be shown as columns and columns will be displayed as rows) so the Summary Table may better fit to page.

Print Options

Defines additional options for printed report.

Print User Column Formulas

Adds calculation formulas used in added User Columns including *User Variables* at the end of the appropriate table to be printed.

Note: For GLP mode formulas are printed automatically, even if the checkbox is disabled.

8.9 Sequence

Determines the parts of the sequence displayed in the report.

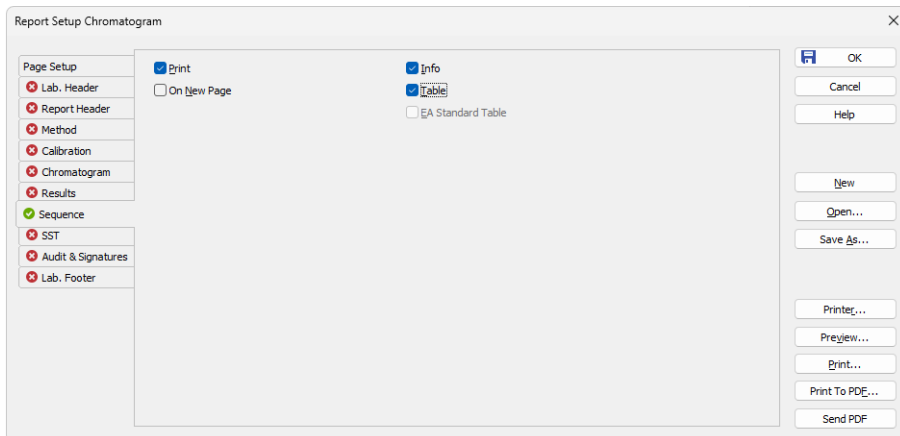


Fig. 232: Report Setup - Sequence

Info

Prints the description of the sequence - namely the **Sequence Name** and **Description**, name of the **User Account** used to create the sequence, date and time when the sequence was **Created** and **Modified**, the **Type** of the sequence (**ACTIVE** or **PASSIVE**) and the **Idle Time** parameter set. All these parameters are described in the chapter describing the [Sequence](#) window (for more details see the chapter **Sequence** on pg. 385).

Table

Prints the sequence table.

8.10 Audit & Signatures ✓ Full version

Governs the print of local audit trails and electronic signatures.

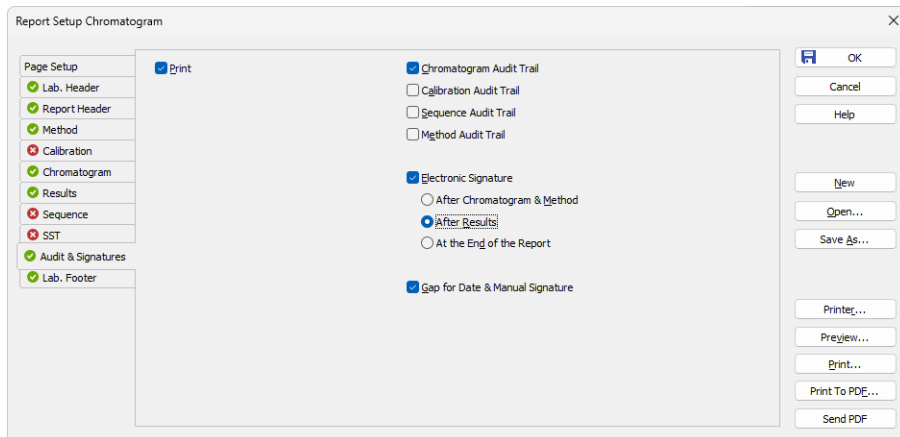


Fig. 233: Report Setup - Audit & Signatures

Chromatogram Audit Trail

Prints the operations made with the **Active Chromatogram** logged in the [Chromatogram Audit Trail](#) window.

Calibration Audit Trail

Prints the operations made with the **Calibration** file logged in the [Calibration Audit Trail](#) window.

Note: This option invokes print of complete audit trail of [Calibration](#) linked to current active chromatogram if the print is requested from [Chromatogram](#) window.

Sequence Audit Trail

Prints the operations made with the **Sequence** logged in the [Sequence Audit Trail](#) window.

Note: This option invokes print of complete audit trail of last opened sequence file in [Sequence](#) window if the print is requested from [Chromatogram](#) window.

Method Audit Trail

Prints the operations made with the **Method** file logged in the [Method Audit Trail](#) window.

Note: This option is solely operational in case the print is requested from [Method Setup](#) dialog only. If the print is requested (with this option enabled) from another location than *Method Setup* dialog (for example from [Chromatogram](#) window) there will be nothing printed.

Electronic Signature

Determines the placement of the electronic signature:

After Chromatogram & Method

Places the signature after the chromatogram and its method.

After Results

Places the signature after the result tables.

After the End of the Report

Places the signature at the end of the report.

Gap for Date and Manual Signature

Prints a pre-printed blank line at the end of the report so that the date and signature may be filled in by hand after the printout.

Note: Printing the entire station's logs (**Session Audit Trail** and **Daily Audit Trail**) can only be done directly and manually from the [Audit Trail](#) window using the *File - Print* command.

8.11 Lab. Footer

Specifies the page footer.

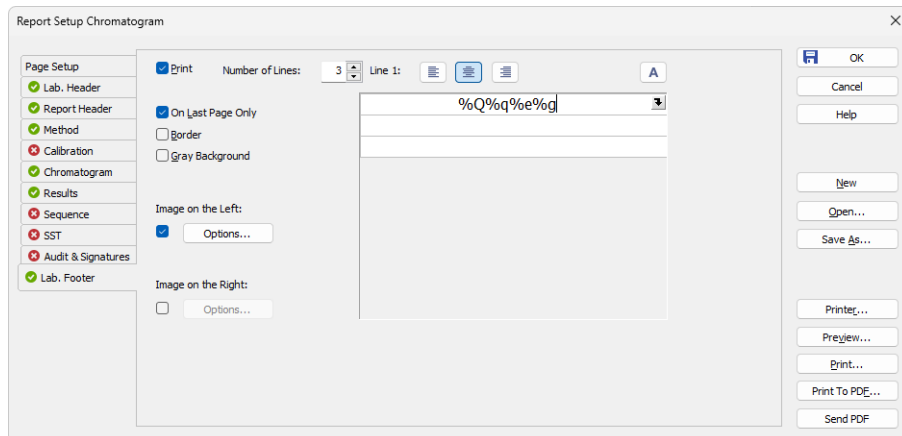


Fig. 234: Report Setup - Lab. Footer

On Last Page Only

Sets the print of the footer on the last page only.


Border

When checked, places the footer in a frame made of thin lines.

Gray Background

When checked, prints the footer with a gray background (blue when using a color printer).

Number of Lines

Defines the number of lines in the footer. New lines will be appended/removed to/from the end of the current list. Maximum number is 9. After clicking on any row, icon for selecting  appears in the right corner of the row. Upon clicking it, a list where you can pick available variables for additional details to be placed in the footer is invoked. Variables that can be used:

Tab. 32: Variables to display on the Report Setup - Lab. Footer tab





Name	Variable	Description
<i>Analyst</i>	%g	Inserts name of the <i>Analyst</i> who acquired the chromatogram.
<i>Sample</i>	%Q	Inserts name of the <i>Sample</i> .

Name	Variable	Description
<i>SampleID</i>	%q	Inserts value of the <i>SampleID</i> .
<i>Method</i>	%J	Inserts name of the method that was used to acquire the chromatogram.
<i>Chromatogram</i>	%C	Inserts name of the chromatogram and path to the chromatogram.
<i>Instrument Name</i>	%e	Inserts value of the <i>Instrument Name</i> .
<i>The per cent sign %</i>	%%	Inserts per cent sign.

Line 1(...9)

Indicates the current line for the purpose of formatting. Use arrows or click a line to make it current, then use one of the icons to change the alignment or format of the text:

Tab. 33: Description of icons on the Report Setup - Lab. Footer tab

Icon	Description
	Left-aligns the text on the current line.
	Centers the text on the current line.
	Right-aligns the text on the current line.
	Selects the font for the current footer line. Invoking the command will open the standard <i>Font</i> dialog.

The changes in the footer are then shown in the preview. Click the corresponding line and enter the required text, or click the existing text to edit it.

Image on the Left (Right)

Mark the checkbox to print an image on the left (right) side of the page footer. Use the *Option...* button to define the picture.

Options...

Invoking this button opens the *Set Image Options* dialog where the desired image and its dimensions can be set.

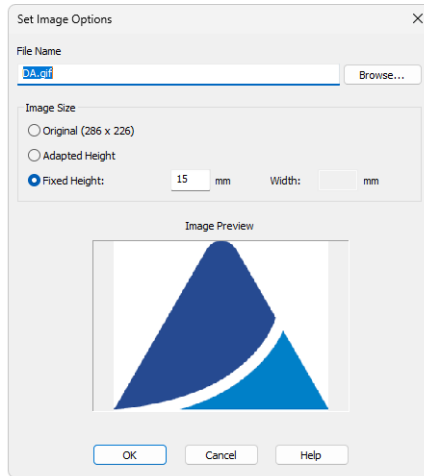


Fig. 235: Set Image Options

File Name

Displays the filename of the image including its path (relative to the **Clarity** root directory). **Clarity** supports various image files formats. It is recommended to use preferably *.PNG, *.JPG or *.JPEG image files.

Image Size

The image size can either correspond to the specifications in the file (*Original*) or can be resized to the height of the footer (*Adapted Height*) or to explicitly specified dimensions (*Fixed Height*).

If the image and text do not fit to the page width, **Clarity** will provide a warning when opening the [Print Preview](#) dialog, divide the footer in thirds (halves when only one image is selected) and print its contents without respect to the actual dimensions.

Caution: Check the page footer using the *Preview* button to see whether the image and text fits on the page.

Caution: The size of the page depends on the selected printer. Re-check the page when you switch to another printer.

8.12 Print Preview

Invoking the *Preview* button in the [Report Setup](#) dialog or using the *Print Preview...* command opens the *Print Preview* dialog which displays a preview of the report prior to printing it.

Note: If there is no printer installed in MS Windows the *Print* and *Print Preview* commands will be disabled.

The screenshot shows a 'Print Preview' window for a chromatogram report. The report title is 'Clarity - Chromatography SW' by DataApex. It includes a header with the company logo and website. The main content is divided into three sections: 'Chromatogram Info', 'Printed Version Info', and 'Sample Description'. Below these is a chromatogram plot showing voltage over time with several peaks labeled. At the bottom, there is a 'Result Table (ISTD - Data|PERS01)' with columns for Retention Time, Response, Amount, Amount%, Peak Type, and Compound Name.

Chromatogram Info:

- File Name : C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm
- Origin : Save File C:\Clarity\Alpha\DEMO1\Data\Pers01.PRM As C:\Clarity\Alpha\DEMO1\Data\Pers01x.PRM
- File Created : 26.01.2024 10:04:54
- Acquired Date : 16.01.1995 14:16:00
- By : DataApex Ltd.

Printed Version Info:

- Printed Version : 1 - #11: 21.04.2023 8:04:47, 1A: Wave rev. 1 Recent (Linked Calibration)
- Report Style : C:\Clarity\DataFiles\Common\Chromatogram.sty
- Calibration File : C:\Clarity\DataFiles\DEMO1\Calib\Ethanol.cal
- Project : DEMO1
- Printed Date : 31.01.2024 11:35:51
- By : Administrator

Sample Description:

- Sample ID : Mr. X.Y.
- Sample : DEMO Example - ethanol in blood

Chromatogram Plot: The plot shows Voltage [mV] on the y-axis (0 to 15) and Time [min] on the x-axis (0 to 6). Peaks are labeled with their retention times: 1.19, 1.75, 2.30 ETHANOL, 2.55, and 2.857 T-BUTANOL. The peak at 2.30 min is the largest, reaching approximately 14 mV.

Result Table (ISTD - Data|PERS01)

	Reten. Time [min]	Response	Amount [g/kg]	Amount% [%]	Peak Type	Compound Name
1	1,187	0,768	0,000	0,0		
2	1,752	0,612	0,000	0,0		
3	2,302	33,096	0,648	16,2	Ordnr (by ISTD1)	ETHANOL
4	2,552	1,623	0,000	0,0		
5	2,857	44,570	ISTD	ISTD	ISTD1	T-BUTANOL
Total			4,000	16,2		

Fig. 236: Print Preview

Print

Initiates the print of the report. When invoked, the standard [Print](#) dialog is opened.

Print to PDF

Prints the report to the *.PDF file. Using the button invokes the *Print to PDF* dialog (similar to [Open Method](#) dialog) where the user can select filename and location of the resulting *.PDF file.

Note: *.PDF files can be read by freely available Adobe Acrobat Reader.

Send PDF

Sends *.PDF file as an email attachment. The command will automatically print the report to *.PDF file, create new message in your default email client and enclose the created *.PDF file as an attachment. Then you can fill in the remaining information (recipient, text of the message, etc.) into the email message and send it.

Caution: In case you opened a preview of a chromatogram which contains unsaved changes, the printed results may be different in the end as the chromatogram is automatically saved when printed. Saving a chromatogram causes a recalculation which may affect printed data.

Next Page ▶

Displays the next page of the report. Only active for reports consisting of more than one page and when the last page is not already displayed.

Previous Page ◀

Display the previous page of the report. Only active for reports consisting of more than one page and when the first page is not already displayed.

Two Page/One Page 📄

This button switches between the display of one page and the display of two pages of the preview on one screen. Only active for reports with more than one page.

Zoom In 🔍

Enlarges the size of the preview by one step. If the maximum enlargement has already been reached, switches to the least enlargement possible instead.

Zoom Out 🔍


Reduces the size of the preview by one step. If the maximum reduction of the size has already been reached, switches to the maximally enlarged view instead.

Close

Closes the preview.

8.13 Print

Invoking the *Print...* command, pressing Ctrl + P combination or using the *Print...* button from the [Report Setup](#) or [Print Preview](#) dialogs will opens the *Print* dialog, which is used for specifying the printer and starting the actual printing. The layout of this dialog will vary depending on which version of Windows operating system is installed and the local settings being used.

Pressing the  directly from toolbar will print out the report immediately, according to actual settings.

Note: If there is no printer installed in MS Windows the *Print* and *Print Preview* commands will be disabled.

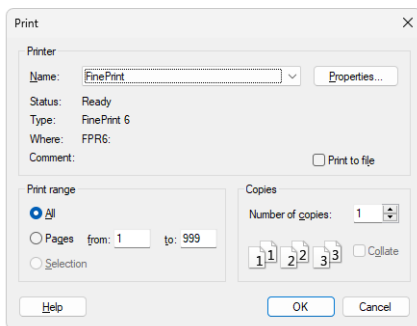


Fig. 237: Print

8.14 Print to PDF - Errors

There are some known limitation for using function *Print to PDF*. Known issues and how to solve them is described below.

Fonts

When selected font does not contain required symbols, *Print to PDF* will produce incomplete file, where some symbols are replaced by squares. In such case following message is displayed:

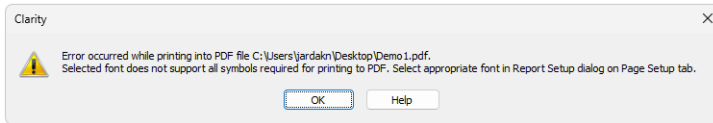


Fig. 238: Font with missing symbols

This issue can be solved by selecting a font with needed symbols on [Page Setup](#) tab of [Report Setup](#) dialog.

Note: Problem with fonts can mainly occur while using Chinese localization, selecting fonts *Microsoft Yahei* or *SimSun* should resolve the issue.

Alternative solution is to use function *Print* and using a virtual PDF printer like *Microsoft Print to PDF*.

Control Modules

Print to PDF of information from some control modules can result in incomplete file. This can be solved by using *Print* function and selecting a virtual PDF printer like *Microsoft Print to PDF*.

9 Troubleshooting

This section briefly overviews possible error messages and the procedures which will lead to the identification of the problem and its solution.

9.1 Clarity Error Messages

9.1.0.1 List of error messages:

An unknown error occurred while accessing C:\Users\\AppData\Local\Temp\Clarity\\${ch1}run.raw

It can be displayed during the start of the acquisition, probably when the User does not have writing rights into C:\...\Clarity.

Attempted an unsupported operation.

It may occur when accessing a broken dialog or window. Please contact our support and describe in which window it happened.

Board malfunction

Probably there is an error in communication with DataApex converter. See a manual of INT7 or INT9 - chapter Troubleshooting, table List of Error Messages.

Blocked HW key

Your HW key has for some reason been blocked. Contact our support for help.

Cannot add device group

When trying to drag the whole group of devices (AS, GC, ...) over to the Instrument.

Cannot add some subdevices. - DEMO - 1 was configured on Instrument XX

If the number of DEMO detectors in configuration exceeds a certain number. Up to 10 is definitely still fine.

Cannot connect with communication library CswHP1100.dll. Install Agilent IO Library Suite version 15.

Libraries for GPIB are not installed (e.g. when switching the station from Clarity Demo mode with 1100 over GPIB in configuration). We do not include the libraries, see the Agilent website. Also note that GPIB communication is no longer supported since Windows 7.

Cannot create Detector

This error message can occur while using a DataApex A/D converter. Probably an unregistered library. Please contact our support.

Cannot create RAW file

Cannot create raw file C:\Users\\AppData\Local\Temp\Clarity\\${ch1}temp.raw is an error message which occurs due to very specific circumstances.

After starting the analysis, the file \${ch1}run.raw is created. When the analysis finishes, it is then renamed to \${ch1}last.raw from which the chromatogram *.prm is created. The file \${ch1}temp.raw gets created in case the renaming is not possible - usually due to a modal error message which awaits confirmation.

Cannot create temporary files

At **Clarity** startup if the user cannot write to C:\Clarity (installed without administrator rights).

Can't create ... (device name)

Usually a problem with the control module library (*.dll file). See FAQ - Question "I get an error message (Error on setup, Can't create ...) when I want to add an hardware to **Clarity** Configuration".

Cannot determine the number of bytes in input queue for Serial communication. System Error Information : 31. A device attached to the system is not functioning

If Multicom is unplugged from the USB of the PC (ECOM LCO connected over Multicom).

Cannot determine the number of bytes in input queue for Serial communication. System Error Information : 1167. The device is not connected

If Multicom is unplugged from the USB of the PC (ECOM LCO 102 connected over Multicom).

Cannot establish communication with XXXX SN xxx! XXXX SN xxx might not be connected, installed properly or it might be malfunctioning

In an attempt to open Instrument which has an uncommunicative device in configuration (e.g. unplugged U-PAD2 or Colibrick).

Cannot find driver file

From version 2.8 and later - this message pops up if an DataApex internal A/D (INT7, INT9) card is configured but physically unplugged. Also if the device is disabled in the Device Manager. See a manual of INT7 or INT9 - chapter Troubleshooting, table List of Error Messages.

Cannot find first board

This message may occur when a user wants to configure more A/D cards than is present in the PC.

Cannot find RAW file

This message has occurred while ending the analysis (Agilent 7890). Cause unknown yet.

Cannot find second board

If the user tries to add a second board which is, however, not present in the PC. See a manual of INT7 or INT9 - chapter Troubleshooting, table List of Error Messages.

Cannot load device driver

This message could have occurred on older versions of **Clarity** (for example on 2.5.6.99), probably due to a missing DataApex INT7 card. See a manual of INT7 or INT9 - chapter Problems with INT7.

Cannot load script xxx server execution failed (Ruby control modules)

Problem is caused by recent Windows 10 update (Build 1809), which is blocking the used RUBY script interpreter library version used due to a vulnerability issues. For remedy, please update to Clarity version 8.1 or higher, the affected library was updated in it.

Cannot open File Open Dialog. An unknown error occurred during this operation

This message seems to be related to exhausted Windows resources. Make sure you are using the latest version of **Clarity** and a fully functional Windows installation.

Cannot open file XXX The file is already open on Instrument YYY.

If you attempt to open a method that is already opened on another instrument.

Cannot open USB communication for XY

For example U-PAD2/Colibrick. Possible causes are if the A/D converter is connected over a USB hub or if there is a problem with DLL registration.

Cannot send data in serial communication

If you have, for example, a GC connected over a NetPAD and in configuration you first remove the NetPAD and then try to perform something with the GC.

Changing project requires to restart instrument. (You will be prompted to save modified files.) Is this OK ?

If you have unsaved changes in the Chromatogram window and you also want to change a project on the instrument.

Clarity is already running!

Appears during the startup of clarity.exe if another instance is already running.

Clarity is unable to find HW key

Appears if Clarity has lost communication with the **HW Key**. The dialog is displayed for a predefined period of time and then the application is closed. The option *Retry* checks again for the **HW Key** and resumes to Clarity upon detection. Clicking *Close* closes Clarity.

Clarity.psw file has been changed. Please see help file for possible reasons.

When upgrading Clarity from versions older than 8.0, this dialog may occur at first run and be logged in Station Audit Trail. It is a standard behavior caused by security improvements in newer versions of Clarity.

When manipulation with the *.psw file has been detected, it appears during the start of Clarity . This manipulation may mean a *.psw file from another station was copied to the Clarity configuration folder (C:\CLARITY\CFG by default) or when Clarity closed unexpectedly (Clarity crash, PC power failure, ...) when the *.psw file was modified but not yet saved.

When the *.psw file found does not contain a record about station running in the Regulated Environment, station will normally continue working and no message will be displayed on further Clarity station starts. If the *.psw file contains the record about station running in the Regulated Environment, station will not start at all. An empty *.psw file from the \CFG\BACK\LAST_INSTALLATION\ subfolder can be used, all user accounts must be recreated and all GLP options must be re-selected.

Clarity.psw file has been corrupted. Clarity will now terminate. Replace the corrupted Clarity.psw file in Clarity folder (C:\Clarity\Cfg) with default file

from the backup folder C:\Clarity\Cfg\Back\Last installation. All user accounts will be lost.

Appears during the start of Clarity when *.psw file is corrupted (illegible). Clarity will not start at all. An empty *.psw file from the \CFG\BACK\LAST_INSTALLATION\ subfolder can be used, all user accounts must be recreated and all GLP options (if used) must be re-selected.

Configuration file C:\Clarity\Cfg\Clarity.cfg is not valid. The file was either damaged or created with a later version of the software. The backup copy will be used.

Appears when starting Clarity with a non-compatible *.cfg file.

Configuration file C:\Clarity\Cfg\Clarity.cfg is not valid. The file was either damaged or created with a later version of the software. Contact support for help.

Appears when starting Clarity with a non-compatible *.cfg file. Backup cannot be restored in this case.

Detector 1 (= NAME OF SIGNAL) is not acquiring any data

In case of high load on a low performance PC. This error may also occur due to physically damaged card during acquisition.

Encountered an improper argument

In version 3.0.3.295, this message appeared when the PDA tab in Report Setup was moved from the initial position.

Error Occurred During Setup.

This message can happen during the configuration of a control module.

Error 1008 V-2500 (Upchurch) (SN N/A): Not Connected

If the valve from a COM port is disconnected, it is switched from Waiting to Communication Error.

FAILED to send method to device (Thermostats)

When thermostat is unplugged from RS232 and then "Send Method" is pressed manually.

FAILED to send method to sub-device

If the device stops communicating with several parts (e.g. 7890).

Fraction table contains overlapping time intervals. Please amend the table so that the time intervals don't overlap.

This error occurs if the user creates a wrong table for a fraction collector with overlapping times. It is a warning for the user that the fraction table needs to be corrected in order to avoid presence of the overlapping time segments in the table.

HW Key test Failed

Your HW key is not working correctly. Contact our support for help.

Incompatible device driver

The kernel driver and the driver in the Clarity do not match.

Invalid rows detected in the Method Setup - Event Table. The invalid rows will be marked out and skipped from events processing

This message appears during the opening of a method whose Event Table uses something that is not in the configuration.

Method file XXX does not exist. For more information about errors on the other rows, point mouse cursor over "Sts." Column for each row.

This happens when opening or checking a sequence which contains a name of a non-existent method.

Method file XXX was prepared with different instrument configuration and cannot be sent into HW. Open Edit Method Dialog and press OK to adapt it to the new configuration (non-matching parameters will be replaced by defaults).

If the instrument or method being opened does not correspond to the hardware which is currently present in the configuration.

Microsoft Visual C++ 2005 Redistributable Package (x86) installation failed. Exit code: 1618. Installation of Windows update or another program is already in progress. Let it finish first, restart the PC if necessary, and then start Clarity installation again.

This can happen when Windows update or another program is already being installed, in rare cases this is caused by Windows installer process not being terminated properly. Waiting for installation to finish and restarting PC should resolve the issue.

Missing keylock drivers

The drivers for the HW key are missing or corrupted. They need to be reinstalled. See FAQ on our website - HW key (re)installation.

Net-PAD (SN Error) Cannot send sockets.

Net-PAD is not communicating. This may be due to a faulty cable or that when using a direct connection the PC does not have a static IP address set up.

NETPAD malfunction

This message appears if the data do not arrive within 7.5 seconds.

No data received for 10 s.

This message may occur during an acquisition if **Clarity** has not received any data for a prolonged period of time. Make sure the PC is not under high load during the acquisition.

No detector has been found and not even DEMO detector has been found

The control modules may be incorrectly registered. Please check the IQ Report of **Clarity**.

Please enter valid Data Size. Minimum is 2.

The content of the imported file is too short (only one data point on the graph).

Project directory <Project name> already exists but has no project file! Do you want to create the project file?

Project directory with this name already exists but it misses its project *.prj file. Select one of options. It is recommended to select Yes option.

Project file <Project name> already exists but has no project directory! Do you want to create the project directory?

There already exists project *.prj file with given name but it misses its project folder. Select one of options. It is recommended to select Yes option.

Project <Project name> already exists! Choose a different name.

Project with this name already exists. Select another and unique name for newly created project.

Seek failed on C:\..... .csv

The content of the imported file is too short (less than 5000 Bytes). Please update to the latest version of **Clarity**.

Shutdown from Event Table

This message appears after executing the Shutdown command from the Event Table.

Stop time must be larger than Start time for individual fractions.

This message concerns fraction collectors. The Fraction table contains incorrect settings of Start Time and Stop Time for one or more rows. Each row of the Fraction table has to be set such that the Stop Time is always higher than the Start Time on the same row.

The directory specified for instrument x does not exist: C:\..... It is necessary to set correct directory with projects for instrument x in Directories dialog.

This message appears during the opening of an Instrument window while deleting/renameing or damaging the respective directory in the meantime.

The report style "Chromatogram.sty" does not exist or is damaged. Default report style "Noname" will be used instead.

This message appears during the opening of a Chromatogram window while deleting/renameing or damaging the respective .sty file in the meantime.

Too many peaks in chromatogram. Try to increase peak width or threshold
Peak Width was set to a low value (e.g. to 0.001 minutes in a 80 minute noise chromatogram).**Too much data for FFT. Max. number of samples in interval is 2E6**

FFT applied to a too large interval.

Unable to lock instrument in unprotected mode!

When no user is created and you attempt to set Lock on an opened instrument.

UPAD (SN...): Cannot send data in USB communication.

For example when you unplug a USB cable during acquisition and confirm the displayed error, the Instrument then switches to a Communication Error.

UPAD device malfunction

This appears during the test of a UPAD when it does not provide any data. In other words, during the start of **Clarity** an acquisition signal 10V/100Hz is sent to the first UPAD channel and if there is nothing received from the UPAD in 1 second, this error message appears. See the manual of UPAD - chapter Troubleshooting.

■ User accounts file load error

The file **Clarity.psw** failed to load. Happens, for example, if you downgrade from 3.0 to 2.8 and leave the old files in place.

■ You are attempting to paste incompatible or out of range values

This message may occur while copying a sequence table prepared in Excel. Make sure the form of the table and its values are correct.

■ You do not have sufficient privileges to read file XXX.prj.

This message occurs if the user tries to open the project file created by user who has option *No Access* selected in *Other Users Can* setting.

■ You entered 3 times wrong password, you must restart program

If the user submits a wrong password three times in a row prior to closing **Clarity**.

9.1.0.1.1 Error messages in IQ report:**■ wrong checksum (size), probably different version of the file**

Check the IQ Report to see if the **Clarity** installation is correct.

■ Warning: unknown control module

Happens e.g. in **Clarity Lite** for drivers of control modules if the PC finds a full version of **Clarity** installed.

■ Failed: bad size

The file has a different size (compared to iq.chk) - occurs e.g. in **Clarity Full** for **.dll** from Lite, if that one was the last registered.

■ Failed: bad checksum

The file has a different checksum (compared to iq.chk) - occurs for **.dll** which has the right size, but the checksum does not match. For example if you edit the size of iq.chk manually.

9.2 Report error after Clarity crashed

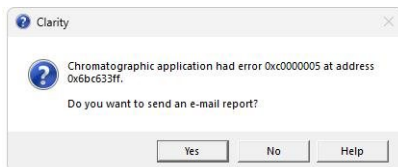


Fig. 239: Send Report dialog

If **Clarity** encounters serious problems and crashes, it will invoke a dialog during the crash that offers the possibility to send report about the problem to **DataApex**. Such report would help us locate the conditions leading to crash and improve **Clarity** accordingly.

However, in some cases, the **Clarity** may crash without producing any message. In such case, similar error message is prompted at the next start of the **Clarity** station. More details about sending an e-mail report can be found in the chapter "**Send Report by E-Mail** " on pg. 56. If you check *Do not send this report in the future* checkbox, **Clarity** will not open this dialog in case of next crashes.

9.3 How to get help

Invoke the help in **Clarity** and try to use fulltext search.

Consult the **Troubleshooting** chapter of the **Getting Started** manual.

If you do not find your answers here, use the www.dataapex.com website where the *Support* menu will navigate you to video tutorials, frequently asked questions (FAQ), and the *Support request form*. Alternatively, you can contact your distributor or the **DataApex** helpdesk via e-mail. Please note that we can request the collection of some configuration files. In case you have an e-mail client installed, you can collect these files using the *Help - Send Report by E-mail* menu in the main **Clarity** window.

Importantly, solutions to problems connected to particular **hardware** can be found in their respective manuals.

As the last option when troubleshooting a problem, **DataApex** also provides remote support via **TeamViewer QuickSupport** to registered customers in case of complicated issues (paid service). For troubleshooting via this option, the user must first contact **DataApex Technical Support** (support@dataapex.com). The **TeamViewer QuickSupport** application can be downloaded by clicking *Help - TeamViewer QS* in the main *Clarity* window. The application is ready to be used directly after downloading.

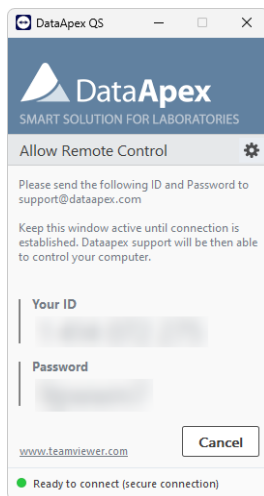


Fig. 240: TeamViewer QuickSupport application

9.4 External Control Module process encountered a problem

Some control modules run in a different process than Clarity itself. This way, it is possible to use memory more effectively and prevent memory problems due to exhausted memory for the 32-bit Clarity process.

In the case the external control module process encountered a problem, this message in Clarity pops up. Communication error is invoked in Clarity. It is necessary to restart Clarity before further usage to prevent unanticipated behavior.

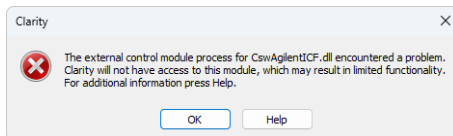


Fig. 241: External control module process error message

Until Clarity is restarted, it is not possible to enter the **System Configuration** dialog to prevent configuration corruption - a different message displays during that time when trying to open **System Configuration** dialog.

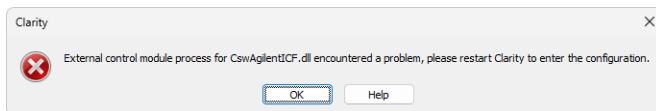



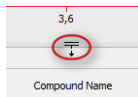
Fig. 242: Entering System Configuration disabled error message


9 Appendices

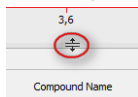
9.5 Adjusting the size of panes

Panes can be adjusted in the [Chromatogram](#) and [Calibration](#) windows. It applies to horizontal as well as vertical splitters.

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



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



9.6 List of terms

To prevent any errors or misunderstandings, the following list of terms (often-used or differing) has been provided.

21 CFR Part 11

A directive which specifies the conditions under which a company may use electronic records and signatures. The directive is mandatory for companies that use computer system designed for the manufacturing or distribution of products which are subject to regulation by the FDA (known as, "regulated products").

Access rights

A system which governs the activities that specified users are allowed to perform. Among other things, a user may be restricted in their authorization to change fundamental station settings, access certain instruments, inspect or change the data of other users, etc.

Active calibration signal

When performing a multi-detector measurement, each calibration file may contain calibration curves for up to 32 signals, the same as with chromatograms. Only one of these signals may be active at a time and this signal is modified.

The active calibration signal (i.e. its table or curve) is recognizable by its name highlighted in the header of the **Calibration Summary Table** or its curve. At the same time, all values that are signal specific will be displayed in the same color as the active signal.

Active chromatogram

The chromatogram name which is displayed in the header of the [Chromatogram](#) window. All data being displayed and operations performed will only relate to this

active chromatogram. The name of the active chromatogram is highlighted in the key by bold letters.

Active chromatogram signal

When performing a multi-detector measurement, each chromatogram file may contain a record from up to 32 detectors (this is what we call “signals”). The active signal in the chromatogram is the signal whose name is being displayed behind the name of the chromatogram in the window header and header of the tables (divided by a hyphen).

The name of the active signal together with the name of the chromatogram are highlighted in the graph key by bold letters.

Active detector

A detector whose measurement and calculation parameters are displayed in the [Acquisition](#) or [Calculation](#) tabs in the [Method Setup](#) dialog with the help of the *Select Detector* field. The field is visible only when performing a multi-detector measurement.

Analogous *Select XXX* fields may be present for other devices than detectors - for example valves on the *Method Setup - Valve* tab if more than one valve is present.

AIA format

Also named NetCDF format, export format serving as a common format for chromatographic data. The data are saved in the vector format with the header containing the information on the data type and chromatogram information. **Clarity** only exports and imports raw data, not the results.

Calibrated group

A group of peaks calibrated as a single component.

Calibration file (Calibration)

Contains calibration curves and further data for calibrated calculations. When performing a multi-detector measurement, each substance will have its own calibration curves for all detectors.

Calibration standard

A chromatogram containing known amounts of some compounds that is used to calibrate/recalibrate at a specified calibration level.

Channel

Part of the converter which enables the independent collection of data from one single detector. **DataApex** produces A/D converters that has 1, 2 or 4 channels.

Clarity Offline (used to be Clarity EVAL)

A version of the **Clarity** station that, although otherwise fully functional, does not allow the data acquisition.

Clipboard

A **Windows** tool that uses the *Copy*, *Cut* and *Paste* commands for the simple transfer of data between items, including those in other applications.

Closed window

A closed window is invisible and its activity has been terminated. A window is usually closed using the *Close* or *Close Window* command (see also the **Hidden window** term).

Configuration of the station

Sets the number of Instruments, the allocation of the A/D converters, directly controlled chromatographs, autosamplers, pumps and other devices.

Data processing string

A series of operations comprising the entire procedure used for everything from processing data from an analysis to printing the report. This procedure is shown graphically in the Instrument window using icons representing the main commands.

Desktop file - extension DSK

A file used to store the size, location and appearance of all windows and parameters of the Instruments.

Direct control of chromatograph (autosampler, pump)

An integrated additional module for selected chromatographs (pumps, autosamplers etc.) enabling the direct control and monitoring of selected parameters. For example, directly controlled detectors (GC or LC chromatographs with detectors) might not need A/D converter as they gather digital data directly from the controlled instrument.

Electronic signature

An electronic signature is a substitution of the handwritten signature for electronic documents. These electronic signatures thus must fulfil the same function and prerequisites. Meaning that it is a similar process of marking a document for protection and that it must be unique, clear and ensure the immutability of the document.

File sharing


Clarity enables file sharing between multiple stations. Any changes (saving) of such files are only enabled in the station that first opened it. Modifications performed with the shared file will take effect in the other stations only after the file has been reloaded. **Clarity** does not enable file sharing between Instruments of a single station. On the other hand, **Clarity** does enable projects to be shared between multiple Instrument of the same station.

Note: It is still not possible to use the same file on multiple Instruments even if they share the same project. The same project on two Instruments of the same station are useful when one instrument is *OFFLINE* and used to prepare methods for the other Instrument.

GLP

Good Laboratory Practice (GLP) is an internationally agreed upon system for ensuring and monitoring the quality of laboratory work. This is verified and its fulfillment confirmed by the issuance of a certificate.

Hidden window

A window which is not visible or has been "hidden". Its activity has not been terminated but rather suspended or is proceeding in the background. Click the minimize button  to hide a window (see also the **Closed window** term).

Information table

A table in the [Instrument](#) window displaying the Instrument name, the measurement methods and the identification of the measured chromatogram.

Instrument

(a) A part of the program designated to measure and evaluate analyses that share a common time base (from one chromatograph). The Instrument is indicated by the [Instrument](#) window, from which further windows and dialogs can be opened, e.g. [Chromatogram](#), [Calibration](#), etc. Detectors and control modules can be configured into individual Instruments. **Clarity Lite** has only one Instrument available. In this meaning, the word "Instrument" is written with the capital I.

(b) Sometimes also a chromatograph or generally any piece of equipment in the laboratory.

Instrument directory

The directory identified in the main [Clarity](#) window for each Instrument, where projects (i.e. project directories) are sought.

Integration Table

Constitutes a part of the method and contains a list of all modifications of the baseline or peaks that have been or will be effected in the chromatogram measured by that method.

Locked file (READ ONLY)

A file that can only be read and never modified. The file may be *READ ONLY* for several reasons, including (but not exclusive to) chromatogram measured in *GLP mode* and opened outside it, chromatogram opened with a version from the history, a user account not having user rights to modify method/chromatogram/sequence etc.

Locked instrument

An Instrument in the protected mode with locked control. Lock mode can be activated using a command from the *Lock* submenu in the main [Clarity](#) window. An Instrument is unlocked with the same password as was used to log on to the Instrument.

Main station directory

The directory where the executable file of the station CLARITY.EXE is stored (C:\CLARITY\BIN by default). Supporting *.DLL and other binary files are stored in the C:\CLARITY\BIN. Configuration and system files are stored in the C:\CLARITY\CFG directory. User's data files are stored in the C:\CLARITY\DATAFILES directory which holds individual projects, PROJECTS directory holding the project files, COMMON directory with print styles and other files.

Method file - extension MET

A template method file with a description of all parameters affecting the analysis.

Model Method

A chromatogram method marked as **Model Method** that can be easily used with other chromatograms by invoking the *Copy from Model* command.

Multi-detector configuration (measurement)

Setting of the station so that it measures, saves and evaluates one analysis by simultaneously using a signal from multiple detectors.

Password

A string of several characters which are necessary for working in the **Protected Mode** of the station. Each user has his own password. The minimal length of the password may be set centrally in the [User Accounts](#) dialog.

Printout

The layout of individual parts of analysis results and the setting of parameters controlling the resulting report. The layout is defined by the employed report style.

Project directory

Directory used to store all working files of an Instrument in which the homonymous project has been opened.

Project file - extension PRJ

The file that specifies the directories in which all user files will be stored.

Protected mode

A regime which enables only authorized users (users who have an account assigned in the [User Accounts](#) dialog) to work with the station and access data.

Raw data file - RAW

A file used in previous versions of the **CSW10 - 17** and for the external PAD unit to save non-analyzed and non-adjusted data from the analysis. The **CSW32** and **Clarity** stations save raw data directly into the chromatogram file, the *.RAW data file is used only for the gathering of the data during the acquisition (chromatogram file (*.PRM) is created only after the acquisition ends).

Report style

An outline determining which analytical results will be incorporated into a report and subsequently printed. Each report style will be stored in a separate report style file.

Report style file - extension STY

A file storing information which determines what to print and how to print it.

Sequence file - extension SEQ

A file that defines an automatic sequence of analyses.

Splitter

A resettable bar dividing certain windows (e.g., the [Chromatogram](#) or [Calibration](#) windows) into several panes. The bar can be moved to change the size of individual panes - "Adjusting the size of panes" on page 472.

SST

The **System Suitability Test** is an Extension module designated to validate the chromatographic system on the basis of evaluation of chromatograms obtained from the **Clarity** station.

Station configuration

Determines the number and arrangement of Instruments and their interconnection to possible A/D converter board(s) and directly controlled chromatographic equipment. Also allows to name the connected detectors and set signal units for them.

Status table

A table displayed in the [Instrument](#) window containing the names of system files, the status of the analysis currently in progress, potentially the retention time and identification number of a sample.

System files

The decisive files for working with the station and individual data files: **project**, **method**, **report style**, **sequence** and **calibration** files.

Tabs

Tab is the term for a section of the window or dialog where several layers of control elements are "stacked" on itself. The system is frequently used in dialogs and also in the [Chromatogram](#) and [Calibration](#) windows. Click the only visible part of the tab - that with the tab name - to switch to the corresponding tab.

Template method

A method file that serves as a template for new analyses. Its name is displayed in the **Information Table** of the [Instrument](#) window and its contents are always copied to the newly created chromatogram.

Toolbar

A block of icons symbolizing a set of commands. Each toolbar can be situated anywhere on the screen and be configured by accessing the *View - Customize...* command in the window or by right clicking the mouse button on any toolbar to access the local menu.

Unprotected mode

A regime of the station that enables any user to work with the station and access its data. No passwords are necessary for opening the Instruments.

Window title bar

Title bar is the upper band of each window. It is comprised of the button which activates the control menu of the window, the window name, the minimize button and the maximize button.

9.7 Shortcuts

MS Windows shortcuts:

Enter

Applies or implements the selected command. The command that has been selected will be highlighted in the menu; in a dialog the borderline of the button will be emphasized by a continuous or broken line).

From the menu the required command can be selected using the cursor keys, and from a window using the Tab key.

Esc

In a dialog, the Esc key substitutes for the Cancel key and will close a dialog without saving the changes.

Hides an expanded menu.

Tab

Gradual selection of commands, parameters, edit lines and buttons in the active window. A selection is usually completed using the **Enter** key.

Space bar

Rapidly switches between selected parameters by checking or unchecking them.


Alt

Selects the first menu item.

Alt + letter

Rapidly selects a command or parameter that has the selected letter underscored.

Tab. 34: Clarity shortcuts:

Shortcut	Command from menu	Description	Validity
F1	<i>Help</i>	Open new Help window	Everywhere
F2	<i>Edit</i>	Enter into edit mode of the selected cell	
Ctrl + N	<i>New file</i>	Create a new file	
Ctrl + A		Select all items in the list/table	
Ctrl + O	<i>Open</i>	Open file	
Ctrl + S	<i>Save</i>	Save file	
Ctrl + Shift + S	<i>Save As...</i>	Save file as	
Ctrl + W	<i>Close</i>	Close current file	
Ctrl + Shift + W	<i>Close All</i>	Close all opened files	
Ctrl + P	<i>Print</i>	Print	
Ctrl + X	<i>Cut</i>	Cut selected values	
Ctrl + C	<i>Copy</i>	Copy selected values	
Ctrl + V	<i>Paste</i>	Insert from clipboard	
Ctrl + Z	<i>Undo</i>	Cancel the last command	
Ctrl + Shift + Z	<i>Redo</i>	Repeat the last command	
Ctrl + I	<i>Paste Insert</i>	Insert and create lines	
Delete		Erase the table field	
Alt + ↓		Work when cell contains  , the shortcut opens corresponding options.	

Shortcut	Command from menu	Description	Validity
Ctrl + E		Automatic export of data from Chromatogram window according to settings in Export Data dialog	
(Ctrl) + F7	<i>(First) Previous</i>	Browse through chromatograms: open the previous (first) chromatogram from the current directory.	Chromatogram
(Ctrl) + F8	<i>(Last) Next</i>	Browse through chromatograms: open the next (last) chromatogram from the current directory.	
Ctrl + ⏪	<i>Previous Zoom</i>	Display the previous cut-out	
Ctrl + ⏩	<i>Next Zoom</i>	Display the next cut-out	
Shift + Mouse wheel		Move the cut-out Left & Right	
Mouse wheel		Move the cut-out Up & Down	
Ctrl + Mouse wheel		Zoom In/Out	Chromatogram Calibration
+	<i>Zoom In</i>	Enlarge graph	Data Acquisition
-	<i>Zoom Out</i>	Reduce graph	
Ctrl + Shift + Mouse wheel		Enlarge/reduce the cut-out of the chromatogram in the dimension of the Y-axis only	
Ctrl + *	<i>Unzoom</i>	Display graph in original size	
Ctrl + R	<i>Run Single</i>	Start an analysis	Data Acquisition

Shortcut	Command from menu	Description	Validity
Ctrl + Q	<i>Start, Run Sequence</i>	Start a sequence	Sequence Data Acquisition
Ctrl + Space bar	<i>Pause / Resume</i>	Pause a sequence / Resume running of a set sequence	
Ctrl + B	<i>Abort</i>	Immediately terminate a sequence	
Ctrl + H	<i>Snapshot</i>	Process the sample currently being measured without terminating the analysis	
Ctrl + T	<i>Stop</i>	Terminate a sequence after the completion of a sample measurement	Sequence
Ctrl + ↓	<i>Skip</i>	Skip the current sample	
Ctrl + ←	<i>Repeat Injection</i>	Repeat an injection from the current vial	
Ctrl + E	<i>Reset Status (Status)</i>	Reset the flags in the Status column	

10 Technical Specification

10.1 Declaration of Software Validation

You can find **Declaration of Software Validation** certificate on the **Clarity** installation USB in \DOCUMENTATION\DATASHEETS\D021- CLARITY-DECLARATION-OF-SW-VALIDATION.PDF.

Note: Actual version of this certificate is available for download as the D021 datasheet from www.dataapex.com.

10.2 Command line parameters

It is possible to specify command line parameters for automating certain functions. If not specified otherwise, CLARITY.EXE file can be run with the same or different set of parameters again and again. This creates new instance, which is temporary and just passes new parameters into **Clarity** station that is already running.

Some of the command line parameters may be also defined in the OTHERS.INI file (by default located in C:\CLARITY\CFG). Used settings will override any of the same parameters used in the command line. OTHERS.INI file supports the use of following command line parameters: *bad_trace_cnt*, *create_emf_during_pdf*, *dump_memory*, *enable_asserts*, *mail_dump*, *report_cmdline_in_bad_trace*.

All command line parameters are processed in the order they are set on the command line. It is thus usually necessary to open the file first, before making any changes to it (for example, open calibration, open chromatogram, recalibrate the calibration on the given level, close chromatogram and close calibration, in this order).

Each use of command line for controlling **Clarity** is recorded in [Audit Trail](#) including all parameters called.

No wildcards (*, ?) are allowed in the command line.

All parameters (but not file paths etc.) are case-sensitive, unless stated otherwise. No spaces are allowed between the command and the argument and in the argument itself.

Example: *clarity.exe command=value* is correct while *clarity.exe command = value* is wrong.

If you want to use spaces or other white space in parameters, you may use the quotation marks to do so.

Example: *clarity.exe c="C:\Documents and Settings\Smith\Desktop\Ethanol in blood.met"* or *clarity.exe user="John Doe"*.

10.2.1 List of commands

abort

description: Stops the single analysis/sequence measurement on the specified Instrument. This parameter is suitable for automatic testing. Does the same as **stop** command line parameter, but it does not store the chromatogram measured up to the time of abort.

syntax: `abort=VALUE`

possible values: 1 (for Instrument 1), 2 (for Instrument 2), 4 (for Instrument 3), 8 (for Instrument 4), and their binary combinations.

implicit value: None.

example: `clarity.exe abort=7` (will abort single analysis/sequence on Instruments 1, 2 and 3)

bad_trace_cnt

description: Sets the number of lines in the BADTRACE.TXT file. Maximum value is 10 000 (exceeding value will be converted to 10 000). This parameter may be also used (and is overwritten by settings) in DATAAPEX.INI file.

syntax: `bad_trace_cnt=VALUE`

possible values: 0 - virtually any number

implicit value: 100

example: `clarity.exe bad_trace_cnt=1000`

cal_apply

description: Applies the specified calibration to the active chromatogram. It is recommended to use absolute paths because the calibration file will not be searched for in the working directory but in the calibration directory of the active project.

syntax: `cal_apply=PATHFILENAME`

possible values: A valid path to the calibration (*.CAL) file.

implicit value: None.

example: `clarity.exe cal_apply=C:\CLARITY\DataFiles\WORK1\Calib\1.cal`

cal_save

description: Saves the active calibration. Use together with the **instrument** parameter to specify the Instrument whose [Calibration](#) window holds the calibration file you are interested in. Calibration file can be opened by specifying its path and filename. It is recommended to use absolute paths. This command is ignored in GPC mode - use **gal_save** instead.

syntax: `cal_save`

possible values: None.

implicit value: None.

example: `clarity.exe i=2 cal_save` - saves the calibration opened in the second Instrument.

cal_save_as

description: Saves the active calibration under the specified name. Use together with the **instrument** parameter to specify the Instrument whose [Calibration](#) window holds the calibration file you are interested in. Calibration file can be opened by specifying its path and filename. It is recommended to use absolute paths. This command is ignored in GPC mode - use **gal_save_as** instead.

syntax: `cal_save_as=PATH\FILENAME`

possible values: A valid path to the calibration (*.CAL) file.

implicit value: None.

example: `clarity.exe cal_save_as=C:\CLARITY\DataFiles\WORK1\Calib\results.cal`

cal_type

description: Changes the type of calibration calculation for the active chromatogram. The parameter allows to specify calibration type for each signal of the chromatogram -the first character is corresponding to the first signal, second character to the second signal and so on.

syntax: `cal_type=TYPE`

any combination of _, *U*, *I*, *E*, *N* and *S*. For each signal in the chromatogram, a separate symbol is needed.

Characters used mean:

possible values:

- _ (underline) - do not change
- U - uncalibrated
- I - ISTD
- E - ESTD
- N - NORM
- S - STDADD

implicit value: _ (underline) for each signal.

example: *clarity.exe cal_type=_UIE* (the first signal is left unchanged, the second is set to UNCAL, the third to ISTD, the fourth to ESTD).

cfg or g

description: Opens the **Clarity** with the specified *.CFG file. Must be used when opening **Clarity** for the first time, otherwise it is ignored. Uses just the selected configuration file, not other files present in the \CFG subdirectory.

syntax: *g=PATH\FILENAME*

possible values: The path to *.CFG file.

Empty.

If the path is not specified, the system will look for the *.CFG file in the \CFG directory. If not found, the system will use the default CLARITY.CFG file from the \CFG directory.

implicit value: When the path is specified absolutely, the **Clarity** will start with the *.CFG file specified.

When the path is specified relatively, the *.CFG file will be searched for in the directory relative to the current directory. Working directory will then be set to the new location.

example: *clarity.exe g=C:\CLARITY\Cfg\user1.cfg*

clear_cal

description: Clears the responses in the opened calibration file. When used with **recal_level**, the calibration is cleared first and recalibrated after that.

syntax: *clear_cal*

possible values: None.

implicit value: None.

example: *clarity.exe test.cal clear_cal*

control_devel_folder

description: Adds additional path to be scanned for control module *.DLL files. Can be used only once with one path, the path must be absolute. If both CLARITY\BIN and folder specified by using the *control_devel_folder* contain *.DLL files with the same name or the same GUID, then only the file from *control_devel_folder* will be loaded. This parameter may be also used (and is overwritten by settings) in DATAAPEX.INI file. Note that any control module loaded from the folder specified by using the *control_devel_folder* parameter will be considered unauthorized.

syntax: *control_devel_folder=PATH*

possible values: Absolute folder path.

implicit value: None.

example: *clarity.exe control_devel_folder=C:\Dev\CTRL_Dlls*

create_emf_during_pdf

description: Forces the creation of the *.EMF file from which the *.PDF files are converted. This parameter may be also used (and is overwritten by settings) in DATAAPEX.INI file.

syntax: *create_emf_during_pdf*

possible values: None.

implicit value: None.

example: *clarity.exe create_emf_during_pdf*

delayed_exit

description: Exits **Clarity** after the time specified in seconds if it has no running acquisition and no running background threads (export, printing). This parameter is suitable for automatic testing.

syntax: *delayed_exit=VALUE*

possible values: Numeric.

implicit value: None.

example: *clarity.exe delayed_exit=120*

disable_message_boxes

description: Suppresses the showing of message boxes. If **Clarity** would trigger a message box with a Yes-No-Cancel option then the preselected option will be applied. The Yes-No-Cancel dialog itself will not be shown but the option chosen is recorded to Audit Trail. Must be used when opening **Clarity** for the first time, otherwise it is ignored. This parameter is suitable for automatic testing.

syntax: *disable_message_boxes*

possible values: None.
implicit value: None.
example: `clarity.exe disable_message_boxes`

disable_send_report

description: Suppresses the sending of error reports. If **Clarity** would trigger a message box with a Yes-No-Cancel option then the preselected option will be applied. The Yes-No-Cancel dialog itself will not be shown but the option chosen is recorded to Audit Trail. Must be used when opening **Clarity** for the first time, otherwise it is ignored. This parameter is suitable for automatic testing.

syntax: `disable_send_report`
possible values: None.
implicit value: None.
example: `clarity.exe disable_send_report`

dsk or k

description: Opens the specified Instrument of **Clarity** with the specified desktop (*.DSK) file. Must be used when opening **Clarity** for the first time, otherwise it is ignored, the same command line must contain the number of the Instrument to be opened.

syntax: `k=PATH\FILENAME`
possible values: The path and filename of the *.DSK file.
 Empty.
implicit value: If the path is not specified, the system will look for the *.DSK file in the \CFG directory. If not found, the system will use the default CLARITY.DSK file from the \CFG directory.
example: `clarity.exe k=C:\CLARITY\Cfg\Peter.dsk i=1`

dump_memory

description: Controls whether memory dump will be included in the crash dump (*.DMP file) in case **Clarity** crashes. Presence of the memory dump influences the size of the crash dump - with memory dump the dump file is about 200MB in size, without memory dump the crash dumps are about 1MB. This function can also be set via the DATAPEX.INI file that may be stored in WINDOWS directory. Must be used when opening **Clarity** for the first time, otherwise it is ignored. `dump_memory` command line parameter has no effect if dump files are disabled by certain values of **enable_asserts**. This parameter is suitable for troubleshooting.

syntax: `dump_memory`

possible values: None.
implicit value: None.
example: *clarity.exe dump_memory*

enable_asserts

description: Specifies what to do if an ASSERT (software developer check point) emerges. Must be used when opening **Clarity** for the first time, otherwise it is ignored. This parameter is suitable for troubleshooting, because it can make **Clarity** to create a process dump file that can be used in **Debugging tools for Windows** to solve the problem. This parameter may also be used in DATAAPEX.INI file (though the value will get overwritten if also specified on the command line).

syntax: *enable_asserts=VALUE*
0, 1, 2, ..., 7

The meaning of particular values when ASSERT emerges are:

0 - Obsolete, same as 1.

1 - note is written into *BadTrace.txt*.

2 - note is written into *BadTrace.txt* and process dump file is created. The message box to send report is not displayed.

possible values: 3 - note is written into *BadTrace.txt* and process dump file is created. The message box to send report is displayed. Recommended for testing and troubleshooting.

4 - Obsolete, same as 3.

5 - Obsolete, same as 1.

6 - Obsolete, same as 1.

7 - Obsolete, same as 3.

implicit value: 1 when **enable_asserts** command is omitted in the command line, 1 when **enable_asserts** command is used without a value.

example: *clarity.exe enable_asserts=3*

err

description: Stores the audit trail records also in the specified text file. File name is valid until it is replaced by a new one.

syntax: *err=PATH\FILENAME*

possible values: A valid path and filename.

implicit value: None.

example: *clarity.exe* *err="C:\Users\<user*
name>\AppData\Local\Temp\CLARITY\error.txt"

exit

description: Immediately exits **Clarity**. Does not work if acquisition is running or if any modal window is opened. This parameter is suitable for automatic testing.

syntax: `exit`

possible values: None.

implicit value: None.

example: `clarity.exe exit`

export_emf

description: Exports the currently opened chromatograms into enhanced Windows metafile.

syntax: `export_emf=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe export_emf=C:\CLARITY\DataFiles\WORK1\Data\test.emf`

export_results

description: Exports the results of active chromatogram into the specified *.TXT file and/or CLIPBOARD (for more details see the chapter **Export Data** on pg. 141). Setting of the export is taken from the active *.CFG or *.DSK file.

syntax: `export_results=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe export_results="C:\Users\<user name>\AppData\Local\Temp\CLARITY\results.txt"`

export_results_dbf

description: Exports results of active chromatogram into specified database (*.DBF) file (for more details see the chapter **Export Data** on pg. 141). Setting of the export is taken from the active *.CFG or *.DSK file.

syntax: `export_results_dbf=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe export_results_dbf="C:\Users\<user name>\AppData\Local\Temp\CLARITY\results.dbf"`

export_run_time

description: Exports the *Autostop Run Time* value from the method currently opened on the Instrument as ANSI text into the specified file. Decimal separator is always ".". Exports "-1" when *Autostop* function is not enabled. In case of any error the text "No current method." is exported instead.

syntax: `export_run_time=PATH\FILENAME`

possible values: Any valid file name, including the path.

implicit value: None.

example: `clarity.exe export_run_time="C:\Users\<user name>\AppData\Local\Temp\CLARITY\runtime.txt"`

gal_apply

description: Applies the specified GPC calibration to the active chromatogram. It is recommended to use absolute paths because the calibration file will not be searched for in the working directory but in the calibration directory of the active project.

syntax: `gal_apply=PATH\FILENAME`

possible values: A valid path to the GPC calibration (*.GAL) file.

implicit value: None.

example: `clarity.exe gal_apply="C:\Users\<user name>\AppData\Local\Temp\CLARITY\1.gal"`

gal_save

description: Saves the active GPC calibration. Use together with the **instrument** parameter to specify the Instrument whose [Calibration](#) window holds the GPC calibration file you are interested in. GPC calibration file can be opened by specifying its path and filename. It is recommended to use absolute paths.

This command is ignored when not in the GPC mode - use **cal_save** instead.

syntax: `gal_save`

possible values: None.

implicit value: None.

example: `clarity.exe i=2 gal_save` saves the calibration opened in the second Instrument.

gal_save_as*description:*

Saves the active GPC calibration under the specified name. Use together with the **instrument** parameter to specify the Instrument whose [Calibration](#) window holds the GPC calibration file you are interested in. GPC calibration file can be opened by specifying its path and filename. It is recommended to use absolute paths.

This command is ignored when not in the GPC mode - use **cal_save_as** instead.

syntax: `gal_save_as=PATH\FILENAME`

possible values: A valid path to the calibration (*.GAL) file.

implicit value: None.

example: `clarity.exe gal_save_as="C:\Users\<user name>\AppData\Local\Temp\CLARITY\results.gal"`

gpc

description: Switches the Instrument into the **GPC** or **Standard** mode.

syntax: `gpc=VALUE`

possible values: 0 or 1.

implicit value: None.

example: `clarity.exe gpc=0`

gpc_recal_stdno*description:*

Together with the **gpc_recal_type** parameter enables to recalibrate an opened GPC calibration. The calibration is recalibrated by the active chromatogram at specified standard number and standard type. For successful recalibration it is necessary to specify the calibration file in the same command line as **gpc_recal_stdno** and **gpc_recal_type** parameters, which has to be both set to nonzero value.

syntax: `gpc_recal_stdno=VALUE`

possible values: 0, 1, .. 20, 21 (Blank). Value 0 does nothing.

implicit value: 0

example: `clarity.exe test.gal gpc_recal_stdno=5 gpc_recal_type=1`

gpc_recal_type

description: Together with the **gpc_recal_stdno** parameter enables to recalibrate an opened GPC calibration. The calibration is recalibrated by the active chromatogram at specified standard number and standard type. For successful recalibration it is necessary to specify the calibration file in the same command line as **gpc_recal_stdno** and **gpc_recal_type** parameters, which has to be both set to nonzero value.

syntax: `gpc_recal_type=VALUE`
0, 1, 2.

possible values: The meaning of values are as follows:
0 - does nothing (no recalibration).
1 - narrow calibration type.
2 - broad calibration type.

implicit value: 0

example: `clarity.exe test.gal gpc_recal_stdno=5 gpc_recal_type=1`

hide_splash

description: Suppresses the splash screen that emerges when starting **Clarity**.

syntax: `hide_splash`

possible values: None.

implicit value: None.

example: `clarity.exe hide_splash`

instrument or i

description: Automatically opens an Instrument specified by the number. The command line parameter for user (and password) should follow, otherwise the opening is stopped on the [Login](#) dialog. Alternatively, it can be used as an accompanying parameter for specifying the number of the Instrument to perform other actions on, e.g., to define the Instrument on which a sequence should be imported using the **seq_import** parameter.

syntax: `i=VALUE`

possible values: 1, 2, 3, 4. To open multiple Instruments, the CLARITY.EXE file has to be called separately for each Instrument.

implicit value: 1

clarity.exe i=3

example:

To work with two or more Instruments at once, you should use the MS Batch "START" command. "Examples" on page 504 section below the commands for more information.

mail_dump

description:

Disables the sending of memory dumps via e-mail. Must be used when opening **Clarity** for the first time, otherwise it is ignored. This parameter is suitable for troubleshooting, when users certainly do not want to mail 200MB files. This parameter may be also used (and is overwritten by settings) in DATAAPEX.INI file.

syntax: *mail_dump=VALUE*

possible values: 0 or 1.

implicit value: 1.

example: *clarity.exe mail_dump=0*

met_apply

description:

Applies the specified method to the active chromatogram (for more details see the chapter **Batch** on pg. 129). It is recommended to use absolute paths because the method file will not be searched for in the working directory but in the default directory of the active project.

syntax: *met_apply=PATH\FILENAME*

possible values: A valid path to the method (*.MET) file.

implicit value: None.

example: *clarity.exe met_apply="C:\Users\\AppData\Local\Temp\CLARITY\1.met"*

Open file (*.PRM, *.MET, *.CAL, *.GAL, *.SEQ, *.PRJ, *.SST, *.NGA, *.AUDIT, *.LIB and *.DHA files)

description:

Opens the specified file(s) on the specified Instrument (using the **instrument** parameter).

syntax: *PATH\FILENAME*

possible values: The path and filename of the selected file.

implicit value: Empty.

example: *clarity.exe C:\CLARITY\DataFiles\PROJECTS\Work1.prj*
clarity.exe "C:\CLARITY\DataFiles\DEMO1\Ethanol in blood.seq"

note:

Opened method (*.MET file) is propagated only to [Single Analysis](#) dialog and is not send to instrument unless *Send Method to Instrument* option is selected in [Method Sending Options](#) dialog in [System Configuration](#).

pass_to_existing_process_only

description: In case the further command line parameters are wrong, **Clarity** will not try to open again. Without the parameter, in case the command line parameters are wrong (e.g. error in the link, extra space, ...), **Clarity** tries to run anew, which produces error message because just one instance of running **Clarity** is possible at the same computer.

syntax: `pass_to_existing_process_only`

possible values: None.

implicit value: None.

example: `clarity.exe pass_to_existing_process_only "C:\CLARITY\DataFiles\DEMO1\Ethanol in blood.seq"`

password or p

description: Tries to log the user on using the password specified. The password used is anonymised in the Audit Trail log.

syntax: `p=STRING`

possible values: String.
Empty.

implicit value: If empty, the system will deem that the user has an empty password.

example: `clarity.exe user=someuser p=mypassword`

prm_close

description: Closes the active *.PRM file opened. If any changes were performed on it, creates the dialog box asking whether these changes should be saved or discarded.

syntax: `prm_close`

possible values: None.

implicit value: None.

example: `clarity.exe prm_close`

prm_close_discard

description: Closes the active *.PRM file opened. If any changes were performed on it, discards the changes in the chromatogram without asking.

syntax: `prm_close_discard`

possible values: None.

implicit value: None.

example: `clarity.exe prm_close_discard`

prm_close_save

description: Closes the active *.PRM file opened. If any changes were performed on it, saves the changes to the chromatogram without asking.

syntax: `prm_close_save`

possible values: None.

implicit value: None.

example: `clarity.exe prm_close_save`

prm_export

description: Exports the active chromatogram into the specified file. The type of the exported file is determined by its file name extension - supported file types are *.CDF, *.CHR, *.TXT, *.ASC. To learn more about file types "Export Chromatogram" on page 182.

syntax: `prm_export=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe prm_export="C:\Users\\AppData\Local\Temp\CLARITY\1.chr"`

prm_import

description: Imports the specified file as a chromatogram. The type of a file imported is determined by its name extension - supported file types are *.CDF, *.CHR, *.TXT, *.ASC. To learn more about file types "Export Chromatogram" on page 182. Imported chromatogram is stored in windows \TEMP directory under the name IMPORT.PRM. Existing *.PRM file is overwritten without warning.

A method must be used on and saved to the resulting chromatogram during import - we use the method currently selected in the Single Analysis window, so its **Integration Table** parameters, linked calibration etc. are defined by it. Imported chromatogram is made active.

syntax: `prm_import=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe prm_import="C:\Users\\AppData\Local\Temp\CLARITY\1.chr"`

prm_import_ex*description:*

Imports the specified file as a chromatogram. The type of a file imported is determined by its name extension - supported file types are *.CDF, *.CHR, *.TXT, *.ASC. To learn more about file types "Export Chromatogram" on page 182. Imported chromatogram is stored in the \DATA directory of the current project under the name FNAME.PRM, where *fname* is file name part of the imported file. Possible existing *.PRM file with the same name is overwritten without warning.

A method must be used on and saved to the resulting chromatogram during import - we use the method currently selected in the Single Analysis window, so its **Integration Table** parameters, linked calibration etc. are defined by it. Imported chromatogram is made active.

syntax: `prm_import_ex=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe prm_import_ex="C:\Users\<user name>\AppData\Local\Temp\CLARITY\1.chr"`

prm_save*description:*

Saves the active chromatogram. Use together with the **instrument** parameter (which is ignored by **Clarity Lite**) to specify the Instrument whose [Chromatogram](#) window holds the chromatogram file you are interested in. Chromatogram file can be opened by specifying its path and filename. It is recommended to use absolute paths.

syntax: `prm_save`

possible values: None.

implicit value: None.

example: `clarity.exe prm_save`

prm_save_as

description: Saves the active chromatogram under the specified name. Use together with the **instrument** parameter (which is ignored by **Clarity Lite**) to specify the Instrument whose [Chromatogram](#) window holds the chromatogram file you are interested in. Chromatogram file can be opened by specifying its path and filename. It is recommended to use absolute paths.

syntax: `prm_save_as=PATH\FILENAME`

possible values: A valid path to the chromatogram (*.PRM) file.

implicit value: None.

example: `clarity.exe prm_ save_ as=C:\CLARITY\DataFiles\Work1\Data\Test.prm`

recal_level

description: Recalibrates the opened calibration file at the specified level with an active chromatogram. The calibration file must be specified in the same command line as **recal_level**. Value 0 does nothing.

syntax: `recal_level=LEVEL`

possible values: 0, 1, ... 20, 21 (Blank)

implicit value: 0

example: `clarity.exe test.cal recal_level=5` Recalibrates the TEST.CAL calibration on the 5th level.

register

description: Registers **Clarity** file extensions.

syntax: `register`

possible values: None.

implicit value: None.

example: `clarity.exe register`

report_last_only

description: Suppresses the BADTRACE.TXT file at the start of **Clarity** and sends only one dump file. This function can also be set via the DATAAPEX.INI file that may be stored in WINDOWS directory. Must be used when opening **Clarity** for the first time, otherwise it is ignored. This parameter is suitable for troubleshooting.

syntax: `report_last_only`

possible values: None.

implicit value: None.

<i>example:</i>	<i>clarity.exe report_last_only</i>
resume_seq	
<i>description:</i>	Resumes the sequence on specified Instrument (the Instrument and sequence file must be opened separately). This parameter is suitable for automatic testing or for LIMS interfacing in combination with seq_import.
<i>syntax:</i>	<i>resume_seq=VALUE</i>
<i>possible values:</i>	1 (for Instrument 1), 2 (for Instrument 2), 4 (for Instrument 3), 8 (for Instrument 4), and their binary combinations.
<i>implicit value:</i>	None.
<i>example:</i>	<i>clarity.exe resume_seq=3</i> (will resume sequence measurement on Instruments 1 and 2)
run	
<i>description:</i>	Runs a single analysis on specified Instrument (which must be opened separately). Single analysis has higher priority than sequence run. This parameter is suitable for automatic testing.
<i>syntax:</i>	<i>run=VALUE</i>
<i>possible values:</i>	1 (for Instrument 1), 2 (for Instrument 2), 4 (for Instrument 3), 8 (for Instrument 4), and their binary combinations.
<i>implicit value:</i>	None.
<i>example:</i>	<i>clarity.exe run=7</i> (will run single analysis on Instruments 1, 2 and 3)
run_seq	
<i>description:</i>	Runs the sequence run on specified Instrument (the Instrument and sequence file must be opened separately). This parameter is suitable for automatic testing or for LIMS interfacing in combination with seq_import.
<i>syntax:</i>	<i>run_seq=VALUE</i>
<i>possible values:</i>	1 (for Instrument 1), 2 (for Instrument 2), 4 (for Instrument 3), 8 (for Instrument 4), and their binary combinations.
<i>implicit value:</i>	None.
<i>example:</i>	<i>clarity.exe run_seq=7</i> (will run sequence measurement on Instruments 1, 2 and 3)
seq_export	
<i>description:</i>	Exports the active sequence into the specified *.TXT file.
<i>syntax:</i>	<i>seq_export=PATHFILENAME</i>
<i>possible values:</i>	A valid path and filename.
<i>implicit value:</i>	None.

example: `clarity.exe seq_ export="C:\Users\<user name>\AppData\Local\Temp\CLARITY\seq.txt"`

seq_export_utf8

description: Exports the active sequence into the specified *.TXT file using UTF8 encoding.

syntax: `seq_export_utf8=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe seq_ export_ utf8="C:\Users\<user name>\AppData\Local\Temp\CLARITY\seq.txt"`

seq_import

description: Imports the specified *.TXT file as a sequence. Current sequence is replaced by imported one, [Sequence](#) window is opened. The command is ignored when the sequence is running. [Sequence Options](#) dialog is never opened after command line import. Import settings are the same as the last saved ones during manual import. File name of imported sequence is NONAME, so it is necessary to use **seq_save_as** to store imported sequence before run.

syntax: `seq_import=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe seq_ import="C:\Users\<user name>\AppData\Local\Temp\CLARITY\seq.txt"`. "Examples" on page 504 section below the commands for more information.

seq_import_append

description: Imports the specified *.TXT file as a sequence. Current sequence will be appended with lines from the imported file, [Sequence](#) window will be opened and the sequence file will be saved. Can be performed when the sequence is running. [Sequence Options](#) dialog is never opened after command line import. Import settings are the same as the last saved ones during manual import.

syntax: `seq_import_append=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe seq_ import_ append="C:\Users\<user name>\AppData\Local\Temp\CLARITY\seq.txt"`

seq_save

description: Saves the active sequence. Use together with the **instrument** parameter to specify the Instrument whose [Sequence](#) window holds the sequence file you are interested in. Sequence file can be opened by specifying its path and filename. It is recommended to use absolute paths.

syntax: `seq_save`

possible values: None.

implicit value: None.

example: `clarity.exe i=2 seq_save` - saves the sequence opened in the second Instrument.

seq_save_as

description: Saves the active sequence under the specified name. Use together with the **instrument** parameter to specify the Instrument whose [Sequence](#) window holds the sequence file you are interested in. Sequence file can be opened by specifying its path and filename. It is recommended to use absolute paths. Command is ignored when sequence is running.

syntax: `seq_save_as=PATH\FILENAME`

possible values: A valid path to the sequence (*.SEQ) file.

implicit value: None.

example: `clarity.exe seq_save_as="C:\Users\\AppData\Local\Temp\CLARITY\results.seq"`

set_sample_name

description: Sets sample name parameter for the next single analysis run. It is possible to set the Instrument by the `i=(number of Instrument)` parameter.

syntax: `set_sample_name=text`

possible values: Any non-empty text.

implicit value: None.

example: `clarity.exe set_sample_name="sample name"`
`clarity.exe i=2 set_sample_name="sample name"`

show_help_id

description: After calling the context help (via the **F1** key or *Help* button) a message box with the help filename and topic ID will be displayed. Hardware and Control modules need to be configured to the Instrument, otherwise a classical help will be displayed for its dialogs.

syntax: `show_help_id`

possible values: None.

implicit value: None.

example: `clarity.exe show_help_id`

sno or o

description: Uses the specified serial number (*.SNO) file. Must be used when opening **Clarity** for the first time, otherwise it is ignored.

syntax: `o=PATH\FILENAME`

possible values: The path and filename of the serial number (*.SNO) file.
Empty path.

implicit value: If the path is not specified, the system will look for the serial number (*.SNO) file in the \CFG directory. If not found, the system will then look for the file in the \BIN directory where the CLARITY.EXE file is located.

example: `clarity.exe o=C:\CLARITY\Cfg\clarity.sno`

stop

description: Stops the single analysis/sequence measurement on the specified Instrument. This parameter is suitable for automatic testing. In case of sequence it stops both current acquisition and sequence itself.

syntax: `stop=VALUE`

possible values: 1 (for Instrument 1), 2 (for Instrument 2), 4 (for Instrument 3), 8 (for Instrument 4), and their binary combinations.

implicit value: None.

example: `clarity.exe stop=7` (will stop single analysis/sequence on Instruments 1, 2 and 3)

unregister

description: Unregisters **Clarity** file extensions.
syntax: `unregister`
possible values: None.
implicit value: None.
example: `clarity.exe unregister`

user or u

description: Logs on the specified user.
syntax: `u=STRING`
possible values: String.
implicit value: Empty.
If empty, the system will show the [Login](#) dialog.
example: `clarity.exe u="John Doe"`
Clarity will automatically log in the user account called "John Doe".

10.2.2 Examples

10.2.2.1 Example 1:

This batch file will subsequently open **Instrument 1** and **Instrument 2**. On **Instrument 1** it will open the DEMO1 project, load the 2506MULTI.PRM chromatogram and ETHANOL IN BLOOD.SEQ sequence. On **Instrument 2** it will open PAH_EPA.CAL calibration file.

This batch file can be found in the UTILS subdirectory of the C:\CLARITY\Bin directory under the name CLARITY_COMMANDLINE_EXAMPLE.BAT.

```
start          C:\CLARITY\Bin\clarity.exe          i=1          u=Administrator
C:\CLARITY\DataFiles\PROJECTS\Demo1.prj
C:\CLARITY\DataFiles\DEMO1\DATA\2506multi.prm
C:\CLARITY\DataFiles\DEMO1\Ethanol in blood.seq
C:\CLARITY\Bin\UTILS\delay.exe 5
start          C:\CLARITY\Bin\clarity.exe          i=2          u=Administrator
C:\CLARITY\DataFiles\PROJECTS\Demo2.prj
C:\CLARITY\DataFiles\DEMO2\CALIB\Pah_epa.cal
```

10.2.2.2 Example 2:

This batch file will open the **Instrument 1**, import 1.CHR file as a chromatogram, apply a calibration on it, export the chromatogram and chromatogram results and close the chromatogram (single line command), then it closes **Clarity** itself. This can be useful when **Clarity** has to cooperate with other programs, such as LIMS.

```
start C:\CLARITY\Bin\clarity.exe i=1 u=Administrator
C:\CLARITY\Bin\UTILS\delay.exe 5
start      C:\CLARITY\Bin\clarity.exe      prm_  import_  ex="C:\Users\<user
name>\AppData\Local\Temp\CLARITY\1.chr"          ca_
apply="C:\CLARITY\DataFiles\WORK1\Calib\1.cal"  prm_ export="C:\Users\<user
name>\AppData\Local\Temp\CLARITY\export.chr"          export_
results="C:\Users\<user name>\AppData\Local\Temp\CLARITY\export.txt"  prm_
close_discard
C:\CLARITY\Bin\UTILS\delay.exe 5
start C:\CLARITY\Bin\clarity.exe exit
```

10.2.2.3 Example 3:

This batch file will open **Instrument 1** as *Administrator*, import sequence file stored in C:\CLARITY\DataFiles\WORK1\SEQUENCE.TXT and save it in the same directory in **Clarity** file format (*.SEQ) and finally start the sequence. Before trying this example create the SEQUENCE.TXT file in the given folder, e.g. using *File - Export* command in the [Sequence](#) window to save existing **Clarity** sequence to *.TXT.

```
start C:\CLARITY\Bin\clarity.exe i=1 u=Administrator
C:\CLARITY\Bin\UTILS\delay.exe 15
```

```

C:\CLARITY\Bin\clarity.exe                               seq_
import=C:\CLARITY\DataFiles\WORK1\sequence.txt
C:\CLARITY\Bin\UTILS\delay.exe 3
C:\CLARITY\Bin\clarity.exe                               seq_       save_
as=C:\CLARITY\DataFiles\WORK1\sequence.seq
C:\CLARITY\Bin\UTILS\delay.exe 10
C:\CLARITY\Bin\clarity.exe run_seq=1

```

10.2.2.4 Notes:

It is possible to call-up the CLARITY.EXE file when another instance of **Clarity** is already running. The new instance must quit (because only one running instance of **Clarity** is allowed at a time). Before quitting this new instance passes parameters to the instance already running. If CLARITY.EXE is already running, the **sdk**, **sno**, and **cfg** parameters will be ignored. If CLARITY.EXE is already running and the specified Instrument is opened, parameters **user**, **password** and **dsk** will be ignored. For all opening files some restrictions apply:

- A sequence must not be running.
- There must not be an opened modal dialog.
- Permission must be obtained to open a method.
- It must be allowed to change project.

Delay is not a regular batch command, it is a utility that waits a specified amount of time (set in seconds). DELAY.EXE file can be found in the UTILS directory.

Note: The necessary delay time that has to be set in the batch file is dependent on the configuration of the station and command line parameters used.

Several restrictions apply to the command line parameters used in the command line or a batch file:

- Only one project file (*.PRJ) can be accepted from the command line (actually the first one) for one Instrument.
- Only one method file (*.MET) can be accepted from one command line (actually the first one).
- Only one sequence file (*.SEQ) can be accepted from one command line (actually the first one).
- Multiple chromatograms (*.PRM) can be accepted for opening from one command line.
- Maximum number of characters per command line is limited to 126 characters. Any commands after this limit will not be carried out and **Clarity** will issue a warning message.
- Configuration files such as *.CFG, *.SNO, *.PSW and *.DSK should be located in the same directory as they are interlinked. Placing them each in a different place may result in incorrect behavior.

When opening an Instrument, the first project, method, sequence, calibration and then the chromatogram(s) are opened.

10.3 OTHERS.INI file

The OTHERS.INI file located in the Clarity installation directory (C:\CLARITY\CFG by default). It contains keys for in-depth tuning of the **Clarity** Chromatography Station. The file in plain text format, is structured into sections introduced by brackets, e.g. [General]. Each section can contain keys with values. Some sections are dependent on specific control modules and description of their keys can be found in appropriate manuals.

Note: Use e.g. Notepad program to edit this file. Using MS Word may result in destroying the proper format of the file.

Lines starting with semicolon (;) are comments.

[General]

The parameters common to all acquisition modules are set in this section.

PulseTime

Sets the length of the pulse in ms. Pulse on selected digital output of the A/D converter can be triggered by specified event from the **Event Table** found in the [Method Setup - Event Table](#) dialog (for more details see the chapter **Event Table** on pg. 85).

Use60Hz

Set the *Use60Hz* parameter to 1 if the power supply frequency in your country is 60Hz (countries in both Americas). Default setting 0 indicates the 50Hz power supply frequency (rest of the world).

EventThreshold = 1

Sets the hysteresis (minimal necessary change) value of the detector signal as an input of the event enabling to trigger the event again. For the detector signal, the value is set in mV or equivalent units as set in configuration of acquisition device. Events are usually defined in the **Event Table** found in the [Method Setup - Event Table](#) dialog (for more details see the chapter **Event Table** on pg. 85).

EventThresholdAuxPressure = 0.01

Sets the hysteresis value of the Auxiliary Signal for Pressure as an input of the event enabling to trigger the event again. For the Auxiliary Signal for Pressure, the value is set in MPa and the default value is 0.01. Events are set in the **Event Table** found in the [Method Setup - Event Table](#) dialog.

EventThresholdAuxTemperature = 1

Sets the hysteresis value of the Auxiliary Signal for Temperature as an input of the event enabling to trigger the event again. For the Auxiliary Signal for Temperature, the value is set in degrees Celsius and the default value is 1. Events are set in the **Event Table** found in the [Method Setup - Event Table](#) dialog.

EventThresholdAuxFlow = 0.01

Sets the hysteresis value of the Auxiliary Signal for Flow as an input of the event enabling to trigger the event again. For the Auxiliary Signal for Flow, the value is set

in mL/min and the default value is *0.01*. Events are set in the **Event Table** found in the [Method Setup - Event Table](#) dialog.

EventThresholdAuxCurrent = 1

Sets the hysteresis value of the Auxiliary Signal for Current as an input of the event enabling to trigger the event again. For the Auxiliary Signal for Current, the value is set in mA and the default value is *1*. Events are set in the **Event Table** found in the [Method Setup - Event Table](#) dialog.

EventThresholdAuxVoltage = 1

Sets the hysteresis value of the Auxiliary Signal for Voltage as an input of the event enabling to trigger the event again. For the Auxiliary Signal for Voltage, the value is set in V and the default value is *1*. Events are set in the **Event Table** found in the [Method Setup - Event Table](#) dialog.

EventThresholdAuxPower = 1

Sets the hysteresis value of the Auxiliary Signal for Power as an input of the event enabling to trigger the event again. For the Auxiliary Signal for Power, the value is set in W and the default value is *1*. Events are set in the **Event Table** found in the [Method Setup - Event Table](#) dialog.

EventThresholdAuxOther = 1

Sets the hysteresis value of the Auxiliary Signal for type Other as an input of the event enabling to trigger the event again. For the Auxiliary Signal for type Other, the value is set as defined by user and the default value is *1*. Events are set in the **Event Table** found in the [Method Setup - Event Table](#) dialog.

TestLostPackets=0

Tests the completeness of data from the A/D converter. When set to *1* **Clarity** will report any lost packets to the BADTRACE.TXT file located in the **Clarity** installation folder (C:\CLARITY\CFG\DEBUG_LOGS by default).

FirstRun=dd.mm.yyyy

Shows the date of the first running of the station after installation.

[PDA]**VertexCountLimit**

Specifies how many vertices will 3D view of PDA data use for display. The lower the value, the faster the PDA 3D view will render but the more degraded will be resulting image quality. Higher value will give better quality but slow responsiveness. Warning: setting value too high can cause communication failures with hardware and/or "Virtual memory too low." error. Default value is 120000.

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