



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.

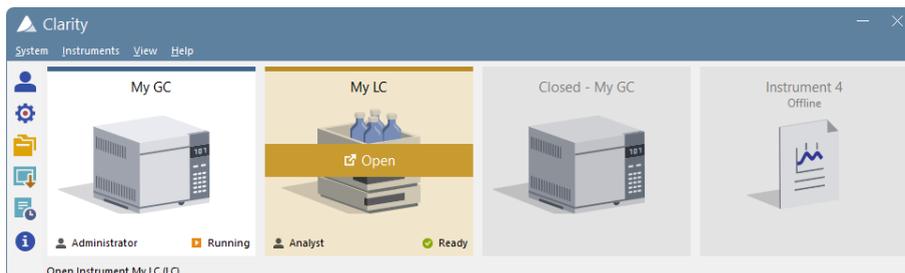


Fig. 1: Main Clarity window

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. 37..

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

A 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. 40)..

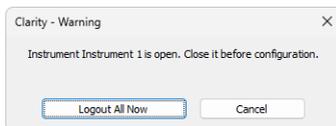


Fig. 3: Logout all instruments

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.

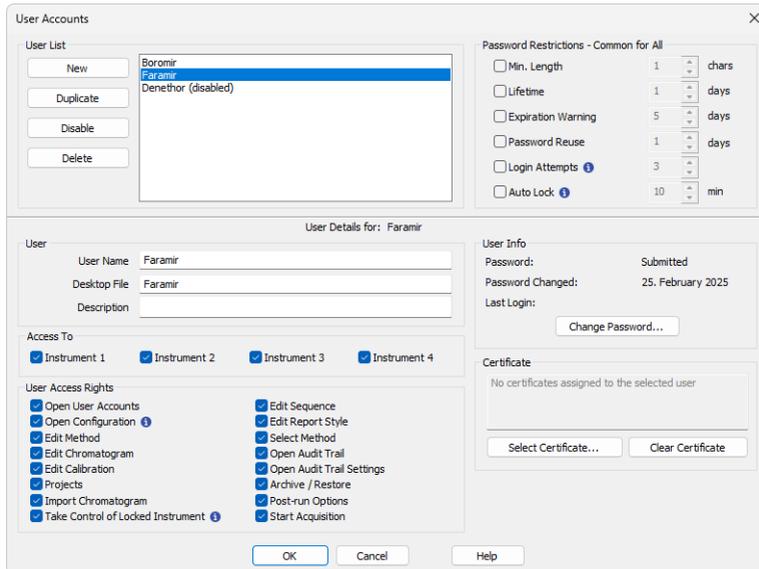


Fig. 4: User Accounts

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 highlighted user has their details displayed below. Disabled users are listed in the bottom of the list with (disabled) after their name.

New

Adds a new user with blank *User Name*, that must be filled in, and with all access rights enabled.

Duplicate

Duplicates the selected user account from the user list. Rights from section *Access To* and *User Access Rights* are copied from the original user. *User Name* is blank and must be filled in manually.

Disable/Enable

Disables the selected active user account. Disabled user account cannot be used to login anywhere in Clarity. To use disabled account again, it has to be enabled here.

Delete

Erases the 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. Once user is deleted and changes are saved this operation cannot be reverted (user must be created manually from scratch).

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.

Lifetime

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. The period is calculated from the time of password creation not from its expiration.

Login Attempts

The maximum number of failed login attempts allowed. After reaching this limit, user account will be disabled permanently. Exception is an account with the right to access the *User Accounts* dialog. Such account is locked only temporarily for one hour.

Auto Lock

If the user does not show any activity in Windows for the specified time duration, all opened Instruments will be locked. All windows opened on Instruments will be hidden and the user has to unlock the [Instruments](#) upon return.

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

User Details for:

The fields displayed in the lower part of the window always relate to the selected user in the *User List*.

User

User Name

User name is used to login to different parts of Clarity. User name will be automatically placed in all headers of files that are created while working with 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 and user settings (such as toolbar layouts, custom calculations etc.). 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.

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, disable, 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: "System Configuration" on page 10, "Units Setup" on page 22, "Instrument Directories for Projects" on page 24 and "Digital Outputs" on page 34.

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.

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 an Instrument that has been locked by another user. The Instrument can be locked either using the Auto Lock or by the *Instrument - Lock Instrument X* command in the *Main* or *Instrument* window. All actions will be logged into *Audit Trails* under the newly logged user. If the new user does not have the *Start Acquisition* rights, the running analysis or sequence will be finished but the next analysis will not be started.

Caution: All unsaved changes in files made 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 the desktop of the first logged user will be used for all users that take control over the Instrument, until the Instrument is closed again. It is also recommended to set the same *Edit...* rights for users that plan to take over Instruments (other rights might differ between the users).

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

Enables access to all Audit Trail (e.g., Station, Chromatogram Audit Trail) dialogs to view the audit trails.

Open Audit Trail Settings

Enables access to the Audit Trail settings dialog.

Archive/Restore

Enables access to *Backup* accessible via *Instrument - Archive/Restore* commands.

Post-run Options

Enables the user to change the post run settings in the [Single Analysis - Post-run Options](#) tab, [Sequence](#) window and the [Batch](#) dialog. Option does not prevent user from performing those actions.

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. Different certificate can be selected manually during the signing process, selecting certificate here just preselects it in the [Sign](#) dialog to minimize manual actions needed. 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.

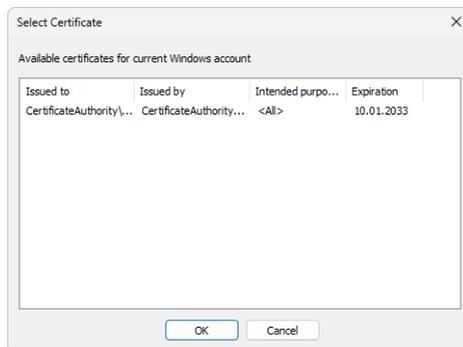


Fig. 5: Select Certificate

Select Certificate

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

Clear Certificate

Cancels the assigned certificate.

Note: DataApex does not issue certificates nor can mediate their purchase. Certificates are issued by independent companies.

1.1.2 User Details

In the *User Details* dialog (accessible from [Clarity](#) window using the *System* menu), every user can view their own user account settings and change the password to their own account. Here, they may also select a certificate for digital signing.

Note: If there is no user 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.

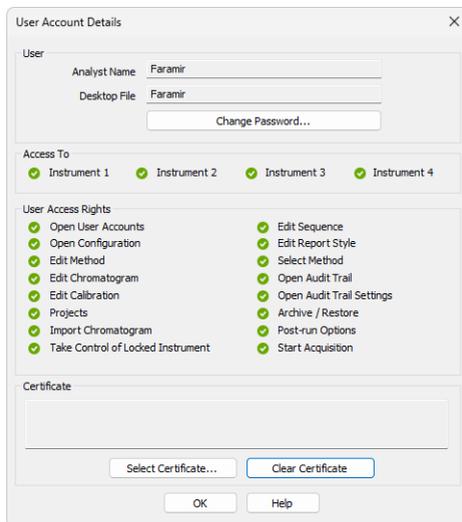


Fig. 6: User Account Details

1.1.3 System 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](#)).

The [left section](#) of the dialog  is used to configure equipment in the **Clarity** station, while the [right section](#)  is where the equipment is allocated to individual Instruments.

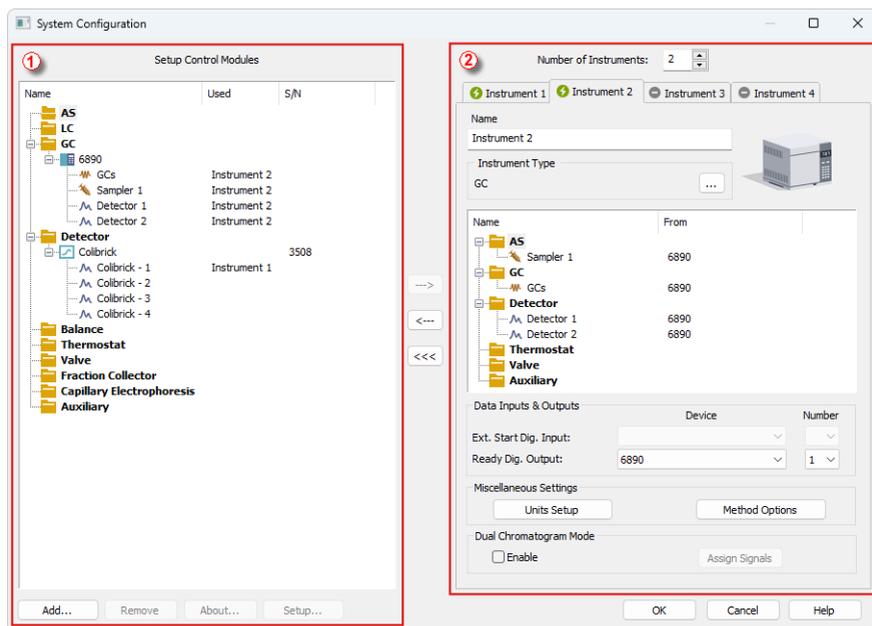


Fig. 7: System Configuration

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.).

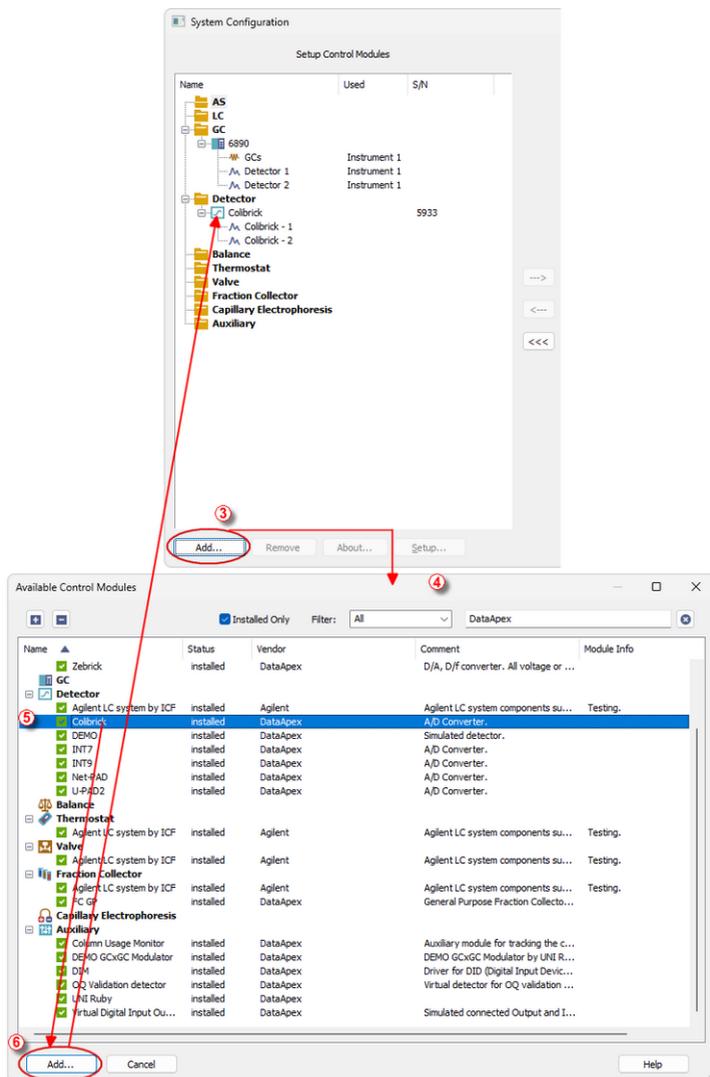


Fig. 8: System Configuration - left part and Available Control Modules dialogs

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. 13).

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 on this, see the Help of the particular control module).

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.

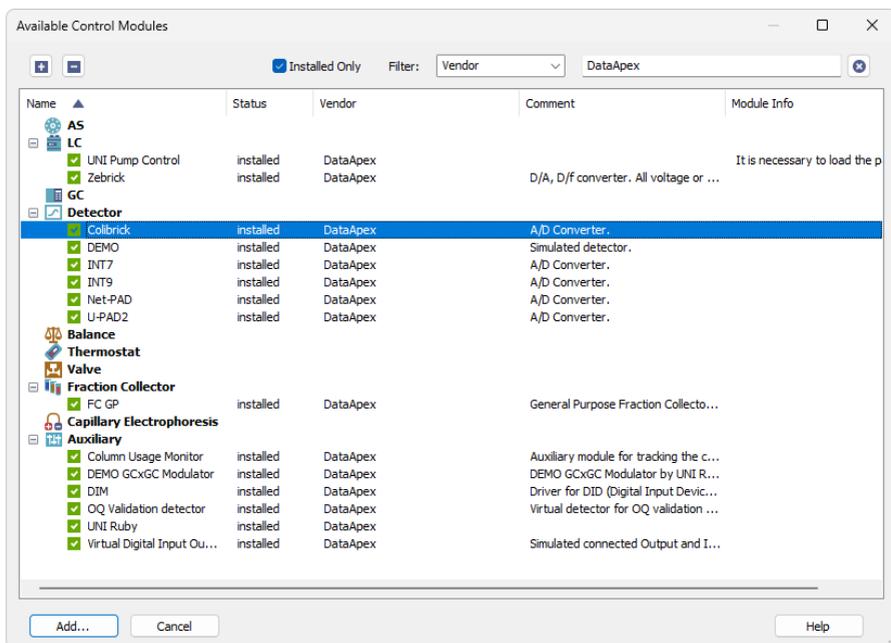


Fig. 9: Available Control Modules

+ / - 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. 13. 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. **13**). 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.

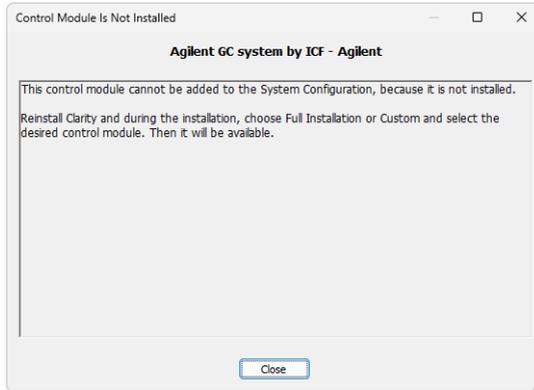


Fig. 10: Control module is not installed dialog

1.1.3.3 Right section of System Configuration dialog

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

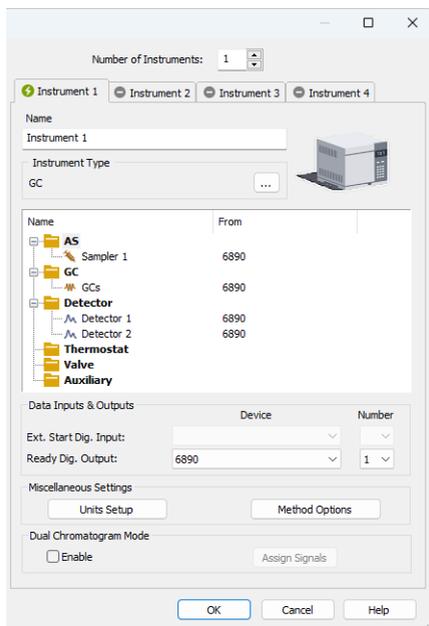


Fig. 11: System Configuration - right section

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 a selected Instrument. |
| <--- | Removes selected equipment from a selected Instrument. |
| <<< | Removes all equipment from a selected 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.

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



Fig. 12: 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 (purchased) 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. The tab (s) of any offline Instrument(s) will have the “Offline” inscription on them. To use it for the data acquisition Add-on Instrument for Clarity license has to be purchased.

 icon indicates not active Instrument. It is not possible to login to this Instrument. The corresponding chromatograph symbol is not displayed in the main [Clarity](#) window.

Name

Holds Instrument Name 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 select your own image. Unchecking the checkbox return the displayed image to the default value.

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.

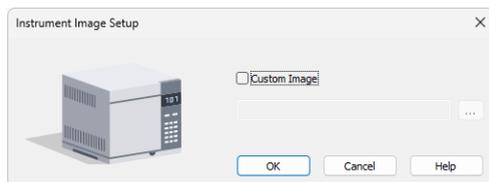


Fig. 13: Instrument Image Setup dialog

Instrument Type

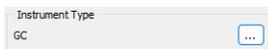


Fig. 14: GC Instrument Type

Left mouse click on the (...) button invokes the *Instrument Type Setting* dialog where the user can select a combination of instrument types. 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, MS-MS, DHA, NGA and PDA).

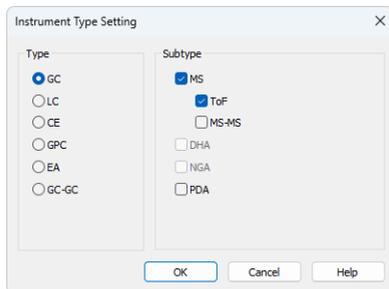


Fig. 15: Instrument Type Setting dialog

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

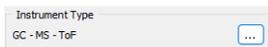


Fig. 16: GC-MS-TOF Instrument Type

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*.

List of the Equipment Connected to the Instrument

| Name | From |
|---------------|-------|
| AS | |
| Sampler 1 | Alias |
| GC | |
| GCs | 6890 |
| Detector | |
| A1_Detector 1 | 6890 |
| A1_Detector 2 | 6890 |
| Thermostat | |
| Valve | |
| Auxiliary | |

Fig. 17: List of equipment connected to an Instrument

AS

Sets direct control of the used autosampler.

GC/LC

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

Detectors

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

Note: Other categories may appear, including Thermostats, Valves, Fraction Collectors, and other auxiliary 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. 18: Digital Outputs for external Start/Stop

The START synchronization between Clarity and the autosampler (eventually other devices such as Detectors, 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 **User Guide** 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* combo-box 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

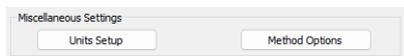


Fig. 19: Miscellaneous Settings

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.

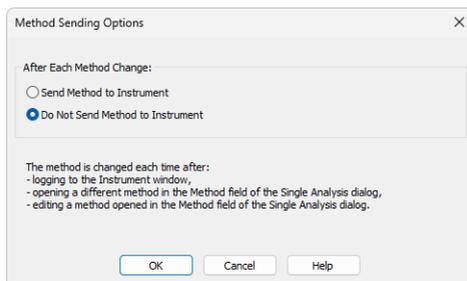


Fig. 20: Instrument Method Sending

This dialog sets whether the method is sent to the instrument (device) at each change of the method set in the *Single Analysis* dialog.

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

After Each Method Change

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 method to the devices automatically without prompt.

Do Not Send Method to Instrument - **Clarity** will **not** send method to instrument devices each time a change occurs. Prior to running single analysis, method must be sent manually.

Regardless of the setting, the method will be sent:

- From the running *Active Sequence* according to the *Sequence Table*.
- Manually using the *Send Method* button from the [Method Setup](#) 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.

Dual Chromatogram Mode

This section enables and sets up Dual Chromatogram mode on the Instrument. For more details see the *Dual Chromatogram Mode* manual.

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.

| Title | Units | Custom Units |
|-------|----------------|--------------|
| Time | Time - minutes | |

Fig. 21: 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 Instrument Directories for Projects

The *Instrument Directories for Projects* dialog allows users to change the location of [Project](#) directories for the instrument and the [Audit Trail](#) directory from the default location to any other desired location. These directory settings are shared across all users. To open this dialog, use the *Directories...* command or click the  icon in the main Clarity window.

Installation Folder Structure

Clarity installation folder contains four directories:

- BIN - Stores supporting *.DLL files and other essential programs for proper functionality.
- CFG - Stores configuration files, including *.CFG, *.DSK, *.INI, *.PSW and *.SNO files. Also contains the AUDIT_TRAILS directory for daily logs, as well as BACK, BUG_REPORTS, DEBUG_LOGS and IMAGES directories.
- DATAFILES - Stores project folders, the PROJECTS directory and the COMMON directory. All measured data is stored here by default.
- DOCUMENTATION - Contains documentation such as manuals, datasheets, and WHATSNEW.TXT and ABOUT.TXT files.

Instrument Directory for Projects

The *Instrument Directory for Projects* is the *DataFiles* ① folder. By default, this folder is located in the Clarity installation directory, but it can be redirected to any other location.

Inside the *DataFiles* folder, the *PROJECTS* directory ② contains a list of all available projects. Each project is represented by a *.prj file ③, which defines specific subdirectories for storing data. Within each project, there are further subdirectories ④ used for organizing calibration and measurement data. Additionally, the *COMMON* directory ⑤ stores shared report styles for all projects within the same *DataFiles* directory.

Note: In the above image the **Instrument 2** DataFiles folder is set to the network drive where can be accessed from different PCs.

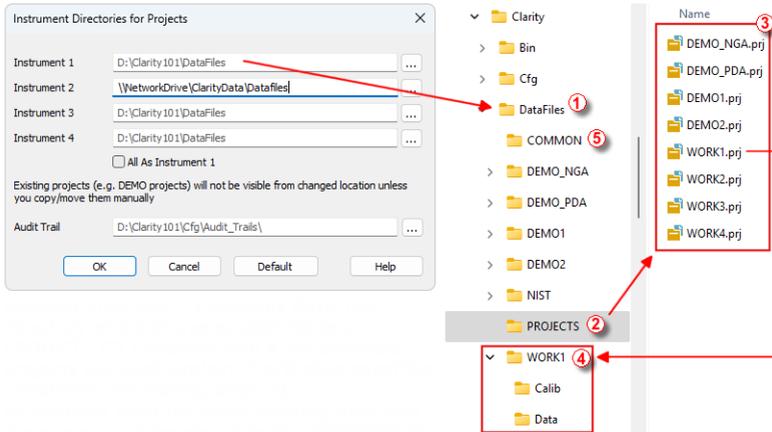


Fig. 22: Instrument Directories

The *DataFiles* directory can be set individually for each *Instrument*. Use the ... button to select the required directory. The directory name cannot contain following characters / : * ? " < > | and also cannot end with a space or a dot.

If the selected directory does not already contain a *DataFiles* structure, Clarity will prompt the user to create the necessary *COMMON* and *PROJECTS* subdirectories.

All As Instrument 1

Sets directories for all instrument as it is set for the first instrument.

Default

Restores the working directories for all Instruments to the one set as the Data Location during installation, and the Audit Trails directory to its default location in Cfg folder.

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.

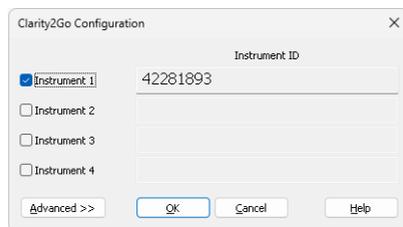


Fig. 23: Clarity2Go Configuration dialog

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.

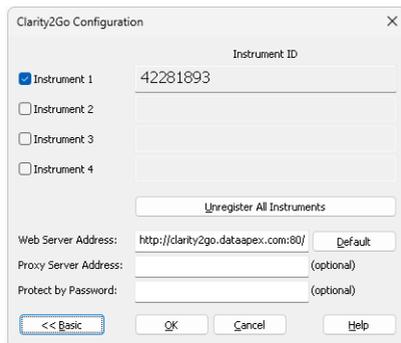


Fig. 24: Clarity2Go Configuration - Advanced dialog

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

In this dialog, the GLP (Good Laboratory Practice) options for the entire **Clarity** software can be configured. After prompting the *System - GLP Options...* command, the user is asked to log in. 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.

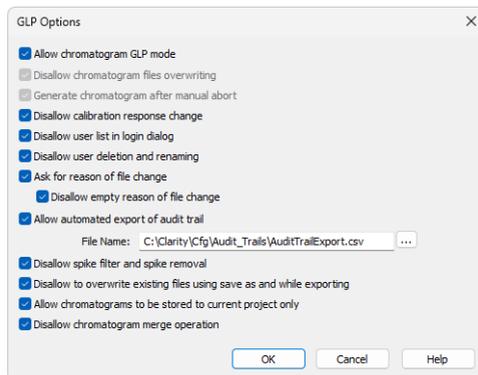


Fig. 25: GLP Options dialog

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 manual abort* checkboxes will be checked automatically. If you open a chromatogram created in the *GLP Mode* on a [Clarity](#) station without the *GLP Mode* enabled, it will always be opened as a read-only.

Note: Chromatograms acquired by an "Unauthorized Control Module" on page 465 or a "Development version of Control Module" on page 464 will contain a record in the *Chromatogram Audit Trail* regarding the fact that they were acquired by such a device to comply with GLP.

Disallow chromatogram files overwriting

This checkbox prevents the possibility of overwriting a chromatogram if one with the same name already exists in the selected directory. The behavior varies based on the action causing the overwriting. If it is a user action (e.g., using the *Save As* command or starting an analysis), the user will be prompted to choose a different file name. If the overwriting is caused by an automatic action (e.g., creating a new chromatogram during measurement), a unique 4- to 6-digit number is added at the end of the original filename.

Generate chromatogram after manual abort

This feature will cause chromatogram generation if a user aborts the analysis manually.

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

Disallow calibration response change

This checkbox prevents the manual change of response in the [Calibration](#) window.

Note: If allowed, any manual changes are logged in the [Calibration Audit Trail](#). Manually changing the responses breaks the link between the calibration standard and the calibration itself. The chromatograms linked to the calibration file will not indicate that manual changes have been made.

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 (i.e., user name and password) to successfully log in.

Disallow user deletion and renaming

This checkbox disables the option to delete or rename an existing user. The renaming is then possible only right after the creation of the user (before saving the *User Accounts*).

Ask for reason of file change

This checkbox enables to fill in the reason for any file change. When saving a file (e.g., chromatogram, method), the *Reason for Chromatogram (Method, ...) Change* dialog will appear. The user can (but is not obliged to) fill in the reason for the change.

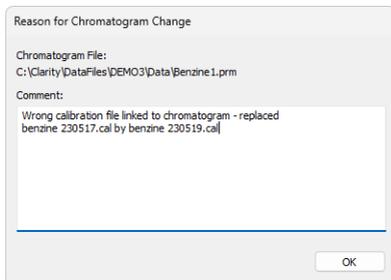


Fig. 26: Reason for Chromatogram Change

Note: The reasons for 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 for change. No empty reason field nor reasons solely composed of spaces are allowed.

Allow automated export of audit trail

This checkbox sets the automatic export of station audit trail file to the file and location specified in the *File Name* field. To specify the location, use the  button and navigate

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

Disallow spike filter and spike removal

This checkbox disables the *Spike Filter* and *Spike Removal* functions in the [Chromatogram](#) window.

Disallow to overwrite existing files using save as and while exporting

This checkbox prevents users from overwriting any existing file. This feature applies to any file (method, calibration, chromatogram, exported documents, etc.) created by **Clarity**. Exporting in the form of appending to an existing file is still allowed.

Allow chromatograms to be stored to current project only

This checkbox restricts storing any newly generated chromatograms outside of the current project directories (typically *Data* and *Calib*).

This feature disables:

- storing any newly generated chromatogram directly into the root of current *Project*
- automated creating of new subfolders directly in the root of current *Project*

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

When defining the destination of a newly generated chromatogram, **Clarity** constantly evaluates the user's input regarding where to store the new chromatogram, and provides feedback to the user. In the [Single Analysis](#) window, the feedback provided to the user is displayed above the *Chromatogram File Name* field. If the given destination is allowed, it is displayed in standard black; if it is prohibited, it is displayed in red.

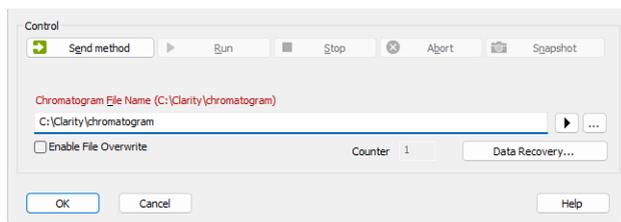


Fig. 27: Single Analysis - Allow chromatograms to be stored to current project only - Prohibited destination

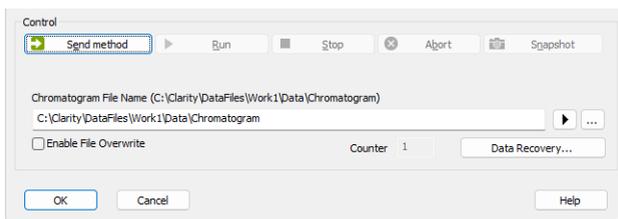


Fig. 28: Single Analysis - Allow chromatograms to be stored to current project only - Allowed destination

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

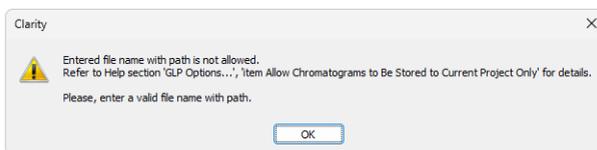


Fig. 29: Single Analysis - Allow chromatograms to be stored to current project only - Prohibited destination - Error message

In **Sequence**, the user is informed about a prohibited destination via a  indication in the **Status** column of the incorrectly set row. If a prohibited path is used, the user is prevented from starting any new analyses and the corresponding error message is displayed. This event is also recorded in **Audit Trail**.

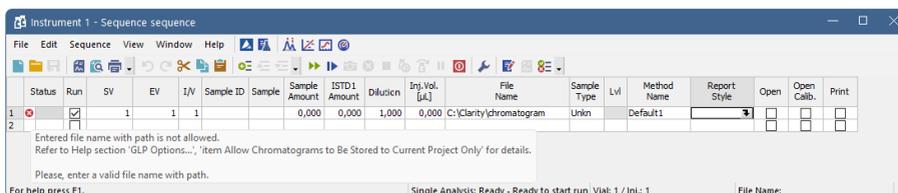


Fig. 30: Sequence - Allow chromatograms to be stored to current project only - Prohibited destination

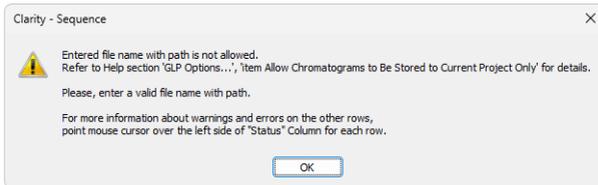


Fig. 31: Sequence - Allow chromatograms to be stored to current project only - Prohibited destination - Error message

The following image provides an overview of the allowed and prohibited destinations.

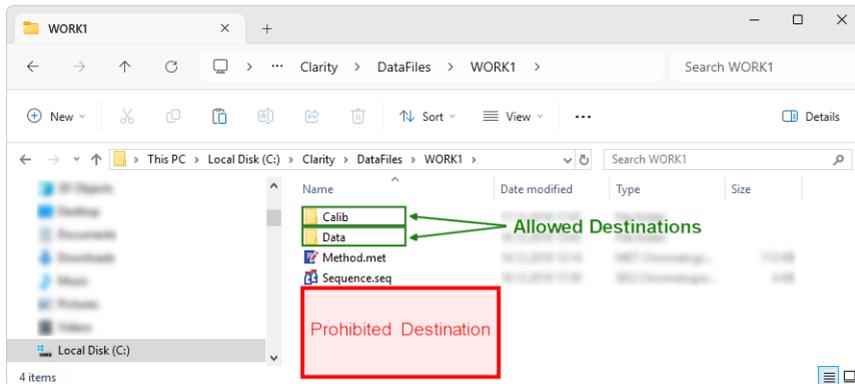


Fig. 32: Allow chromatograms to be stored to current project only - Destinations

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

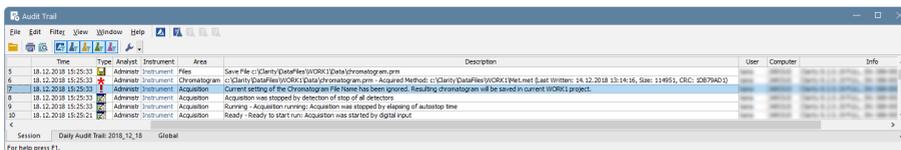


Fig. 33: Audit Trail - Allow chromatograms to be stored to current project only - Fallback Mechanism

The option *Allow chromatograms to be stored to current project only* should also be used if transferring the given [Project](#) among various computers is planned. 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 the use

absolute paths to store chromatograms is recommended. If it is still desired to save a new chromatogram to a specific location, keep in mind that Clarity (and the Windows user) need the write access right to this location. Typical examples of problematic destinations are the root folder of the system hard drive (e.g., C:\) or the root folder of a server (e.g., \\server\).

Disallow chromatogram merge operation

This checkbox prevents users from using the "Merge" on page 268 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. 82), 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).

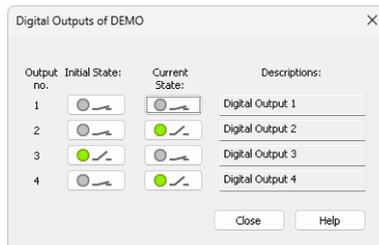


Fig. 34: Digital Output Control

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.

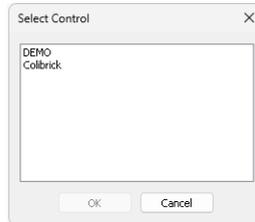


Fig. 35: Select Control

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

1.2 Instruments

A submenu with commands for access to individual instruments. Items in the menu are displayed dynamically, depending on how many instruments are configured, whether any user is logged on any instrument and/or whether any instrument is locked. Furthermore each command is accompanied by the name of the instrument, e.g., *Login to My GC....*

 **Login / Open** *Login / Open* the respective instrument.

 **Logout** *Logout* from the respective instrument.

 **Lock** *Lock* the respective instrument.

Close All Instruments Closes all opened Instruments at once (available only if no instruments are locked).

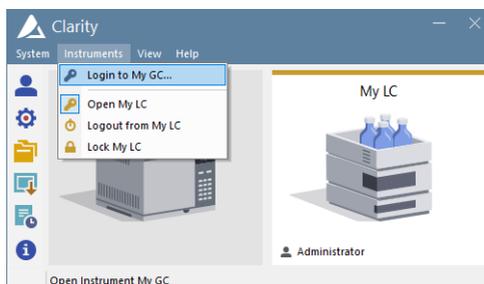


Fig. 36: Menu Instruments

1.2.1 Login

A command for opening the respective Instrument. 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).

After selecting an Instrument to be opened *Login Dialog* is displayed. It always contains *Select Project* list, where a project can be selected or a new one can be created (pre-selected project is based on desktop file). The other contents vary slightly based on the presence of user account and GLP settings done in [GLP Options](#)

If station has at least one user account, the *Login Dialog* contains the drop-down list where user account can be selected. Afterwards, the related password must be filled in to log in to the **ClarityInstrument**. User accounts that are permanently disabled are not displayed in the list. If the option *Disallow user list in login dialog* is enabled in [GLP Options](#) drop-down list is not present and both user name and password must be entered manually.

If the station has no user accounts configured, the login dialog only contains field to enter a name (no password field). The entered name will be saved in all files that you create or modify during your session.

In case **Clarity** 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.

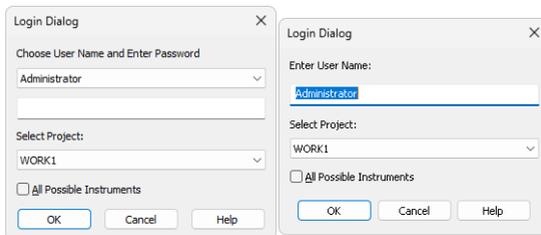


Fig. 37: Login dialog and Username dialog

All Possible Instruments

If you have checked the *All Possible Instruments* box, 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.

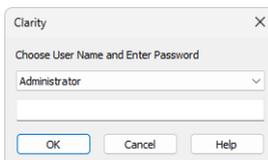


Fig. 38: Login dialog when opening System Configuration or User Accounts

Initial password

After receiving your user name 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.

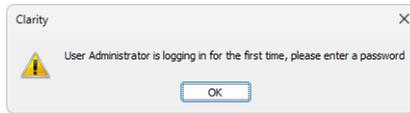


Fig. 39: Initial password warning

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



Fig. 40: New Password dialog

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

In the case that the failed log in attempts exceed the number set in the *User Accounts* dialog, the user will be disabled permanently, except for those with the right to access the *User Accounts* dialog. Such accounts are locked only temporarily for one hour. Disabled user accounts can be enabled via the *User Accounts* dialog.

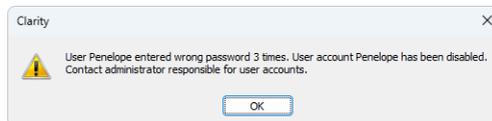


Fig. 41: Account disabled message

1.2.2 Logout

A command for closing the respective Instrument (available only for opened Instruments). The user will be notified of an analysis or sequence in progress as well as of all modified files that have not been saved yet. Unsaved modifications are denoted by a MODIFIED tag next to the filename in the window header.

Close All Instruments

Closes all opened Instruments at once. This command is visible only when it is possible to close all instruments, i.e., if more than one configured instruments are opened and none is locked.

1.2.3 Lock

A command for locking and unlocking the respective Instrument (only available if at least one user account exists). This enables the users to prevent unauthorized actions on an Instrument during their absence. Locked Instruments are denoted with a gray stripe labelled as **Locked**. The name of the user who is logged on the locked instrument is displayed in the left bottom corner of the respective Instrument icon. Locking an Instrument does not affect the running data acquisition nor sequence. An Instrument can be unlocked by entering the password of the user who has locked it.

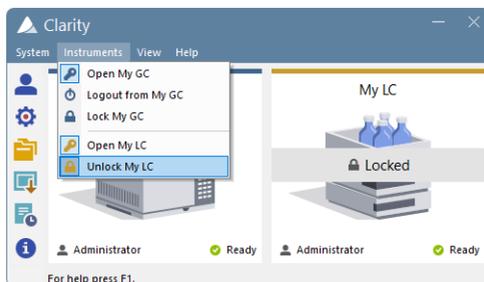


Fig. 42: Opened "My GC" and locked "My LC" Instruments

Note: Instrument locked by any user can be unlocked also by the user that has the *Take Control of Locked Instrument* option in the *User Accounts* allowed. This action is recorded into the [Station Audit Trail](#), and the person that unlocked the locked Instrument becomes logged on this Instrument

It is possible to lock an Instrument at any given moment. If there are any modified documents present at the moment the *Lock* command is invoked, the user will be notified that the changes will be discarded if the Instrument is unlocked by a different user.

If any Instrument is locked, the **Clarity** station cannot be closed, as modified documents could potentially be present or measurements running on the locked Instrument(s). Similarly, accessing the *User Accounts*, *System Configuration*, and *Directories* is not possible if any Instrument is locked.

Note: It is possible to take control of a locked Instrument using the "Command line parameters" on page 477. The user (*user=...*) and password (*p=...*) parameters must be included for each command. Although commands can be run on the locked Instrument this way, the Instrument remains locked.

1.3 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 | <p>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.</p> <p>Tablet Mode is not accessible in Clarity Lite.</p> |
| Toolbars | <p>Displays commands for toolbars.</p> <ul style="list-style-type: none">• 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. <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**.

1.3.1 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

1.3.1.1 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.

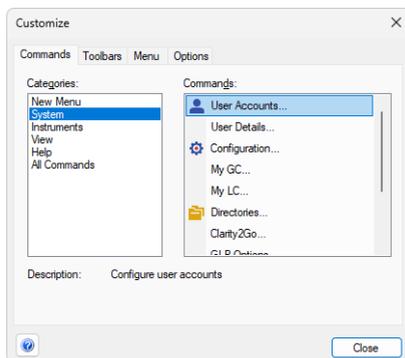


Fig. 45: Customize - Commands

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.

1.3.1.2 Toolbars

The *Toolbars* tab lists all created toolbars for the respective window.

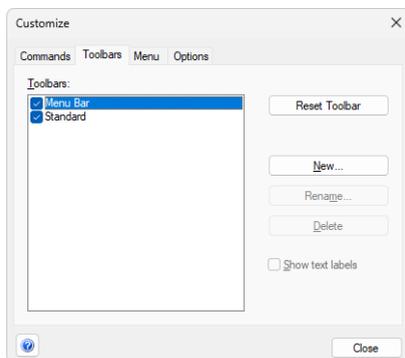


Fig. 46: Customize - Toolbars

- To display/hide a toolbar check/uncheck the box next to its name. The *Reset Toolbar* command restores the original settings.
- The *New...* command will create a new, empty custom toolbar - use the *Commands* tab to drag icons to the toolbar.
- The *Rename...* command invokes *Toolbar Name* dialog for the renaming the toolbar.
- *Delete* command deletes selected toolbar and its contents.
- When checkbox *Show text labels* is checked, corresponding toolbar will display both; icon and description.

Note: *Rename...* and *Delete* commands work only with user defined toolbars. It is not possible to rename nor delete default toolbars.

To reposition a toolbar, left mouse click on the toolbar, and then drag the mouse pointer to the place on the screen where you want the toolbar to be positioned. Alternatively it is possible to place the toolbar out of the window in an individual panel.



Fig. 47: Toolbar panel

1.3.1.3 Menu

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

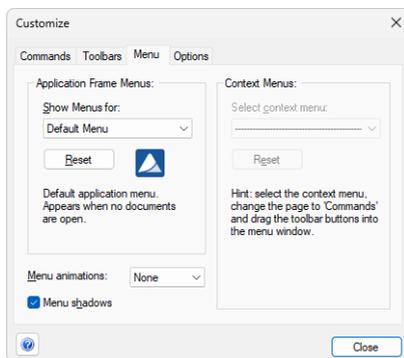


Fig. 48: Customize - Menu

- *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.

1.3.1.4 Options

Options tab displays options for toolbars.

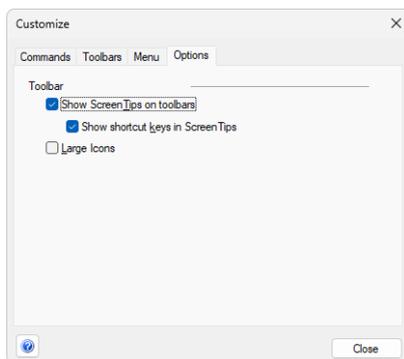


Fig. 49: Customize - Options

- 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

1.4 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. |
| IQ Report | Runs Installation Qualification (IQ) and displays IQ Report. |
| About... | Displays information about Clarity . |

1.4.1 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.

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](#)

LOGIN

Don't have a user account yet?

Create a user account and register your chromatography software.

REGISTER

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.

1.4.1.1 Register Clarity question

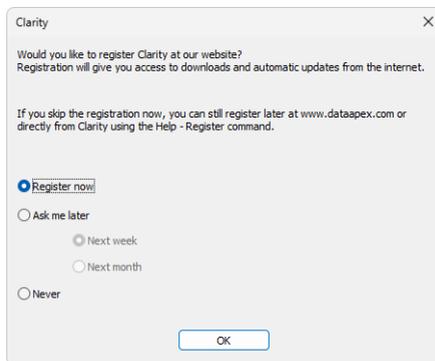


Fig. 52: Clarity registration message

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.

1.4.2 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.

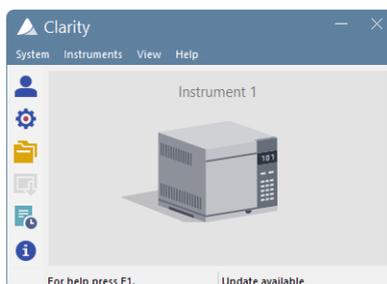


Fig. 53: Update available in the main Clarity window

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.

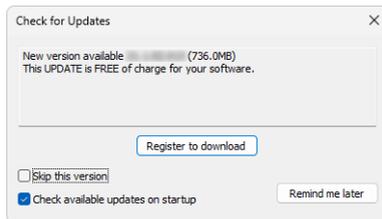


Fig. 55: Check for Updates dialog - Register to download

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. 47.. Once you switch back to Clarity, you will be notified that you have to confirm your registration from your email.

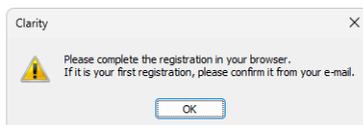


Fig. 56: Confirm your registration from your e-mail

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

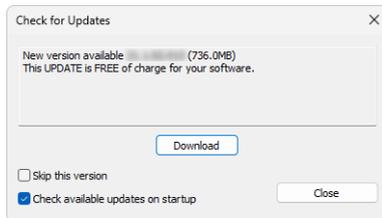


Fig. 57: Check for Updates dialog

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.

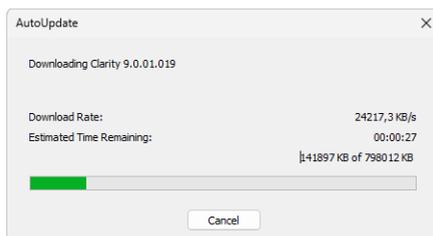


Fig. 58: AutoUpdate dialog

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.

1.4.3 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.

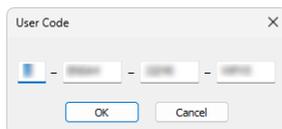


Fig. 59: User Code dialog

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.

1.4.3.1 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.

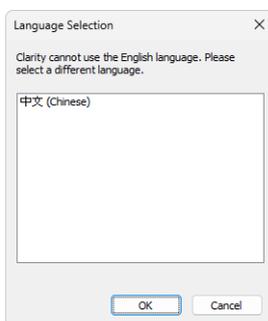


Fig. 60: Language Selection dialog

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

1.4.4 Trial Prolongation...

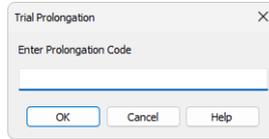


Fig. 61: Trial Prolongation dialog

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**.

1.4.5 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.

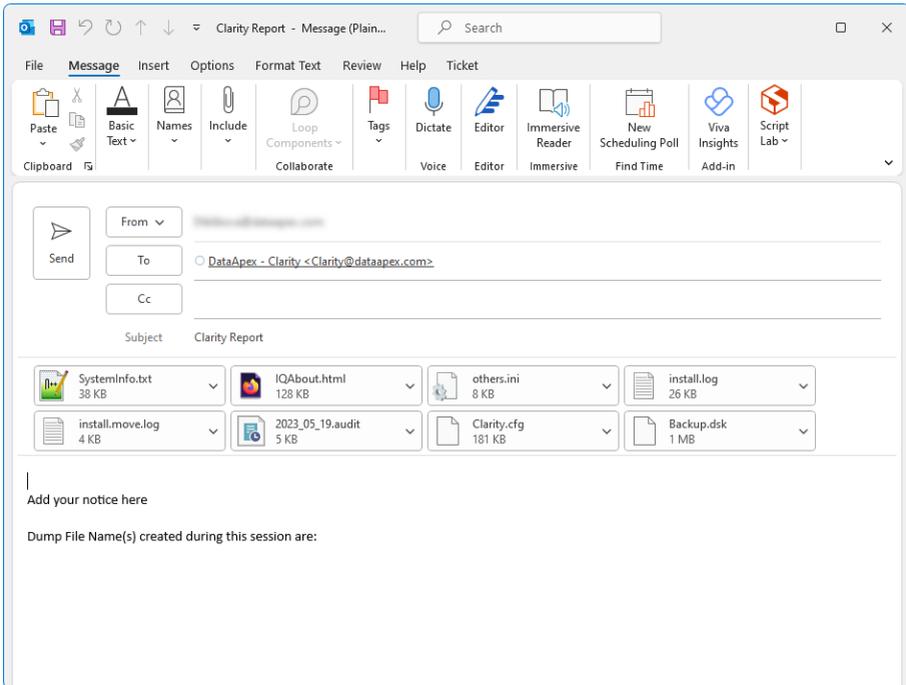


Fig. 62: E-mail message with information about Clarity

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. 411).

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. 142.

1.4.6 Installation Qualification

One of the requirements for ensuring the reliability of generated results is the validation of all instrumentation and procedures that are used to acquire data.

1.4.6.0.1 Levels of Qualification

For chromatography datastations, usually three levels of validation (qualification) are relevant:

Installation Qualification: a procedure confirming, that the datastation was successfully installed and that the installation contains all needed files of correct version. Installation qualification is an integral part of the **Clarity** Chromatography datastation installation procedure.

Operational Qualification: a procedure confirming, that the datastation is performing according to the manufacturer's specification. Chromatography data are acquired and analyzed with prepared procedures and the acquired results are compared with expected values. **System Suitability Test (SST)** module is required for this type of qualification.

Performance Qualification: a procedure confirming, that the analytical system is fit for a given type of analysis. Usually, the overall system performance is tested by this procedure with respect to the requirements of the desired application. The **Clarity** datastation offers many tools in the **System Suitability Test (SST)** module to efficiently evaluate the system performance.

1.4.6.0.2 Installation Qualification of Clarity datastation

This manual describes the **Installation Qualification** of **Clarity** datastations. This qualification can be performed following anytime from the Clarity main window.

Performing Installation Qualification of Clarity is very easy: it consists of launching the *IQ Report* via *Help - IQ Report* command in the main window of Clarity, printing the results and signing them. In case the overall result is *"Failed"*, there is some inconsistency in files which are necessary for proper function of datastation. In that case the user has to check the list of files (in the lower part of page) and find the row containing a red coloured inscription in its *Status* field.

1.4.6.0.3 Possible messages in the Status field

Passed

The file is correctly installed and registered.

Warning: Unknown control module

Possible reasons:

- The control module is located and registered in a different folder than in the current installation. Other installation of Clarity was probably not correctly uninstalled. The solution is to find the old installation folder and delete it

manually.

- The control module is located in the current installation folder, but registered for another EXE file than the current one. The UNINSTAL.LOG file was damaged or corrupted in the previous installation and the files were not uninstalled. Find and delete all DLL and OCX files from the current installation folder before a new installation.
- The file is located in the current installation folder, a control module not present in the installation was added and registered. No remedy needed when it was done on purpose, in other case delete the file manually.

In case this warning is displayed, the overall result of Installation Qualification will be "*Passed (with warnings)*". This means the installation was performed successfully and there is no file missing, however, there are some discrepancies and it is recommended to fix the problem with indicated files.

Failed: file does not exist

The file is registered but not physically present. Possible reasons:

- The previous installation was deleted without proper uninstallation. Clean up the registers for unused entries before a new installation.
- The file was deleted manually from the current installation.

Failed: bad size

File size does not match.

Failed: bad checksum

The module file is corrupted, its size or checksum differs from the proper value for particular version of **Clarity** datastation.

In case some of the files are displayed, the overall result of Installation Qualification will be "*Failed*". This means the proper function of the datastation cannot be guaranteed and the new installation is strongly recommended.

Failed: does not have record in certification file

The file is present in the default installation folder, however according to our certification file it is not supposed to be there, if it is a control module, it will trigger *Unauthorized control module* yellow stripe in the *Instrument* window.

1.4.6.0.4 Troubleshooting

In order to get "*Passed*" for IQ of your station, it is necessary to uninstall the old installation, then check for problem-causing files on your computer and, eventually, delete them manually. Exact suggestions are listed in *Possible Messages* section above. However, a general procedure consists of searching for the problematic files, deleting them and installing the station anew. After deleting the old files, cleaning of the Windows registry has to be performed. It is possible to search for the registry key dealing with the deleted file and remove it too, however, the easiest way is to use some software intended for cleaning the registry.

1.4.7 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.

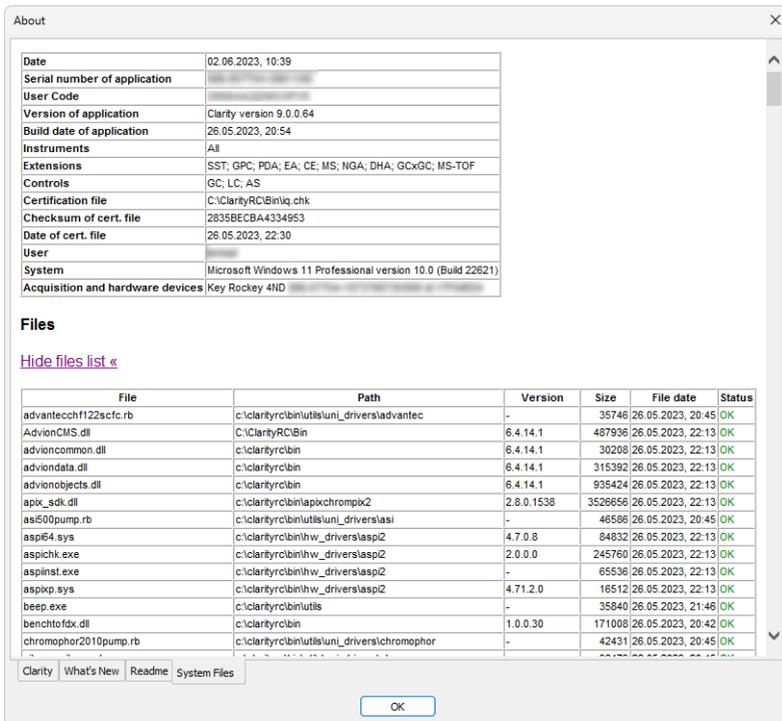
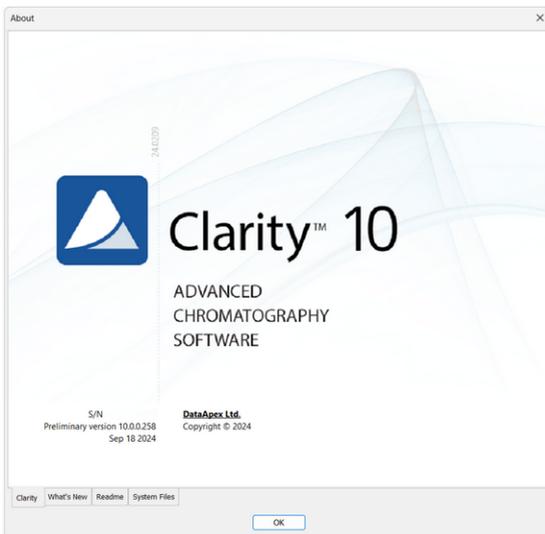


Fig. 63: About - Clarity & System Files

2 Instrument

Caution: In **Clarity Lite** the *Instrument* window is called the *Main* window and slightly differs from the standard *Clarity Instrument* window. For more details, see [Clarity Lite Window Specifics](#) topic.

The *Instrument* window is the central interface for chromatogram measurement and evaluation. To open it, select *Login to Instrument* from the *Instruments* submenu or click the corresponding icon in the main window. The instrument's name is set in the configuration settings (for more details see the chapter **Right section of System Configuration dialog** on pg. 17).

Clarity supports up to four *Instrument* windows displayed simultaneously. Each *Instrument* window has a unique header color for easy identification. The number of open *Instrument* windows can exceed the number of purchased instruments, but additional windows function only as *Offline Instruments*. These are commonly used for method development or evaluating previously measured analyses, but they cannot perform data acquisition.

The *Instrument* window presents a logical sequence of operations and commands needed for comprehensive analysis processing. The simplified workflow is represented by navigation icons, guiding users through method preparation, sample injection, data acquisition, and chromatogram evaluation.

Simplified workflow

| | Icon | Name of Window | Description |
|--|---|-------------------------|---|
| |  | Method Setup | Open Method Setup dialog to create a new method or modify existing. |
| |  | 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. |

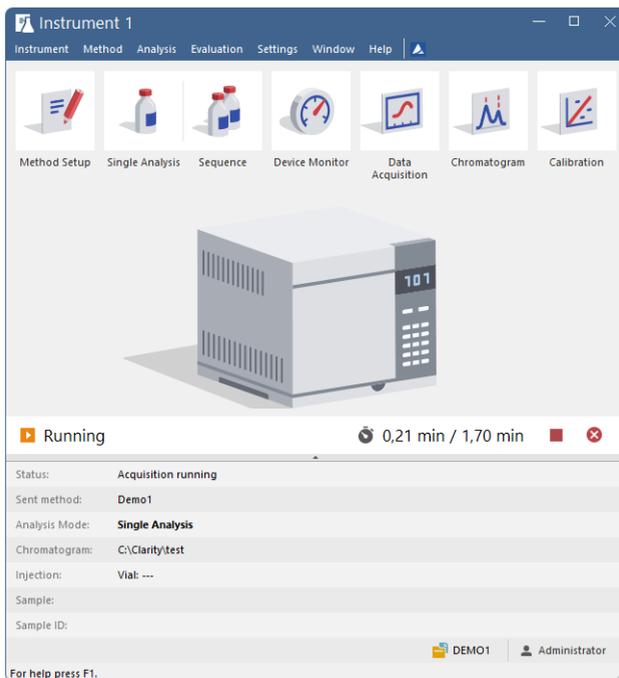


Fig. 64: Instrument

Analysis status bar

The *Analysis Status* bar, located below the workflow icons in the *Instrument* window, provides real-time information about the instrument's state, such as elapsed time during a running analysis or sequence and the current measurement status.



Fig. 65: Analysis statuses

It also contains acquisition control buttons, which change dynamically based on the current operation:

- **Send Method** - Sends the method selected in the [Single Analysis](#) dialog to the connected hardware.
- **Run Sequence** - Starts measuring the sequence opened in the [Sequence](#) window.
- **Stop Acquisition** - Stops the ongoing acquisition.
- **Abort Acquisition** - Immediately aborts the running acquisition.

Information table

Below the status line is the *Information Table*, which provides details about the currently running analysis. When no analysis is running, only the Status and Sent Method fields are displayed, while the rest remain hidden. The table can be collapsed or expanded using the small arrow below the status line.

| Parameter | Description |
|---------------|---|
| Status | Displays complementary information to the status displayed above it. |
| Sent Method | Displays which method was sent to the instrument. If an analysis is running, this method is used for the current acquisition. If no analysis is running, this is the method that will be used when a <i>Single Analysis</i> starts. |
| Analysis Mode | Indicates whether <i>Single Analysis</i> or <i>Sequence</i> is running. If a sequence is running, it displays its name. |
| Chromatogram | Displays the name of the resulting chromatogram. |
| Injection | While a sequence is running, details about <i>Row</i> , <i>Vial</i> , and <i>Injection</i> are displayed. During <i>Single Analysis</i> , only <i>Vial</i> is shown if available. |
| Sample | Displays the content of the <i>Sample</i> field. |
| Sample ID | Displays the content of the <i>Sample ID</i> field. |

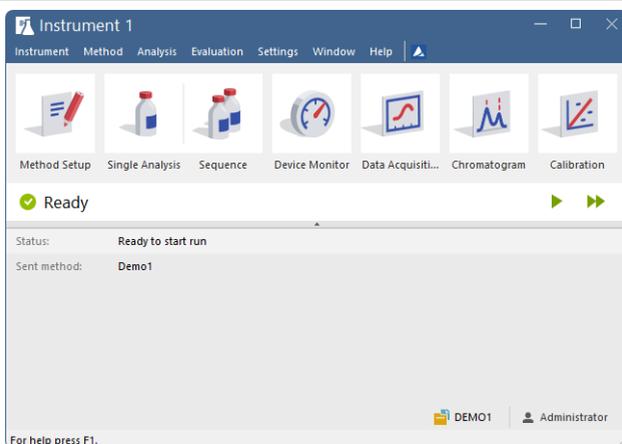


Fig. 66: Instrument Ready

Project and user

The lower end of the *Instrument* window displays information about the currently opened *Project* and the name of the *User* logged into the instrument. Clicking the project name opens the [Project Setup](#) dialog.

Tablet Mode

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

When *Tablet Mode* is enabled and the general scale in Windows is set higher than 100%, some UI elements adjust to improve touch accessibility:

- Workflow icons are arranged into two rows for easier interaction.
- The analysis status line is divided into two rows to remain legible.

These adjustments ensure optimal usability when using Clarity on touchscreen devices.

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.

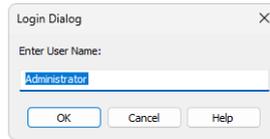


Fig. 67: Username dialog

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> | <p>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.</p> <p>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.</p> |

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.

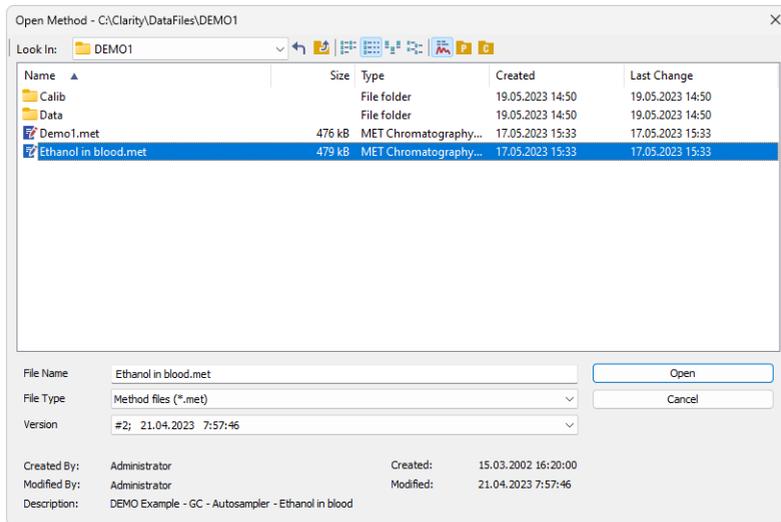


Fig. 68: Select Method

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 Project Setup

To open the *Project Setup* dialog, use the menu *Instrument - Project...* command (icon ) or click the project name in the bottom-right corner of the [Instrument](#) window. The *Project Setup* dialog allows users to modify the current project settings, open an existing project, or create a new one.

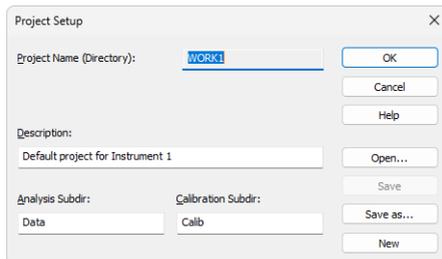


Fig. 69: Project Setup

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 "**Instrument Directories for Projects**" on pg. 24.

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. \/:*?"<>|.

2.2.2.1 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.

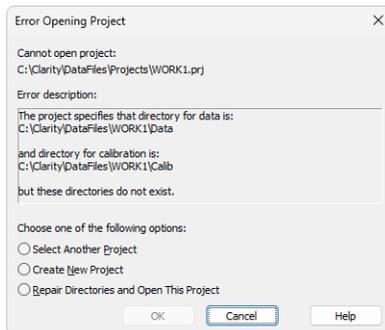


Fig. 70: Error Opening Project

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.

2.2.3 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.

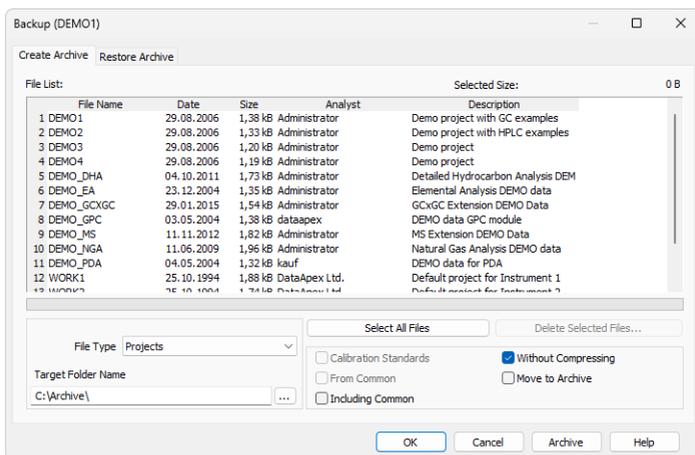


Fig. 71: Backup - Create Archive

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 Files*, *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.

2.2.4 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.

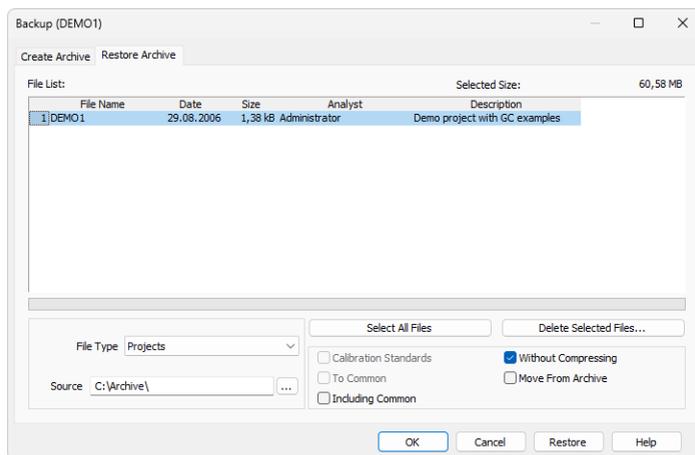


Fig. 72: Backup - Restore Archive

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 Files*, *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.

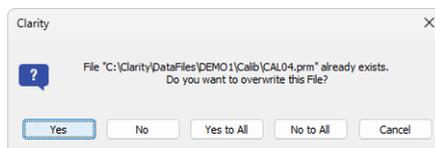


Fig. 73: Warning message when the filename already exists

2.2.5 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:

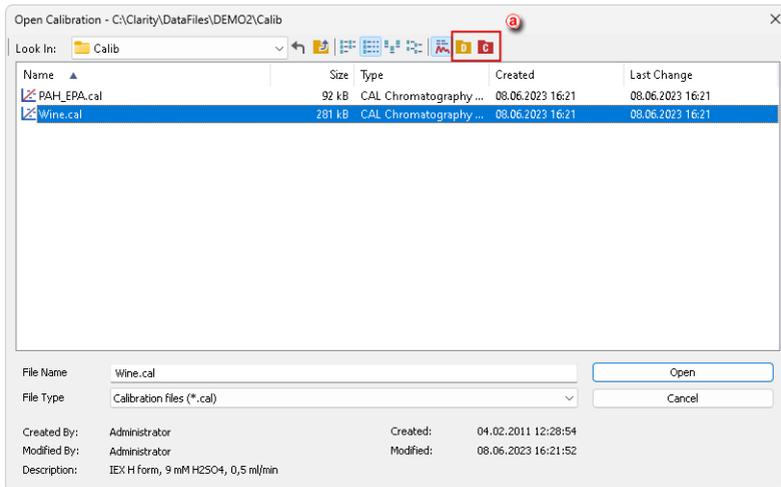


Fig. 74: Open Calibration

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.

2.2.6 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.

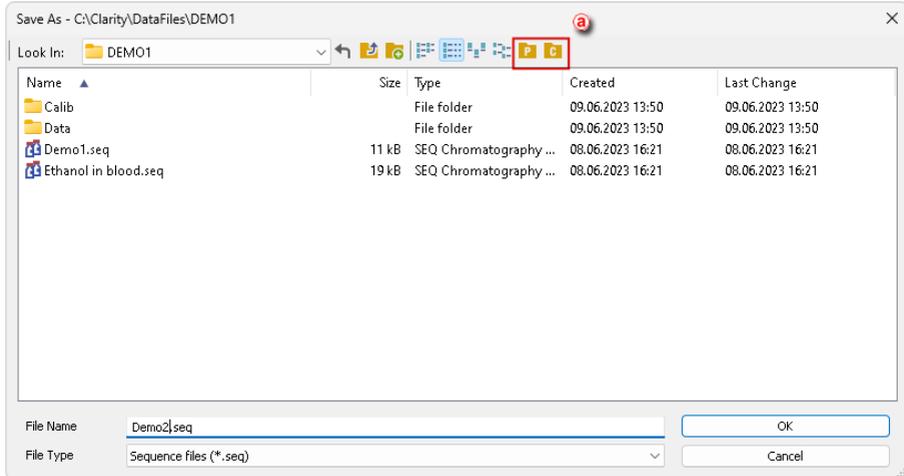


Fig. 75: Save As Dialog

Icons in the upper right corner  serve for quick navigation through useful folders, e.g. DATA, CALIB, COMMON. What folders are shown here depends 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 according to the previous settings. The layout can be changed using the  button to access the *Detailed View*. In the *Detailed View* layout, you can change the sorting order by clicking on the header cell of the desired column. Repeated clicking 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 the 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 of the selected file. It 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 matching the already entered letters in the 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 they are 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.

2.2.7 Send File by Email

This command creates a new email message in your default email client with the currently displayed file attached. It functions uniformly across various Clarity windows, allowing you to send different types of files, such as methods, calibrations, chromatograms, sequences, and reports, directly via email.

Note: For this command to function properly, a working email account configured in your default email client is required.

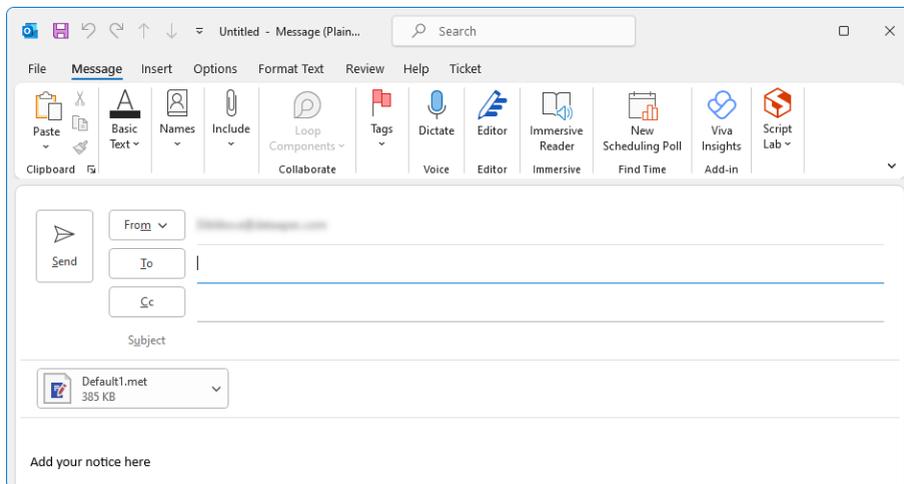


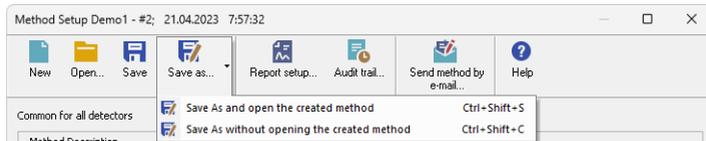
Fig. 76: New email with the selected method in the MS Outlook

2.3 Method Setup

The *Method Setup* dialog is used to define and edit all parameters of the method. The method includes both acquisition and processing parts, organized into several tabs. Each tab covers a different area of the method, such as general instrument parameters, detector setup, data acquisition, peak integration, and result calculation.



The dialog can be accessed from the icon in the *Instrument* window, or from several other locations within Clarity.



Header

At the top of the dialog, the current method name and version are displayed. The date and time indicate when the currently opened version was created (method was last saved).

The format is as follows: *[Method Name] - #[Version Number]; [Date] [Time]*

Date and time are displayed according to the current system locale settings in Windows.

If a method created in an older version of Clarity (without method versioning) is opened, it will be automatically converted to version 1.

Command Bar

The top row of the dialog contains command buttons for common method-related actions, such as creating, opening, or saving a method. A full list of available commands is provided in the table below.

| Icon | Command | Description |
|---|---------|---|
|  | New | Creates a new method (Noname) and closes the current one (a warning appears if there are unsaved changes). This action can also be triggered using the Ctrl + N shortcut. |
|  | Open... | Opens a method file and simultaneously closes the currently opened one (a warning appears if there are unsaved changes). Using this command or pressing the Ctrl + O shortcut opens the Open Method dialog. |

| Icon | Command | Description |
|--|--|---|
|  | Save | Saves the current method file. This command can also be triggered using the Ctrl + S shortcut. If saving a new file for the first time, the <i>Save As</i> dialog will appear, requiring a file name to be specified. The default name <i>Noname.met</i> is reserved for new unsaved files only. |
|  | Save as... | Saves the method file under a chosen name and opens it. Using this command or pressing the Ctrl + Shift + S shortcut opens the <i>Save As</i> dialog. If the selected file name already exists, a confirmation message appears before the file is overwritten. Clicking the arrow next to the button offers an alternative: save the method under a new name without opening it (Ctrl + Shift + C). Method saved this way contains one version, history from the source method is not saved. |
|  | Report setup... | Opens the <i>Report Setup</i> dialog (Ctrl + Alt + P). If there are unsaved changes in the method, you will be prompted to save them first. Reports can only be generated from a saved version of the method. |
|  | Audit trail... <small>✓ Full version</small> | Opens the <i>Method Audit Trail</i> window showing the full change history of the current method. If there are unsaved changes, you will be prompted whether to save them before opening the window. |
|  | Send Method by Email | Sends method file as an email attachment. |
|  | Help... | Opens contex help for the currently active tab. |

Available Tabs

The *Method Setup* dialog contains several tabs, each covering a specific aspect of the method. Some tabs are common to all configurations, while others are only available when specific control modules (e.g., *Thermostat*, *Fraction Collector*) are present.



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

| Tabs | Contents of the tab |
|--|--|
| Event Table | Allows triggering actions during the analysis, such as switching valves. |
| Measurement | Contains run time, external start handling and general settings for measurement conditions, including column, flow rate, and temperature serving only informational value. |
| Acquisition | Detector-specific parameters for acquiring the signal. |
| Integration | Settings defining how the signal is integrated and how the baseline is modified. |
| Calculation | Parameters for calculating final results from the integrated data (calibration, etc.). |
| Advanced <input checked="" type="checkbox"/> Full version | Contains <i>Subtraction Chromatogram</i> function, <i>Column Calculation</i> and <i>User Variables</i> parameters. |
| GC (LC) Control <input checked="" type="checkbox"/> Full version | GC (LC) Control – Direct control parameters for the chromatograph. |
| AS Control <input checked="" type="checkbox"/> Full version | AS Control – Injection control settings for directly controlled autosamplers. |

Footer - Buttons

In addition to the tabs, the lower part of the *Method Setup* dialog contains a set of buttons available on every tab. These buttons are present on every tab.

OK

Saves all changes to the current method and closes the dialog. If acquisition using the opened method is running, only *Enable Autostop* checkbox and *Run Time* parameter in the *Measurement* tab can be modified; the rest of the method is locked. For newly created methods, pressing *OK* opens the *Save As* dialog.

Cancel

Discards all changes and closes the dialog without saving.

Send Method

Sends the currently opened method to all connected control modules and sets it in the [Single Analysis](#) dialog. This button is disabled during data acquisition or if the method is not saved (marked as *MODIFIED* or *Noname*).

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. 88).
- 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.

| Name | Input | | Output | | | | | | |
|-----------|----------------|----------|-----------------|-------|-------|-------------|------------------|-----------|-------------------------------------|
| | Type | Source | Input | Value | Units | Output Type | Output | Parameter | Store |
| 1 Collect | Dig. Input Run | Colbrick | Digital Input 1 | Up | --- | Colbrick | Digital Output 1 | High | <input type="checkbox"/> |
| 2 Waste | Dig. Input Run | Colbrick | Digital Input 1 | Down | --- | Colbrick | Digital Output 1 | Low | <input type="checkbox"/> |
| 3 Next | Dig. Input Run | Colbrick | Digital Input 2 | Up | --- | Colbrick | Digital Output 2 | Pulse | <input type="checkbox"/> |
| 4 V1 | Run Time > | --- | --- | 0,500 | min | Valve 1 | Position | 1 | <input checked="" type="checkbox"/> |
| 5 V2 | Dig. Input Run | Colbrick | Digital Input 1 | Up | --- | Valve 1 | Position | 2 | <input checked="" type="checkbox"/> |
| 6 | | | | | | | | | <input type="checkbox"/> |

Fig. 77: 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. **84.**:

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. This happens after method is sent (outside of sequence or in it). |

| Name of the event | Condition on when the event is triggered |
|-------------------------|---|
| <i>Run Begin</i> | Run has begun. In the Sequence measurement, start of the sequence row (after method was sent and received by hardware, before the injection instructions were sent). In the Single Analysis measurement invoked whenever the <i>Run</i> (or <i>Inject & Run</i> button) was used, or appropriate start signal was triggered. Not invoked during Single Analysis or Passive Sequence measurement when acquisition is restarted (see <i>Restart Acq</i>). |
| <i>Injection</i> | In the sequence row with injection (row with <i>Sample Type</i> other than <i>Bypass</i> value set), injection instructions has been sent to hardware. Also possible during Single Analysis measurement while using autosampler. |
| <i>Bypass Injection</i> | In the bypassed sequence row (row with <i>Sample Type</i> = <i>Bypass</i> value set), injection instructions have just been skipped. |
| <i>Acq Begin</i> | Acquisition has begun. In the Sequence measurement or Single Analysis while using the sampler, injection operation has been finished, detectors start to provide run data. In the Single Analysis measurement without using autosampler, invoked on pressing the <i>Run</i> button or appropriate start signal being triggered very shortly after the <i>Run Begin</i> event is triggered. Not invoked during Single Analysis or Passive Sequence measurement when acquisition is restarted. |
| <i>Restart Acq</i> | Invoked when acquisition is restarted (analysis is already running and new analysis trigger arrives, with method starting conditions set to <i>Start-Restart</i>). Only possible in Single Analysis or Passive Sequence measurements. |
| <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. |

| Name of the event | Condition on when the event is triggered |
|-------------------|--|
| SST OK | On the end of acquisition, when SST resulted with OK. |
| SST Unknown | On the end of acquisition, when SST resulted with Unknown. |
| SST Failure | 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. 398).

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. 90). |
| <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). |

| Name of the command | Meaning of the command |
|-----------------------|---|
| <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. **398**.

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. **502**).

- 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 *Measurement* tab defines the measuring conditions and sets the total duration of the analysis. It is shared across all signals in multi-detector measurements. Using the *Method – Measurement...* command from the [Instrument](#) window opens the *Method Setup* on this tab.

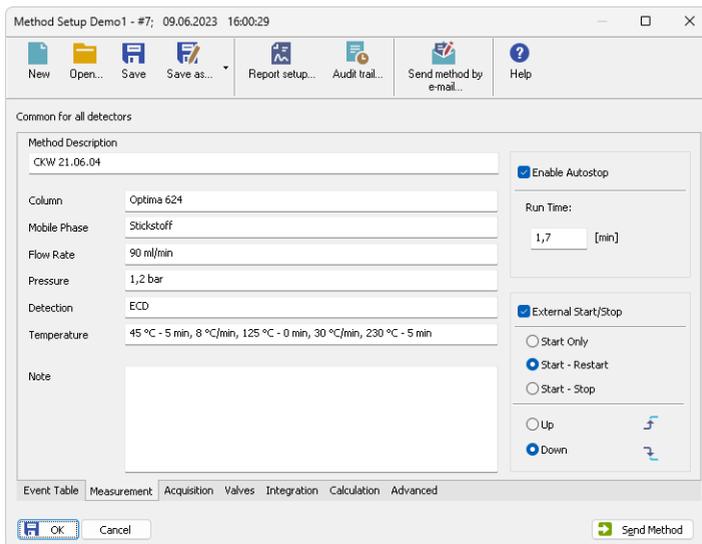


Fig. 78: Method Setup - Measurement

Method Description

Displays a description of the method. When opening the method, this text appears in the *Description* field of the [Open Method](#) dialog.

Informational Fields

The following fields serve for recording descriptive information about the method. Their content has no influence on the actual course of the analysis.

- *Column* – Describes the column used.
- *Mobile Phase* – Describes the mobile phase used.
- *Flow Rate* – Indicates the mobile phase flow rate.
- *Pressure* – Indicates the mobile phase pressure.
- *Detection* – Describes the detector used.
- *Temperature* – Describes temperature parameters.
- *Note* – Optional field for entering any additional method-related information.

Enable Autostop

Enables automatic termination of the analysis once the time set in the *Run Time* field is reached.

Run Time

Specifies how long the analysis should run, in minutes. Once the set time has elapsed, the analysis is automatically finished and the chromatogram is created. This field is only available if *Enable Autostop* is checked. Valid values range from 0.2 to 9999 minutes.

The *Run Time* must be set for all methods used in an [Active sequence](#), as it defines the cycle duration.

External Start/Stop

Enables external synchronization of the analysis using an external start signal. Three operation modes are available:

- *Start Only* – A single external signal starts the analysis. Any further signals received during the run are ignored. This is the default mode used when a new method is created.
- *Start – Restart* – The external signal not only starts the analysis but can also restart it. The first signal starts the analysis, and the second signal stops the current run and immediately starts a new one. This allows continuous measurement. This mode is not supported by most directly controlled instruments.
- *Start – Stop* – Each external signal alternates the state of the analysis. The first signal starts it, the second stops it, the third starts it again, and so on.

The station can respond to two types of signal edge changes:

- *Up* – Triggered when the voltage changes from low (< 0.7 V) to high (> 3 V), typically corresponding to an opened contact.
- *Down* – Triggered when the voltage changes from high (> 3 V) to low (< 0.7 V), typically corresponding 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.

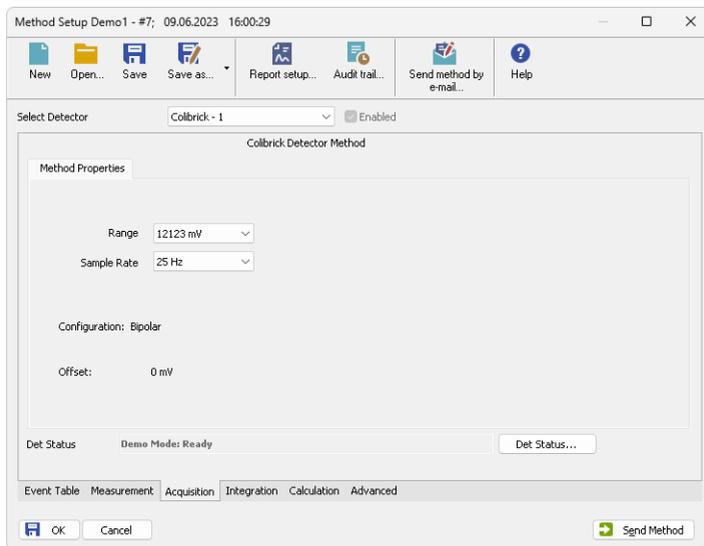


Fig. 79: Method Setup - Acquisition

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.

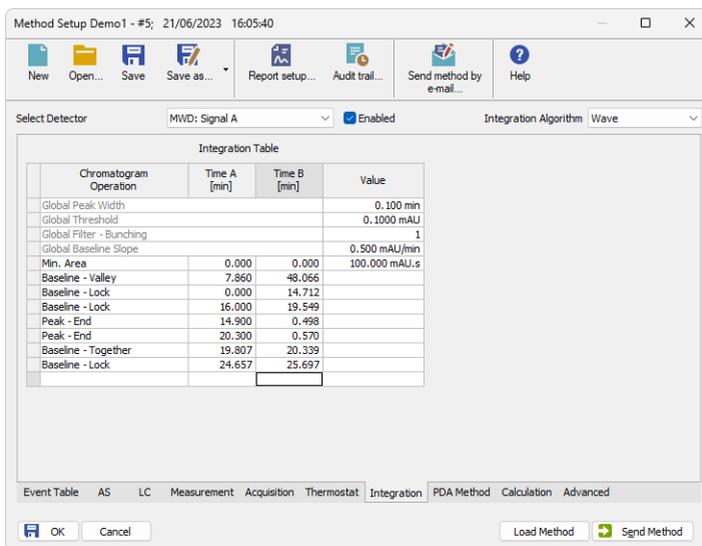


Fig. 80: Method Setup - Integration

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

2.3.5 Calculation

Sets the calculation parameters of the method. It links the method to a calibration file, specifies the calculation type, and includes additional settings such as units, response factor for unidentified peaks, and result display options.

When invoked by the menu command or via the  icon, the *Method Setup* dialog on the *Calculation* tab will open. When utilizing a multi-detector chromatogram, the tab is common for all signals.

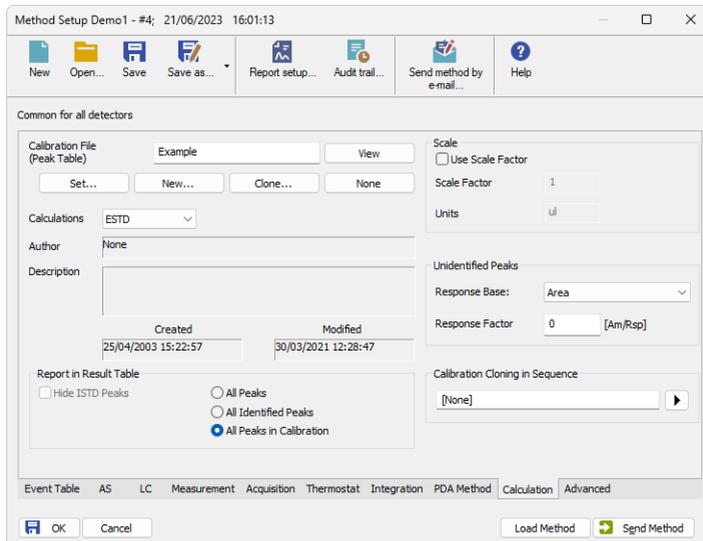


Fig. 81: Method Setup - Calculation

Calibration File (Peak Table)

Specifies the calibration file to be used when evaluating chromatograms measured with this method. Chromatograms will be automatically calibrated using the selected file.

Note: If the calibration file or method is located outside the default project structure, **Clarity** stores the file path as absolute. When such files are moved or copied, the path may no longer be valid and must be manually updated.

The section includes the following buttons:

View

Opens the calibration file in the [Calibration](#) window. As the *Method Setup* is a modal window, the *Calibration* window opens beneath it. To access it fully, you need to close the *Method Setup* dialog first.

Set...

Assigns an existing calibration file to the method.

New...

Creates a new empty calibration file and opens the *Save As* dialog to specify its name and location.

Clone...

Creates a copy of the current calibration file using the *Save As* dialog. The cloned file is then linked to the method. If you want to keep only *Compound Names* and *Retention Times* (without *Responses*), check the *Clear Responses* option in the *Save As* dialog.

None

Removes the calibration file from the method and switches the calculation type to Uncal (uncalibrated).

Calculations

Selects the calculation type:

Uncal

Uncalibrated chromatogram, no calibration file is used. The result is a percentage share of the individual peaks 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 the *Sample Amount* is not filled in. 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. It calculates compound amounts in the unknown sample by extrapolating the calibration curve to the point where $Y = 0$. Results are displayed as absolute values.

To use standard addition correctly, first set the name of the cloned calibration file in the *Calibration Cloning in Sequence* section. Then, in the [Sequence Options](#), in *Calibration and Sequence Usage* section select the *Standard Addition Measurement* option.

Details of Calibration file

Author

Name of the user who created the calibration.

Description

Informative description of the calibration.

Created

Date of the calibration file creation. When copying or moving a calibration file, the *Created* field contains the date of this copy or move operation.

Modified

Date of the last modification.

Report in Result Table

Specifies which peaks should be displayed in the [Result Table](#) when a calibration is used. If the *Calculations* setting is set to *Uncal*, this section will be inactive (grayed out).

Hide ISTD Peaks

Hides peaks identified as internal standards from the Result Table.

All Peaks

Displays all integrated peaks found in the chromatogram.

All Identified Peaks

Displays only the peaks that were identified based on the calibration file.

All Peaks in Calibration

Displays all peaks from the calibration file, regardless of which peaks are found in the chromatogram. This creates a fixed table format based on the number of calibrated compounds.

Scale

Provides parameters for scaling calculated results. If the *Calculations* setting is set to *Uncal*, this section will be inactive (grayed out).

Use Scale Factor

Enables the use of the *Scale Factor* and *Units* fields.

Scale Factor

Multiplies all values in the *Amount* column in the *Result Table* by the specified factor.

Units After Scaling

Replaces the original amount units from the calibration file with the defined units in the *Result Table*.

Unidentified Peaks

Defines how to treat unidentified peaks. If the *Calculations* setting is set to *Uncal*, this section will be inactive (grayed out).

Response Base

Selects whether to use Area or Height as the base for response.

Response Factor

Multiplies the selected response base to estimate the *Amount* of unidentified peaks. This effectively acts as a single-point calibration.

Calibration Cloning in Sequence

Sets the name for the cloned calibration file created during a sequence. This feature is used with the *Standard Addition measurement*, during *Calibration Bracketing*, or when the *Clone on first recalibration (safe calibration usage)* option is enabled in [Sequence Options](#).

You can enter any text as the name of the target calibration file. However, it is recommended to use variables (accessible via the arrow button next to the field) to ensure that each cloned calibration gets a unique and meaningful name. For details on available variables, see the [Chromatogram File Name](#) chapter.

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.

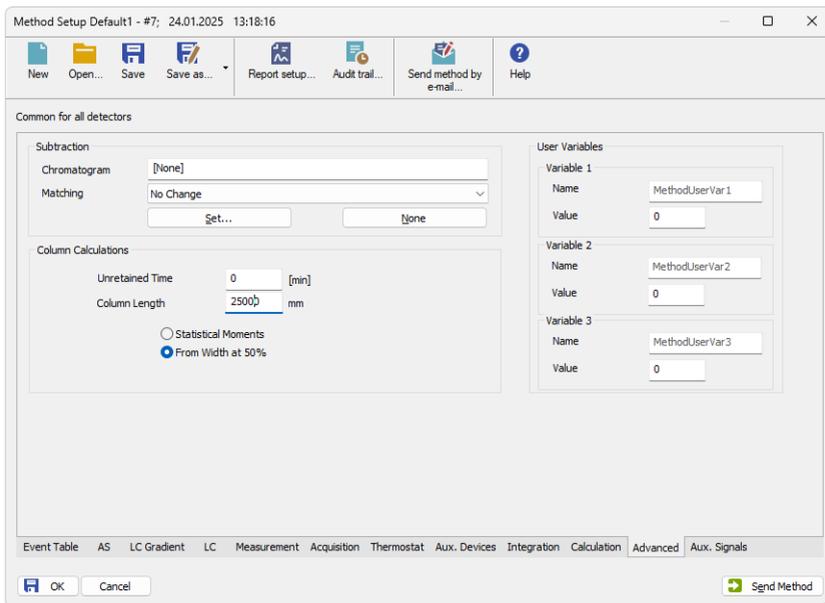


Fig. 82: Method Setup - Advanced

Subtraction

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

The subtracted chromatogram has to be always present in the defined path. The change in the subtracted chromatogram influences the resulted subtraction in the current chromatogram.

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: In the [Data Acquisition](#) window, the subtracted chromatogram may be displayed during a measurement in the background as a grey chromatogram. To display the chromatogram in the background without automatic subtraction (e.g., the solvent) use the *File - Set Background Chromatogram...* command.

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 - “Offsets” the measured chromatogram with the subtraction chromatogram by shifting it on the axis X (time axis) before the actual subtracting.

Scale Subtraction Chromatogram - “Scales” the measured chromatogram before subtracting by scaling the subtraction chromatogram on the time axis.

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.

Set...

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

None

Cancels subtraction of the chromatogram.

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.

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 Aux. Signals ✓ Full version

Sets the auxiliary signals storing and possible display. The tab is present only when the Auxiliary signals are available, and is common to all signals while performing multidetector measurement.

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

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.

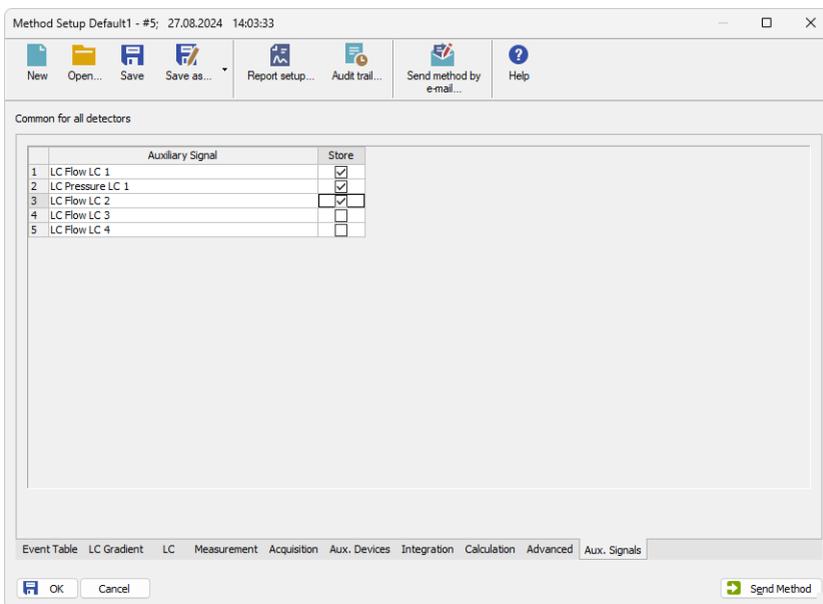


Fig. 83: Method Setup - Aux. Signals

Auxiliary signal

List of available auxiliary signals.

Store

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

2.3.8 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.

2.3.8.1 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. 84: 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. 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.

2.3.8.1.1 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.

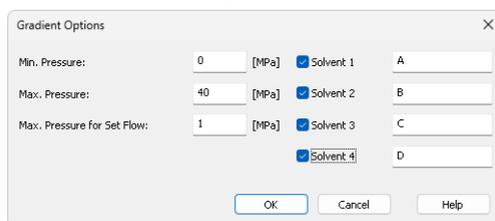


Fig. 85: Gradient Options

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 128.

Solvent 1 (..4)

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

2.3.9 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:

| Icon | Command | Description |
|---|---|--|
|  | Single... | Opens the <i>Single Analysis</i> dialog, allowing users to prepare and perform a single analysis. |
|  | Sequence | Opens the <i>Sequence</i> window, allowing users to prepare and measure a series of analyses. |
|  | Batch... <small>✓ Full version</small> | Opens the <i>Batch</i> dialog, allowing users to reprocess previously performed analyses. |
|  | Data Acquisition | Opens the <i>Data Acquisition</i> window, displaying the signals of connected detectors. |
|  | Device Monitor | Opens the <i>Device Monitor</i> window, allowing users to monitor the status of the connected devices. |

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" below
- "Single Analysis - Post-run Options" on page 114
- "Single Analysis - User Variables" on page 117

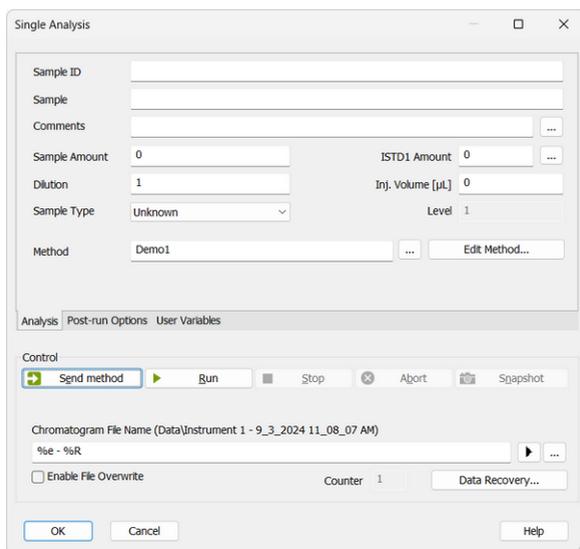


Fig. 86: Single Analysis - Analysis tab

Note: The *Analysis* tab can contain different items based on used Extensions (such as **GPC** or **EA**), refer to the corresponding manual for their description.

Analysis

Comprises the description and parameters of single analysis. All entered values are transferred to the chromatogram header during chromatogram creation.

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. 118).

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. 118).

Comments

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

Sample Amount

The value is used in calculations of individual components percentage. For samples with *ISTD*, enter the sample amount without the *ISTD* amount. 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

The 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

Specifies the dilution factor of the sample, representing the total volume of the solute and solvent combined. Each calibrated amount in the *Amount* column of the *Result Table* is multiplied by this value. The default value is 1.

Inj. Volume

The 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. 20.).

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 - specifies the calibration standard. Samples marked as *Standard* can have the calibration level filled in the *Lvl* field. Chromatograms marked as calibration standards in the time of creation will be stored in the CALIB subdirectory instead of the DATA subdirectory. If the *Lvl* is filled, calibration (or recalibration) of the calibration file specified in the method is performed.

Blank - in fact a calibration standard with no amount of added sample. Calibration file needs to be specified 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. Calibration file needs to be specified in the method on the [Calculation tab](#).

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 selected in the *Method* field to the device(s).

Note: The *Send Method* button is visible only when the detector is configured on the Instrument.

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 which does not exist, for example *%B_%Y%e - %R\%e - %R*, then the confirmation dialog about creating the directory will be displayed. When *No* is selected, the measurement is not started. You can then change or correct the file name and press *Run* again.

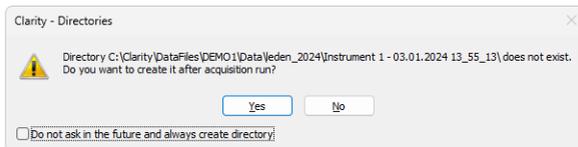


Fig. 87: Clarity - Directories dialog when the subdirectory does not exist

Stop

Terminates the running analysis and processes the results - a chromatogram is created with the name entered in the *Chromatogram File Name* field. Followed by post-run events as specified by items from the "Single Analysis - Post-run Options" on page 114 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 compose the title of the file by selecting the required variables (for more details see the chapter **Chromatogram File Name** on pg. 118).

It is also possible to include 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 recommended 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.

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...

Allows recovering 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 available.

Invoking the command opens the *Rescue Data* dialog where you select from the **LAST.RAW* and **RUN.RAW* files. If no raw file is available, the items are disabled.

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

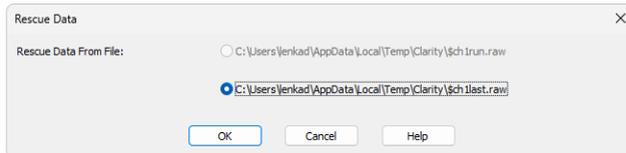


Fig. 88: Rescue Data

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\

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

During the analysis data is saved to the raw file periodically. Frequency of these updates varies based on the detector frequency, it is generally done once per 10-90 seconds (e.g., 20 seconds for detector set to 50 Hz). If a failure occurs before the first data packet is saved to the raw file (soon after analysis start) it only contains the header, trying to recover such file will result in an error.

2.4.1.1 Single Analysis - Post-run Options

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

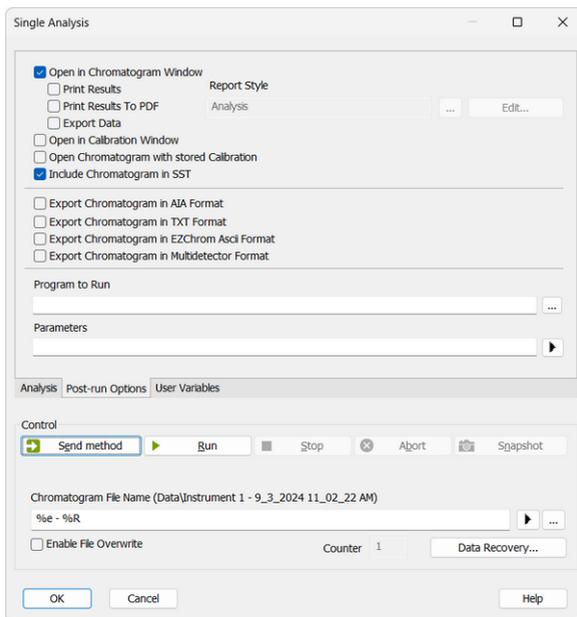


Fig. 89: Single Analysis - Post-run Options

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. 135).

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. 175).

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. 175).

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 the *File - Export Chromatogram* command in the [Chromatogram](#) window (for more details see also chapter **Export Chromatogram** on pg. 175).

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. 175).

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.

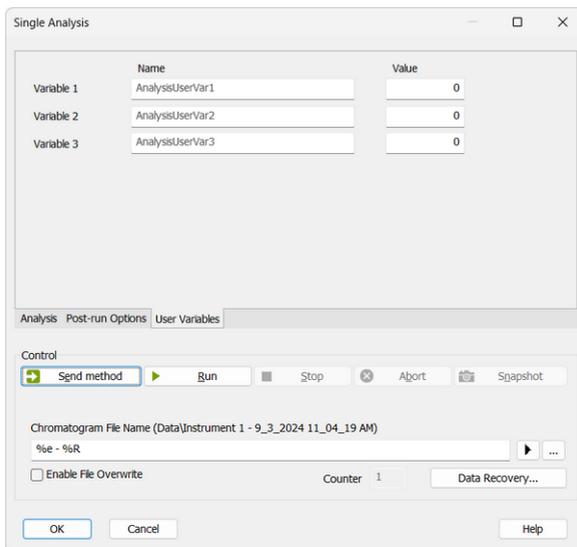


Fig. 90: Single Analysis - User Variables

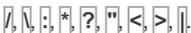
Name

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 users to enter and format text using standard text processing functions, such as bold, italics, underline, text alignment, text color, font selection, text size, and bullet points.

A comment can be assigned to each sequence row or single analysis measurement. It is accessible before the analysis from [Single Analysis](#) (using the  button) or Sequence dialog (using  icon), or after the analysis has ended in the [Measurement Conditions - Instrument](#) tab of the *Chromatogram* window.

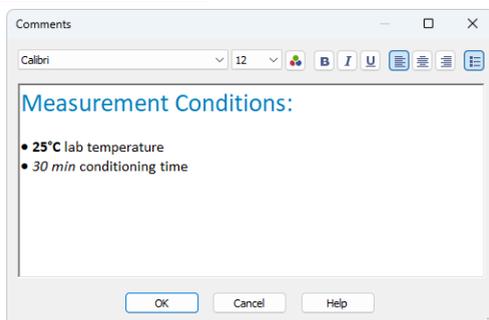


Fig. 91: Comments dialog

2.4.2 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.

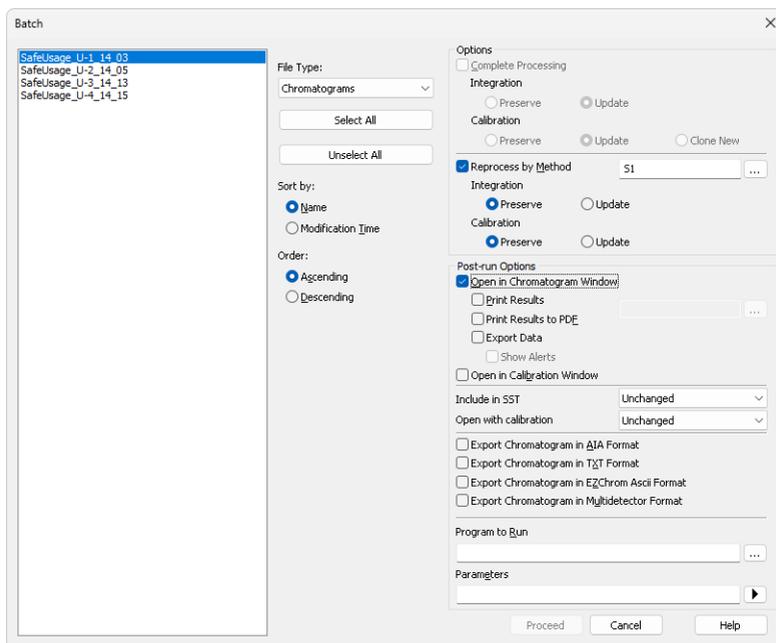


Fig. 92: Batch

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 *Post-run Options*) 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 the particular sequence row during the reprocessing.

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 actions 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. 135).

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. 175).

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. 175).

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. 175).

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. 175).

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.

2.4.3 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.

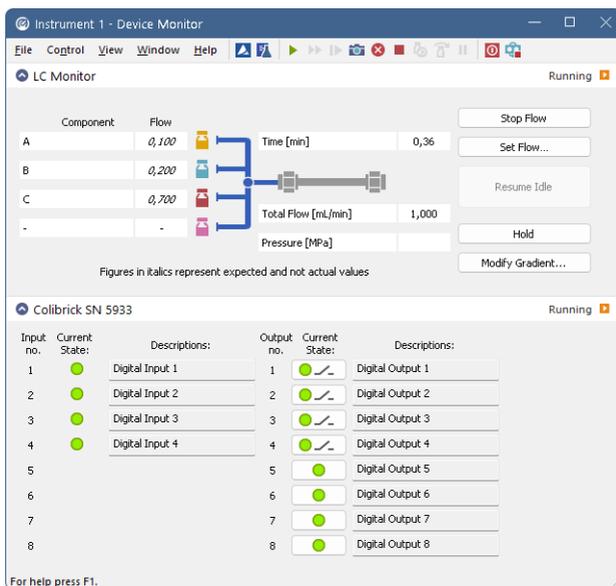


Fig. 93: Device Monitor

Menu

[File](#) Submenu for controlling the *Device Monitor* window.

[Control](#) Submenu for controlling the device.

[View](#) Submenu of commands for setting up the appearance of the *Device Monitor* 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. 108. and the chapter "**Sequence**" on pg. 382.). 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.

LC Monitor

LC Monitor appears on any LC Instrument where directly controlled pumps are configured in the [System Configuration](#) dialog. It is common for all pumps from all vendors in basic functionality, but particular pumps may differ in options that can be performed with them.

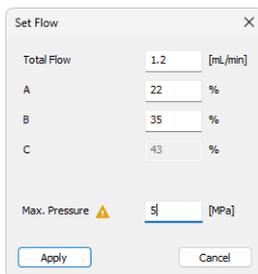
The LC Monitor contains a solvent-mixing diagram, fields for following the actual analysis time, flow and pressure and also a set of buttons for direct control of the gradient composition.

Stop Flow

The pumps can be stopped from this window using the *Stop Flow* button. This action will stop the pump only, the analysis run will continue and must be stopped or aborted from the [Data Acquisition](#) window or [Single Analysis](#) dialog.

Set Flow...

After pressing the *Set Flow...* button the *Set Flow* dialog emerges. This dialog is the same for all LC control modules and allows to set the flow and composition of mobile phase. *Max. Pressure* allows to set a different pressure than set in the "Gradient Options" on page 105 of a given method. More details about this dialog can be seen in the appropriate control module help. Once a method is sent the value is set according to the method. It is usually used to purge systems, i.e. setting the flow and pressure while purge valve screw is open.



| Parameter | Value | Unit |
|---------------|-------|----------|
| Total Flow | 1.2 | [mL/min] |
| A | 22 | % |
| B | 35 | % |
| C | 43 | % |
| Max. Pressure | 5 | [MPa] |

Fig. 94: Set Flow

Resume Idle

Returns the pumps to *IDLE* state as defined in the appropriate field on the [LC Gradient](#) tab of the [Method Setup](#) dialog.

Hold / Resume

Pauses / resumes 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, which returns the method to the original **Gradient Table** again.

Note: Availability of this command depends on the capabilities of pumps used in the gradient. The command is only available during the analysis run.

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 this command depends on the capabilities of pumps used in the gradient. The command is only available while an analysis is running.

2.4.3.1 File

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

2.4.3.2 Control

Send Method Sends method, that is displayed in the [Single Analysis](#) dialog on the *Method* row, to controlled devices.

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 manual 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.

2.4.3.2.1 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.

2.4.3.3 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. 41).</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... - 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. |

2.4.3.4 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. 59). |

2.4.3.5 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 Settings

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 Options](#) 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.

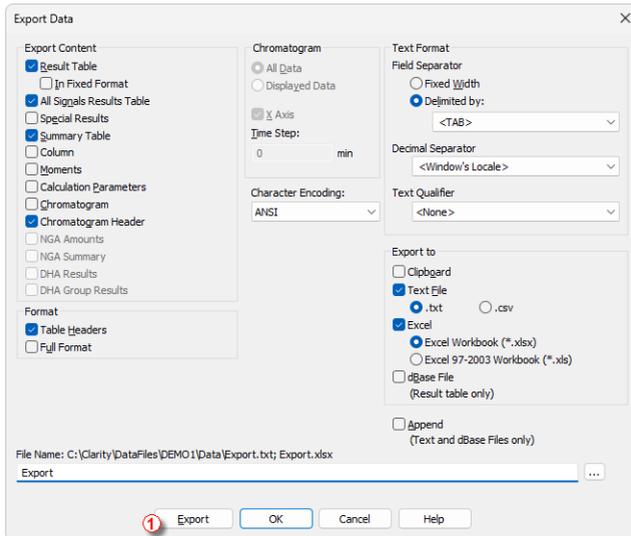


Fig. 96: Export Data

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. 175).

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.

Format

Determines the shape of each table - presence of headers or additional information.

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 the [Global Filter - 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.

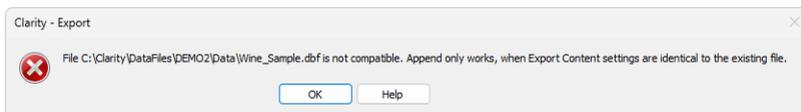


Fig. 97: File is not compatible

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.

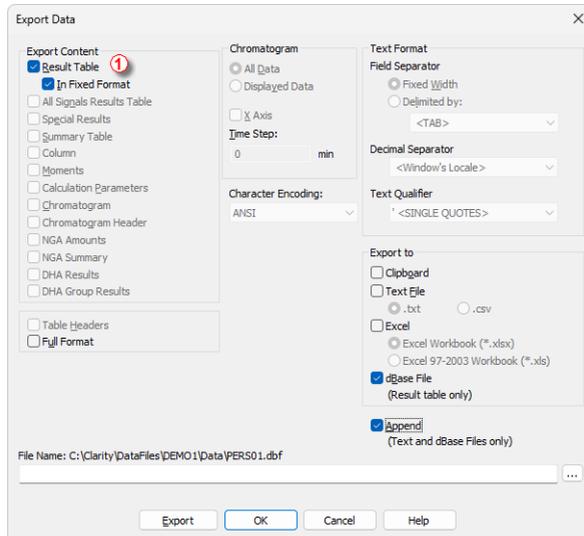


Fig. 98: Export Data - Export to dBase File

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. **142**. 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

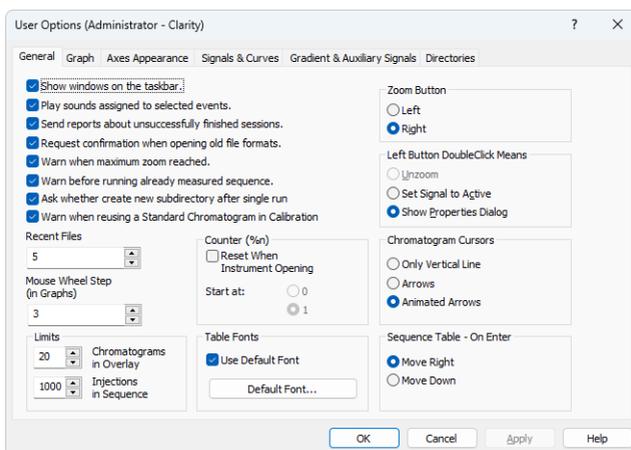


Fig. 100: User Options - General

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 (%)

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. 403).

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 graphs. This selection applies to all graphs when the local setting in the [Graph Properties - Graph](#) dialog has the *Use User Options* checkbox selected.

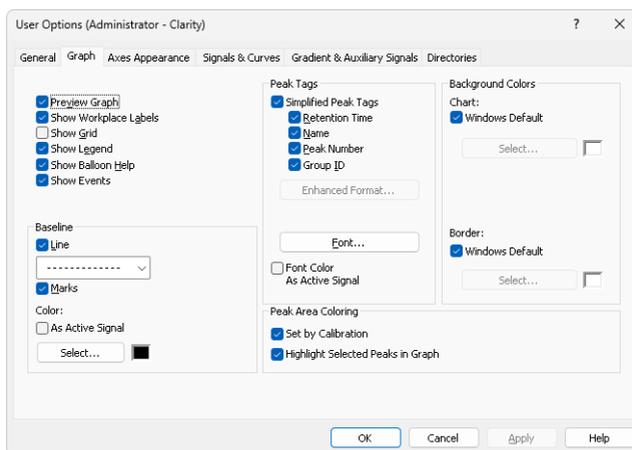


Fig. 101: User Options - Graph

Preview Graph

Shows/hides a preview graph.

Show Workplace Labels

Shows/hides labels and lines assigned to the *Workplace* using the *Create Label* command.

Show Grid

Shows/hides a grid for simplified graph reading.

Show Legend

Shows/hides a legend displaying signal names, their corresponding chromatogram names, and their colors in the graph.

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

Shows/hides visual representation of events from the [Event Table](#) tab of the [Method Setup](#) dialog.

Baseline

Line - Shows/hides the baseline.

Marks - Shows/hides marks of peak starts and ends.

Color

As Active Signal - Determines whether baseline color will be the same as the signal color. If not, it will be the color set by the *Select* button.

Select - Button for color selection.

Peak Tags

Allows to shows or hide peak tags or set enhanced format of tags.

Simplified Peak 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 belongs.

Enhanced Format...

Displays the [Peak Tags Format](#) dialog which allows to set custom format of peak tags. Available only if the *Simplified Peak Tags* checkbox is unchecked. By default the format is empty, so when *Simplified Peak Tags* are unchecked and user does not set the enhanced format, no tags are displayed.

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 active signal 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 - When checked, selecting a peak in either the chromatogram graph or the *Result Table* (including the *All Signals Result Table*) highlights it in both places. When unchecked, the peak is highlighted only in the tables, not in the 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 **Windows OS** 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**.

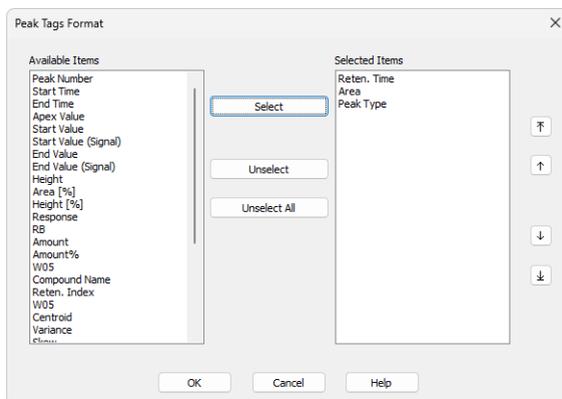


Fig. 102: Peak tags format dialog

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

Sets appearance options for the graph axes.

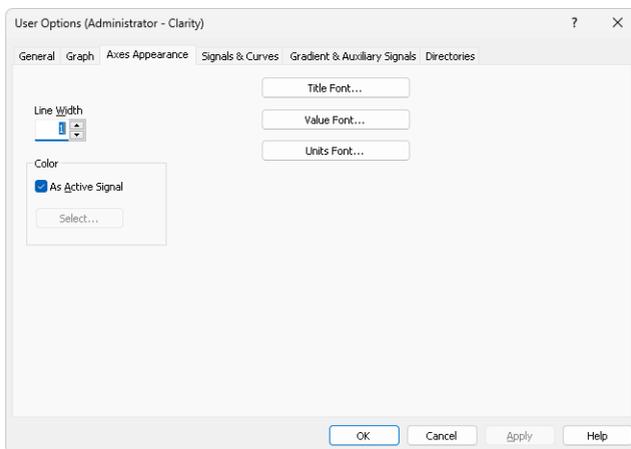


Fig. 103: User Options - Axes Appearance

Line Width - Axis width in pixels. Enter value between 1 and 10.

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 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.

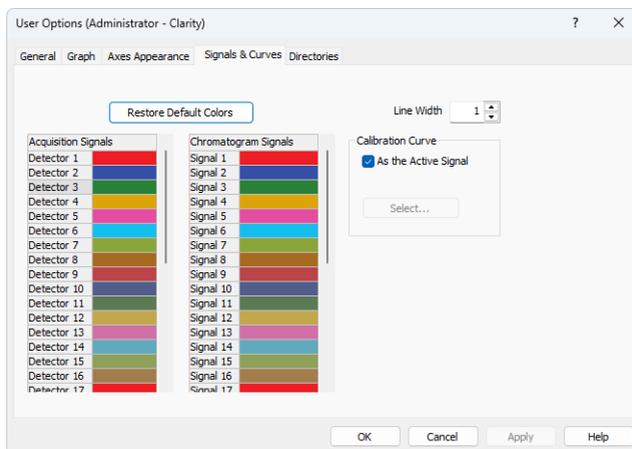


Fig. 104: User Options - Signals & Curves

Line Width

Selects the default curve width.

Restore Default Colors

Resets colors to default ones.

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

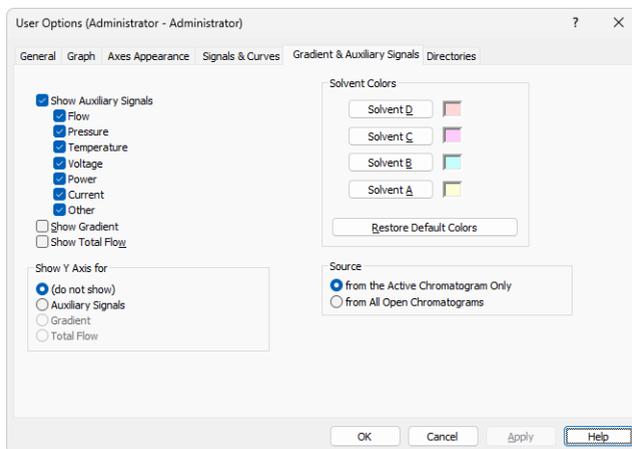


Fig. 105: User Options - Auxiliary Signals

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

Shows/hides auxiliary signals and activates the possibility to select the Auxiliary Signals axis as the right Y axis. Each auxiliary signal is included in one of the following categories: *Flow, Pressure, Temperature, Voltage, Power, Current* and *Other*.

Show Gradient

Shows/hides gradient in the graph and activates the possibility to select the gradient as the right Y axis.

Show Total Flow

Shows/hides the total flow line and activates the possibility to select the total flow as right 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 [Units Setup](#) dialog accessible from the [System Configuration](#) dialog.

Solvent Colors

Selects colors for the display of individual gradient components.

Restore Default Colors

Resets 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

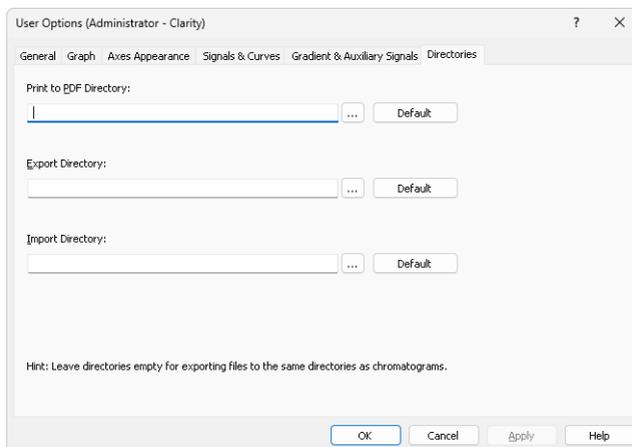


Fig. 106: User Options - Directories

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. |
|  | Show All | Displays all hidden windows. |
|  <small>✓ Full version</small> | Main | Displays the main Clarity window described on pg. 1 . |
|  | Chromatogram | Displays the Chromatogram window described on pg. 156 . |
|  | Calibration | Displays the Calibration window described on pg. 313 . |
|  | Single Analysis | Displays the Single Analysis dialog described on pg. 108 . |
|  | Sequence | Displays the Sequence window described on pg. 382 . |
|  <small>✓ Full version</small> | Station Audit Trail | Displays the Audit Trail window described on pg. 414 . |
|  | Data Acquisition | Displays the Data Acquisition window for online monitoring of a signal from detector(s) described on pg. 366 . |

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 Options" on page 114 or alternatively "Sequence" on page 382.

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. 289 . |
| Default | the chapter " All Signals Result Table " on pg. 297 . |
| Default | the chapter " Summary Table " on pg. 299 . |
| Default | the chapter " Performance Table " on pg. 302 . |
| Default | the chapter " Integration " on pg. 277 . |
| Default | the chapter " Measurement " on pg. 283 . |
| SST Extension | See SST Manual - M020 |
| <i>Note:</i> Extension appears only with purchased Extension license. | |

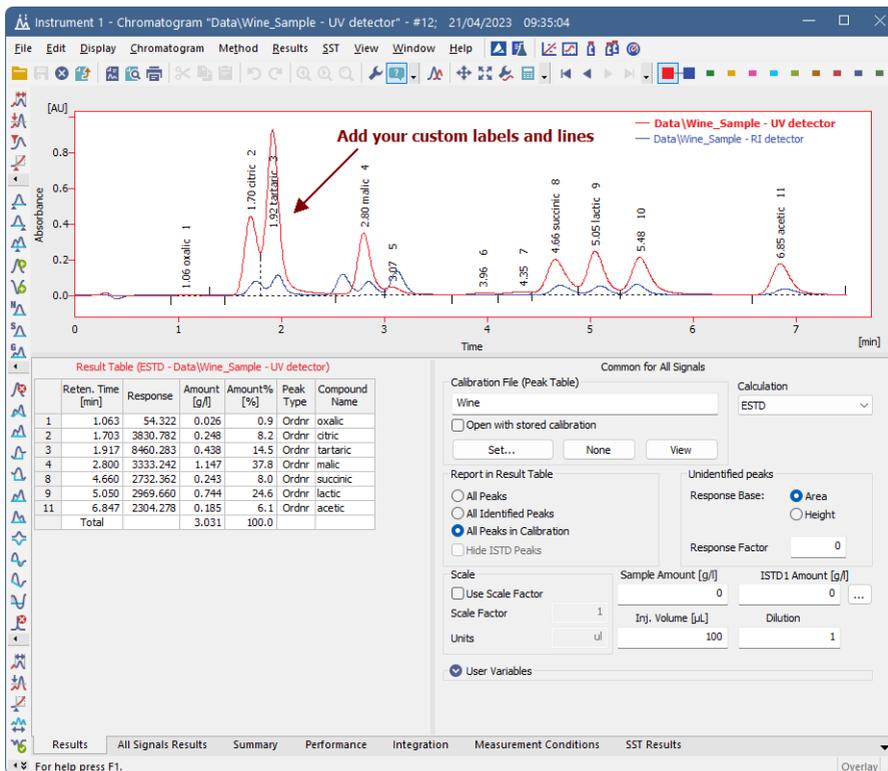


Fig. 107: Chromatogram

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.

| Icon | Command | Description |
|---|---|--|
|  | 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 <i>Project</i> or from the selection made using <i>Browse Selected Chromatograms</i> in <i>Open Chromatogram</i> dialog. In <i>Overlay</i> mode, it browses through currently opened 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 in the header. |
| | Close All | Closes all opened 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 in the header. |
|  | Save | Saves the active chromatogram (Ctrl + S). |
|  | Save As... | Saves active chromatogram under selected name (Ctrl + Shift + S). For existing filenames, message box about file overwriting pops up. |
| | Send Chromatogram by Email | Creates a new email in the default email client with the currently displayed chromatogram attached. In <i>Overlay</i> mode, all displayed chromatograms will be included as attachments in the email. |
| | Import Chromatogram... | Imports chromatograms in the text, AIA or EZChrom ASCII format. |
| | Export | Initial submenu for the following Export commands: |

| Icon | Command | Description |
|---|--|--|
| | Export Data... | Exports results and data of the active chromatogram. After selection, the <i>Export Data</i> dialog will be displayed. By using the Ctrl + E shortcut it is possible to export the data without opening the <i>Export Data</i> dialog. |
| | Export Chromatogram... | Exports chromatographic curve into AIA, text or EZChrom ASCII format. |
| | Export Summary Table... | 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. Individual items of the summary table are divided in the file by a tabulator. Chromatograms containing unsaved modifications will be saved before exporting. Export is logged in the Audit Trail . |
| | Export as Picture to Clipboard | Copies currently displayed chromatogram into clipboard as a vector picture. |
| | 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...  | Displays Sign dialog to electronically signs the active chromatogram. |
| | Verify...  | Displays Verify dialog for verification of electronic signatures of active chromatogram. |
|  | Report Setup... | Selects print configuration (Ctrl + Alt + P). After selection, the <i>Report Setup</i> dialog will be displayed. |
|  | Print Preview | Previews selected print configuration before printing (Ctrl + Shift + P). After selection, the <i>Print Preview</i> dialog 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. |

| Icon | Command | Description |
|---|------------------------------------|--|
|  | Print... | Command for selecting printer and actual printing (Ctrl + P). After selection, the Print dialog described on pg. 456. 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 Post-run Actions... | Command for performing the post-run operations from the Chromatogram window. After selection, the Post-run Options (From Chromatogram Window) dialog 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. The number of files shown is determined by the <i>Recent Files</i> setting in the General tab of the <i>User Options</i> dialog. |
| | 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 in the header. |

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.

When closing multiple chromatograms at once, where some of them are modified, changes can be saved or discarded for all of them by one click using *Yes for All/No for All* buttons. If not used, message will be displayed for every modified chromatogram.

Note: *Yes for All/No for All* buttons are present even when only one of the multiple chromatograms is modified. In such case there is effectively no difference between *Yes* and *Yes for All* buttons (similarly for *No* buttons).

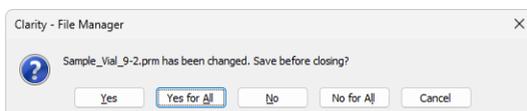


Fig. 108: Saving changes to all chromatograms that are being closed

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  and CALIB folder  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](#).

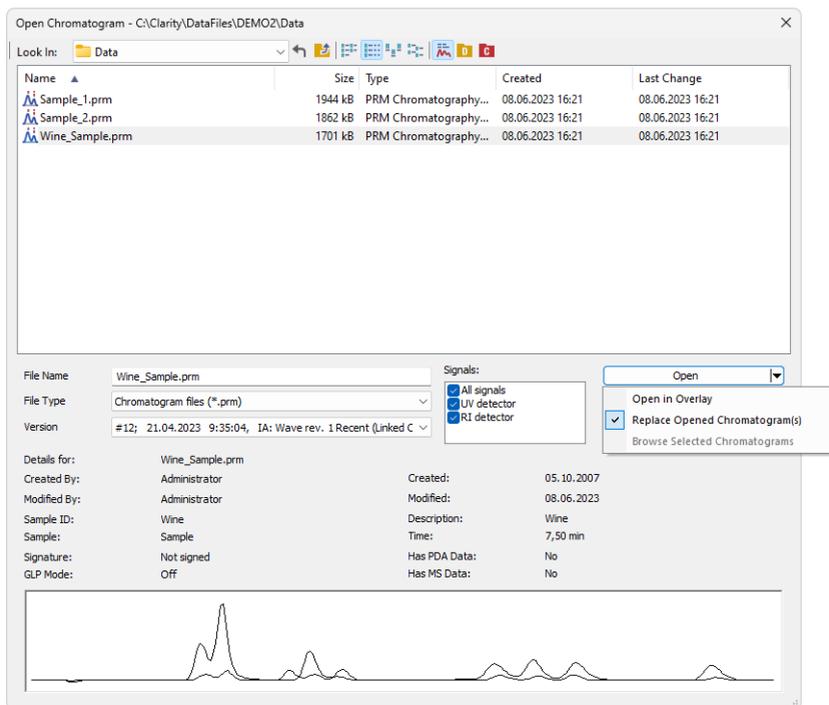


Fig. 109: Open Chromatogram

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)

The default opening selection is governed by *Open with stored calibration* option on [Results](#) tab of [Chromatogram](#) window. When unchecked chromatogram is opened 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.

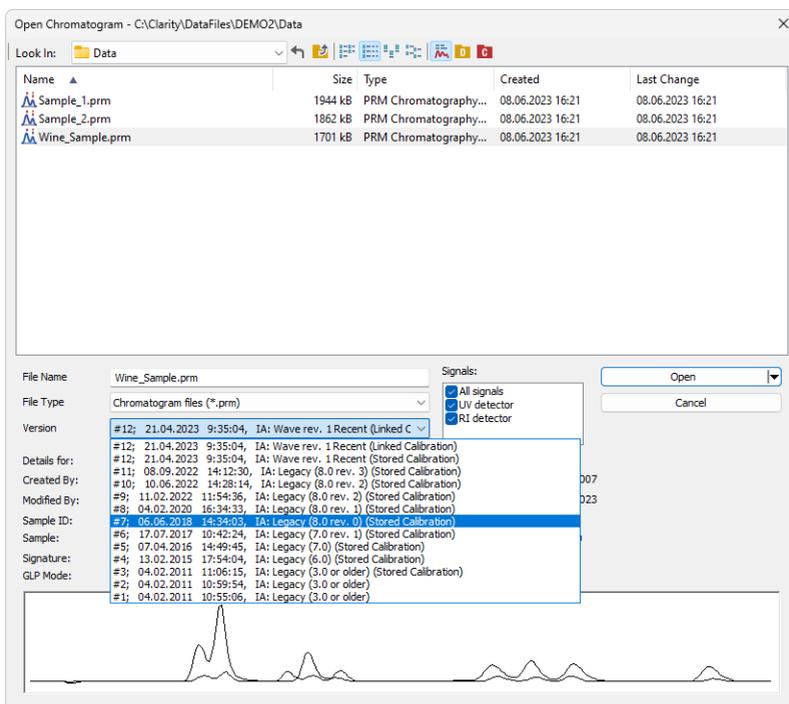


Fig. 110: Open Chromatogram with Stored Calibration

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 and name of user who made the last modification, Sample ID and Sample, if there is signature present, information about GLP Mode, date of creation and last modification, duration of the analysis, presence of PDA or MS data, 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 overlaid files (Ctrl + F7) |
|  Previous | Opens the previous chromatogram from current folder or currently selected chromatograms or currently overlaid files (F7) |
|  Next | Opens the next chromatogram from current folder or currently selected chromatograms or currently overlaid files (F8) |
|  Last | Opens the last chromatogram from current folder or currently selected chromatograms or currently overlaid 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.

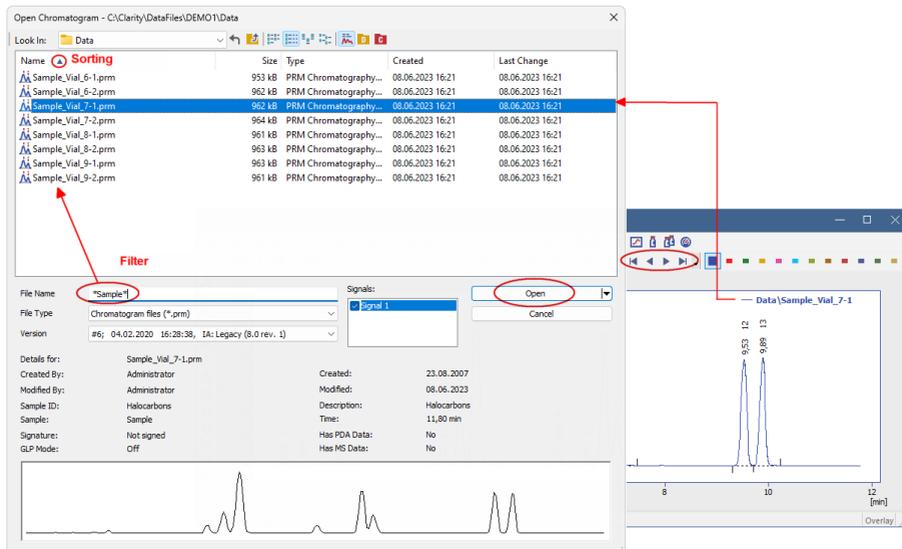


Fig. 111: Browse Through Chromatograms

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).

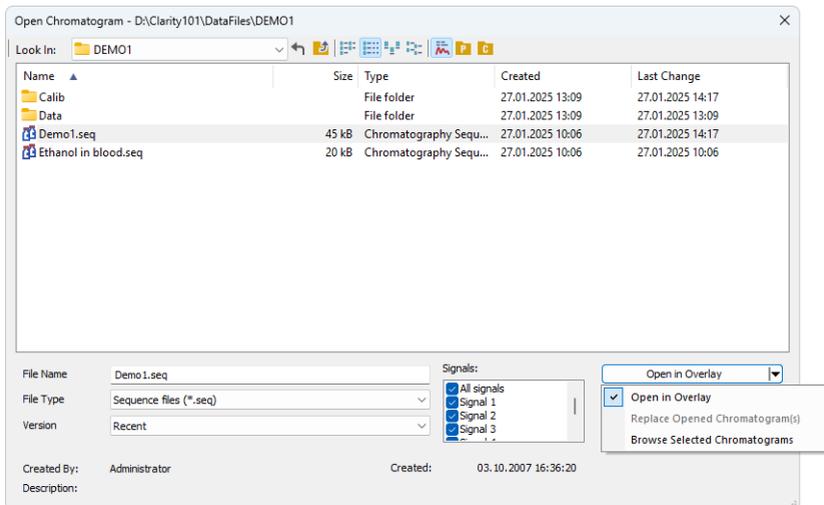
3.1.4 Open Chromatogram from Sequence

Opens chromatograms measured in one sequence.

Using the command invokes the *Open* dialog. In the dialog, select the sequence file, and typically all chromatograms measured in this sequence will be opened.

In the case the *Reset* sequence command was used, only chromatograms measured after the last reset will be opened.

In the case number of chromatograms measured in the selected sequence is bigger than the *Chromatograms in Overlay Limit* set in the [User Options](#) dialog, only a limited number of chromatograms will be opened.



Note: This command is particularly suitable for a fast evaluation of a series of chromatograms in the summary table.

File Name

This field contains the name of the selected file. The name can be entered directly or selected from the list of filenames.

File Type

This field contains the type of the selected file.

Version

In this combo-box it is possible to choose in what version you want to open chromatograms, and if the calibration file should be stored in chromatogram or linked.

Signals

In this section, it is possible to choose what signals of chromatograms should be shown and hidden after the opening.

Sequence Details

Additional information regarding the sequence file.

Opening Options

It is possible to open all of the chromatograms in *Overlay* together, or choose option *Browse Selected Chromatograms* to open them one-by-one.

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.

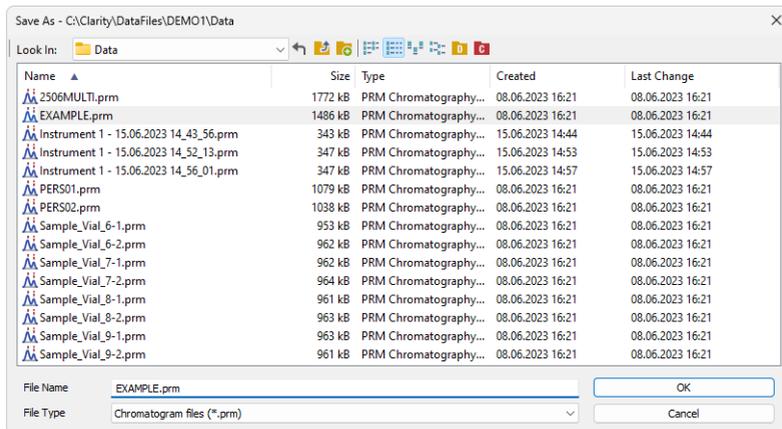


Fig. 112: Save As (Chromatogram)

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.

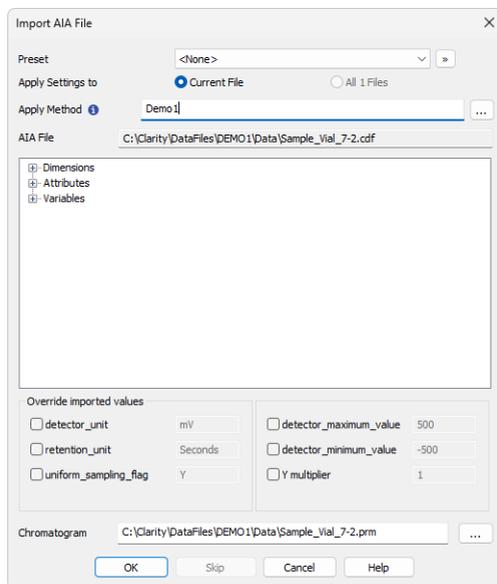


Fig. 113: Import AIA File

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 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** and the **EZChrom** softwares.

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.

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 *Removepresets*. Presets are stored as part of **Clarity** Desktop file.

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 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.

Import Text File

Preset: <None>

Apply Settings to: Current File All 1 Files Prefer Detected Settings

Apply Method: Demo 1

Current Text File: C:\Clarity\DataFiles\DEMO1\Data\Sample_Vial_7-2.txt

Import From Line: [] Import To Line: []

Separator: <TAB> Decimal Separator: <Window's Locale>

Analyst: Administrator

Sample ID: Halocarbons

Sample: Sample

Sample Date: 8/31/2004

Sample Amount: 0

Dilution: 1

ISTD Amount: 2

Injection Volume: 1

Imported Data: Time + Signal + Time + Signal...

Number of Detectors: 1

| 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 | 7080 |

Save as Chromatogram: C:\Clarity\DataFiles\DEMO1\Data\Sample_Vial_7 ... Load Defaults

OK Skip Cancel Help

Fig. 114: Import Text File

Analyst, Sample ID, Sample, Sample Date, Sample 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. 108.

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.

Signal Name

Sets the signal name for further display.

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 our A/D converter or enter your own value.

Signal Units

Determines the units in which the signal values are stated. Entered unit must match the unit which is used in imported file.

Autoscale

Sets the possibility to automatically scale the signal units in graphs.

Signal Axis Name

Sets the identification of the Y axis.

Time Units

Determines the units in which time values are stated.

Possible values are: *ms* - milliseconds, *s* - seconds, *min* - minutes. 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. 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.

To select another name 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 you can get the number of the line selected. 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.

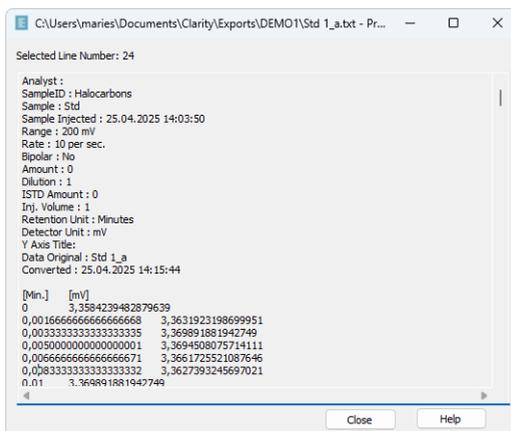


Fig. 115: Import Preview

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. 66.). 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.

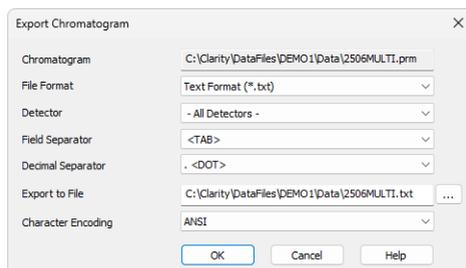


Fig. 116: *Export Chromatogram*

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

This command allows you to apply an electronic signature to the current version of the chromatogram. After selection, the *Sign* dialog will be displayed, where you can choose to sign the chromatogram either as a Clarity user or using a digital certificate. You can also specify a reason for the signature.

After a chromatogram which is opened with a linked calibration is signed the option *Open with stored calibration* on [Results](#) tab is checked automatically to ensure consistency of displayed results. However, if the chromatogram is already opened with a stored calibration the option is not automatically checked. This prevents creation of a new potentially unwanted 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 is READ-ONLY mode e.g., as a result of opening historical chromatogram version or not having rights to edit it.

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. Default certificate is preselected according to setting in the [User Accounts](#) dialog. It's possible to select different certificate by using the *Select Certificate* command. User name according to *Choose User* field is still displayed in the final signature alongside the used certificate when using this option.

The image shows a 'Sign' dialog box with the following elements:

- Title:** Sign
- Choose User:** Analyst John (dropdown menu)
- User Description:** (empty text box)
- Sign As Current User:** (selected radio button)
- Sign Using Certificate:** (unselected radio button)
- Analyst John:** (text box)
- Purpose of Signature:** authorship (dropdown menu)
- Time Stamp:** 16.06.2023 14:03:38 (text box)
- Password:** ***** (text box)
- Buttons:** Select Certificate..., OK, Cancel

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*.

3.1.9 Verify

Opens *Verify Signatures* dialog that displays a list of the active chromatogram's electronic signatures.

The list contains all existing signatures for all existing versions of given chromatogram. Each version of chromatogram may be signed several times, in such case signatures are ordered from the oldest to the most recent one.

Each signature is represented in the list by the name and description of the user who authorized the signature, name of the used certificate (if used) and the purpose of signature.

Icon before each signature differs based on whether it is a signature done as a user  or using a certificate . When at least one of the signatures for given chromatogram version has been done using certificate the icon for the entire version is changed to the certificate icon. If there is a problem with the signature the icons are amended by  or  symbol depending on the severity of the issue.

Caution: Timestamps in the list correspond to the time when chromatogram was saved NOT to the time of a signature. Such info can be viewed in the *Signature Details* dialog.

Current State

Displays signature for opened version of the active chromatogram. Number after "#" symbol corresponds to the chromatograms version. Time stamp corresponds to the time when given version was saved. If the current version does not have signature, *Not signed* is displayed.

- When current state of chromatogram is modified, the time stamp is replaced by *MODIFIED* text. Such state is always reported as *Not Signed*.
- When chromatogram is opened with linked calibration text *Linked Calibration* is displayed behind the time stamp. Such state is always reported as *Not Signed*. To view signatures for this version, chromatogram must be opened with stored calibration.
- When historical version of chromatogram is opened text *Chromatogram is not opened in the latest version* is displayed behind the time stamp. This only has an informational values, there is no difference in how the individual signatures are displayed compared to the latest version.

History of signatures

Contains list of all signatures for all versions (including the latest one). Versions that were not signed are not displayed. Versions are listed in descending order.

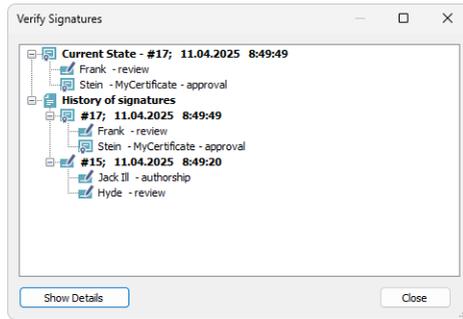


Fig. 118: Verify Signatures

Double-clicking on a signature or clicking on the *Show Details* button will display all details about the currently selected signature.

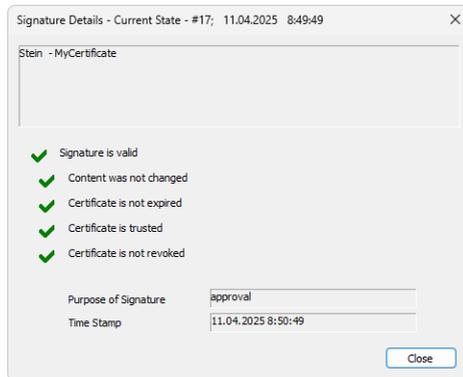


Fig. 119: Signature Details

Text field

Contains the user name and the description of the account that authorized the signature and the name of the certificate (if used).

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).

Certificate is not expired

Confirms that the certificate validity duration has not passed (only displayed for signature done using a certificate).

Certificate is trusted

Confirms that the certificate source is validated as trusted by Windows (only displayed for signature done using a certificate).

Certificate is not revoked

Confirms that the validity of certificate has not been revoked (only displayed for signature done using a certificate).

Purpose of signature

Displays the purpose of signature as filled in while signing.

Time Stamp

Displays the date and time of signature.

3.1.10 Post-run Options (From Chromatogram Window)

Post-processing of an already measured chromatogram. This dialog can be invoked using the *Perform Post-run Actions...* command from the *File* menu of the [Chromatogram](#) window. When prompted, the *Post-run Options (From Chromatogram Window)* opens, where the selected actions can be manually performed on the active chromatogram.

The same function can be executed by the  icon (hidden by default), as long as the *Post-run Options (From Chromatogram Window)* dialog is unset. When some actions are checked in the dialog, the  icon only performs the set actions, without opening the dialog.

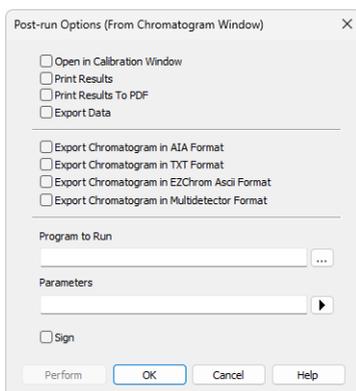


Fig. 120: Post-run Options (From Chromatogram Window)

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. 135).

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. 175).

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. 175).

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. 175).

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. 175).

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 post-run 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

A sub-menu of commands for working with clipboard and tables.



Undo

Cancels the last modification made in a field or table (**Ctrl** + **Z**). This can be used repeatedly as the station remembers all changes done in tables from the initial start-up. Each field and table maintains its own independent list of operations, so the *Undo* command will be performed according to the command history of the selected table.

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

Cancels the last *Undo* command in the *Integration table* (**Ctrl** + **Shift** + **Z**). This can be used repeatedly as the station remembers all changes done in tables from the initial start-up. Each table maintains its own independent list of operations, so the redo command will be performed according to the command history of the selected table.



Cut

Removes the selected text and stores it in clipboard (**Ctrl** + **X**).



Copy

Copies the selected text to clipboard (**Ctrl** + **C**).



Paste

Pastes the clipboard content to the selected field or table (**Ctrl** + **V**). If the table area is larger than the content, the copied content will fill all the selected cells. This can be used to fill multiple fields with identical content or with several periodically repeating fields.

Select All

Selects all fields of the 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...  Adds column as defined by the user.

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.

Delete User Column...  Deletes all user columns.

To delete only some of the user columns use the *Setup Columns...* command. In the [Setup Columns](#) dialog then delete the selected user columns using the *Delete* button.

Note: If you wish to remove a user column only temporarily, use the *Hide Column(s)* command (available from the local menu of the table or from the [Setup Columns](#) dialog).

Restore Default Columns...

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.

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 *Summary* 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 *Common* tab of the [Summary Columns Setup](#) dialog) loads the default set of visible columns.

Note: By contrast to the *Delete User Columns* 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 *Summary* 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 <i>Hide column(s)</i> 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:

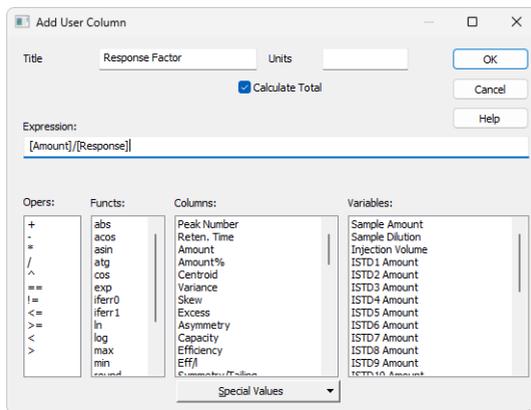
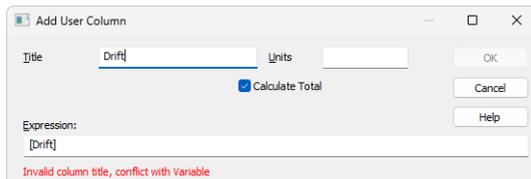


Fig. 121: Add User Column

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.

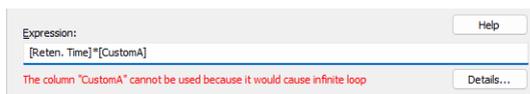
Calculate Total

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*, *Funcs*, *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. The first five operators (+, -, *, /, ^) denote operations of addition, subtraction, multiplication, division and power, while the remaining six operators (==, !=, <=, >=, <, >) are used for logical tests and return values of 0 (if not true) or 1 (if true) and can thus be used for complex calculations. It is only possible to evaluate numerical values, not text values such as *Compound Name*.

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. |
| iif | - Returns specified value when logical condition is true or not true. Syntax is iif(logical condition; value if true; value if not true) e.g., iff ([Reten. Time]<10;8;5) returns 8 when <i>Retention Time</i> is lower than 10 and returns 5 when it is higher (or equal to) than 10. |
| ln | - Natural logarithm |
| log | - Logarithm |
| max | - Maximum value of parameter of a function. E.g. MAX (1; 5; 3) returns value 5. |

| Function | Explanation |
|---------------|---|
| 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 | | |

Fig. 122: 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. |
| 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 columns of the tables in the *Calibration*, *Chromatogram*, and *Sequence* windows.

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.

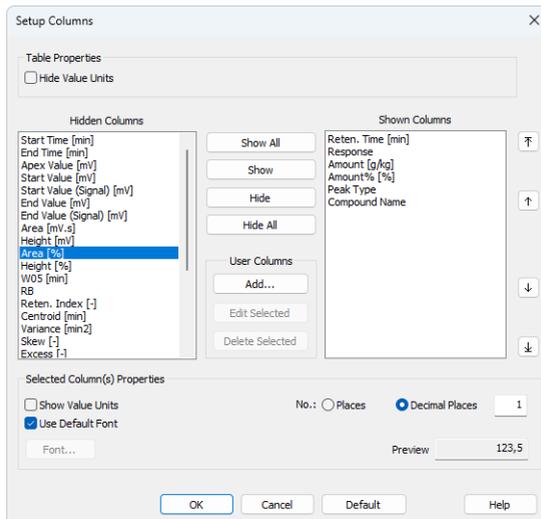


Fig. 123: Setup Columns

Table Properties

This section is not present in the dialog invoked from the *Sequence* window.

Hide Value Units

Hides value units in the cells in columns where they were previously shown by the *Show Value Units* checkbox in the *Selected Column(s) Properties* section.

Hidden Columns

Shows the list of all hidden columns.

Shown Columns

Shows the list of all displayed columns.

Show All

Displays all existing columns by transferring hidden columns from the left *Hidden Columns* list to the right *Shown Columns* list.

Show

Shows the selected hidden column(s) by transferring them from the left list to the right list. The displayed columns are added to the *Shown Columns* list in the fixed order, but may be moved forward/backward via the arrow icons on the right of the *Shown Columns* list.

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 ✓ Full version

This section is present only in the dialog invoked from the *Chromatogram* window.

Add...

Opens the [Add User Column](#) dialog (for more details see the chapter **Add User Column** on pg. 188). to add a new column with user-defined calculation.

Edit Selected

Modifies the selected user column.

Delete Selected

Deletes the selected user column.

Selected Column(s) Properties**Show Value Units**

Shows the values with units right in the cell for the selected column. This option is not present in the dialog invoked from the *Sequence* window.

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 *Settings - User Options...* command).

Font

Opens the *Font* dialog, which prescribes the font for the column selected.

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.

Custom Name

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. 382..

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. 186).

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*:

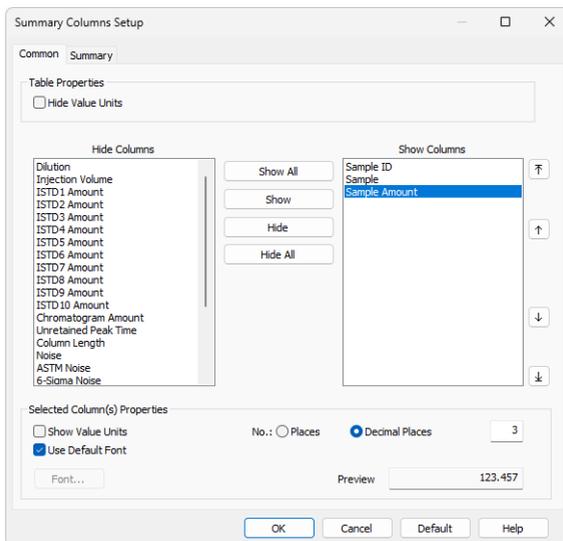


Fig. 124: Summary Columns Setup - Common

The *Common* tab in the *Summary Columns Setup* is used to customize the common columns for the chromatogram or signal.

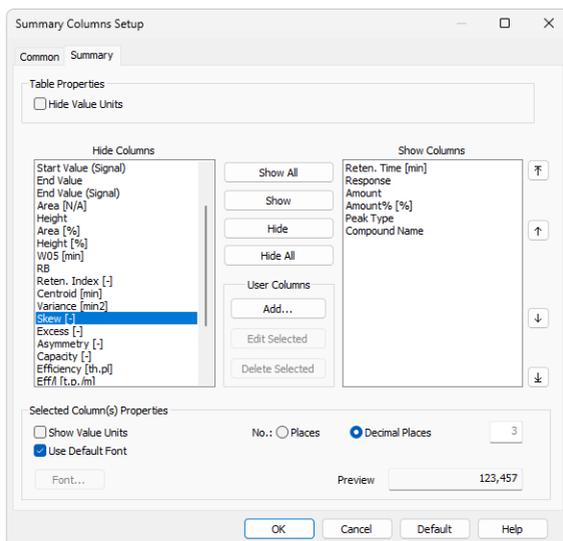


Fig. 125: Summary Columns Setup - Summary

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. 188). 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. 186). 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.

| Icon | Command | Description |
|---|--------------------------|--|
| | 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.

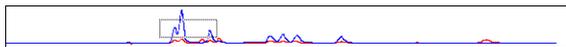


Fig. 126: Auxiliary Graph

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

Configures the appearance and behavior of graphs and chromatograms. After selection, the [Graph Properties](#) dialog will be opened. Some tabs in this dialog are the same as in User Options described in the chapter "[User Options...](#)" on pg. 142.. User Options apply to both the *Chromatogram* and the *Data Acquisition* windows. If *Use User Options* is checked, those settings apply to the chromatogram; otherwise, the settings in Graph Properties take effect.

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. 146.

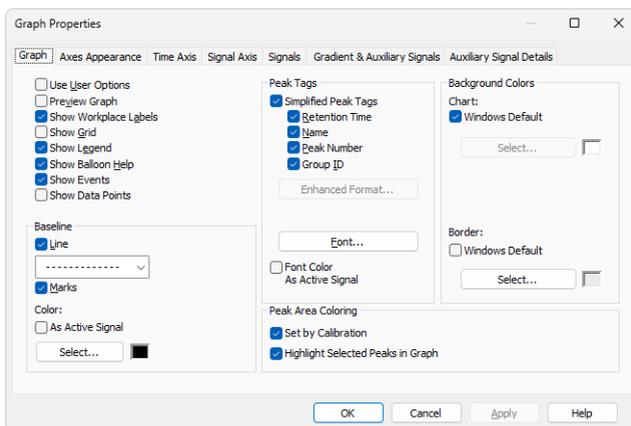


Fig. 127: Graph Properties - Graph

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 *Settings - User Options...* command).

Show Data Points

When checked, shows the individual data points in the graph. These data points may be inspected while zoomed in the investigated 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

Sets appearance options for the 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. 149.

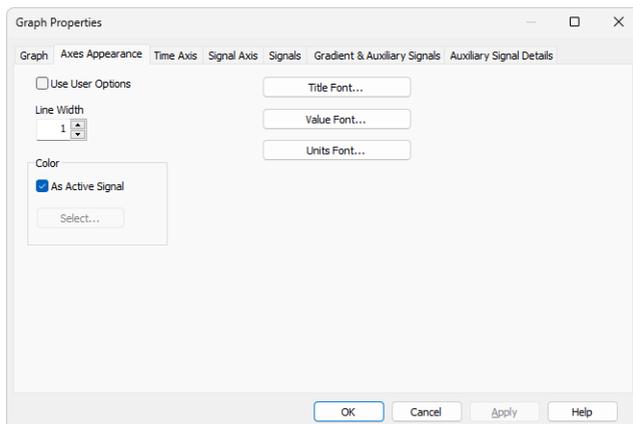


Fig. 128: Graph Properties - Axes Appearance

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 *Settings - User Options...* command).

3.3.2.3 Graph Properties - Time Axis tab

Sets the display scale and the time units on the horizontal axis of the graph.

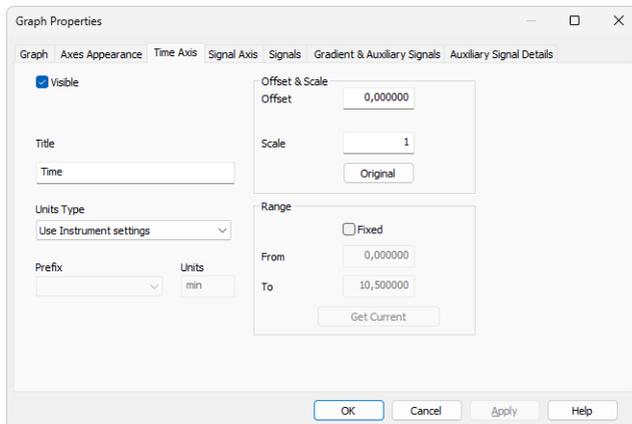


Fig. 129: Graph Properties - Time Axis

Visible

Shows/hides the 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 unit 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 length 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 display scale and signal 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.

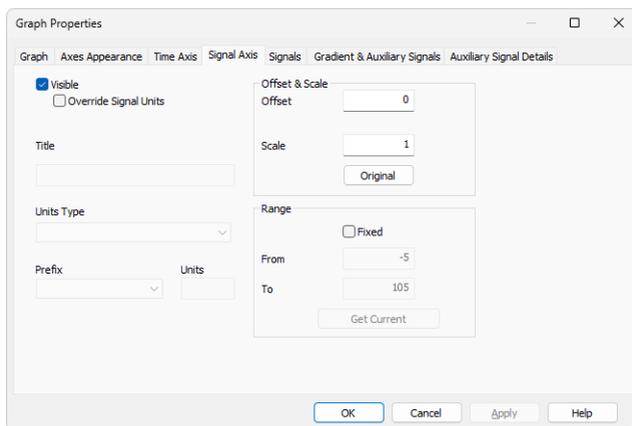


Fig. 130: Graph Properties - Signal Axis

Visible

Shows/hides 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

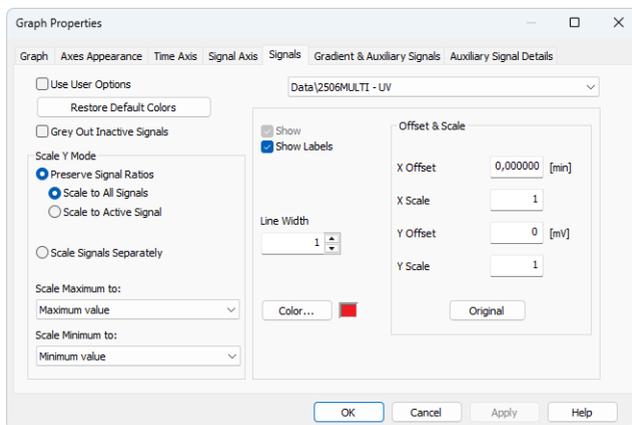


Fig. 131: Graph Properties - Signals tab

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).

Restore Default Colors

Sets colors back to the default ones. *Restore Default Colors* button is disabled when option *Use User Options* is checked.

Grey Out Inactive Signals

When checked, all signals from opened chromatograms except 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 signals. These 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 signal value.

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

Scales 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 signal selected in this field.

Show

Shows/hides selected signal. 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

Shows/hides labels and lines assigned to the *Active Signal* using the *Create Label* command. Labels assigned to the *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 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. **261**).

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.

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 tab lets you set the visibility of the particular Auxiliary Signals, as well as scale their signal axis.

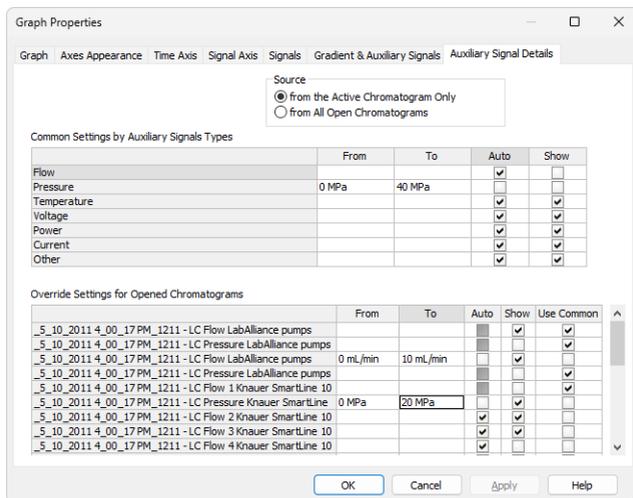


Fig. 132: Graph Properties - Auxiliary Signals

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

Shows/hides specific type of auxiliary signal and sets the auxiliary signal axis range for each type. When the *Auto* checkbox is checked, the range of the auxiliary signal axis starts at a minimum value and expands according to the auxiliary signal's course. While unchecked, the axis range is fixed on the values entered in the respective *From* and *To* columns. Checkbox *Show* shows/hides respective auxiliary signal type in the graph.

Override Settings for Opened Chromatograms

Overrides the settings for any particular auxiliary signal from currently opened chromatogram only when *Use Common* checkbox is unchecked. This table contains line for every auxiliary signal available in the opened chromatograms. The settings of axis and show checkbox works the same way as in the table above. If checkbox *Use Common* is checked, parameters from the **Common Settings by Auxiliary Signals Types** table will be used instead of overriding.

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. 151.

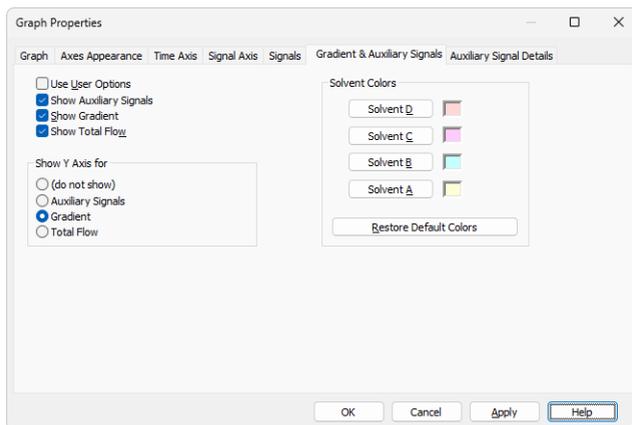


Fig. 133: Graph Properties - Gradient

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 *Settings - User Options...* command.

3.4 Chromatogram

A submenu of commands for working with chromatograms.

| | |
|---|--|
|  Global Peak Width | <p>This command or the  icon sets the <i>Peak Width</i> parameter for the whole chromatogram based on the interactively selected interval. The <i>Global Peak Width</i> can also be set manually in the first row of the <i>Integration Table</i> found on the Chromatogram - Integration tab.</p> <p>Detailed description of the <i>Peak Width</i> parameter can be found in the chapter "Integration" on pg. 247.</p> |
|  Global Threshold | <p>This command or the  icon calculates the <i>Threshold</i> parameter for the whole chromatogram based on the interactively selected interval. The <i>Global Threshold</i> can also be set manually in the second row of the <i>Integration Table</i> found on the Chromatogram - Integration tab.</p> <p>Detailed description of the <i>Threshold</i> parameter is in the chapter "Integration" on pg. 246.</p> |
|  Global Filter - Bunching | <p>This command or the  icon calculates the <i>Global Bunching</i> parameter for the whole chromatogram based on the set <i>Global Peak Width</i> value and the data acquisition frequency. The automatically provided <i>Global Bunching</i> parameter value is calculated so that the peak as defined by the <i>Global Peak Width</i> has approximately 30 datapoints. The <i>Global Filter - Bunching</i> can also be set manually in the third row of the <i>Integration Table</i> found on the Chromatogram - Integration tab.</p> |
|  Global Baseline Slope | <p>This command or the  icon calculates the <i>Global Baseline Slope</i> parameter for the whole chromatogram based on the 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 <i>Integration Table</i> found on the Chromatogram - Integration tab. The command is only available if the <i>Wave</i> integration algorithm is used.</p> |

| | |
|---|--|
| Baseline | Commands for baseline correction. Detailed description of <i>Baseline</i> parameters can be found in the chapter " Baseline " on pg. 215 . |
| Peak | Commands for operations with peaks. Detailed description of operations with peaks can be found in the chapter " Peak " on pg. 231 . |
| Integration | Commands for adjustment of integration parameters. Detailed description of <i>Integration</i> options can be found in the chapter " Integration " on pg. 246 . |
| Separation | Commands for adjustment of separation parameters. Detailed description of <i>Separation</i> parameters can be found in the chapter " Separation " on pg. 257 . |
| 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. 258 . |
|  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. 260 . |
| 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: Values displayed by *Show Slope/Level* function are influenced by the set *Global Filter - Bunching* value in the *Integration Table*. If you need to display *Show Slope/Level* values in order to fill them in the *Fraction table* for the fraction collectors, is necessary to have the same values set for the *Global Filter - 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. 266.

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.

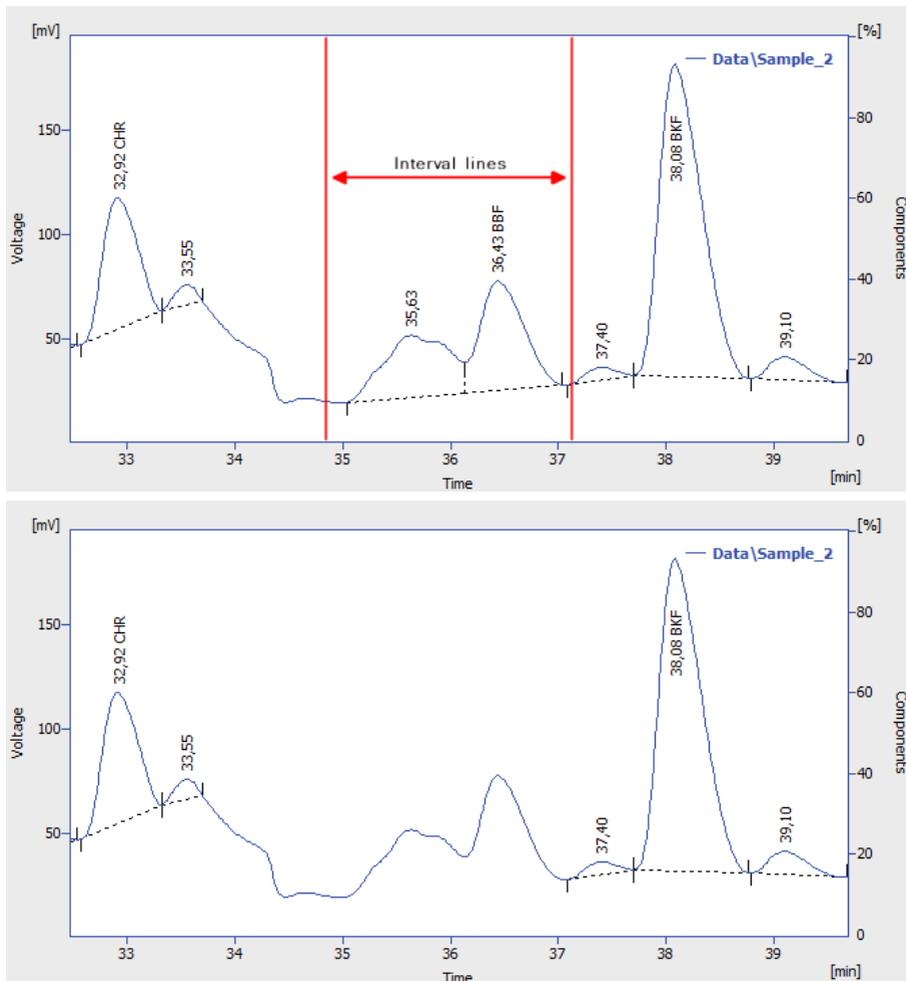


Fig. 135: Peak deletion using Lock

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.

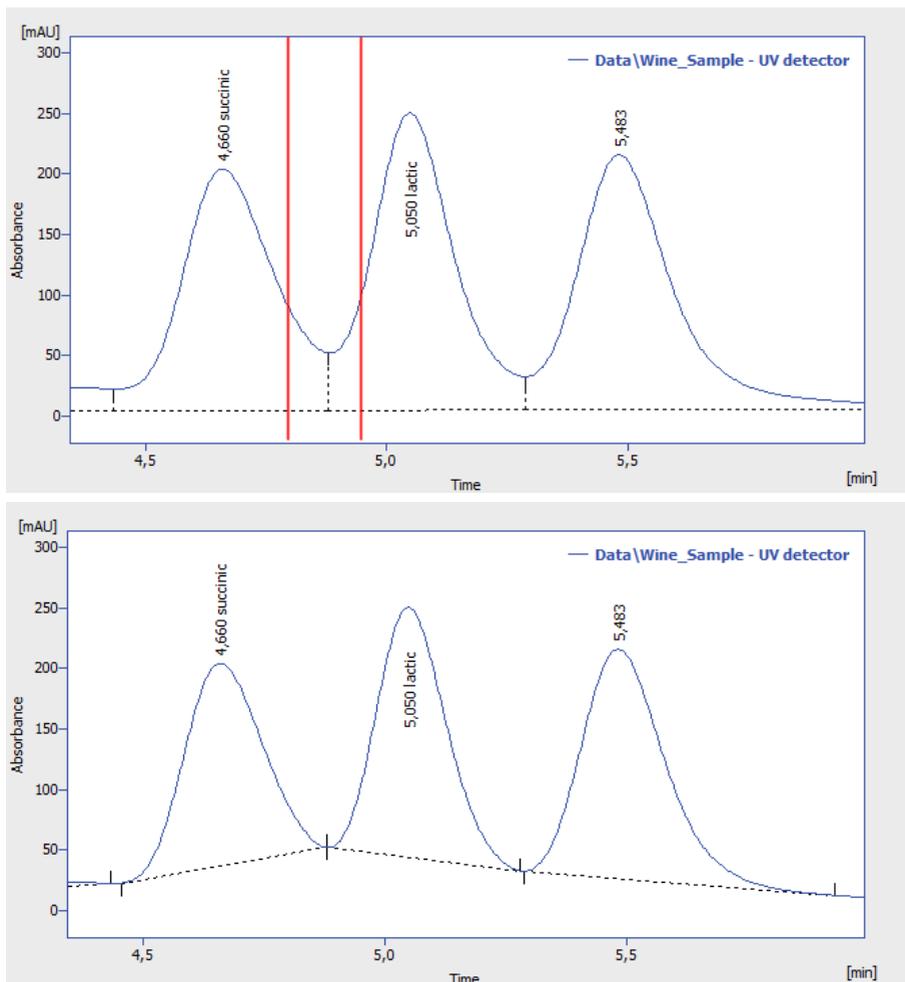


Fig. 136: Baseline into valley

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.

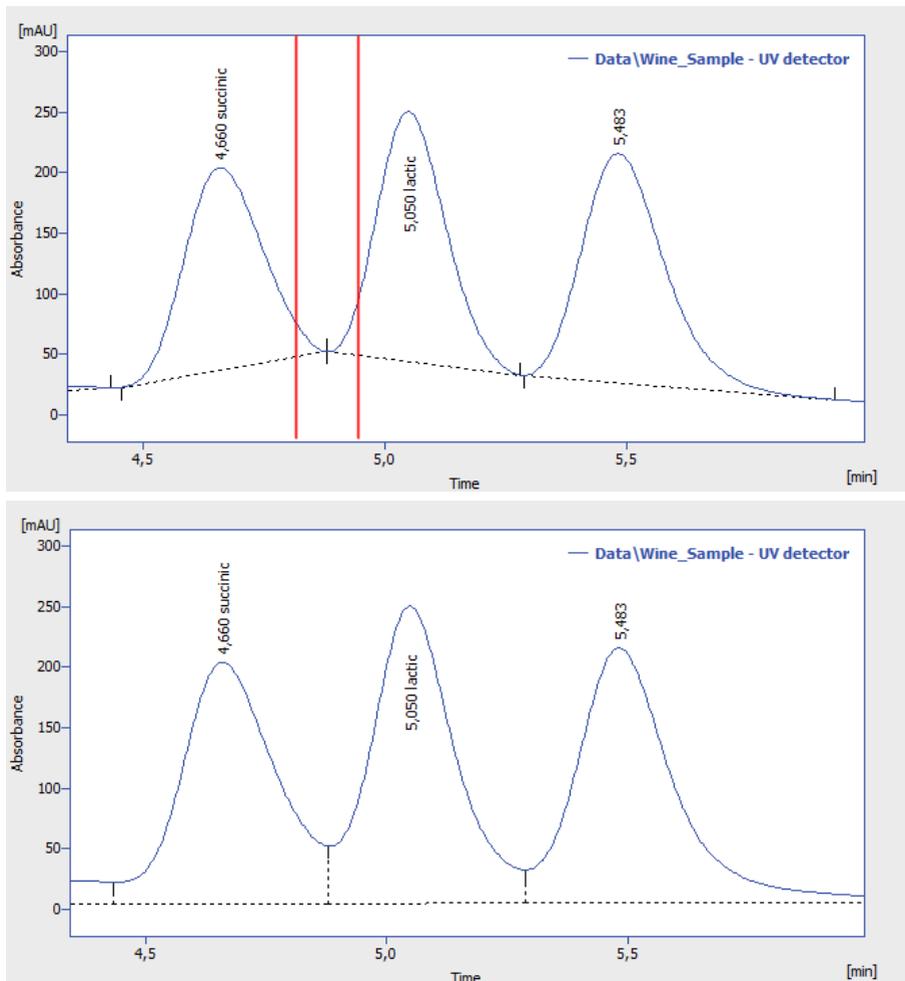


Fig. 137: Vertical separations to all valleys

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.

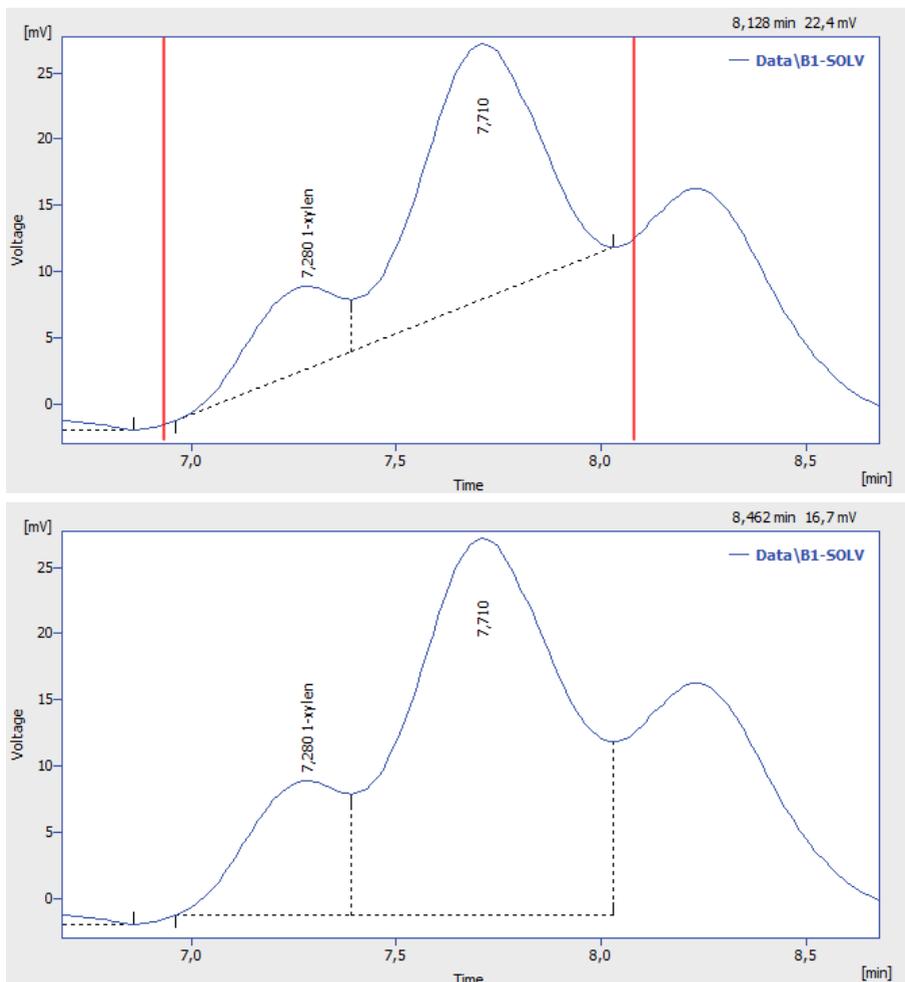


Fig. 138: Forward horizontal baseline

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.

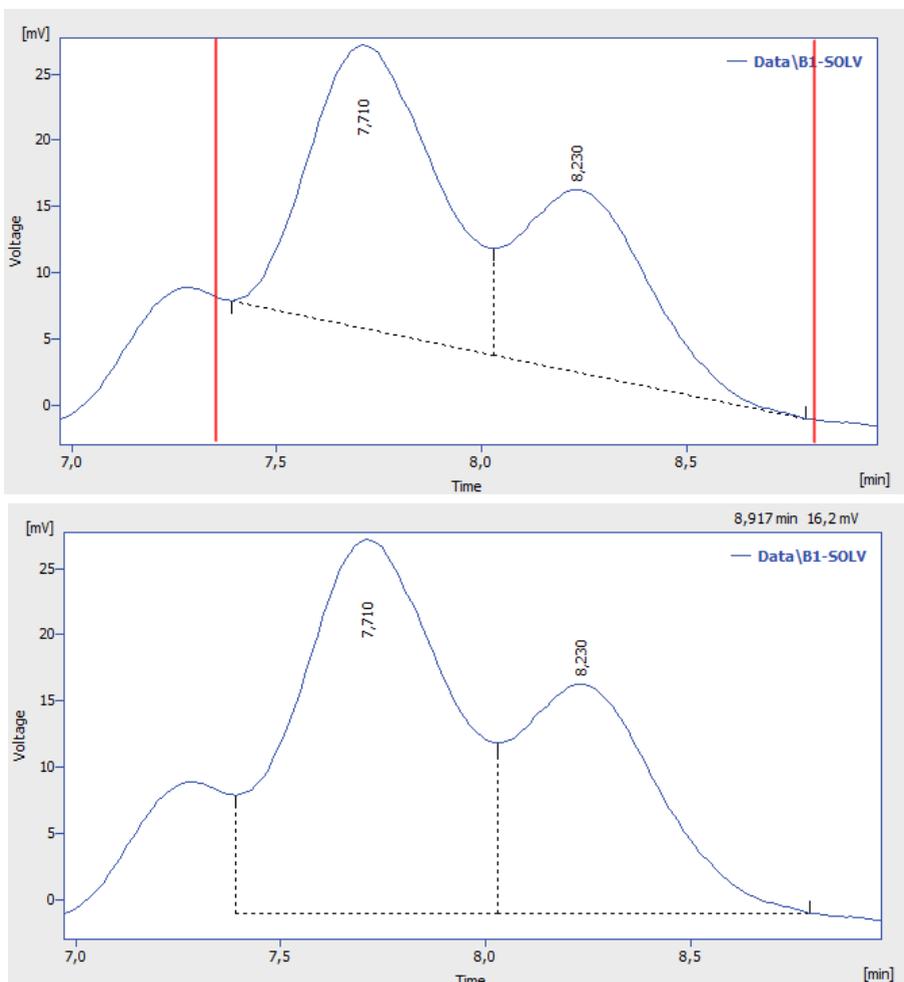


Fig. 139: Backward horizontal baseline

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.

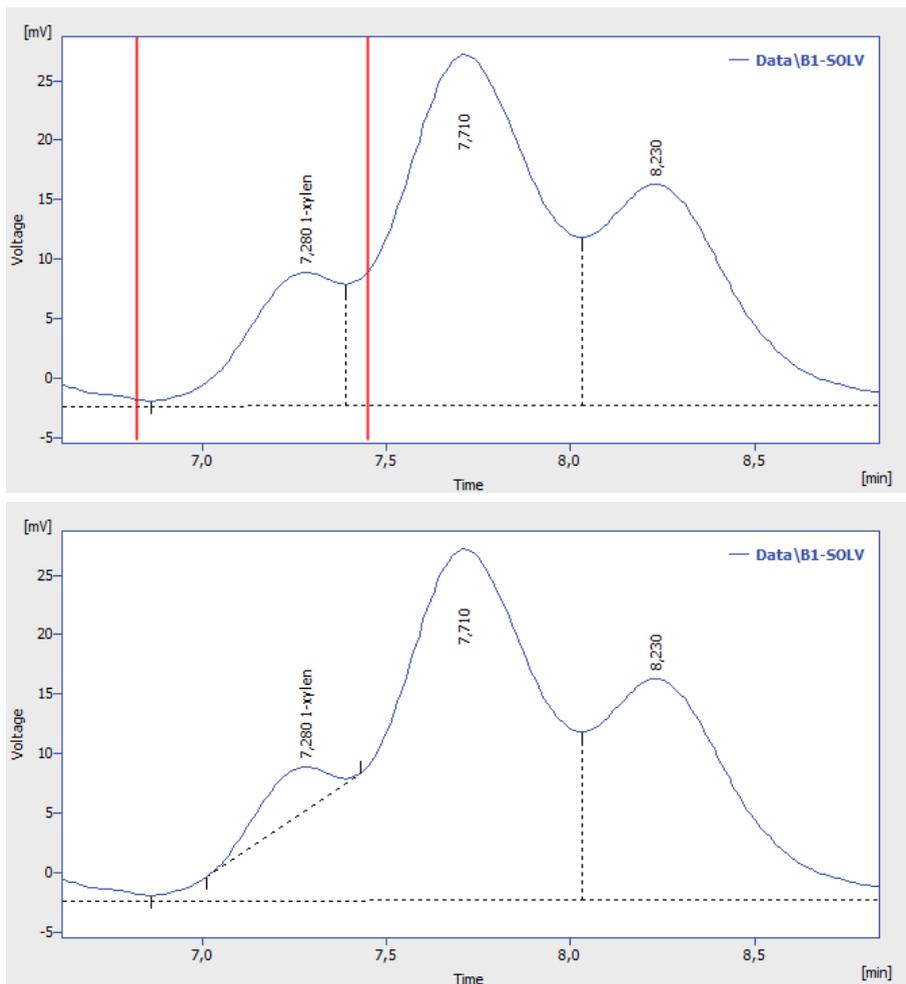


Fig. 140: Front tangent

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 your wish to separate. Place the right interval borderline behind the end of last rider to be separated.

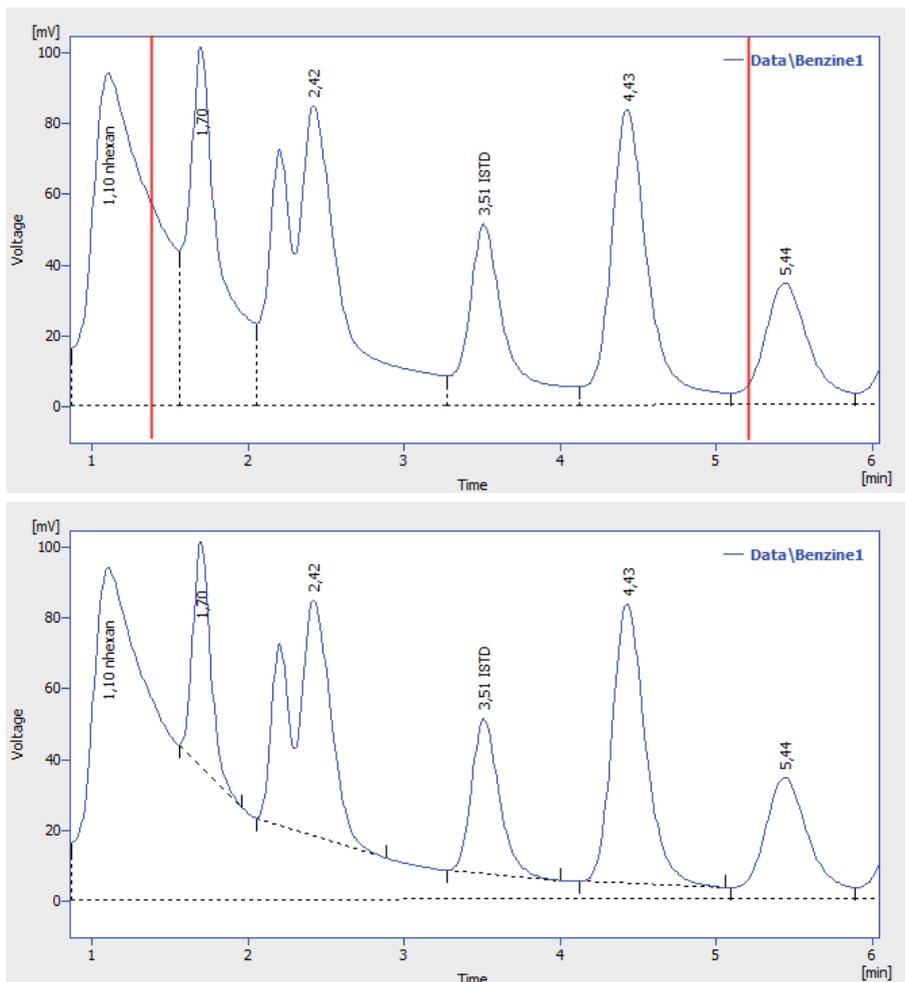


Fig. 141: Tail tangent

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).

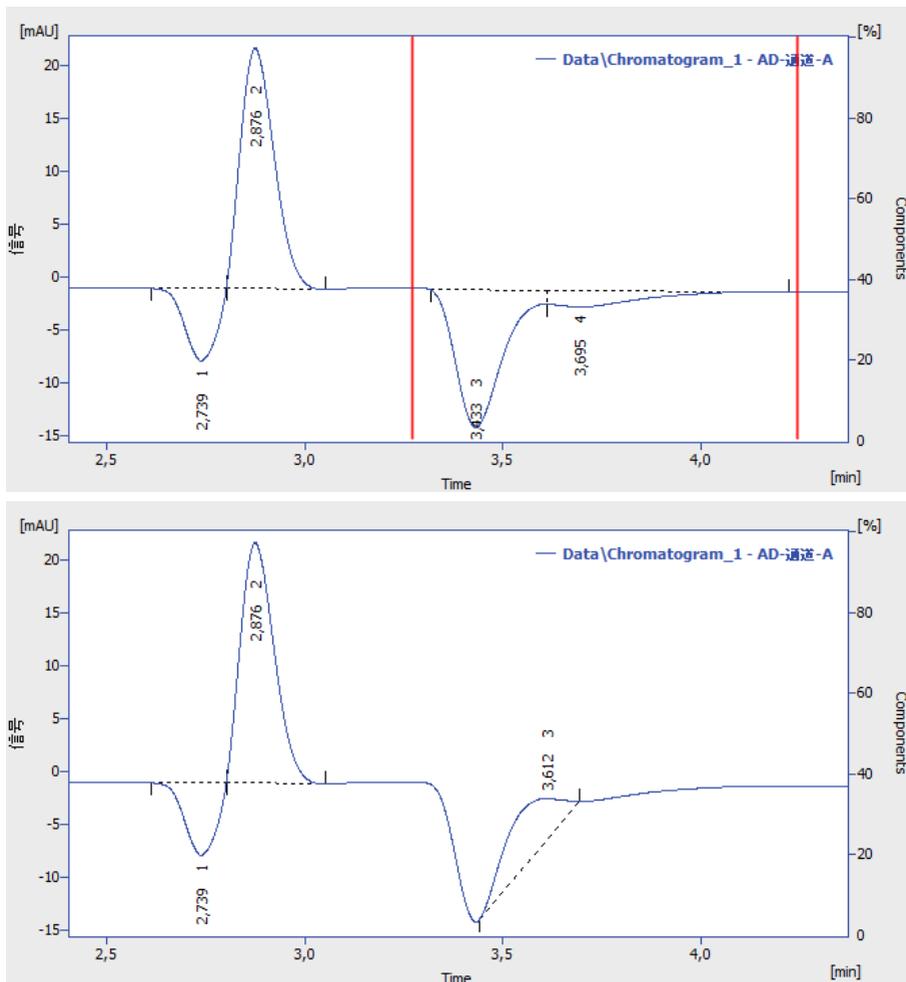


Fig. 142: Clamp negative

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.

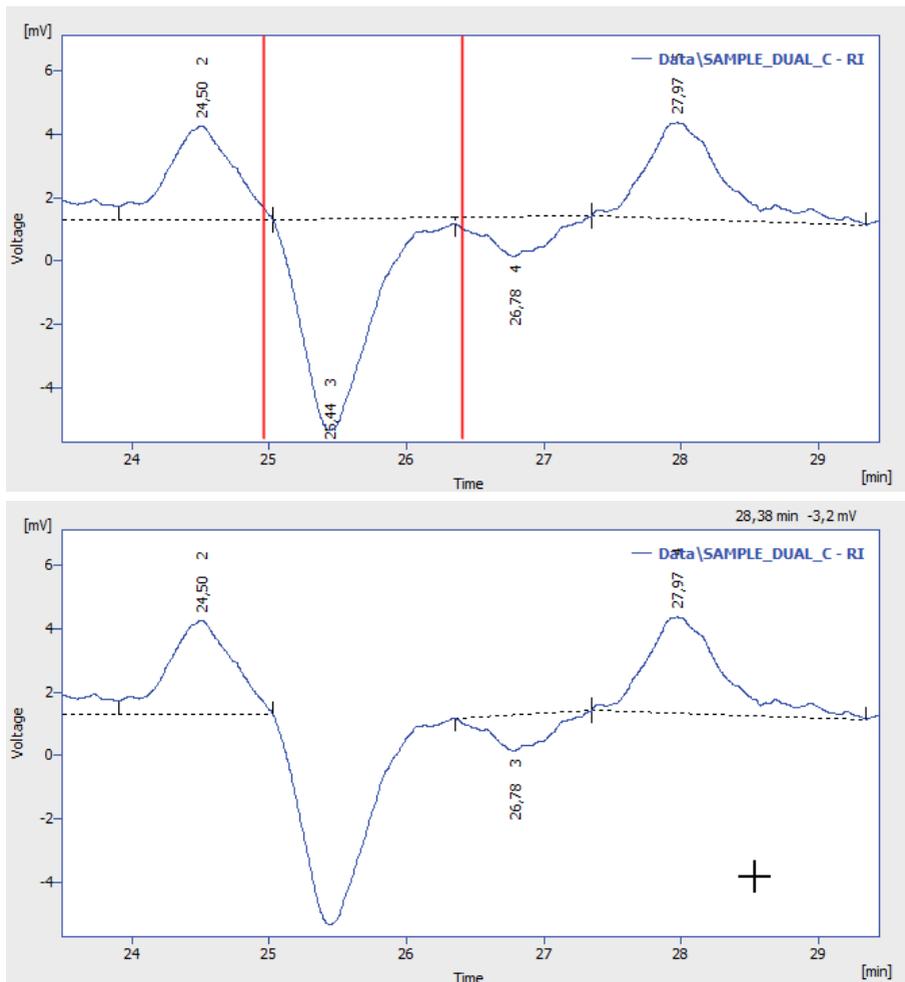


Fig. 143: Cut negative peaks

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.

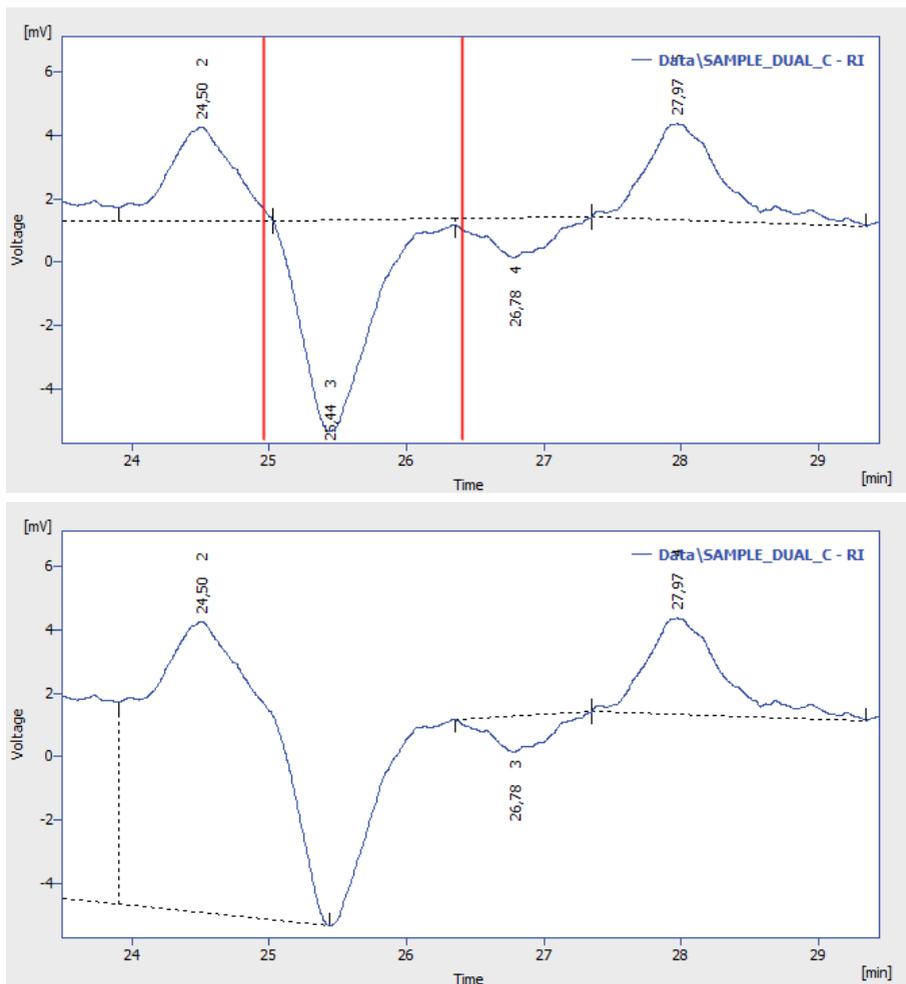


Fig. 144: Cut negative peaks

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.

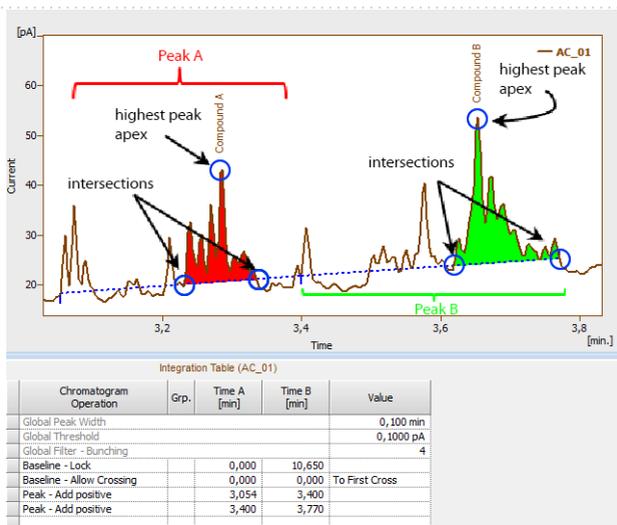


Fig. 146: To First Cross

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.

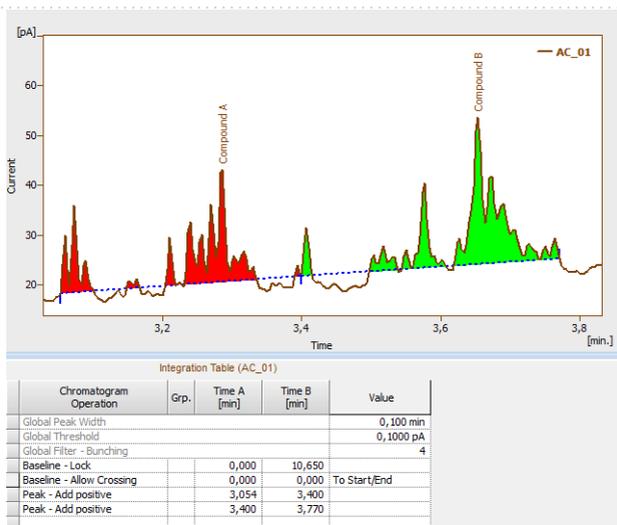


Fig. 147: To Start/End

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.

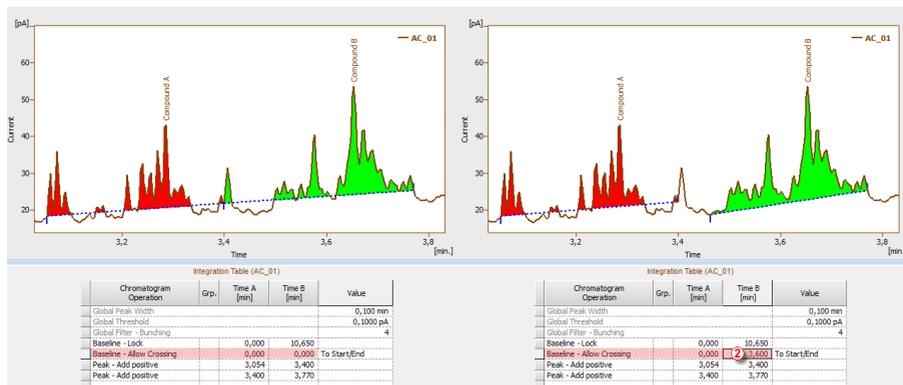


Fig. 148: Comparison of different time intervals set for Allow Crossing

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. 28).

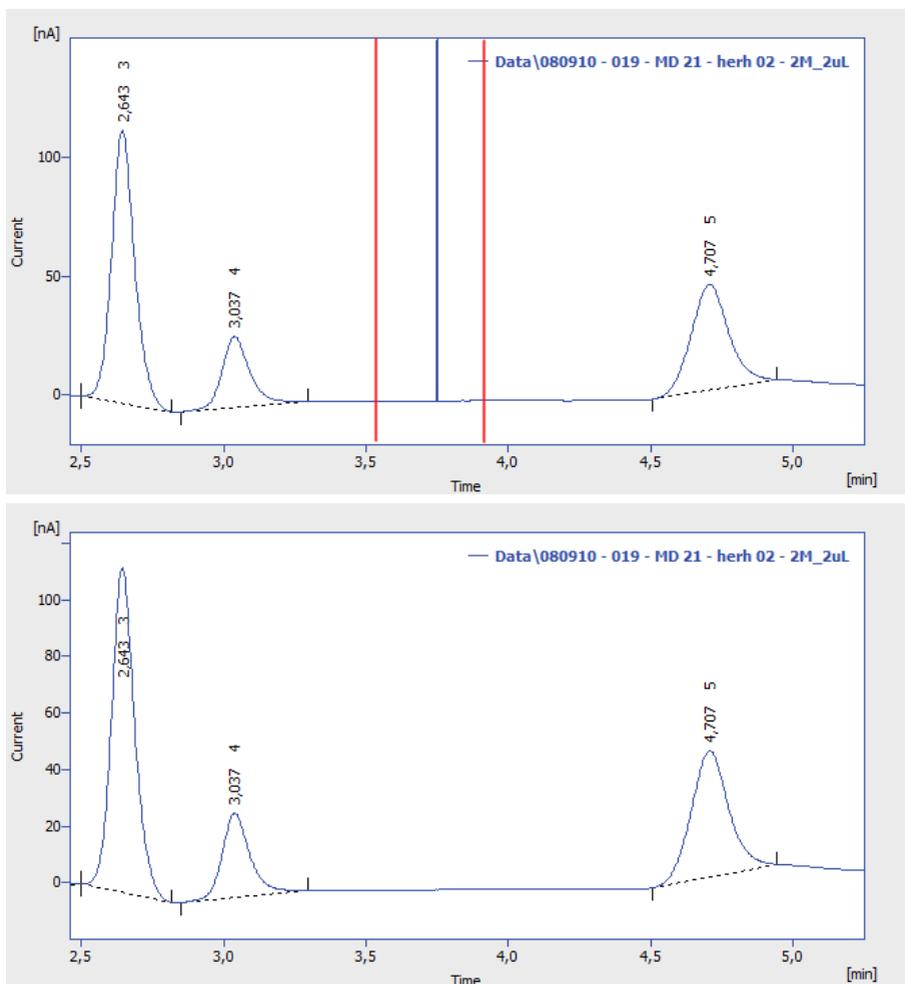


Fig. 149: Spike removal

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.

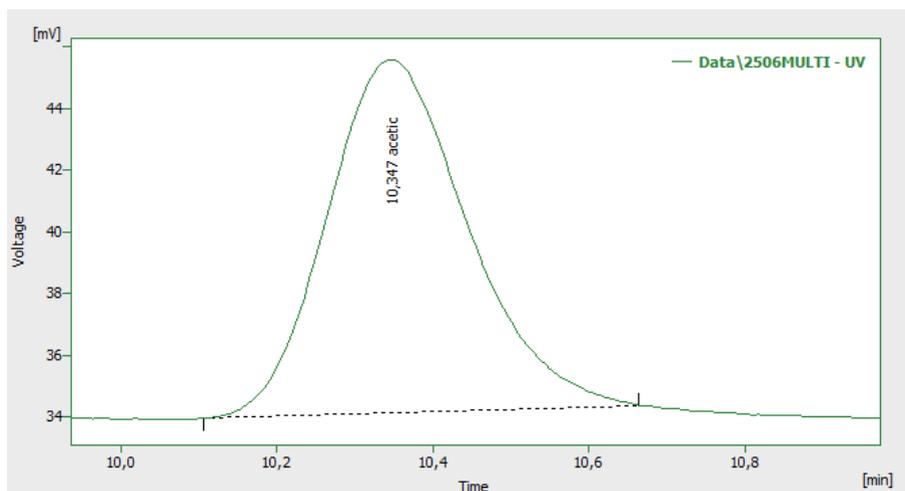
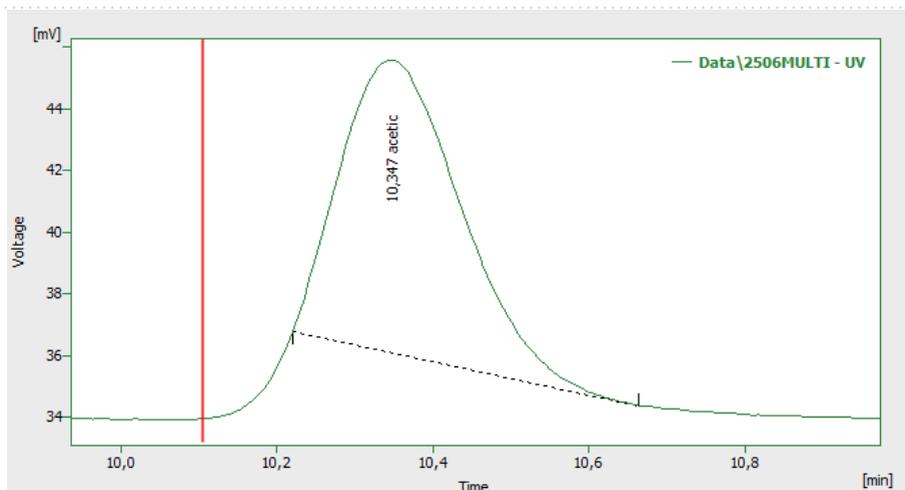


Fig. 151: Shift peak start

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.

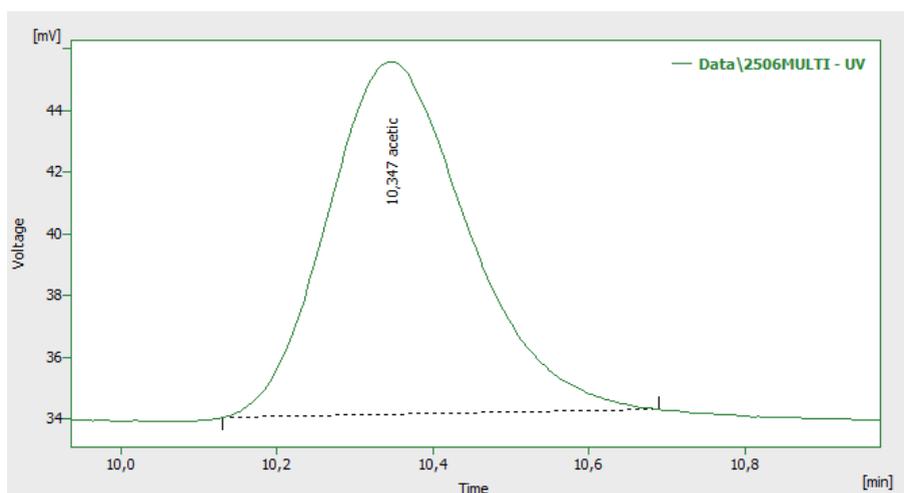
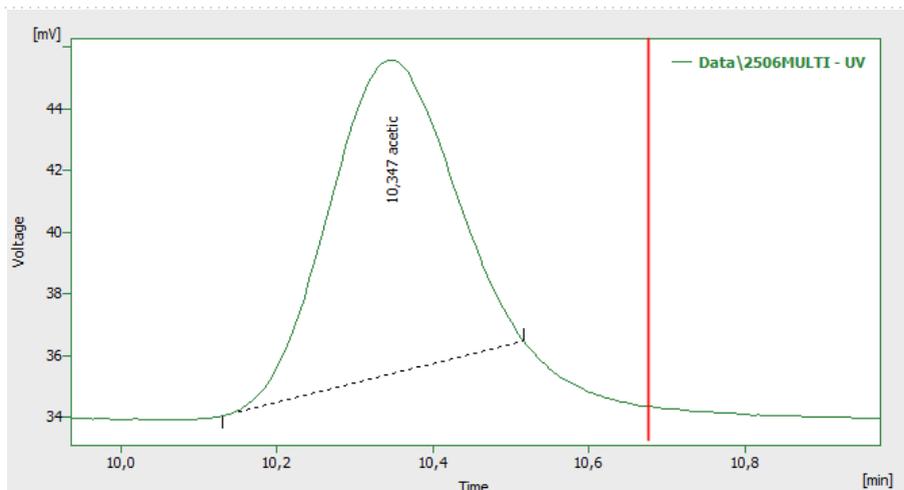


Fig. 152: Shift peak end

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.

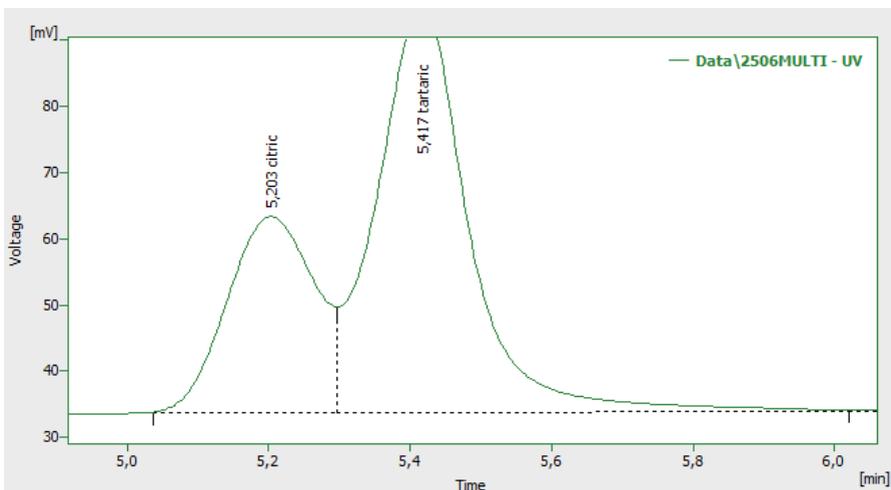
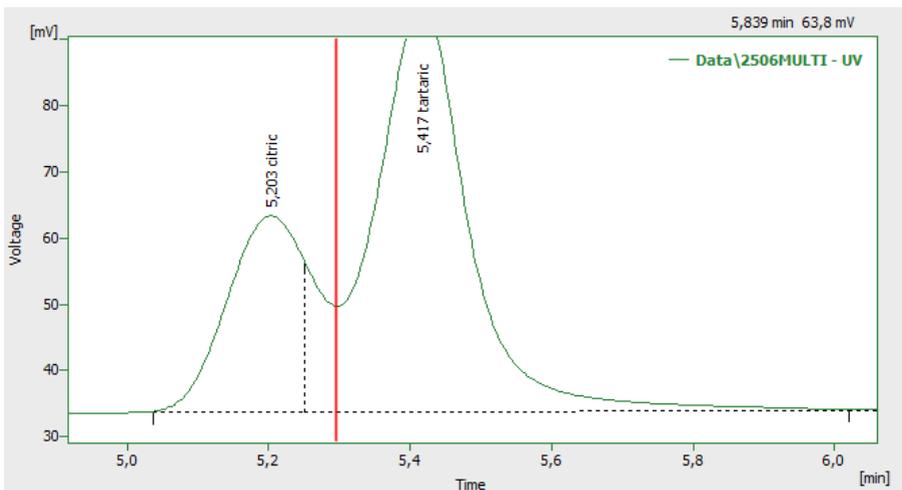


Fig. 153: Shift valley line

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.

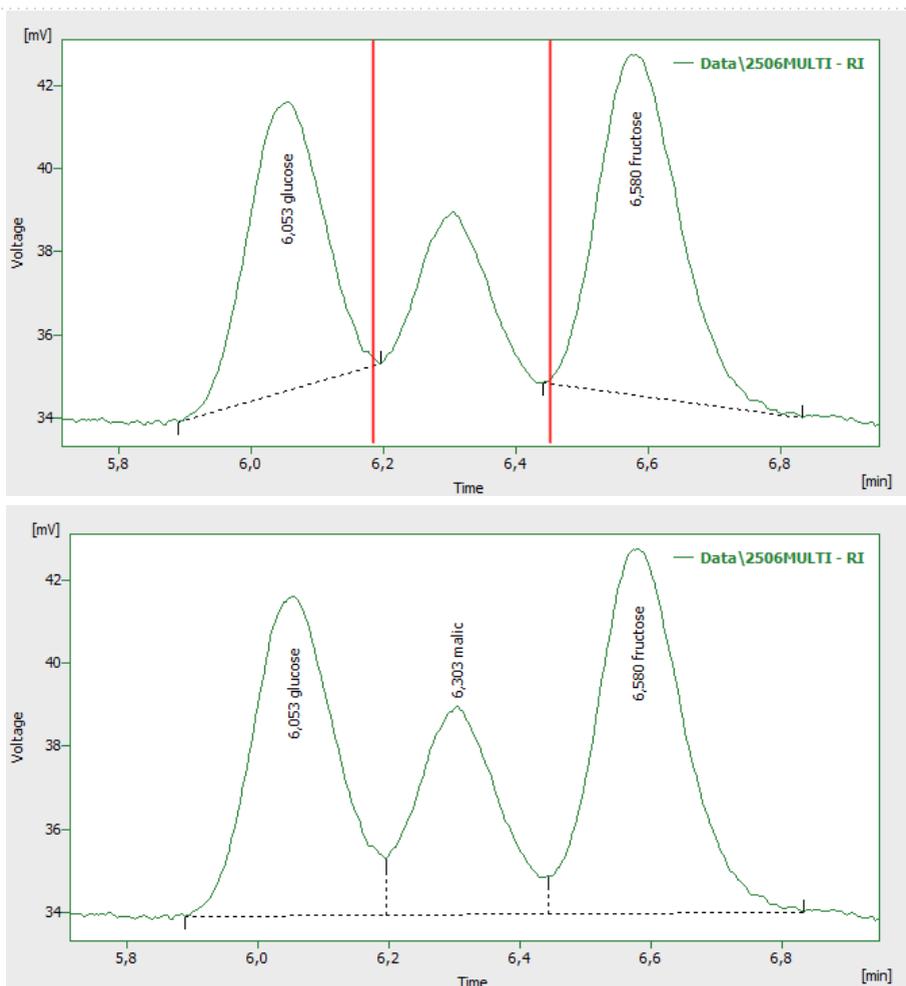


Fig. 154: Add a positive peak

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.

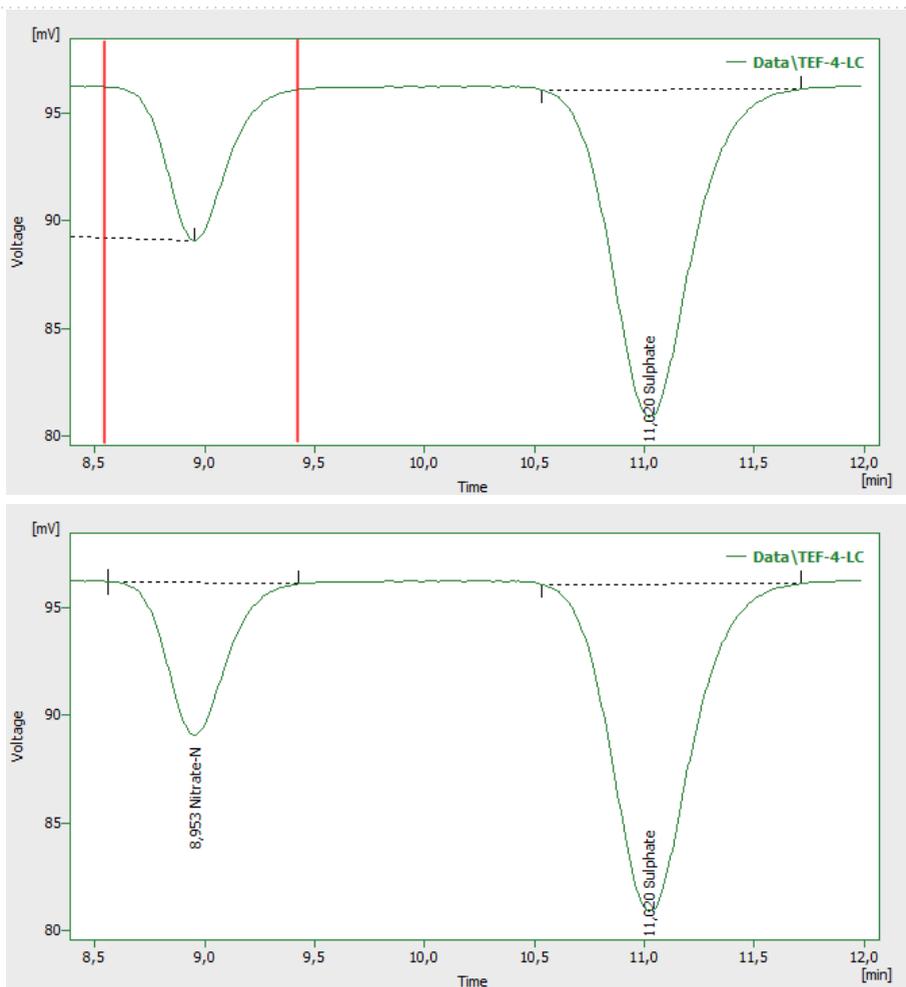


Fig. 155: Add a negative peak

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.

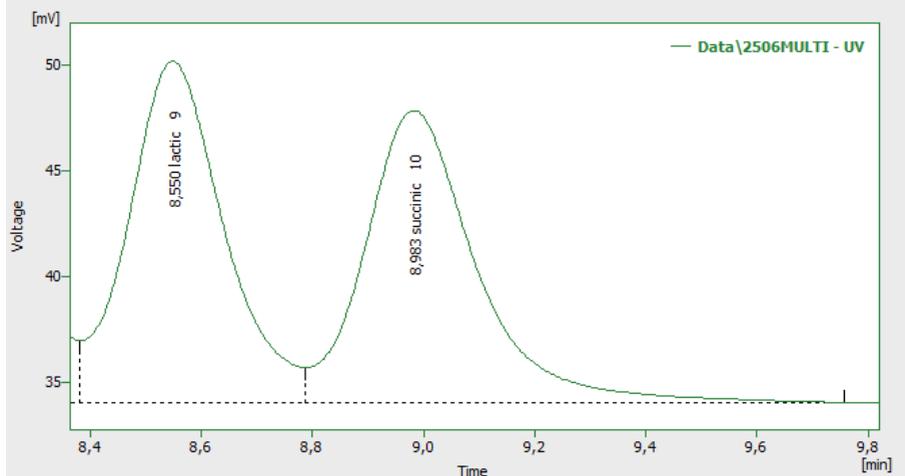
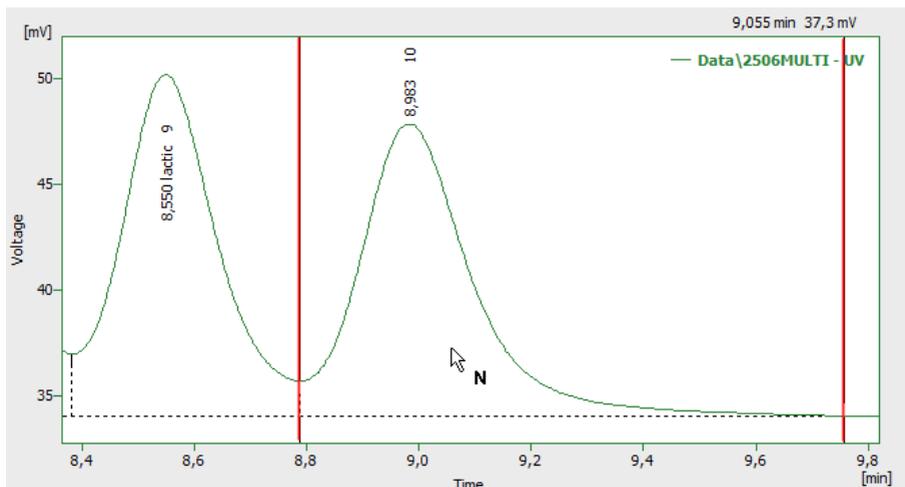


Fig. 156: Override peak name from calibration

Fig. 157:

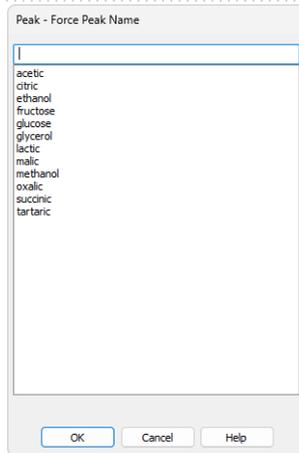


Fig. 158: Force Peak Name

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.

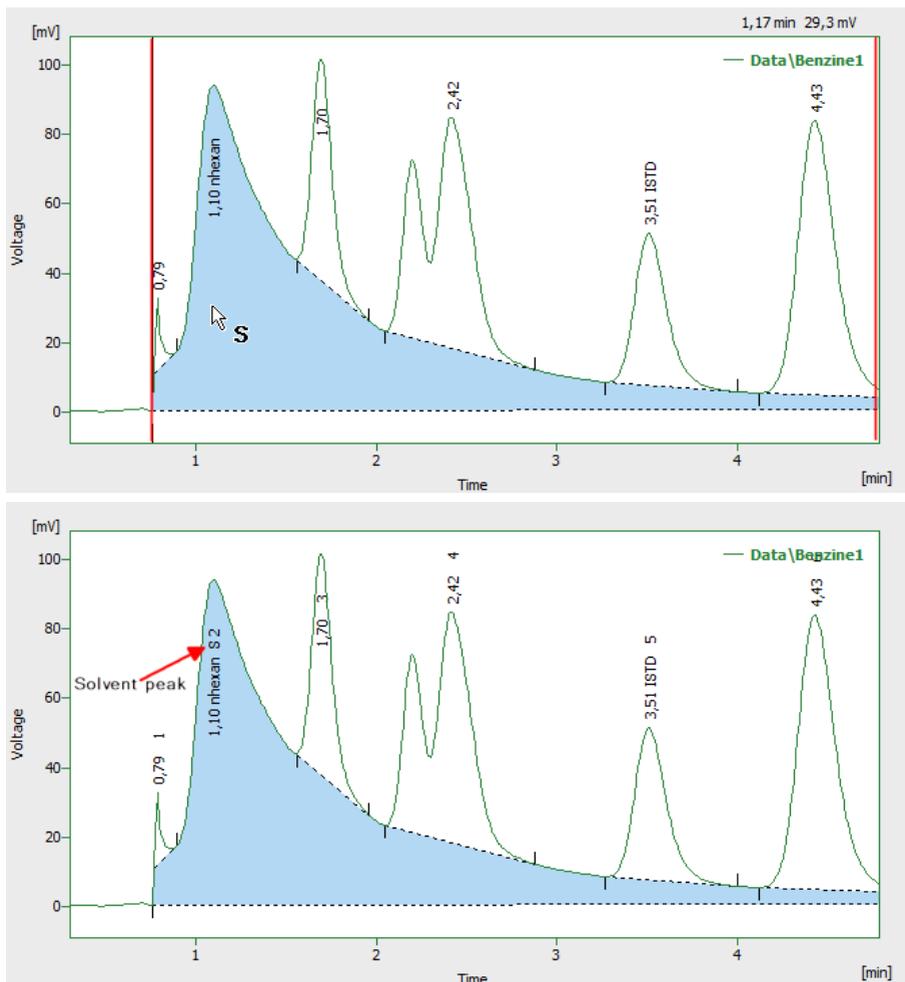


Fig. 159: Set a solvent peak

3.4.2.8 Groups

Invoking this command or the *Group* icon  opens the *Groups* dialog used for the operations with peak groups.

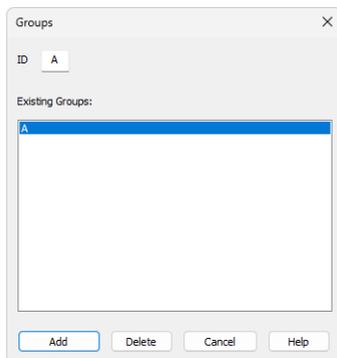


Fig. 160: *Groups*

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.

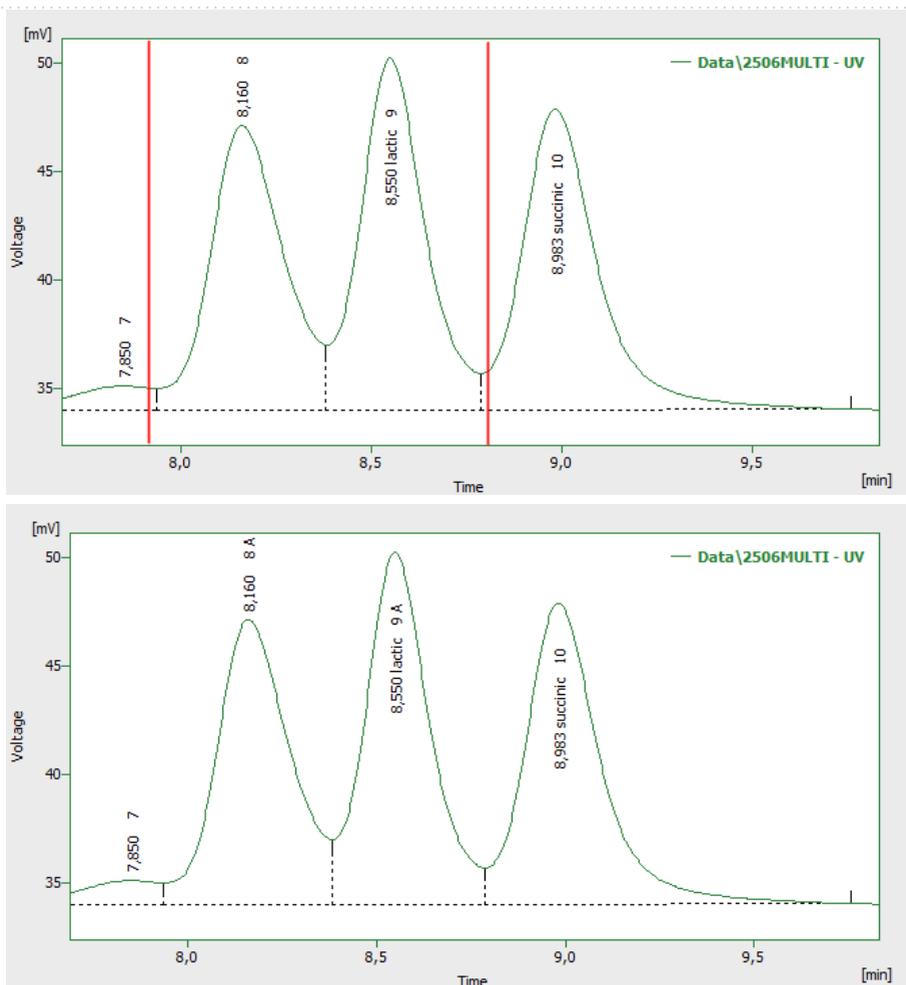


Fig. 161: Add peaks into a group

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. 277). 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

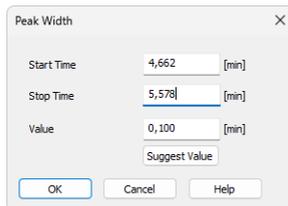
| | | |
|---|------------------------------|--|
|  | Local Peak Width | Defines minimum width of peak. |
|  | Local Threshold | Describes the threshold of noise. |
|  | Local Baseline Slope | Defines the position of automatically found peak starts and peak ends. The command is only available if <i>Wave 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.



The image shows a dialog box titled "Peak Width" with a close button (X) in the top right corner. It contains three input fields: "Start Time" with the value "4,662" and "[min]" unit; "Stop Time" with the value "5,578" and "[min]" unit; and "Value" with the value "0,100" and "[min]" unit. Below the "Value" field is a "Suggest Value" button. At the bottom of the dialog are three buttons: "OK", "Cancel", and "Help".

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. 211).

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 $1 \mu\text{V} - 10 \text{V}$.

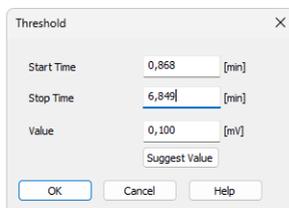


Fig. 164: Threshold

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. 211).

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).

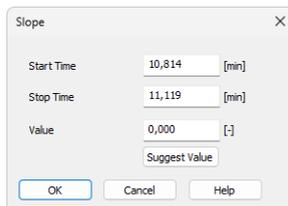


Fig. 165: *Slope*

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. 211).

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.

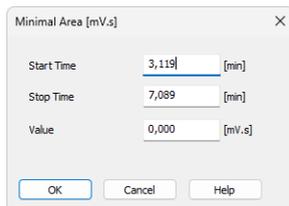
Caution: It is not true that the *Integration Interval* command is an opposite to the *Baseline - Lock* command. Although their logic is opposite (the first command will permit the integration in the interval and in the second will prohibit it) there is a significant difference between using the *Integration 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. 28).. 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.

3.4.6.1 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. 206). 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.

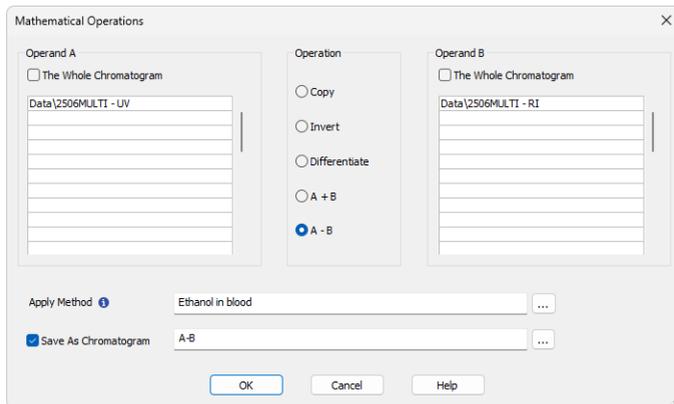


Fig. 170: *Mathematical Operations*

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> At least 2 opened signals are required to have this option available. |

| Operation | Effect |
|-----------|---|
| A-B | - Difference of signals or chromatograms. <i>Note:</i> At least 2 opened signals are required 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. 424.

| 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.

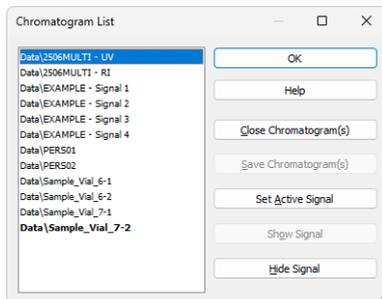


Fig. 172: Chromatogram List

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.

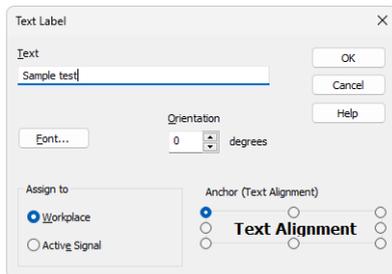


Fig. 173: Text Label

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.

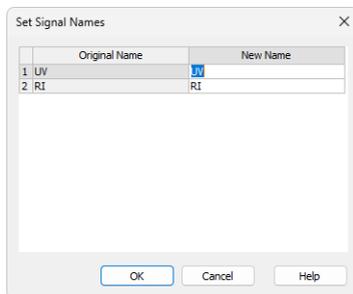


Fig. 175: Set Signal Names

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.

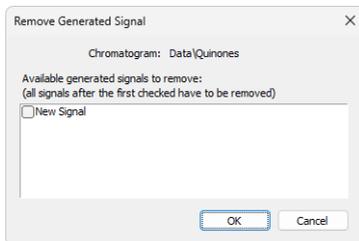


Fig. 176: Remove Generated Signal

Only named signals can be removed. Currently, it is not possible to delete only one signal (except for the last one), every signal following the one selected for deletion will be also deleted.

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 Method... | <p>The command saves the method used for the measurement of active chromatogram as a method file, i.e., a method that can be used for other analyses. Invoking the command displays the <i>Save As</i> dialog, where the name of the new method should be specified.</p> <p>Integration Table is part of method, therefore contents of the Integration Table will be saved to the new method as well.</p> |
|  | <p>Set Model </p> <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> |
|  | <p>Copy from Model </p> <p>Copies a Model Method to another chromatogram. Prior to invoking the command a method must have been marked as model method by the <i>Set Model Method</i> command. The model method can then be applied on any chromatogram opened in the Chromatogram window by using the <i>Copy from Model</i> command.</p> <p>Integration Table from the Model method will be copied into the Integration Table of the active chromatogram.</p> |

Copy from Method... Copies processing part of the selected 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. 74., in which you can select the required method.

Copy from Chromatogram... Copies the processing method from a selected chromatogram to the active chromatogram.
Use this command to open the [Open Chromatogram](#) dialog (described in the chapter "**Open Dialog (Sequence, Chromatogram, Calibration, Method)**" on pg. 74., in which you can select the required chromatogram.

3.5.1 Calculation

This section is located in the right part of the bottom pane of the [Chromatogram](#) window. On the left, there is the [Result table](#), or [All Signals Result table](#).

The parameters stated here are common for all detector's signals of the chromatogram. The displayed values come from the method; they are transferred from the [Calculation](#) and [Advanced](#) tab of the [Method Setup](#) dialog and some fields from the *Single Analysis* or the *Sequence*.

Calibration File (Peak Table)

Name of the calibration file connected to the chromatogram.

Open with stored calibration

When this option is checked, the chromatogram will be opened with the calibration stored in the chromatogram file. To apply this setting, you must re-open the chromatogram using the [Open Chromatogram](#) dialog - simply re-opening the [Chromatogram](#) window is not enough.

This option can also be enabled automatically when the chromatogram is created if the corresponding Post-Run Action is checked, either in [Single Analysis](#) or in [Sequence](#).

Note: The difference between *Stored* and *Linked* calibration is explained in the [Calibration \(stored x linked\)](#) section of Open Chromatogram topic.

Set...

Invokes the *Open Calibration* dialog where the calibration file may be selected.

None

Unlinks calibration file and sets the *Calculation* type to *Uncal* (uncalibrated).

View

Opens the linked calibration file in the [Calibration](#) window. Active chromatogram will be automatically opened in it as a standard.

| 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 | citric |
| 3 | 1.917 | 8460.283 | 0.438 | 14.5 | Ordnr | tartratic |
| 4 | 2.800 | 3333.242 | 1.147 | 37.8 | Ordnr | malic |
| 8 | 4.660 | 2732.362 | 0.243 | 8.0 | Ordnr | succinic |
| 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

Sample Amount [g/l]: 0
Inj. Volume [μl]: 100
Dilution: 1
ISTD1 Amount [g/l]: 0

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. 273.

Tab. 15: List of available calculation types

| Calculation type | Description |
|------------------|--|
| <i>Uncal</i> | Calculation without use of calibration file. The result is percentage representation of individual areas and heights of peaks in the chromatogram. When using this option, sections that are connected to the calculations with calibration file are disabled. |
| <i>ESTD</i> | External standard calculation. The result will be both a percentage and absolute representation of individual substances and their names according to the selected calibration. |
| <i>ISTD</i> | Internal standard calculation. The result will be both a percentage and an absolute representation of individual substances and their names according to the selected calibration. |
| <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 according to the selected calibration. In case any peak found in the Result Table is not present in a calibration and/or the <i>Sample 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 | Description |
|------------------|---|
| <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 section determines which peaks will be displayed in the *Result Table* and included in the sum for the *Total* row.

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

Only the peaks defined in the calibration file will be displayed, regardless of which peaks are present in the chromatogram. This creates a fixed table format based solely on the calibration file.

Hide ISTD Peaks

The peaks identified as the internal standards will not be displayed in the *Result Table*. 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 uncalibrated substances. Amount is set as area/height of peak multiplied by this coefficient. This value serves as a simple single-point calibration.

Scale

Area for entering the auxiliary calculation parameters.

Use Scale Factor

The whole section 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

The units in the results table taken from the calibration file are overridden by the units defined here.

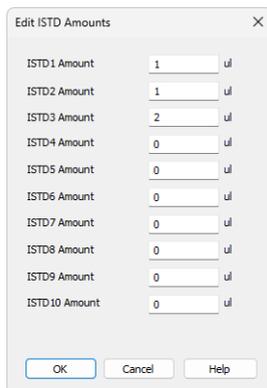
Sample Amount

The actual amount of the sample measured in the laboratory and used for analysis. This value includes both the target compounds and any impurities and is used in ISTD and ESTD calculations to adjust the percentage distribution and total amount. When using the ISTD method, enter the sample amount before adding the internal standard. Always use the same units as in the calibration file.

If the default value 0 is used, the total amount is determined as the sum of the identified compound amounts, which is then considered 100%. Otherwise, the entered sample amount is taken as 100%, and the identified compounds are calculated relative to it.

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

The *Edit ISTD Amounts* dialog allows you to set the internal standard (ISTD) amounts for all ISTDs used in a chromatogram. It can be accessed from the *Single Analysis* dialog, and values can also be entered in the *Sequence* window (in the ISTD1 Amount – ISTD10 Amount columns, with only ISTD1 Amount displayed by default). Enter values in the same units as used in the calibration file.

Note: If the same ISTD amount is used in all calibration standards and unknown samples, it does not need to be entered and can remain 0 in both the calibration and chromatograms. However, if you enter an ISTD amount in one place (calibration file or unknown sample), you must enter it in the other as well. If only one is filled and the second one is empty (zero), no results will be displayed in the *Result Table*, and the compound will be omitted from the *Summary Table*.

Result Table (Uncal - Data (PERSON1))
 !!! Missing ISTD Amount in Sample (ISTD1) !!!

| 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 | | | | | |

Common for All Signals

Calibration File (Peak Table): Ethanol
 Calculation: ISTD

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: g/kg

Amount [g/kg]: 4
 ISTD1 Amount [g/kg]: 0
 Inj. Volume [µL]: 2
 Dilution: 1

User Variables:

Fig. 179: Chromatogram - Calculation - ISTD settings

Inj. Volume

Specifies the injection volume. This parameter affects calculations only if a *Default Injected Volume* is set in the [Calibration Options](#) dialog. If the *Default Injected Volume* is set, the response of all substances in calibrated calculations is adjusted based on the ratio of the *Inj. Volume* to *Default Injected Volume*.

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 factor of the sample, representing the total volume of the solute and solvent combined. Each calibrated amount in the *Amount* column of the *Result Table* is multiplied by this value. The default value is 1.

User Variables

Specifies the Names and Values of *User Variables*, that can be used in *User Columns* calculations.

Analysis Variables

Specifies up to three *Analysis User Variables* originating from the [Single Analysis](#) or [Sequence](#).

Method Variables

Specifies up to three *Method User Variables* originating from the [Method . . . Advanced](#) 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 content of the tab is based on the [Integration tab](#) of the method used to measure the chromatogram. These values can be further modified through operations available in the *Chromatogram* window in the toolbar or the [Chromatogram](#) menu.

Integration Algorithm

Selects the integration algorithm for integration of displayed chromatogram. It 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 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 Clarity 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).

Integration Algorithm (Common for All Signals) Wave

Integration Table
Data\Sample_884002 - Signal 1, Integration Algorithm: Wave rev. 1

| 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-Golay | 10.250 | 14.500 | 20 |
| Baseline - Allow Crossing | 17.700 | 21.700 | To First Cross |
| Peak - End | 19.842 | 1.050 | |

Results All Signals Results Summary Performance Integration

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. 246.

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. 215.

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. 231.

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. 244.

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. 258.

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. 270** - 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 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 | |
|--|--|
| Measurement Conditions | Sample Identification |
| Description: Fluorescence Detector PAH_MZP-PCLYA | Sample ID: 0542 |
| Column: Supelcosil LC_PAH, 25cm x 4.6mm, 5µ | Sample: DEMO Example - PAH |
| Mobile Phase: GRAD ACN/W(2min-50/50, 2min-50/50, 30) | Acquired: 31.01.2024 11:08 |
| Flow Rate: 1.0 ml/min | Analyst: DataApex |
| Pressure: 1300 psi at start | Acquisition Parameters |
| Detection: Fluorescence, prog. | AutoStop: 50 min, enabled |
| Temperature: 25 degree centigrade | Ext. Start: Down |
| Note: time Ex Em 00.00 220 324 (RAP) 17.00 270 324 (ANA-FLU) | Range: 1250 mV, unipolar |
| | Sample Rate: 2 samples/sec |
| | Acquisition Method: N/A |
| | Processing Method: N/A |
| | Subtraction: [Set...] [None] |
| | Chromatogram: [No Change] |
| | Matching: [No Change] |
| | Chromatogram |
| | Comments: [Edit...] |
| | Audit Trail: No Acquisition Messages [Show...] |
| | GLP Mode: Off |

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

Specifies whether and by what change on the relevant input the measurement was started. This corresponds to the *External Start/Stop* section of the [Method Setup - Measurement](#) tab.

Acq. Method

Name of the 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 ✓full version

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](#) tab (for the newly created chromatograms) accessible from

the [Instrument](#) window and *Measurement Conditions - Instrument* tab of the [Chromatogram](#) window.

The subtracted chromatogram has to be always present in the defined path. The change in the subtracted chromatogram influences the resulted subtraction in the current chromatogram.

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: In the [Data Acquisition](#) window, the subtracted chromatogram may be displayed during a measurement in the background as a grey chromatogram. To display the chromatogram in the background without automatic subtraction (e.g., the solvent) use the *File - Set Background Chromatogram...* command.

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.

Matching

Selects the subtraction method.

No change - The chromatogram is subtracted from the measured chromatogram without any additional adjustments.

Offset Subtraction Chromatogram - "Offsets" the measured chromatogram with the subtraction chromatogram by shifting it on the axis X (time axis) before the actual subtracting.

Scale Subtraction Chromatogram - "Scales" the measured chromatogram before subtracting by scaling the subtraction chromatogram on the time axis.

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. 446.

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. 82.

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. 186.

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. 193.

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 ✓ Full version

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. 188.

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. 185.

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*.

| Result Table (ESTD - Data(Wine_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 | citric |
| 3 | 1.917 | 8460.283 | 0.438 | 14.5 | Ordnr | tartaric |
| 4 | 2.800 | 3333.242 | 1.147 | 37.8 | Ordnr | malic |
| 8 | 4.660 | 2732.362 | 0.243 | 9.0 | Ordnr | succinic |
| 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) | | Calculation | |
| Wine | | ESTD | |
| <input type="checkbox"/> Open with stored calibration | | | |
| Set... | | None View | |
| Report in Result Table | | Unidentified peaks | |
| <input type="radio"/> All Peaks | | Response Base: <input checked="" type="radio"/> Area | |
| <input type="radio"/> All Identified Peaks | | <input type="radio"/> Height | |
| <input checked="" type="radio"/> All Peaks in Calibration | | Response Factor: 0 | |
| <input type="checkbox"/> Hide ISTD Peaks | | | |
| Scale | | Sample Amount [g/l] | ISTD1 Amount [g/l] |
| <input type="checkbox"/> Use Scale Factor | | 0 | 0 |
| Scale Factor: 1 | | Inj. Volume [µl] | Dilution |
| Units: ul | | 100 | 1 |
| <input checked="" type="checkbox"/> User Variables | | | |

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, only two will be displayed in a list ①, the remaining messages can be visualized as a tooltip over the visible error messages.

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 (Kováts 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 Kováts Indexes are described in the chapter "[Calibration Options](#)" on pg. 358.

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. 302.

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.

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. 446.

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.

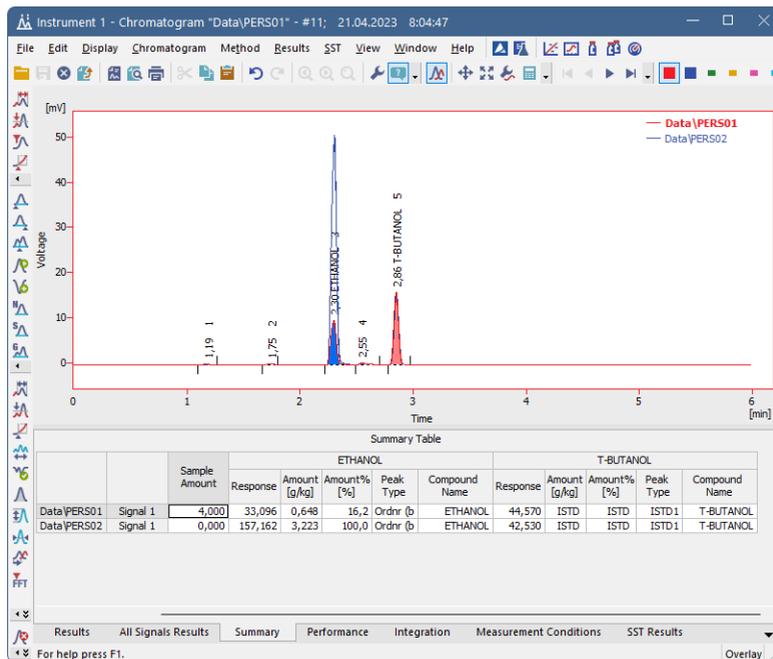


Fig. 185: Chromatogram - Summary

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. 446.

The results table can also be exported using the *File - Export - Export Summary Table* command described in the chapter "File" on pg. 159.

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. 289.

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.

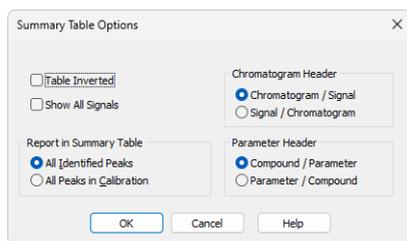


Fig. 186: Summary Table Options

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 on.

Available layouts of Summary Table:

| Summary Table | | | | | | | | | |
|---------------|----------|---------------|-------------|---------------|-------------|---------------|-------------|---------------|-------------|
| | | Chloride | | Bromide | | Nitrate-N | | Sulphate | |
| | | 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 |
| | | Signal 1 | | Signal 1 |
| Chloride | Amount [mg/l] | 0,036 | | 0,289 |
| | Amount% [%] | 1,3 | | 7,7 |
| Bromide | Amount [mg/l] | ISTD | | ISTD |
| | Amount% [%] | ISTD | | ISTD |
| Nitrate-N | Amount [mg/l] | 0,907 | | 2,618 |
| | Amount% [%] | 32,9 | | 70,0 |
| Sulphate | Amount [mg/l] | 1,814 | | 0,832 |
| | Amount% [%] | 65,8 | | 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-4LC | | NYL-3LC |
| | | 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.

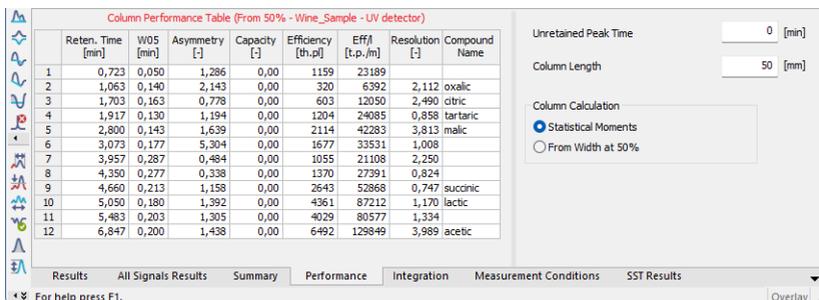


Fig. 187: Chromatogram - Performance

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. |
| 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 |
|---------------|---|
| W05 [min] | - Peak width at half-height in minutes. |
| 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: $Efficiency_i = 5.54 \cdot \left(\frac{RT_i}{W05_i} \right)^2$ |
| 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: $Resolution_i = \frac{1.18 \cdot (RT_i - RT_{i-1})}{(W05_{i-1} + W05_i)}$ |

Tab. 23: Description of used symbols

| Symbol | Description |
|---------------|--|
| RT_i | - is the retention time of the component. |
| $W05_i$ | - 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. Within the mode where ISTD peak can be used from different than active signal, the messages may be enhanced by definition of the signal where the error happens (e.g. instead of "*ISTD (Compound X) is not enabled in the Calibration*" message you would see "*ISTD (Compound X) on signal UV is not enabled in the Calibration*" message instead. 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 <input type="button" value="..."/> 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>ISTD (Compound X) is not enabled in the Calibration</i> | At least one peak in ISTD calculation mode is using ISTD peak which is disabled in the used calibration. The remedy is to select a different ISTD peak or enable the disabled ISTD peak in calibration, which may in turn produce other messages as the disabled ISTD peak was probably not recalibrated. |

| Error message | Detailed description |
|---|--|
| <i>Definition of ISTD compound for X peak is not valid.</i> | In the mode allowing to use the ISTD peak from different signal, a peak from signal not present in the chromatogram should be used as ISTD (e.g. ISTD peak should be set on signal 3, but chromatogram has just 1 signal). |
| <i>Peak(s) ISTDX on signal Y not detected.</i> | One or more of the ISTD peaks defined is not found in its identification window. |
| <i>Chromatogram does not have enough signals - ISTD peak for compound X is not valid.</i> | Calibration file is used in a mode where ISTD peak can be defined on a different signal. Calibration itself has enough signals so that all ISTD peaks are properly defined, but opened chromatogram has fewer signals and at least one of the cross-signal ISTDs is looked for on non-existing chromatogram signal. |
| <i>Some referred ISTD compound not used.</i> | Only possible in version of integration algorithm older than version <i>Wave rev. 4</i> or <i>Legacy (10.0 rev. 2)</i> . One or more of the ISTD peaks has the <i>Used</i> checkbox in the calibration disabled. |
| <i>Calibration curve for X compound could not be constructed</i> | <p>If calibration curve could not be constructed for one compound in calibration, no results are calculated for any compound. The problematic compound is listed in the error message and can be detected in the Peak Type column as "Error". To remedy, 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> |
| <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. |

| Error message | Detailed description |
|------------------------------------|--|
| <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 |
| <i>Quantification signal for X compound cannot be constructed, spectral data are missing at specified time.</i> | Spectral data needed for the compound to create the quantification signal are not defined in the expected retention time (plus minus the Left Window and Right Window) both in the calibration and in the chromatogram's MS Method. |
| <i>Quantification signal for X compound cannot be constructed, signal out of range of spectral data.</i> | Quantification signal that needs to be constructed for a compound is outside the m/z range of the spectral data. |

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. 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 <i>Display - Properties - Signals</i> tab, use the <i>Original</i> button in the <i>Offset & Scale</i> part. |
| <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.

| Command | Description |
|------------------------|---|
| 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 | 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. |
| Show Both | Used to display both parts of the window (the chromatogram and the tabs). |
| Maximize Tables | 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. |
| Show Tables | <p>Opens a submenu for showing or hiding tabs in the Chromatogram window. Tabs with a checkmark are currently displayed.</p> <p>Either the Results or All Signals Results tab must always remain visible - at least one of them cannot be hidden.</p> |

3.9 Window

This is an entry point to a submenu of commands for displaying other main windows.

| | |
|---|--|
| Main <small>✓ Full version</small> | Displays the Clarity main station window described on pg. 1 . |
| Instrument | Displays the Instrument window described on pg. 59 . |
| Calibration | Displays the Calibration window described on pg. 313 . |
| Single Analysis | Displays the Single Analysis window described on pg. 108 . |
| Sequence | Displays the Sequence window described on pg. 382 . |
| Data Acquisition | Displays the Data Acquisition window described on pg. 366 . |
| Device Monitor | Displays the Device Monitor window described on pg. 128 . |
| Station Audit Trail <small>✓ Full version</small> | Displays the Audit Trail window described on pg. 411 . |
| Chromatogram Audit Trail <small>✓ Full version</small> | Displays the Chromatogram Audit Trail window described on pg. 424 . |

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 opened calibration file. The *Compounds* tab contains the main calibration table and graph area for the calibration standard chromatogram. The [Individual Compound](#) tabs contain a table for the displayed compound, several parameters and its calibration curve.

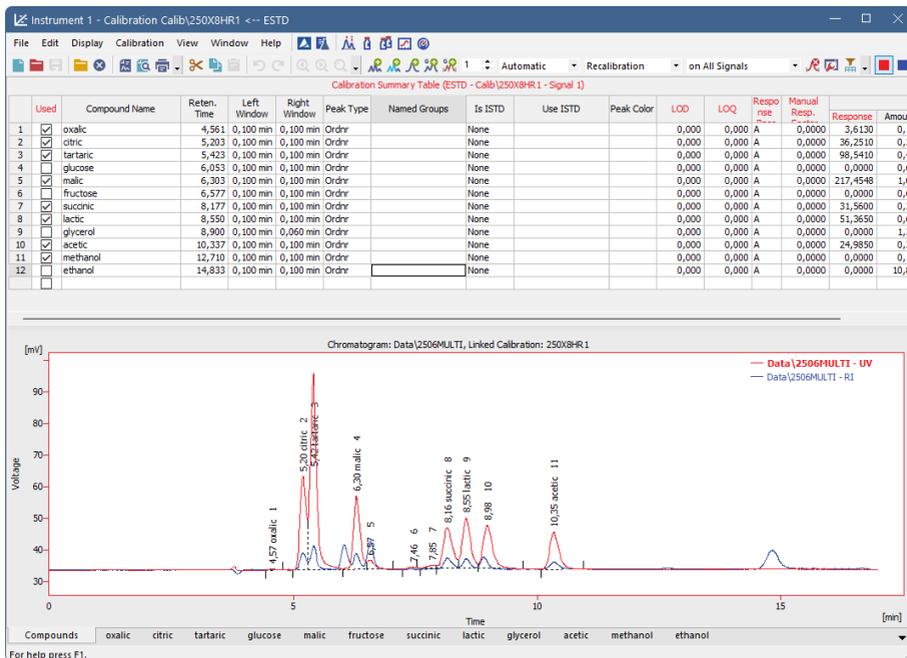


Fig. 188: Calibration - Compounds

4.1 Compounds tab

Overview tab that contains Notification area, Calibration Summary Table and a view of the standard chromatogram.

4.1.1 Notification area

The area above **Calibration Summary Table** contains some basic information on the opened calibration file (calibration name, the display mode and the active signal). Below the information on the table is an area where warning messages appear if something is not set correctly in the calibration file. Up to two lines are reserved for the

warning messages, if more messages should be displayed, they are signaled by ... sign at the end of the last line and can be viewed in a tooltip over the notification area.

Note: Not all problems of the calibration have warning messages at the moment, further warnings will be added in future versions.

4.1.2 Calibration Summary Table

The *Calibration Summary Table* provides an overview of all compounds across all signals. Any row corresponds to one compound or group of compounds. Some columns, such as *Compound Name* and *Reten. Time*, are shared across all signals, while others are specific to the currently active signal and are displayed in its color. Additionally, some of these signal-specific columns apply only to the currently displayed calibration level.

In the table below, there is description of each column present in the *Calibration Summary Table*:

| Column | Description | Applies To |
|-------------|--|---------------|
| | <p>Row header with the numbering of compound according to retention time.</p> <p>A double-click on the row header switches the view to the tab of the corresponding compound.</p> | All signals |
| Used | <p>Controls whether a compound is included in quantification and calibration – only compounds with the Used checkbox checked will be (re)calibrated, while unchecked compounds are excluded.</p> <p>If multiple compounds share the same retention time on a single signal, only one of them can have the Used checkbox checked; otherwise, a warning message is displayed.</p> <p>This column is especially useful in multi-detector chromatograms, where each compound is assessed on one signal and can be hidden from the results table for the remaining signals using this selector.</p> | Active signal |

| Column | Description | Applies To |
|----------------------------|---|-------------|
| Compound Name | <p>Name of the compound.</p> <p>If a compound is added from a standard chromatogram (either using commands like <i>Add All</i> in the <i>Calibration</i> window or automatically after measuring a standard chromatogram) it is named "Peak [retention time]" by default. If a new compound is created directly in the table (e.g., by filling in Retention Time), no default name is pre-filled.</p> | All signals |
| Reten. Time | Retention time of the compound. It is used for compound identification. | All signals |
| Search Window | <p>Defines whether the search window for a compound is specified in absolute values (<i>Abs</i>, set in minutes) or relative values (<i>Rel</i>, set as a percentage of the retention time).</p> <p>When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab. This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | All signals |
| Left (Right) Window | <p>Defines the width of the left (right) window for identification of compounds.</p> <p>At any given time point, only one <i>Search Window</i> can be applied. If multiple search windows are set to overlap, they will be shortened accordingly. This shortening is not reflected in the table.</p> <p>When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab.</p> | All signals |

| Column | Description | Applies To |
|------------------------------|---|--------------------|
| <p>Peak Selection</p> | <p>Determines how the peak is identified when multiple peaks appear within the identification window. The available options are:</p> <ul style="list-style-type: none"> • <i>Nearest</i> – Selects the peak closest to the expected retention time (default for standard peaks). • <i>First</i> – Selects the first peak in the window. • <i>Last</i> – Selects the last peak in the window. • <i>Biggest</i> – Selects the peak with the highest response (default for reference peaks). <p>The <i>Peak Selection</i> setting is ignored if a peak is manually linked to a compound in the calibration using the <i>Force Peak Name</i> function in the <i>Chromatogram</i> window. For more details see the chapter Peak on pg. 231. This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | <p>All signals</p> |

| Column | Description | Applies To |
|-----------|--|-------------|
| Peak Type | <p>Specifies the type of the calibrated compound. This column is shared across all signals and defines whether the entry is treated as an individual peak or a group.</p> <p>Individual Peaks</p> <p>Individual peaks represent single compounds identified as a distinct peak in the chromatogram. These types can be switched between each other at any time. The available types are:</p> <ul style="list-style-type: none"> • <i>Ordnr</i> – A standard peak that is not a reference peak (assigned by default to new compounds). • <i>Refer</i> – A reference peak used to adjust retention times. The retention times of all other peaks are interpolated based on the time shift of the reference peak. If a peak is located between two reference peaks, its shift is determined by the interpolated shift of both reference peaks. For more details, see <i>Using Reference Peak</i> topic in the User Guide. <p>Groups</p> <p>Groups represent a collection of peaks that are treated as a single unit. The available types are:</p> <ul style="list-style-type: none"> • <i>Grp_X</i> – A standard group created in the <i>Chromatogram</i> window, which can later be included in the calibration. The <i>Peak Type</i> consists of Grp_ followed by a letter (A-Z) identifying the group from the standard chromatogram. • <i>Named_Grp</i> – A named group consisting of selected peaks already present in the Calibration Summary Table. <p>Once a group is created in the <i>Calibration Summary Table</i>, its <i>Peak Type</i> cannot be changed. Additionally, individual peaks (<i>Ordnr</i> or <i>Refer</i>) cannot be converted into groups, and groups cannot be changed into individual peaks.</p> | All Signals |

| Column | Description | Applies To |
|---------------------|--|-------------|
| Named Groups | A column for managing <i>Named Groups</i> . If a <i>Named Group</i> is defined, the corresponding row contains an <i>Edit...</i> button, allowing you to modify which compounds belong to it. For individual compounds, this column displays the <i>Named Group</i> they are assigned to. | |
| Is ISTD | Indicates whether the given compound is an Internal Standard (ISTD) peak and assigns an ISTD peak number. Up to 10 compounds in the calibration file can be marked as internal standards. Groups cannot be assigned as ISTD peaks. This setting is applied only if <i>Calculation</i> is set to <i>ISTD</i> in the Chromatogram window for the evaluated chromatograms. | All signals |
| Use ISTD | Specifies which Internal Standard (ISTD) peak is used for the calculation of a given compound. When the first ISTD peak is selected in the <i>Is ISTD</i> column, the <i>Use ISTD</i> column for all other compounds is automatically set to this peak. If a peak is set as ISTD, it cannot <i>Use ISTD</i> peak for calculation. Group (<i>Grp_X</i>) can <i>Use ISTD</i> for calculations. This setting is applied only if <i>Calculation</i> is set to <i>ISTD</i> in the Chromatogram window for the evaluated chromatograms. | All signals |
| Peak Color | Sets the color used to highlight the peak area in the chromatogram. | All signals |
| Reten. Index | Used to enter known Retention (Kováts) Indexes for certain compounds. In the evaluated chromatogram, retention indexes for other compounds are then calculated based on the calculation method set in Calibration Options – Log. Interpolation with Unretained Peak, and the specified <i>Unretained Time</i> . For more details, see <i>How to use Kováts Reten. Indexes</i> topic in the User Guide. This column is hidden by default, For more details see the chapter Setup Columns on pg. 193. | All signals |

| Column | Description | Applies To |
|----------------------------|--|---------------|
| LOD | Limit of Detection (LOD). Used to enter the known Limit of Detection (LOD) for this compound using this method. In the evaluated chromatogram, if the compound is below the detection limit, "< LOD" is displayed in the <i>Peak Type</i> field. | Active signal |
| LOQ | Limit of Quantification (LOQ). Used to enter the known Limit of Quantification (LOQ) for this compound using this method. In the evaluated chromatogram, if the compound is below the quantification limit, "< LOQ" is displayed in the <i>Peak Type</i> field. | Active signal |
| Response Base | Defines what should be used as the <i>Response</i> for the given compound. Options are <i>H</i> (Height), <i>A</i> (Area), <i>P</i> (Area Percent). See Quantification section for more details. When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab. | Active signal |
| Manual Resp. Factor | Used to enter the factor for calculating results for the compound when the <i>Curve Fit Type</i> is set to <i>Free Calibration</i> . It serves as a simple single-point calibration. If <i>Free Calibration Curve Fit Type</i> and <i>Manual Response Factor</i> is set, the entered <i>Amount</i> value for the compound will not be used. In the evaluated chromatogram, the amount is calculated as the response of the peak multiplied by this coefficient. | Active signal |
| Correction Factor | Used to enter a correction factor for <i>Amount</i> , for example, to account for lower recovery. The <i>Amount</i> - whether entered directly, derived from another compound using <i>Calculate By</i> , or calculated from <i>Manual Response Factor</i> based on the response - is multiplied by the <i>Correction Factor</i> to obtain the final <i>Amount</i> . This column is hidden by default, For more details see the chapter Setup Columns on pg. 193. | Active signal |

| Column | Description | Applies To |
|-----------------------|---|---------------|
| Calculate By | <p>Sets a compound whose <i>Calibration Curve</i> will be used for <i>Amount</i> calculation of a given compound in the evaluated chromatogram. Only compounds already added to the calibration can be selected. <i>Named Groups</i> cannot be selected as the <i>Calculate By</i> parameter. A calibration curve constructed with entered Amount and Response values for the compound, that is set to be Calculated By another one will not be used.</p> <p>Do not use <i>Calculate By</i> in combination with ISTD calculations. For ISTD peaks, <i>Calculate By</i> is ignored. For peaks calculated with ISTD, applying <i>Calculate By</i> may lead to unexpected results.</p> <p>This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | All signals |
| Curve Fit Type | <p>Determines the type of the curve used to fit the data. See Quantification section for more details.</p> <p>When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab. This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | Active signal |
| Origin | <p>Specifies the method for including origin zero point into the calibration curve. See Quantification section for more details.</p> <p>When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab. When a valid Blank level is added this option is automatically changed to <i>Ignore Origin</i> for given compound. In case of conflicting setting warning is displayed above the table.</p> <p>This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | Active signal |

| Column | Description | Applies To |
|-------------------------|--|---------------|
| Ending Point | <p>Specifies the maximum interpolation of <i>Sigmoid</i> and <i>Half Sigmoid Curve Fit Type</i>. See Quantification section for more details.</p> <p>This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | Active signal |
| Weighting Method | <p>Determines the value of the weight of individual points when calculating the interposing curve. See Quantification section for more details.</p> <p>When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab. This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | Active signal |
| Linearization X | <p>Sets the X-axis linearization for the calibration curve calculation. See Quantification section for more details.</p> <p>When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab. This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | Active signal |
| Linearization Y | <p>Sets the Y-axis linearization for the calibration curve calculation. See Quantification section for more details.</p> <p>When a new compound is added, the default value is pre-filled based on the Calibration Options - Defaults tab. This column is hidden by default, For more details see the chapter Setup Columns on pg. 193.</p> | Active signal |

| Column | Description | Applies To |
|--------------------|---|-------------------------------|
| Level X | <p>The Level header groups multiple columns related to a specific calibration level. The calibration table consists of 20 standard levels plus a <i>Blank</i> (BL) level. The <i>Blank</i> (BL) level has <i>Amount</i> set to "BLANK" and is treated as a zero-level reference.</p> <p>Each level must be filled separately, and values are displayed according to the level number in the header.</p> <p>In Standard Addition <i>Display Mode</i> (STDADD), the first standard level is transformed into the <i>Unknown</i> level, with <i>Amount</i> set to "UNKNOWN".</p> | - |
| Response | <p>Represents the signal intensity used for quantification, based on the selected Response Base. The Response value is read from the standard chromatogram during the (re)calibration process.</p> <p>Manual adjustment of <i>Response</i> is possible unless disabled in Calibration Options. If a compound's response is manually modified at any level that includes at least one recalibration, the entire recalibration history for that calibration point will be cleared. A warning message will appear before proceeding.</p> | Active signal on active level |
| Amount | <p>Amount of the compound at the selected level, in units specified in Calibration Options dialog. If the Amount or Response of a calibration level (1–20) is 0, the calibration point is not created.</p> | All signals on active level |
| Resp. Fact. | <p>Response coefficient for each level. See Individual Compound Table section for more details.</p> | Active signal on active level |
| Rec No. | <p>Shows number of used recalibrations to number of total recalibrations on the level displayed. See Individual Compound Table section for more details.</p> | Active signal on active level |

| Column | Description | Applies To |
|---------------------|---|-------------------------------|
| Lin Response | Displays calculated value of <i>Response</i> ; the calculation is based on the option selected in <i>Linearization Y</i> . This column is hidden by default, For more details see the chapter Setup Columns on pg. 193 . | Active signal on active level |
| Lin Amount | Displays calculated value of <i>Amount</i> ; the calculation is based on the option selected in <i>Linearization X</i> . This column is hidden by default, For more details see the chapter Setup Columns on pg. 193 . | Active signal on active level |

4.1.3 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 compounds that have the Used checkbox disabled.

Note: Warning is displayed above the Calibration Summary Table when rows are hidden. Clicking *Show all* disables filtering.



Fig. 189: Filtering ON warning

4.1.4 Graph of the calibration standard

This section displays the chromatogram loaded using the *File – Open Standard* command. Its name is shown above the chromatogram, along with information about the linked calibration file.

The view facilitates the transfer of retention times and responses from the chromatogram to the calibration table. It follows the display settings from *User Options*, except for the *Peak Area Coloring* setting, which is ignored.

Peak Color remains visible regardless of display settings if a color is set in the calibration and the calibration is linked to the standard chromatogram. This can also be done directly in this window using the *Link Calibration to Standard* command.

4.2 Calibration - Individual Compound tabs

The *Individual Compound* tabs contain a table for the displayed compound, several parameter sections, and its calibration curve.

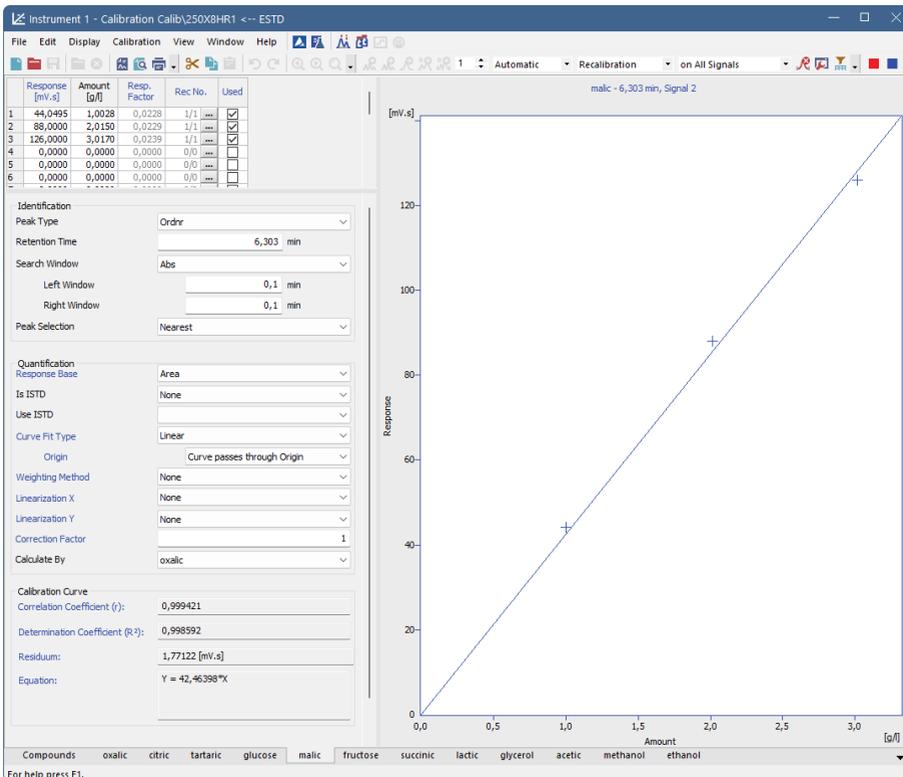


Fig. 190: Calibration - Individual Compound (malic)

4.2.0.1 Compound Table

The table is located in the top left corner of the individual compound tab. It contains a row for each calibration level, including up to 20 standard levels and the Blank (BL) level. The first column displays the level number, while the remaining columns represent the level-specific parameters for the given compound.

First column

Contains the level number of each displayed line.

Response

Represents the signal intensity used for quantification, based on the selected Response Base. The Response value is read from the standard chromatogram during

the (re)calibration process. Manual adjustment of Response is possible, but this option can be disabled in [Calibration Options](#).

Amount

Amount of the compound at the selected level, in units specified in [Calibration Options](#) dialog. If the Amount or Response of a calibration level (1–20) is 0, the calibration point is not created.

Response Factor

The Response Factor at a given level is defined as the reciprocal of the slope of a straight line passing through the origin and the calibration point at that level. It is calculated automatically and cannot be manually edited. By default, it is determined as Amount / Response:

$$LRF_i = \frac{A_i}{R_i}$$

where:

A_i - Amount of the compound at level i .

R_i - Response (height or area) at level i .

The calculation can be switched to the inverse form (Response / Amount) by enabling the Response Factor as Response / Amount option in [Calibration Options](#).

Rec No.

Indicates how many recalibrations with the Used checkbox enabled are included in the calibration, out of the total number of stored recalibrations for the given level. Clicking  opens the [Details of Calibration Point](#) dialog, where you can view and manage individual recalibrations.

The total number of stored recalibrations is limited by the *No. of Points* setting in the [Recalibration](#) section of *Sequence Options*. If this limit is reached, adding a new recalibration permanently deletes the oldest one.

Used

Determines whether a calibration level is included in the calibration curve. If the checkbox is cleared, the level is omitted from the calibration curve and is represented by a circle in the graph.

Deviation [%]

Represents the deviation of the entered Amount of the calibration point from the calculated Amount given by the calibration curve. This column is hidden by default. For more details see the chapter **Setup Columns** on pg. 193.

$$\text{Deviation}[\%] = \left(\frac{\text{Amount} - \text{Amount}_C}{\text{Amount}_C} \right) \times 100$$

where:

Amount - The entered Amount at the concentration level.

Amount_C - The Amount calculated from the constructed calibration curve for the given concentration level.

RSTD [%]

Displays the relative standard deviation (RSD) of the averaged recalibrations used for the respective concentration level. This column is hidden by default, For more details see the chapter **Setup Columns** on pg. **193**.

Lin Response

Displays the calculated *Response* value, determined based on the option selected in *Linearization* Y. This column is hidden by default, For more details see the chapter **Setup Columns** on pg. **193**.

Lin Amount

Displays the calculated *Amount* value, determined based on the option selected in *Linearization* X. This column is hidden by default, For more details see the chapter **Setup Columns** on pg. **193**.

4.2.0.2 Local menu of the Compound Table

In addition to the common commands for the majority of tables, the local menu contains the following items:

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

Opens the [Details of Calibration Point](#) dialog, where you can view and manage individual recalibrations.

Identification section

A section containing parameters used to identify the peak belonging to the given compound.

Peak Type

Specifies the type of the calibrated compound. See [Calibration Summary Table](#) section for more details.

Retention Time

Retention time of the compound. It is used for compound identification.

Search Window

Defines whether the search window for a compound is specified in absolute values (*Abs*, set in minutes) or relative values (*Rel*, set as a percentage of the retention time).

Peak Selection

Determines how the peak is identified when multiple peaks appear within the identification window. See [Calibration Summary Table](#) section for more details.

Quantification section

A section containing parameters related to the quantification of the given compound.

Response Base

Sets which value will serve as Response. The Response is then used for calculating the calibration curve, calibration dependency equation, and response factors. This setting is specific to each signal. Available Options are:

- *Area* – Area is used as the response base.
- *Height* – Height is used as the response base. The height is measured as the vertical distance from the peak apex to the baseline, which may lead to imprecise values for small peaks on steep baselines.
- *Area Percent* – Calibration is based on the percentage of peak area relative to the total peak area of all compounds included in the calibration. This means that all relevant compounds must be added, even if their results are not needed. The recommended calculation type for this method is ESTD.

The selected Response Base affects other fields in the individual compound tabs and the calibration curve. Changing the Response Base will recalculate all dependent values accordingly.

Is ISTD

Indicates whether the given compound is an Internal Standard (ISTD) peak and assigns an ISTD peak number. See [Calibration Summary Table](#) section for more details.

Use ISTD

Specifies which Internal Standard (ISTD) peak is used for the calculation of a given compound. See [Calibration Summary Table](#) section for more details.

Curve Fit Type

Determines the type of curve used to fit the calibration data. If the number of available points is insufficient for the selected curve type, the curve is automatically changed to the next lower type, while the Curve Fit Type selection remains unchanged. In Standard Addition Display Mode, only the *Linear* curve fit is available, and the *Curve Fit Type* selection is disabled.

Curve Fit Types available are:

Free Calibration

No calibration curve is constructed. The calibration equation is in the form:

$$Y = \text{Manual Response Factor} \times \text{Correction Factor} \times X$$

Instead of values interpolated from a calibration curve, calculations use the global Response Factor from the global calibration table. That means the entered

Amount value for the compound will not be used. *Origin* parameter is replaced by *Manual Response Factor*, in the *Individual Compound* tabs.

Point to Point

Calibration points are connected by a broken line, with no common calibration equation. Instead, each segment's equation is used in calculations. The *Point to Point* fit type always includes the origin point (0,0) in the calibration curve, regardless of the *Origin* setting.

Linear

A straight line is fitted through the points.

Quadratic

A second-degree polynomial is used to interpolate the calibration curve.

Cubic

A third-degree polynomial is used to interpolate the calibration curve.

Sigmoid

A sigmoid function is used for curve fitting:

$$z = 2 \cdot \sqrt[b]{\frac{\text{Response}}{d}} - 1$$

$$\text{Amount} = c \cdot \sqrt[a]{\frac{1}{2} - \frac{1}{2k} \cdot \text{sign}(z) \cdot \ln(1 - \text{abs}(z) \cdot (1 - e^{-k}))}$$

where:

c – Maximum Amount

d – Maximum Response

b = 1, a, k – Coefficients optimized through iteration (<0, 1 – 100 >) to best fit the calibration points.

The Ending Point field allows increasing c and d up to 125% (both parameters change simultaneously).

Half Sigmoid

A variation of the sigmoid curve that represents only one half of the function.

Logarithmic Functions:

ln – Interpolates using a natural logarithm function.

log10 – Interpolates using a decimal logarithm function.

Exponential Functions:

exp – Fits an exponential curve.

pow10 – Fits a base-10 exponential curve.

Hyperbola

Uses a hyperbolic function for interpolation.

Origin

Specifies how the zero point (origin) is handled in the calibration curve. This setting is individual for each signal. Available Options are:

- *Ignore Origin* – The origin is not included in the calibration curve. This is the only option where Blank level is included in calibration curve construction.
- *Compute with Origin* – The origin is treated as one of the calibration points. Blank level is ignored with this option.
- *Curve passes through Origin* – The calibration curve is forced to pass through the origin. Blank level is ignored with this option.

In Standard Addition Display Mode, blank is never used for construction of the curve. The Origin field is replaced by the *Unknown* field, which has the same options:

- *Ignore Unknown* – The Unknown point is not included in the calibration curve.
- *Compute with Unknown* – The Unknown point is treated as one of the calibration points.
- *Curve passes through Unknown* – The calibration curve is forced to pass through the Unknown point.

When using the Sigmoid curve fit, the Origin field is replaced by the Ending Point field.

Ending Point

This setting is only applicable when the *Curve Fit Type* is set to *Sigmoid* or *Half Sigmoid*. It allows the sigmoid interpolation to extend beyond the last calibration point. The last calibration point is taken as the limit value, and both its *Amount* (X-coordinate) and *Response* (Y-coordinate) can be increased by a selected percentage according to the *Ending Point* setting.

The available options range from *Last Point* (using the last calibration point as the limit) to *Last Point + 25%* (extending both coordinates by 25%).

This setting is useful when measuring calibration points within a sufficient range is not possible.

Manual Response Factor

Used to enter the factor for calculating results for the compound when the *Curve Fit Type* is set to *Free Calibration*. It serves as a simple single-point calibration.

In the evaluated chromatogram, the amount is calculated as the response of the peak multiplied by this coefficient.

Weighting Method

Determines how individual calibration points are weighted when calculating the interpolated calibration curve.

By default, higher concentration points (with larger Amount and Response) have a greater influence on the calibration curve than lower concentration points. This method helps improve calibration accuracy, especially when dealing with wide concentration ranges.

Weighting allows adjusting this influence:

- $1/x$ – Assigns the same relative influence to each point.
- $1/x^2$ – Gives greater influence to lower concentration points.

Weighting can be applied based on:

- *Amount* – The amount of the compound at the given calibration point ($1/Amount$ or $1/Amount^2$).
- *Response* – The response of the compound at the given calibration point ($1/Response$ or $1/Response^2$).

Linearization X

Applies a transformation to the X-axis values (*Amount*) using the selected formula before calculating the calibration curve equation. This affects only the calibration curve equation itself, not how the curve is displayed. The X-axis and calibration points remain shown with their original (non-linearized) values, meaning the visual representation of the curve does not correspond to the linearized X-axis values, the modified calibration equation, or the linearized calibration points.

To display the curve according to the transformed equation and linearized calibration points, the *Show Linearized Values* checkbox must be enabled in the [Graph Properties](#) dialog.

Available Linearization Formulas:

- *None* – No linearization is applied.
- $1/Amount$ – Uses the reciprocal of the Amount.
- $\ln(Amount)$ – Applies the natural logarithm to the Amount.
- \sqrt{Amount} – Uses the square root of the Amount.
- $1/\sqrt{Amount}$ – Uses the reciprocal of the square root of the Amount.
- $Amount^2$ – Squares the Amount.
- $1/(Amount^2)$ – Uses the reciprocal of the squared Amount.

Linearization Y

Applies a transformation to the Y-axis values (*Response*) using the selected formula before calculating the calibration curve equation. This affects only the calibration curve equation itself, not how the curve is displayed. The Y-axis and calibration points remain shown with their original (non-linearized) values, meaning the visual representation of the curve does not correspond to the linearized Y-axis values, the modified calibration equation, or the linearized calibration points.

To display the curve according to the transformed equation and linearized calibration points, the *Show Linearized Values* checkbox must be enabled in the [Graph Properties](#) dialog.

Available Linearization Formulas:

- *None* – No linearization is applied.
- $1/Response$ – Uses the reciprocal of the Response.
- $\ln(Response)$ – Applies the natural logarithm to the Response.
- $\sqrt{Response}$ – Uses the square root of the Response.
- $1/\sqrt{Response}$ – Uses the reciprocal of the square root of the Response.
- $Response^2$ – Squares the Response.

- $1/(\text{Response}^2)$ – Uses the reciprocal of the squared Response.
- $\log(\text{Response})$ – Applies the base-10 logarithm to the Response.

Correction Factor

Used to enter a correction factor for *Amount*, for example, to account for lower recovery. The *Amount* - whether entered directly, derived from another compound using *Calculate By*, or calculated from *Manual Response Factor* based on the response - is multiplied by the *Correction Factor* to obtain the final *Amount*.

Calculate By

Sets a compound whose *Calibration Curve* will be used for *Amount* calculation of a given compound in the evaluated chromatogram. See [Calibration Summary Table](#) section for more details.

4.2.0.3 Calibration Curve section

This section displays calculated parameters of the calibration curve, including the calibration equation and other derived values. All values in this section are computed based on the settings and data entered in the previous sections. These parameters are read-only and cannot be modified directly.

Correlation Coefficient (r)

Represents a value in the range <0, 1> that characterizes the linearity of data. The value is only relevant if the *Curve Fit Type* is set to *Linear*. In all other cases, the value is displayed but does not reflect the quality of the calibration curve.

$$r = \sqrt{\frac{\left(\sum(x_i - X) \cdot (y_i - Y)\right)^2}{\sum(x_i - X)^2 \cdot \sum(y_i - Y)^2}}$$

where:

x_i - The actual (measured) response at level i .

y_i - The calculated (predicted) response at level i .

X - The mean of all actual responses (including the zero point if *Compute with Origin* or *Curve passes through Origin* is selected, Blank level is ignored when one of these options is selected).

Y - The mean of all calculated responses (including the zero point if *Compute with Origin* or *Curve passes through Origin* is selected, Blank level is ignored when one of these options is selected).

Determination Coefficient (R²)

Also referred to as coefficient of determination. It describes how well the independent variable(s) explain the variability of the dependent variable.

$$R^2 = 1 - \frac{\sum(x_i - y_i)^2}{\sum(x_i - X)^2}$$

where:

x_i - The actual (measured) response at level i .

y_i - The calculated (predicted) response at level i .

X - The mean of all actual responses (including the zero point if *Compute with Origin* or *Curve passes through Origin* is selected, Blank level is ignored when one of these options is selected).

Residuum

Represents the calibration curve fit residuum, which quantifies the average deviation of actual responses from the calculated calibration curve. A lower value indicates a better fit, meaning the calibration points closely follow the curve.

$$\text{Residuum} = \sqrt{\frac{1}{n} \cdot \sum((x_i - y_i) * w_i)^2}$$

where:

n - The number of calibration points (including the zero point if *Compute with Origin* or *Curve passes through Origin* is selected, Blank level is ignored when one of these options is selected).

x_i - The actual (measured) response at level i .

y_i - The calculated (predicted) response at level i .

w_i - Weighting coefficient calculated based on selected *Weighting Method*. It is not used when *Weighting Method* is set to *None* or in cases that would result in dividing by zero e.g., when using *Compute with Origin* and *1/Response* weighting the w_i is not applied for the origin point, it is apply only for all remaining ones.

This value helps assess how well the calibration curve represents the measured data.

Equation

Displays the equation of the calibration curve, which defines the relationship between *Response* and *Amount* based on the selected *Curve Fit Type*. This equation is used to calculate the *Amount* of an unknown sample from its measured *Response*.

The displayed equation provides a mathematical representation of the calibration curve, ensuring consistent quantification of unknown samples.

Note: In case the calibration curve of the compound cannot be constructed because the relevant information is missing (e.g. ISTD peak has no response on any level or is disabled), a warning is displayed instead of the *Equation (ISTD peak unavailable in the mentioned case)*.

Curve Check

Displays the calibration curve linearity check result, performed only if enabled in [Calibration Options](#). To activate the check, enable Deviation and/or Correlation and set the corresponding limits.

The result can be:

- *OK* – The calibration curve meets the selected Deviation and/or Correlation criteria.
- *Error* – At least one of the applied Curve Check tests has failed.

If failed, it is also indicated in evaluated chromatograms in the Chromatogram window (Peak Type column as Error (Curve Check)).

4.2.0.4 Calibration curve graph

The calibration curve for each compound is displayed in the right-hand section of the compound tab. It represents the relationship between Amount and Response.

Name of Compound and Retention Time

Displayed above the graph, this section contains identifying data for the compound, including its *Compound Name*, *Retention Time*, and the *Name of the active signal*.

Graph Overview

The graph shows calibration points for the selected compound along with the calibration curve. Its appearance can be modified using the [Graph Properties](#) dialog.

Graph Symbols and Interpretation

- Calibrated points (levels with only a single calibration value) are displayed as crosses ⑤ .
- Recalibrated points (levels with multiple recalibrations) are displayed as asterisks ⑥ , with a range indicating the recalibration span.
- If the *Used* checkbox is unchecked ① for the entire level in the *Compound Table*, the calibration level is excluded from the calibration curve and displayed as a large circle ② .
- If a single recalibration is excluded from the calibration point calculation by unchecking the *Used* checkbox ③ in the [Details of Calibration Point](#) dialog, it is displayed as a small circle ④ .

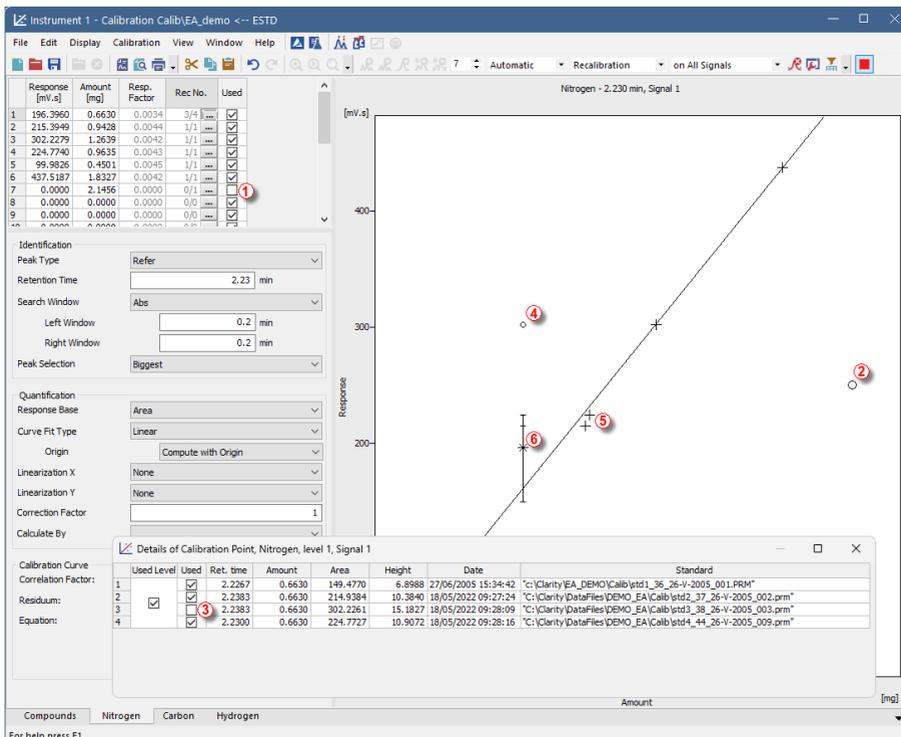


Fig. 191: Representation of different points in the graph

Standard Addition (STDADD) Calibration Curve

In the STDADD calibration type, the Blank sample is represented as a vertical line with a multiplication cross sign. This indicates that the sample amount is not determined from the intersection of the calibration curve with the X-axis at zero response, but rather from the intersection of the calibration curve with the blank horizontal line.

Internal Standard (ISTD) Calibration Curve

When using the ISTD method, the calibration curve is displayed as a relative calibration curve, depending on whether the same or a different amount of the internal standard was used:

- Same Amount of Internal Standard

The relative calibration curve represents the dependence of the response ratio of the compound and the internal standard on the amount of the compound injected:

$$\frac{R_i}{R_{ISTD}} = f(A_i)$$

R_i - Response of the compound

R_{ISTD} - Response of the internal standard

A_i - Amount of the compound

- Different Amount of Internal Standard

The relative calibration curve represents the dependence of the response ratio of the compound and the internal standard on the ratio of their respective amounts:

$$\frac{R_i}{R_{ISTD}} = f \frac{(A_i)}{A_{ISTD}}$$

R_i - Response of the compound

R_{ISTD} - Response of the internal standard

A_i - Amount of the compound

A_{ISTD} - Amount of the internal standard

4.3 File

This is an entry point to a *File* menu of commands for working with calibration files:

| Icon | Command | Description |
|---|--|--|
|  | New | <p>Creates a new calibration file and simultaneously closes the currently opened file (a warning appears if there are unsaved changes). This action can also be triggered using the Ctrl + N shortcut.</p> <p>The new calibration file will be based on the template calibration (TEMPLATE.CAL) located in the COMMON directory (C:\CLARITY\DATAFILES\COMMON\ by default).</p> |
|  | Open | <p>Opens a calibration file and simultaneously closes the currently open file (a warning appears if there are unsaved changes). Using this command or pressing the Ctrl + O shortcut brings up the <i>Open Calibration</i> dialog.</p> |
|  | Save | <p>Saves the current calibration file. This command can also be triggered using the Ctrl + S shortcut.</p> <p>If saving a new file for the first time, the Save As dialog will appear, requiring a file name to be specified. The default name NONAME.CAL is reserved for new unsaved files only.</p> |
|  | <u>Save As</u> | <p>Saves the calibration file under a chosen name. This command can also be triggered using the Ctrl + Shift + S shortcut.</p> <p>If the selected file name already exists, a confirmation message appears before the file is overwritten.</p> |
| | <u>Send Calibration by email</u> | <p>Creates a new email in the default email client with the currently displayed calibration file attached.</p> |

| Icon | Command | Description |
|---|--------------------------------------|--|
|  | Open Standard | Opens a chromatogram in the <i>Standard</i> section of the <i>Calibration</i> window. This command brings up the <i>Open Chromatogram</i> dialog, which by default displays the <i>Calib</i> subdirectory. This action does not directly affect the calibration (only sets the number of signals according to chromatogram) but allows the chromatogram to be used for calibration or recalibration. |
|  | Close Standard | Closes the currently displayed calibration standard. |
| | Open Standard as Chromatogram | Opens the <i>Standard</i> in the <i>Chromatogram</i> window. This option is available only if a <i>Standard</i> is currently opened. |
| | Link Calibration To Standard | Links the currently opened calibration to the currently opened standard chromatogram. This enables the display of peak names as defined in the calibration file. This option is available only if the opened standard chromatogram is editable. |
| | Export | Displays the following export commands, available only in the Individual Compound tabs: <ul style="list-style-type: none"> • <i>Export Calibration Curve as Picture to Clipboard</i> – Copies the calibration curve image to the clipboard, allowing it to be pasted into other applications using the standard <i>Paste</i> command (Ctrl + V). This is useful for quickly inserting the image into spreadsheet or word-processing software. • <i>Export Calibration Curve as Picture...</i> – Opens the <i>Save As</i> dialog to save the calibration curve image as an Enhanced Metafile Format (.emf) file. This format is widely supported by Microsoft Windows and Microsoft Office. Both commands are also available from the context menu by right-clicking in the calibration curve area. |

| Icon | Command | Description |
|---|---|---|
|  | Report Setup | Opens the Report Setup dialog. This command can also be triggered using the Ctrl + Alt + P shortcut. |
|  | Print Preview | Displays a preview of the printout before actual printing. Using this command or pressing the Ctrl + Shift + P shortcut opens the <i>Print Preview</i> dialog. |
|  | Print to PDF | Prints the report to a *.PDF file. The Print to PDF dialog appears, allowing you to set the file name and destination. By default, the file is saved in the same folder as the calibration file. The default <i>Print to PDF</i> location is set in the Directories tab of the <i>User Options</i> dialog. |
|  | Send Printed PDF by Email | Creates a new email in the default email client, prints the report to a *.PDF file, and attaches the generated file to the email. |
|  | Print | Sends the report to a selected printer. Using this command or pressing the Ctrl + P shortcut opens the <i>Print</i> dialog. |
| ----- | | Displays a list of recently opened files for quick access. The number of files shown is determined by the <i>Recent Files</i> setting in the General tab of the <i>User Options</i> dialog. |
| | Close Window | Closes the Calibration window along with all open files. If the calibration file has unsaved changes, a prompt appears asking whether to save them before closing. |

4.3.1 Save As Calibration

The dialog is opened by the *File - Save As...* command or the **Ctrl** + **Shift** + **S** shortcut in the *Calibration* window. It saves the opened calibration file under a newly desired name or to a new selected directory. The dialog is very similar to the generic [Save As](#) dialog.

If you attempt to overwrite an existing file, a warning message appears. The ability to overwrite files can be disabled in [GLP Options](#). Additionally, a file that is currently open elsewhere cannot be overwritten.

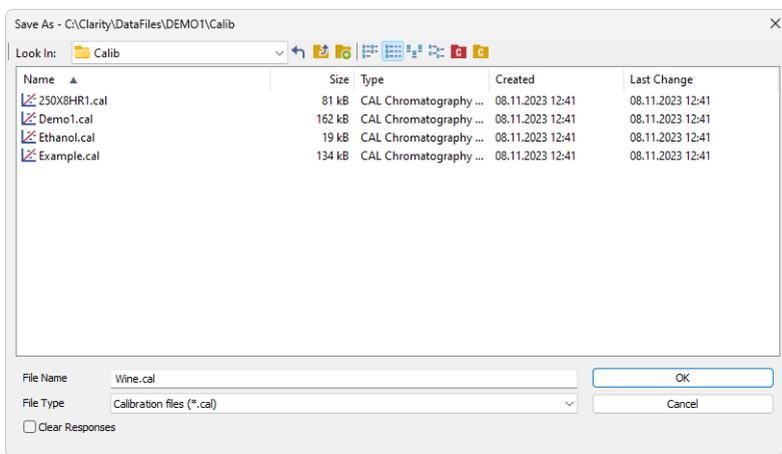


Fig. 192: Save As Calibration

Clear Responses

The *Clear Responses* checkbox enables to clear all responses in the new calibration file.

4.4 Edit

Commands for working with the clipboard and individual tables.

| Icon | Command | Description |
|---|----------------------------------|---|
|  | Undo | Cancels the changes done in tables (shortcut Ctrl + Z). |
|  | Redo | Reverts the last <i>Undo</i> command (shortcut Ctrl + Shift + Z). |
|  | Cut | Moves the selected text to the clipboard (shortcut Ctrl + X). |
|  | Copy | Copies the selected text to the clipboard (shortcut Ctrl + C). |
|  | Paste | Pastes the clipboard content to the indicated place (shortcut Ctrl + V). |
| | Fill Down | Copies the content of the current cell to all directly below it or to a selected range of cells in the same column. This command can also be triggered using the Ctrl + F shortcut. <i>Fill Down</i> only works when the selected range consists of consecutive cells in a single column. |
| | Fill Series... | Opens the <i>Fill Series</i> dialog, allowing incremental values to be filled into all cells below the current one or within the selected range. <i>Fill Series</i> can be used in most input fields where values can be freely entered, except for predefined selection fields such as <i>Peak Type</i> , <i>Use ISTD</i> , and <i>Curve Fit Type</i> . |
| | Select All | Selects all cells in the table (Ctrl + A). |
| | Restore Default columns | Resets all columns to their default settings. This restores the default column widths, displays only the default visible columns, and hides the rest. |
| | Setup Columns... | Using this command invokes the Setup Columns dialog, where you can set the display of columns. |
| | Hide Column(s) | Hides the selected columns. Columns can be selected by left-clicking on the column header, and multiple columns can be selected by holding the Ctrl key while clicking. |
| | Show Hidden Column(s) | Shows all hidden columns. |

4.5 Display

The *Display* menu provides commands for adjusting the appearance of graphs and tables. It includes options for zooming, previewing graphs.

| Icon | Command | Description |
|---|----------------------|--|
| | Preview Graph | Displays or hides the preview graph, which appears above the <i>Standard Chromatogram Graph</i> . It always shows the entire chromatogram. When zooming in on the main graph, the <i>Preview Graph</i> highlights the currently visible section, helping with orientation. The command is also available in the context menu, accessed by right-clicking on the graph area. |
|  | Zoom Out | Zooms out the current view of the chromatogram. This command can also be triggered by pressing the  key. |
|  | Zoom In | Zooms in on the current view of the chromatogram. This command can also be triggered by pressing the  key. |
|  | Previous Zoom | Restores the previous chromatogram cut. (Ctrl + ) |
|  | Next Zoom | Restores the previous zoom level of the chromatogram. This command can also be triggered using the Ctrl +  shortcut. |
|  | Unzoom | Resets the zoom and displays the entire chromatogram. This command can also be triggered using the Ctrl +  . |
| | Tables Up | Swaps the placement of the <i>Calibration Summary Table</i> and the <i>Standard Chromatogram Graph</i> . When enabled (default setting), the table appears above the graph. When disabled, the graph moves to the top, and the table is displayed below. |
|  | Properties | Opens the Graph Properties dialog, which controls the appearance and display settings of graphs. The specific dialog depends on the active tab: <ul style="list-style-type: none"> On the Compounds tab, it opens the Graph Properties dialog for the Standard Chromatogram Graph which is based on the same dialog in the <i>Chromatogram</i> window On the Individual Compound tab, it opens the Graph Properties dialog for the calibration curve graph. <p>This command is also available from the context menu, accessed by right-clicking in the graph area.</p> |

4.5.1 Graph Properties

The Graph Properties dialog for the Calibration Curve Graph allows customization of the graph's appearance and display settings.

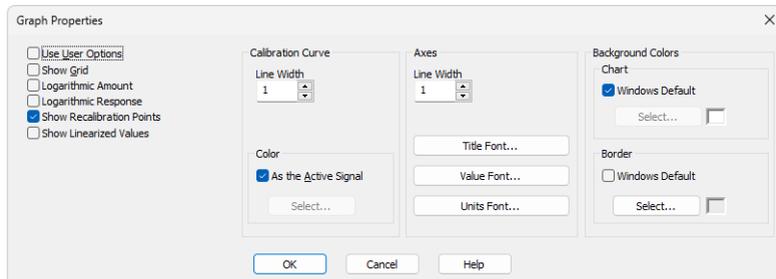


Fig. 193: Graph Properties

Use User Options

Applies global graph settings from the [User Options](#) instead of individual customization.

This option is also available from the context menu, accessed by right-clicking in the calibration curve area.

Show Grid

Displays/hides the grid in the calibration curve graph, helping with visual alignment and reading values more easily.

Logarithmic Amount

Switches the Amount axis to a logarithmic scale, changing how values are displayed and distributed along the axis.

Logarithmic Response

Switches the Response axis to a logarithmic scale, changing how values are displayed and distributed along the axis.

Show Recalibration Points

Displays/hides the spread of individual recalibrations for each calibration point. When disabled, only the averaged calibration point is displayed.

Show Linearized Values

Adjusts the axes and calibration curve in the graph to reflect the applied linearization. When Linearization X or Linearization Y is enabled for a compound, this option updates the graph to display values according to the recalculated calibration curve equation.

Calibration Curve

Line Width - Sets the thickness of the calibration curve in points.

Color - Defines the color of the calibration curve.

As the Active Signal - Uses the color of the currently active signal.

Select... - Opens a color selection dialog to choose a custom color.

Axes

Line Width - Sets the thickness of the axis lines in points.

Title Font... - Selects the font for the axis titles.

Value Font... - Selects the font for the numerical values displayed on the axes.

Units Font... - Selects the font for the units displayed on the axes.

Background Colors

Chart - Sets the background color of the graph (the area between the axes).

Windows Default - Uses the default system color.

Select... - Opens a color selection dialog to choose a custom color.

Border - Sets the background color outside the axes.

Windows Default - Uses the default system color.

Select... - Opens a color selection dialog to choose a custom color.

4.6 Calibration

Contains commands for managing calibration levels, signals, and compounds, including adding, deleting, clearing, and filtering calibration data.

| Icon | Command | Description |
|---|------------------------------|--|
| | Set Level | <p>Sets the calibration level displayed in the <i>Calibration Summary Table</i>, the same way as the tool in the <i>Calibration</i> toolbar.</p> <p>In the <i>Compounds</i> tab, all compounds appear at the chosen level, while individual compound tabs show all levels for the selected compound. The selected level is shown in the header above the last four columns.</p> |
| | Set Signal | <p>Selects the active signal when using multi-detector calibration. The sub-menu lists available signals, and the active one is displayed in the header of the <i>Calibration Summary Table</i> and next to the compound name and retention time in the <i>Calibration Curve Graph</i>.</p> <p>The signal can also be selected using the icon in the <i>Calibration</i> toolbar.</p> |
|  | Add All | Adds all peaks found in the open calibration standard to the calibration or updates their existing entries. |
|  | Add Existing | Adds/Updates all peaks and peak groups already present in the calibration using the data from the calibration standard. Peaks that are not yet in the calibration are ignored. |
|  | Add Peak | Adds the selected peak from the calibration standard to the calibration or updates its existing entry if a matching compound is already present. |
|  | Add Group | Adds or updates a group of peaks selected in the calibration standard into the calibration. |
|  | Add Named Group | Opens the Edit Named Group dialog to create a new named group in the Calibration Table. Named groups are used to sum the amounts of already calibrated peaks for reporting grouped results. |

| Icon | Command | Description |
|---|-----------------------------|---|
|  | Delete Compound | Deletes a selected compound from the calibration file. Compounds can also be deleted by removing the corresponding row from the <i>Calibration Summary Table</i> 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. A warning message will appear before executing the command to confirm this action. This command is also present in the <i>Calibration Summary Table</i> local menu. |
| | Clear All Responses | Clears responses on all calibration levels. A warning message will appear before executing the command, informing you that this action cannot be undone using the <i>Undo</i> command. |
| | Clear All Levels | Clears all responses and amounts on all calibration levels. If used in the <i>Compounds</i> tab, it removes data for all compounds. If used in an individual compound tab, it removes data only for the selected compound. A warning message will appear before executing the command, informing you that this action cannot be undone using the <i>Undo</i> command. |
| | Clear Selected Level | Clears all responses and amounts on the selected calibration level. If used in the <i>Compounds</i> tab, it removes data for all compounds on the selected level. If used in an individual compound tab, it removes data only for the selected compound on the selected level. A warning message will appear before executing the command, informing you that this action cannot be undone using the <i>Undo</i> command. |
| | Show Details | Opens the Details of Calibration Point dialog, displaying a detailed log of the selected calibration level of the compound, including all available recalibrations. |

| Icon | Command | Description |
|---|---|--|
|  | Filter Not Used Compounds | Hides or shows rows in the <i>Calibration Summary Table</i> (and related individual compound tabs) where the <i>Used</i> checkbox is disabled. A warning is displayed above the table when rows are hidden. Clicking <i>Show All</i> disables filtering. |
|  | Options... | Opens the Calibration Options dialog, where various calibration and recalibration settings, and default values can be configured. |

4.6.1 Add All

Adds all peaks from the calibration standard to the calibration, whether for a new calibration level or recalibration. Peaks are identified in the *Calibration Summary Table* based on retention time and identification windows, while groups are identified by a letter.

- *Existing Compound*: If a peak/compound already exists in the calibration within the given *Search Window*, it is identified, and its retention time (if enabled in [Calibration Options](#)) and *Response* are updated for the selected level.
- *New Compound*: If no matching compound is found, a new entry is created with the name *Peak - [Retention time]*. This command also adds new compounds to the calibration during a recalibration of a level.
- *On All Signals / On Active Signal*: Determines whether *Responses* are added to all signals or only to the active signal in the *Calibration Summary Table*. Peak identification is shared across all signals.
- *Automatic Calibration*: All compounds are added to the calibration, and *Responses* are assigned to the first available empty calibration level, regardless of the selected level. The selected level then automatically switches to the newly filled one.
- *Automatic Recalibration*: Compounds are recalibrated at the current level, with further adjustments possible later.
- *Manual Calibration or Recalibration*: The *(Re)Calibrate Peak* or *(Re)Calibrate Group* dialog appears for direct data verification and adjustments.

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

4.6.2 Add Existing

Updates peaks and peak groups that are already present in the calibration using the data from the calibration standard, updating their retention time (if enabled in [Calibration Options](#)) and filling in *Response*. Unlike *Add All*, this command does not introduce new compounds to the calibration. If no peaks are present in the calibration, the command is disabled.

- *On All Signals / On Active Signal*: Determines whether Responses are updated on all signals or only on the active signal in the *Calibration Summary Table*. Peak identification is shared across all signals.
- *Automatic Calibration*: All matching compounds are updated in the calibration, and *Responses* are assigned to the first empty available calibration level, regardless of the selected level. The selected level then automatically switches to the newly filled one.
- *Automatic Recalibration*: Compounds are recalibrated at the current level, with further adjustments possible later.
- *Manual Calibration or Recalibration*: The *(Re)Calibrate Peak* or *(Re)Calibrate Group* dialog appears for direct data verification and adjustments.

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

4.6.3 Add Peak

Adds the selected peak from the calibration standard to the calibration. If a matching compound is already present, its retention time (if enabled in [Calibration Options](#)) and Response are updated.

Invoking the *Add Peak* command or clicking the icon moves the cursor to the calibration standard graph, where the desired peak should be selected. Press **Esc** to cancel the command.

- *On All Signals / On Active Signal*: Determines whether the peak response is added on all signals or only on the active signal. Peak identification is shared across all signals.
- *Automatic Calibration*: When a new standard chromatogram is opened, *Add Peak* always assigns the peak to the first completely empty calibration level. As long as peaks are added from the same chromatogram, they are added to the last active level if they do not already have added responses here. A new calibration level is created if *Add Peak* is used on a peak that is already present on the last active level (even within the same chromatogram) or when a different chromatogram is opened.
- *Automatic Recalibration*: The peak/compound is added or updated at the current level, with further adjustments possible later.
- *Manual Calibration or Recalibration*: The *(Re)Calibrate Peak* dialog appears for direct data inspection and modifications.

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

4.6.3.1 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.

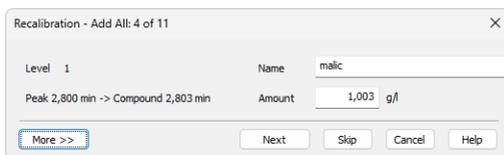


Fig. 194: Calibrate Peak

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. 195: 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* (M+ icon) command.

Cancel

Cancels calibration of the current compound and any remaining (if there are any).

4.6.3.1.1 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 .

4.6.3.1.2 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. 272)..

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.

4.6.3.1.3 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.

4.6.3.1.4 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.

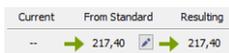


Fig. 196: Cut of Calibrate Peak dialog

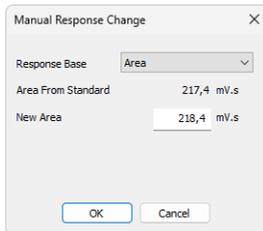
When performing calibration on a new level, the field *Current* will be empty. Field *From Standard* displays response for the given compound from the standard. *Resulting* field displays the new response which will be calibrated when the *OK* button is pressed.

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](#).



4.6.3.1.5 Calibrate Group/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* (📈^{G+}) 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 [\(Re\)Calibrate Peak](#) dialog.

4.6.4 Add Group

Adds or updates a group of peaks selected in the calibration standard into the calibration. To use this command, peak groups must first be defined in the chromatogram, for more details see Add Group topic. Groups are identified by the corresponding letter.

The Calibration - Add Group command or the corresponding 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 any time.

- *On All Signals / On Active Signal*: Determines whether the group response is added on all signals or only on the active signal. Group identification is shared across all signals.
- *Automatic Calibration*: When a new standard chromatogram is opened, Add Group always assigns the group to the first empty calibration level. As long as groups are added from the same chromatogram, they are added to the last active level if they do not already have added responses here. A new calibration level is created if Add Group is used on a group that is already present on the last active level (even within the same chromatogram) or when a different chromatogram is opened.
- *Automatic Recalibration*: The group is added or updated at the current level, with further adjustments possible later.
- *Manual Calibration / Recalibration*: The (Re)calibrate Group dialog opens after selecting the group, allowing modification of previously entered data.

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

4.6.5 Edit Named Group

The Edit Named Group dialog allows users to create and manage named groups in the Calibration Table. Named groups are used to sum the amounts of already calibrated peaks for reporting grouped results.

To create a new *Named Group*, use the *Calibration - Add Named Group* command (or its icon). This opens the *Edit Named Group* dialog, where peaks can be selected for inclusion. All peaks present in calibration are available for selection, and are listed alphabetically. Unlike standard groups, a peak can be part of multiple *Named Groups*.

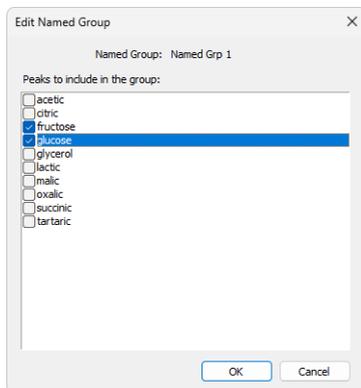


Fig. 197: Edit Named Group

The name of a *Named Group* is set in the *Calibration Summary Table*, the same way as compound names. *Named Groups* do not have an individual compound tabs, as their purpose is solely to sum the amounts of other calibrated peaks.

To edit an existing *Named Group*, click the *Edit...* button in the *Named Groups* column in the selected *Named Group* row of the *Calibration Summary Table*.

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

4.6.6 Details of Calibration Point

This dialog lists all recalibrations recorded for a given calibration level. Based on the enabled recalibrations, the final Calibration Point for the 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.

Used Level

Checkbox that determines whether the calibration level is included in the calibration curve.

Used

Checkbox that determines whether the recalibration is included in the calculation of the *Calibration Point*.

Ret. Time

The retention time recorded for the recalibration.

Amount

The amount of the compound at this level. The value is the same for all recalibrations within the level.

Area

The peak area recorded for the recalibration.

Height

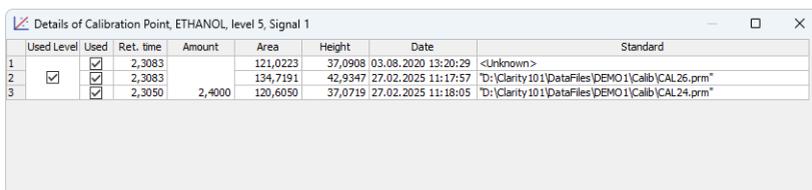
The peak height recorded for the recalibration.

Date

The date and time when the recalibration was added.

Standard

The data file from which the recalibration originates. If unknown, it is marked as *<Unknown>*.



| Used Level | Used | Ret. time | Amount | Area | Height | Date | Standard |
|------------|-------------------------------------|-----------|--------|----------|---------|---------------------|--|
| 1 | <input checked="" type="checkbox"/> | 2,3083 | | 121,0223 | 37,0908 | 03.08.2020 13:20:29 | <Unknown> |
| 2 | <input checked="" type="checkbox"/> | 2,3083 | | 134,7191 | 42,9347 | 27.02.2025 11:17:57 | 'D:\Clarity 101\DataFiles\DEMO 1\Calib\CAL 26.prm' |
| 3 | <input checked="" type="checkbox"/> | 2,3050 | 2,4000 | 120,6050 | 37,0719 | 27.02.2025 11:18:05 | 'D:\Clarity 101\DataFiles\DEMO 1\Calib\CAL 24.prm' |

The number of recalibrations stored is limited to the value set in the [Recalibration](#) section of *Sequence Options*. If a new recalibration is performed after reaching this limit (*No. of Points*), the oldest recalibration will be permanently deleted.

4.6.7 Filter Not Used Compounds

Filter Not Used Compounds function can be turned on/off from toolbar , *Calibration* menu  and local menu of *Calibration Summary Table*.

When active, all rows of *Calibration Summary Table* that have the *Used* checkbox unchecked are hidden along with the corresponding individual compound tabs.

When some rows are hidden, warning "Filtering ON - Not Used Compounds are hidden."  is displayed above the *Calibration Summary Table*. Same warning is also displayed in reports. Clicking *Show all* switch off *Filter Not Used Compounds* function and show all hidden rows.

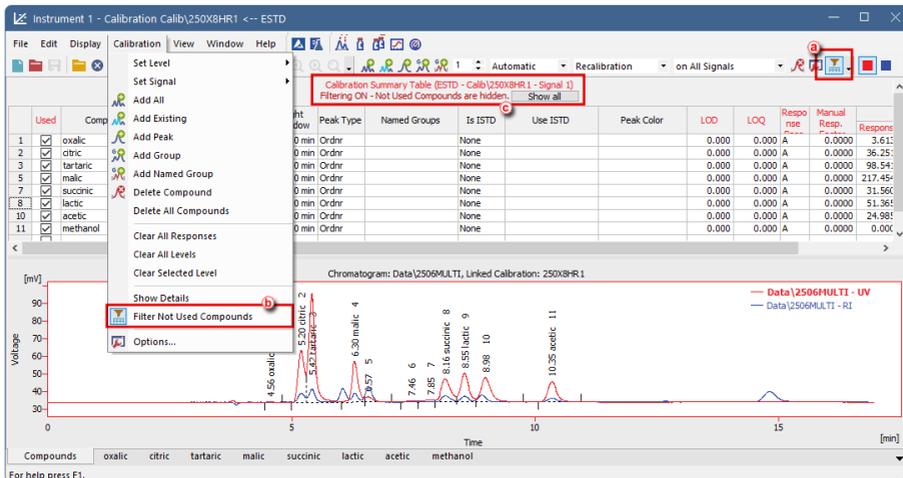


Fig. 198: Filter Not Used Compounds

4.6.8 Calibration Options

The *Calibration Options* dialog contains various settings that influence calibration. It can be opened via the *Calibration - Options...* menu item or by clicking the  icon. The settings configured here are stored in the calibration file.

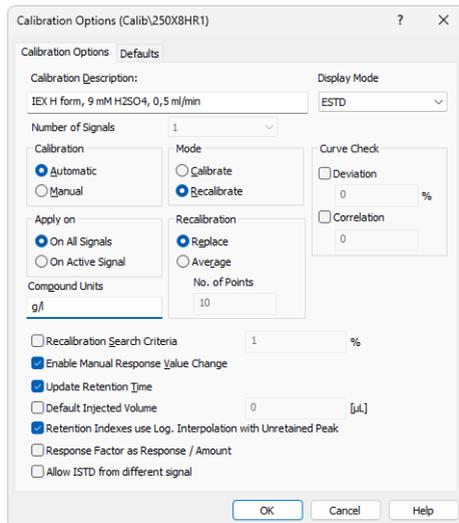


Fig. 199: Calibration Options - Calibration Options

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](#) dialog; it is also shown in the *Description* field of the [Method Setup - Calculation](#) tab when a calibration is loaded there.

Display Mode

Sets the method of the calibration curve display (suitable for different types of calibration curve use):

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.

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

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 the *Sample Amount* is not filled in. 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

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.

Number of Signals

Selects the number of displayed signals when a multi-detector calibration is used. The default 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, so the field is disabled.

Calibration

Sets the calibration or recalibration method for the *Add All*, *Add Peak* and *Add Group* commands. It can be also changed in the toolbar of the [Calibration](#) window. 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

Determines how the calibration process is performed. This setting applies only when working manually in the *Calibration* window. When calibration is performed from *Single Analysis* or *Sequence*, the specified calibration level is always recalibrated according to the settings in *Recalibration* options. It can be also changed in the toolbar of the [Calibration](#) window. For *Standard Addition* calibrations, this selection is disabled.

Calibrate

Transfers data from the standard chromatogram into the first available empty calibration level. If all 20 calibration levels are filled, the responses in the last

(Blank) calibration level will be overwritten.

Recalibrate

Recalibrates the level currently selected in the calibration window with the data from the standard chromatogram.

Curve Check

Enables verification of the calibration curve's linearity based on two following parameters. If either parameter fails for a given compound, the entire *Curve Check* for that compound is considered failed. This is indicated in the *Calibration* window on the compound's tab and reflected in the *Result Table* of the *Chromatogram* window, where the *Peak Type* column will display *Error (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 compound.

Apply On

Specifies where the (re)calibration will be performed. This setting can also be changed in the toolbar of the *Calibration* window.

On All Signals

Calibration or recalibration is performed on all signals. When *Add All* is clicked, all peaks from the currently active signal are added to the *Calibration Summary Table*. For subsequent signals, responses for these peaks are filled in if they are found. However, any additional peaks present in these signals are not added automatically - they must be added separately by switching to the respective signal and using *Add All* or other functions again.

All added peaks have the *Used* checkbox checked on all signals. This option is selected by default when creating a new calibration.

On Active Signal

Calibration or recalibration is performed only on the currently active signal. When *Add All* is clicked, all peaks from the active signal are added to the *Calibration Summary Table*. The responses for these peaks are filled in only for the active signal, even if they are found on other signals. On all other signals, the *Used* checkbox for these peaks is unchecked. In this mode automatically created compound name is amended by signal name to the form "Peak [retention time] [signal name]".

Recalibration

Defines the conditions for recalibration mode:

Replace

Each new response replaces the previous one, ensuring that only one response of each compound is stored for each calibration level.

Average

The average response value is calculated as the arithmetic mean of the responses from the last X recalibrations for the given level, where X is defined by the *No. of Points* setting.

No. of Points

Specifies how many last recalibrations are used for averaging. The *No. of Points* can be set between 0 and 100, with a default value of 10.

Note: Changing the *No. of Points* setting does not retroactively affect existing recalibrations - it only applies to 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 [Result Table](#) in the *Chromatogram* window, unless other units are specified by *Scale Factor* and *Units after Scaling* fields.

Recalibration Search Criteria

Specifies the maximum allowed percent deviation of response for recalibration. The allowed deviation range is 1 to 50%.

When Calibration option is set to Automatic

If the deviation in the response exceeds the set threshold, recalibration is not performed, and the event is logged in the audit trail.

When Calibration is set to Manual

If the deviation in the response exceeds the set threshold, the *Over* is stated in the dialog for manual recalibration. After confirmation, recalibration is still performed.

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 (re)calibration. The retention time of the compound is adjusted to the current value of the peak identified as that compound.

Default Injected Volume

Corrects response values for differences in injected volume by comparing the actual injection (from the *Inj. Volume* in the chromatogram) with the *Default Injected Volume*. The response is adjusted based on their ratio, assuming a direct proportionality between amount and response.

When the *Inj. Volume* in the standard chromatogram is set to the actual injected amount, and the *Default Injected Volume* is defined in calibration before (re)calibrating, the response for each level in calibration is corrected accordingly. This ensures that the calibration reflects response values as if the default volume had been used. The corrected response is recorded in *Calibration Point Details* in the format: Corrected by Injection Volume (Default X ml, Actual X ml).

Changing the *Default Injected Volume* setting does not retroactively affect previous (re)calibrations. The response values in the calibration table remain unchanged, only

the values in the evaluated chromatogram in the *Chromatogram* window are corrected.

Retention Indexes use Log. Interpolation with Unretained Peak

Uses *Unretained Time* value (set on the [Method Setup - Advanced](#) tab) for retention index calculation. By default, this checkbox is unchecked and retention indexes are calculated using the linear interpolation. When it is checked, then the logarithmic interpolation with unretained peak time is used instead.

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 = Kováts 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 = Kováts 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 = Response / Amount (by default : RF = Amount / Response). This setting changes the format of RF in [Calibration](#) window as well as on [Results](#) tab of the [Chromatogram](#) window.

Allow ISTD from different signal

Enables the usage of ISTD peaks that are found on a different signal of the same chromatogram. When checked, the *Use ISTD* column in the **Calibration Summary Table** will contain separate entries for the ISTD peaks defined on particular signals in addition to their generic entries. Generic entries (without the *Signal X* part in the name) mean "use the given ISTD peak on the active signal", while entry with the *Signal X* part in the name means "use the given ISTD peak calibration curve from Signal X, regardless for which signal the results are calculated." Using this option will also modify some warning messages in the [Chromatogram](#) window above the **Result**

Table and in [Calibration](#) window above **Calibration Summary Table** by adding information on the signal for which the message is relevant.

4.6.8.1 Defaults

The [Calibration Options](#) dialog tab that defines the default parameters that will be used for new compounds.

For description of the parameters for which default values can be set, please see the topics regarding [Calibration Summary Table](#) and [Individual Compound tab](#).

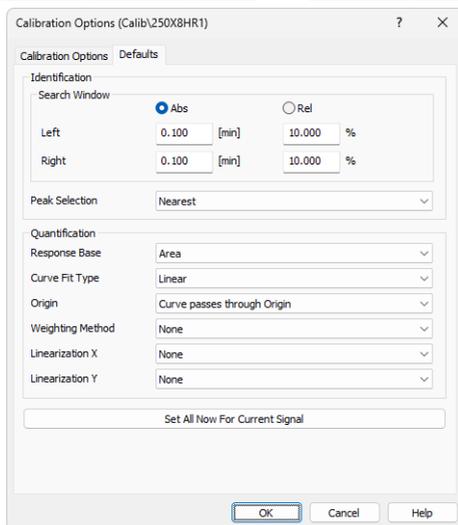


Fig. 200: Calibration Options - Defaults

Set All Now For Current Signal

Immediately applies the selected parameters to all compounds in the current calibration for the active signal. In contrast, pressing **OK** only saves the parameters as defaults for future signals and compounds.

4.7 View

This menu contains commands for setting up the appearance of the [Calibration](#) window.

| Command | Description |
|-----------------------|--|
| 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"> • <i>Standard, Edit, Calibration, Signals</i>: Hides/shows the respective toolbar. • <i>Customize...</i>: Customization of items in the toolbars. • <i>Reset All</i>: Returns all menus and default toolbars in the <i>Calibration</i> window into their initial state. <i>Reset All</i> does not display hidden toolbars, even if they were displayed by default. To show them invoke <i>Customize... - Toolbars</i> menu. |
| Maximize Graph | <p>Enlarges the graph section over the whole window and hides <i>Compound Summary Table</i> completely. This action can also be performed by double-clicking on the edge of the graph near the splitter when the cursor changes to . This command is only available in the Compounds tab.</p> |
| Show Both | <p>Displays both parts of the window (chromatogram and tabs). This command is only available in the Compounds tab.</p> |
| Maximize Table | <p>Enlarges the <i>Compound Summary Table</i> section over the whole window and hides the graph completely. This action can also be performed by double-clicking on the edge of the table section near the splitter when the cursor changes to . This command is only available in the Compounds tab.</p> |

4.8 Window

This menu contains commands for displaying other main windows:

| Command | Description |
|--|---|
| Main  | Displays the Clarity main station window described on pg. 1 . |
| Instrument | Displays the Instrument window described on pg. 59 . |
| Chromatogram | Displays the Chromatogram window described on pg. 156 . |
| Single Analysis | Displays the Single Analysis window described on pg. 108 . |
| Sequence | Displays the Sequence window described on pg. 382 . |
| Data Acquisition | Displays the Data Acquisition window described on pg. 366 . |
| Device Monitor | Displays the Device Monitor window described on pg. 128 . |
| Station Audit Trail  | Displays the Audit Trail window described on pg. 411 . |
| Calibration Audit Trail  | Displays the Calibration Audit Trail window described on pg. 424 . |

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.

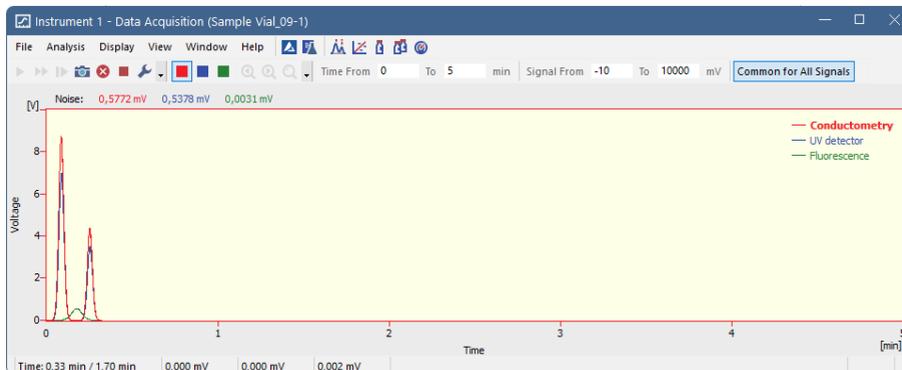


Fig. 201: Data Acquisition

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. 377).

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](#) tab 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. 399). |

| | | |
|---|---|--|
|  | 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. 108.

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.

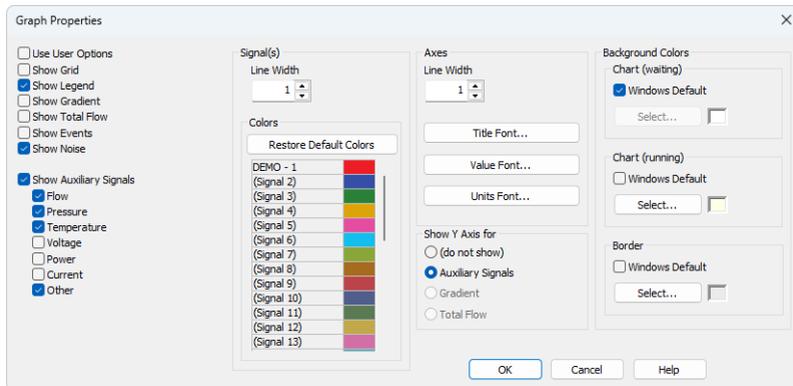


Fig. 203: *Graph Properties*

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 *Settings - User Options...* command.

Show Grid

Shows/hides auxiliary grid for easier reading of values in graph.

Show Legend

Shows/hides names of the individual signals including the eventual subtraction chromatogram and background chromatogram.

Show Gradient

Shows/hides gradient when using direct control of LC pumps.

Show Total Flow

Shows/hides total flow when using direct control of LC pumps.

Show Events

Shows/hides the events from the **Event Table** in the [Data Acquisition](#) window.

Show Noise

Shows/hides the **Noise** value (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*. Note those options are only available if they are available in the configured devices.

Signal(s)

Line Width

Selects the curve width in points.

Colors

Selection of color of the signal .

Restore Default 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. ± 20 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 Signal(s) | Switches the display of the Data Acquisition window to showing the detector signals. Only available on the PDA or MS instrument types (requires PDA Extension or MS Extension). |
| Show MS Spectrum | Switches the display of the Data Acquisition window to showing the actual MS spectra. Only available on the MS instrument types (requires MS Extension). |
| Show PDA Spectrum | Switches the display of the Data Acquisition window to showing the actual PDA spectra. Only available on the PDA instrument type (requires PDA Extension). |
| Show Isoplot | Switches the display of the Data Acquisition window to showing the isoplot from the PDA spectra. Only available on the PDA instrument type (requires PDA 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 | | | |
|-----------------|---------|----------|----------|
| | Fixed | | Floating |
| | From | To | Range |
| Time Axis | 0 min | 5 min | 1 min |
| Signal Axis | -10 mAU | 1000 mAU | 5 mAU |

| Individual Settings | | | |
|---------------------|---------|----------|----------|
| | Fixed | | Floating |
| | From | To | 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.

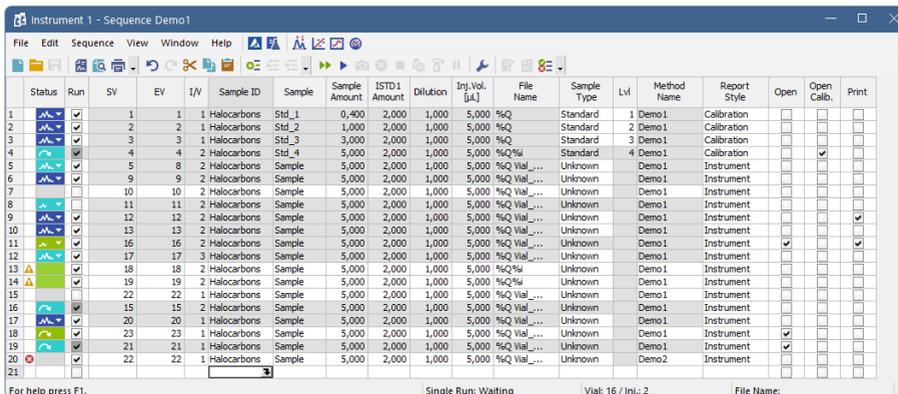
5.5 Window

This is an entry point to a submenu of commands for displaying other main windows.

| | |
|--|---|
| Main <small>✓ full version</small> | Displays the Clarity main window described on pg. 1 . |
| Instrument | Displays the Instrument window described on pg. 59 . |
| Chromatogram | Displays the Chromatogram window described on pg. 156 . |
| Calibration | Displays the Calibration window described on pg. 313 . |
| Single Analysis | Displays the Single Analysis window described on pg. 108 . |
| Sequence | Displays the Sequence window described on pg. 382 . |
| Device Monitor | Displays the Device Monitor window described on pg. 128 . |
| Station Audit Trail <small>✓ full version</small> | Displays the Audit Trail window described on pg. 411 . |

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 | Dilution | Inj. Vol. [µL] | File Name | Sample Type | Lvl | Method Name | Report Style | Open | Open Calib. | Print |
|--------|-----|----|----|-----|--------------------|--------|---------------|--------------|----------|----------------|-----------|-------------|------------|-------------|--------------|------|-------------|-------|
| 1 | 1 | 1 | 1 | 1 | Halocarbons Std_1 | 0,400 | 2,000 | 1,000 | 5,000 | %Q | Standard | 1 | Demo1 | Calibration | | | | |
| 2 | 2 | 2 | 1 | 1 | Halocarbons Std_2 | 1,000 | 2,000 | 1,000 | 5,000 | %Q | Standard | 2 | Demo1 | Calibration | | | | |
| 3 | 3 | 3 | 3 | 1 | Halocarbons Std_3 | 3,000 | 2,000 | 1,000 | 5,000 | %Q | Standard | 3 | Demo1 | Calibration | | | | |
| 4 | 4 | 4 | 2 | 1 | Halocarbons Std_4 | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Standard | 4 | Demo1 | Calibration | | | | |
| 5 | 5 | 8 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 6 | 9 | 9 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 7 | 10 | 10 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 8 | 11 | 11 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 9 | 12 | 12 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 10 | 13 | 13 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 11 | 16 | 16 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 12 | 17 | 17 | 3 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 13 | 18 | 18 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 14 | 19 | 19 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 15 | 22 | 22 | 1 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 16 | 15 | 15 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 17 | 20 | 20 | 1 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 18 | 23 | 23 | 1 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 19 | 21 | 21 | 1 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo1 | Instrument | | | | | |
| 20 | 22 | 22 | 2 | 1 | Halocarbons Sample | 5,000 | 2,000 | 1,000 | 5,000 | %Q | Unknown | Demo2 | 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 injection per vial I/V parameter indicates number of injections from one vial.

Status

Status of the row in the sequence.

 Indicates a row with one or more errors, such row blocks the measurement of the sequence.

 Indicates a row with one or more warnings, measurement will still be carried out.

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. |

| Status | State | Description |
|---|----------------------------|--|
|  | 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. |

Note: A text description will be printed in the printouts instead of colored tags in the *Status* column.

Already measured rows will be blocked against changes (dimmed) in all columns except for *Run*, *Sample Type*, *Lvl*, *Report Style*, *AnalysisUserVar1-AnalysisUserVar3*, and *Post-run Options*, columns which can be changed for reprocessing in Batch dialog.

If there is a chromatogram resulting from a row, small arrow 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 options to open the chromatogram(s). See **Fig. 206** on pg. **384**..

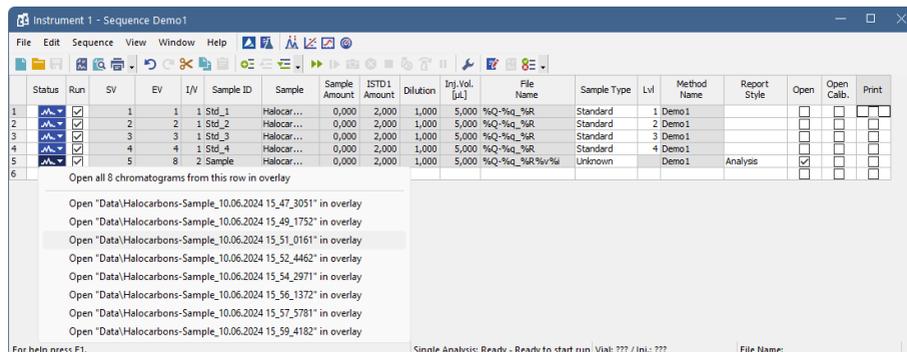


Fig. 206: Open chromatograms in overlay

It is possible to open one specific chromatogram or open all chromatograms measured in this row in overlay.

Selected row(s) will return to their initial *Status* (all fields green) when the sequence is reset:

- 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**).

If the Sequence is reset, also its audit trail is reset. In GLP it is recommended to clone measured sequences using *Save As* option.

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 line 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. All vials between SV and EV (these included) are measured.

If *Sequence Options - Solve conflict of filename* is set to *Automatically* (default value), then for more than one vial or injection, the File Name pattern is extended by %v and/or %i variables.

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 *Sequence Options - Solve conflict of filename* is set to *Automatically* (default value), then for more than one vial or injection, the File Name pattern is extended by %v and/or %i variables.

Sample ID

The sample identification field serves for information only. Maximum number of characters in this field is limited to 64. The parameter corresponds to the *Sample ID* field of the [Single Analysis](#) dialog. *Sample ID* is saved in the chromatogram and can be viewed or edited on *Measurement Conditions - Instrument* tab.

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. 108.

Sample

The Sample description field serves for information only. Maximum number of characters in this field is limited to 64. The parameter corresponds to *Sample* field of the [Single Analysis](#) dialog. *Sample* is saved in the chromatogram and can be viewed or edited on *Measurement Conditions - Instrument* tab.

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. *Comments* are saved in the chromatogram and can be viewed or edited on *Measurement Conditions - Instrument* 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. *Sample Amount* is saved in the chromatogram and can be viewed or edited on *Calculation - Common for all signals* section of *Results* tab.

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 *ISTD1 Amount* field of the [Single Analysis](#) dialog. *ISTDs*

Amounts are saved in the chromatogram and can be viewed or edited on *Calculation - Common for all signals* section of *Results* tab.

Dilution

This field holds the sample dilution factor - its value is used to multiply each calculated *Amount* in the *Result Table*. The default value is 1. The parameter corresponds to *Dilution* field in the [Single Analysis](#) dialog. *Dilution* is saved in the chromatogram and can be viewed or edited on *Calculation - Common for all signals* section of *Results* tab.

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. The units are set in the [Instrument Units](#) dialog. *Injection Volume* is saved in the chromatogram and can be viewed or edited on *Calculation - Common for all signals* section of *Results* tab.

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, the row of the sequence will be in error state.

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.

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. The same variables may be used as in the [Single Analysis](#) dialog, plus %v and %i variables for numbering 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. Variables are described in the *Chromatogram File Name* section of the [Single Analysis](#) dialog described on pg. 108.

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, it will be created when creating the chromatogram.

When the information on the sequence row are valid (the analysis from the row could proceed), the tooltip over the *File Name* cell will display the name(s) of the chromatogram file(s) (as it would look if the analysis started right away, with respect to time variables) and also the name of the calibration that will be created as a clone during the first analysis on that row (if calibration cloning is used and the row is the place where the cloning will occur).

Note: If variable %n is being used, it will be independent from the same variable [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* can have the calibration level filled in the *Lvl* column. Chromatograms marked as calibration standards in the time of creation will be stored in the CALIB subdirectory instead of the DATA subdirectory. If the *Lvl* is not filled, calibration (or recalibration) is not performed, chromatograms are only stored in the CALIB subdirectory.

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). Chromatograms marked as blanks in the time of creation will be stored in the CALIB subdirectory instead of the DATA subdirectory.

Bypass - 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..

The row indicates an error and prevents running the sequence, if *Standard* (with filled *Lvl*) or *Blank Sample Types* are selected, and in the selected *Method* there is not defined the calibration file.

Caution: In the case, the finishing of the analysis results in calibration (or recalibration) of calibration file, which is at the same time modified in the Calibration window, any unsaved changes are discarded, and the (re)calibration is performed.

Lvl

Indicates the number of the calibration level that will be (re)calibrated. Cells in this columns are enabled only when *Sample Type* on the same row is set to *Standard*. If the *Lvl* is not filled, calibration (or recalibration) is not performed.

Method Name

Indicates the name of the method governing all analyses set on a given line. If you point the mouse cursor to the cell, a tooltip will open, in which the name of the method including the entire path will be displayed.

Report Style

Sets the report style to be used for printing. If printing is checked on the row, the report style has to be selected. After clicking on the cell in this column the  icon will appear. Using it opens the *Select Report Style* dialog. If you point the mouse cursor to the cell, a tooltip will open, in which the name of the report style including the entire path will be displayed.

Post-run Options

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 Options](#) tab. All of these columns contain checkboxes, with the exception of the *Program to Run* column and the *Parameters* column.

Note: When there is *Print*, *Print to PDF* or *Export Data* set in the *Post-run Options*, the *Open* chromatogram post-run option 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 if opened in the chromatogram window.

Stored Calib.

This checkbox causes the created chromatogram to be opened with the latest 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 *Calculation - Common for all signals* section of *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 currently measured chromatogram will be opened in *Chromatogram window*. Other post-run operations always follow after *Close all* command.

Line Info

This column serves for any information that belongs to the sequence only and is not transferred to the chromatograms.

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 currently being measured.

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 *Solve conflict of filename* section in the [Sequence Options](#) dialog described on pg. **403**.

6.1 File

This is an entry point to a submenu of commands for working with sequence files.

| Icon | Command | Description |
|---|--|---|
|  | New | <p>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 <i>ACTIVE</i> 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.</p> <p>The first row in a new sequence takes its settings from the Method and Report setup currently loaded to the Instrument, the Post-run information is loaded from the actual setting of the Single Analysis - Post-run Options tab. By checking the <i>Run</i> checkbox for further rows, the settings are copied from the previous line.</p> |
|  | Open | <p>Selects and opens a sequence file. Invoking the command or using the Ctrl + O shortcut opens the <i>Open Sequence</i> dialog.</p> <p>The same particular sequence cannot be opened on multiple Instruments at once.</p> |
|  | Save | Saves changes in the currently opened sequence. |
|  | Save As | <p>The command invokes the <i>Save As</i> 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 <input checked="" type="checkbox"/> full version only), you are not allowed to change a file without the appropriate access rights (see <i>System - User Accounts...</i> command).</p> <p><i>Note:</i> For existing filenames, message box about file overwriting pops up.</p> |
| | Send Sequence by Email | <p>Creates a new email in the default email client with the currently displayed sequence file attached.</p> <p>The sequence will automatically be saved prior to sending.</p> |

| Icon | Command | Description |
|---|----------------------------------|--|
| | Import... | Imports the sequence table from a text file (for more details see the chapter Import... on pg. 392). |
| | 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. 429 . |
|  | Print Preview | Displays a preview of the printout prior to actual printing. The command opens the Print Preview dialog described on pg. 454 . |
|  | 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. 456 . |
| | ----- | 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.

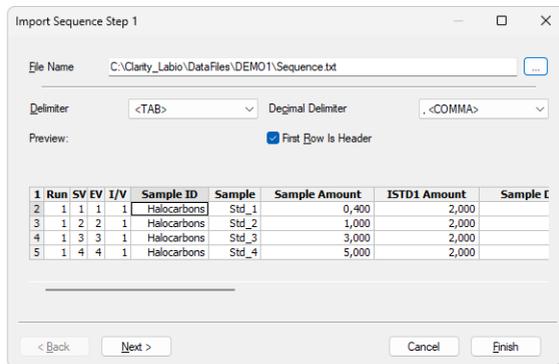


Fig. 207: Import Sequence Step 1

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.

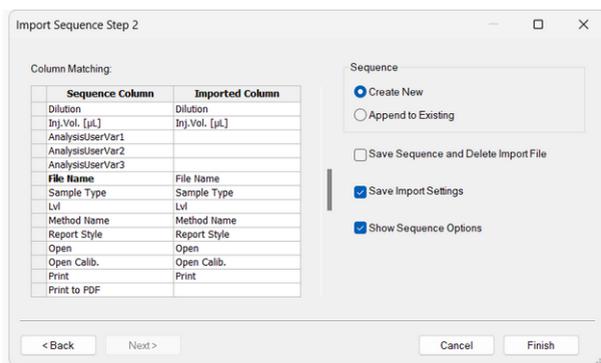


Fig. 208: Import Sequence Step 2

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. **403**.

6.2 Edit

Provides access to commands for working with the clipboard and table editing in the [Sequence Table](#). Commands from this menu can also be accessed from the local table menu by right-clicking on the table.

The movement direction of the focus after pressing **Enter** can be adjusted in [User Options](#).

| Icon | Command | Description |
|---|------------------------|---|
|  | 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. |
| | 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 for the <i>End Vial (EV)</i> column or when multiple cells in the same row are selected. |

| Icon | Command | Description |
|---|--------------------------------|---|
| | 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 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. |
| | Delete | 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. |
| | Mark for Run | Checks the checkbox in the <i>Run</i> column for selected lines. These rows will be processed when the sequence will be run. |
| | Clear Run Marks | Unchecks the checkbox in the <i>Run</i> column for selected lines. These rows will not be processed when the sequence will be run. |
| | Invert Run Marks | 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). |
|  | Reset Status | 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. |
| | Restore Default Columns | Restores the default columns setting (for more details see the chapter Edit on pg. 186). |
| | 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

The Fill Series dialog fills a series of values in a selected column, either by incrementally generating values or copying an existing value to all selected cells below. It can only be used in one column at a time; if multiple columns are selected, the command is disabled. When a selection is made, the series is applied within that range, starting from the first cell. If no selection is made, it fills all remaining cells in the column below the current one.

The Fill Series dialog can be accessed via the right-click menu in tables, including the [Gradient Table](#).

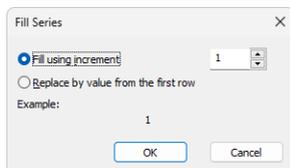


Fig. 209: Fill Series dialog

Fill using increment

This option fills the selected cells by increasing values step-by-step using the specified increment. The starting value is taken from the first selected cell. If the cell contains a number at the end of a string, only the numerical part is incremented.

Replace by value from the first row

This option copies the value from the first selected cell and applies it to all other selected cells below. It functions the same way as the *Fill Down* command.

Example

The *Example* preview at the bottom of the dialog shows how the first and second cells in the selected column will be filled.

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.

| Icon | Command | Description |
|---|------------|---|
|  | Run | <p>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 <i>RUNNING</i> state. Before the sequence is run, the validity check is performed. All methods used in <i>ACTIVE</i> sequence must:</p> <ul style="list-style-type: none"> • have <i>External Start/Stop</i> option in the Method _ Setup _ - _ Measurement dialog checked. • have <i>Enable Autostop</i> checkbox in the Method _ Setup _ - _ Measurement dialog selected and <i>Run Time</i> field filled. <p>The <i>Run</i> command invokes dialog with options to: <i>Reset</i>, <i>Resume</i> or <i>Cancel</i>. <i>Reset</i> command, resets the status of all lines in the Sequence Table (all fields in the <i>Status</i> column will turn green). Running a partially measured sequence using the <i>Resume</i> command starts the measurement from the first non-measured line, while running it using the <i>Run</i> command the entire sequence will be measured again.</p> <p>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.</p> <p>User has to have <i>Start Acquisition</i> right to be able to perform this option.</p> |

| Icon | Command | Description |
|---|--------------------------------------|---|
|  | Pause | <p>Using the <i>Pause</i> 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 <i>Pause</i> command depends on the status of the sequence before invoking the command: <i>WAITING</i>, <i>IDLE</i> sequence is turned to <i>PAUSED</i> status. <i>RUNNING</i> sequence is turned to the <i>PAUSED</i> status only after the data acquisition of the current analysis is completed (the intermediate status is <i>RUNNING/PAUSE</i>).</p> |
|  | Resume | <p>Using this command,  icon or the Ctrl + Space bar shortcut resumes the operation of a suspended sequence. The sequence status becomes <i>IDLE</i> or <i>WAITING</i> 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 <i>IDLE</i> state, the sequence counts the time from the moment it was set to the <i>PAUSED</i> state.</p> <p>When the <i>Resume</i> command is used while in the <i>RUNNING/PAUSE</i> state, the planned pause of the sequence will be canceled.</p> <p>If you run a partially measured sequence using the <i>Resume</i> command, measurement continues from the first line that wasn't measured yet. If you run it using <i>Run</i>, the entire sequence will be measured again.</p> <p>User has to have <i>Start Acquisition</i> right to be able to perform this option.</p> |
|  | Abort Sequence or Acquisition | <p>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.</p> |

| Icon | Command | Description |
|---|---------------------------------------|---|
|  | Stop Sequence or Acquisition | 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>). If the <i>Stop</i> command is used for the second time, it will stop the running analysis. |
|  | Repeat Injection | 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. User has to have <i>Start Acquisition</i> right to be able to perform this option. |
|  | Skip Vial | 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. The line containing skipped injections will be indicated in the <i>Status</i> column by light blue color. Potential re-measurement of skipped vials has to be done manually (e.g. by creating a new line in the Sequence Table). User has to have <i>Start Acquisition</i> right to be able to perform this option. |
|  | <u>Check Sequence</u> | This command performs a check of every row in the <i>Sequence Table</i> for potential errors. |

| Icon | Command | Description |
|---|-------------------------------------|--|
|  | Snapshot | 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. 108 . The snapshot chromatogram will be automatically replaced by another snapshot or the final chromatogram after the analysis is finished. Sample counter <i>%n</i> , 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. |
|  | Options... | When invoked, opens the Sequence Options dialog used for defining the sequence parameters (for more details see also chapter Sequence Options on pg. 403). |
|  | Edit Current Method... | 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. 90 . 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 . |
|  | Edit Current Report Style... | 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. 429 . 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 . |

6.3.1 Resume/Reset Sequence

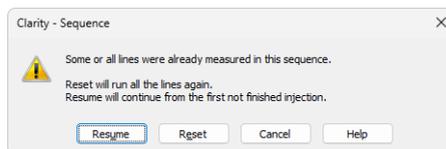


Fig. 210: Dialog to Resume or Reset Sequence

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 Check Sequence

The Check Sequence function verifies the sequence before execution. It can be triggered manually from the toolbar or runs automatically when attempting to start a sequence. If any issues are detected, an error message appears, always displaying the first detected issue in the sequence. Rows containing an error or warning are also marked in the Status column.

6.3.2.1 Error Messages

Below are notable error messages (it is not an exhaustive list) that may appear during the sequence check:

| Error message | Detailed Description |
|--|---|
| <p>Calibration file must be defined in method [Method Name] for successful recalibration.</p> | <p>If you set the Sample Type to Standard (and filled in Lvl column) or Blank, a calibration file must be set in the method used to measure this row.</p> |
| <p>Open checkbox must be selected to perform Print, Print to PDF, and/or Export Data.</p> | <p>To proceed with printing or exporting, ensure that the Open checkbox is checked for the relevant sequence rows.</p> |

| Error message | Detailed Description |
|--|---|
| <p>Calibration [Calibration Name] already exists.</p> | <p>This warning occurs when a cloned calibration has a non-unique name. To resolve this, adjust the Cloned Calibration Name setting in Method Setup - Calculation to include a unique identifier (e.g., sequence name, time, or counter).</p> |

6.3.3 Sequence Options

The *Sequence Options* dialog serves for defining the sequence parameters. It can be opened using the  icon or the *Sequence - Sequence Options* command of the [Sequence](#) window.

Fig. 211: Sequence Options

Description

The description of the displayed sequence.

Sequence mode

Defines the operation mode of the sequence — whether it is fully controlled by Clarity (*Active*) or triggered externally without further checks (*Passive*). For more details on how to connect autosamplers, see the *Connecting Autosamplers* topic in the *User Guide* manual.

Passive

In *Passive* mode, the autosampler (or other source of a start signal) initiates the start of each analysis. Clarity waits for the external start signal and begins the sequence and data acquisition once the signal is received.

In this mode, the behavior of the *External Start/Stop* setting in the *Method Setup - Measurement* tab of the method is respected as configured (*Start Only*, *Start-Restart*, or *Start-Stop*). The *Autostop* setting is not required.

If *Autostop* is defined in the method, Clarity will wait for the next start signal after it has elapsed. The analysis can also be manually ended using the *Stop* button twice, or via the external input if the *External Start/Stop* setting is set to *Start - Restart* or *Start - Stop*.

Active

In *Active* mode, Clarity controls the start of the sequence. When all devices are ready, it sends a signal to the autosampler to initiate an injection process. The autosampler performs the defined operations and then signals Clarity that the injection is complete. Data acquisition begins only after this signal is received. No further injections are allowed until the current one is completed and all devices are ready again.

Autostop and *External Start/Stop* must be enabled in the *Method Setup - Measurement* tab of the selected method. In this mode, the *External Start/Stop* setting is always interpreted as *Start Only*, regardless of the selected option.

Input/output assignments can be modified in the [System Configuration](#) dialog, under the corresponding *Instrument* tab (*Ext. Start Dig. Input* and *Ready Dig. Output* fields). *Active* sequence mode can be used even without an autosampler controlled by Clarity. Proper synchronization using the Start In and Ready Out synchronization cables is sufficient.

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 using *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 multiple chromatograms with the same *File Name* would be created on a single row. This only influences the pattern for the *File Name*. If a conflict in chromatogram name is left unsolved by user, the set name is appended by counter to prevent file overwriting.

Automatically

The pattern will be automatically modified by addition of *%v* and/or *%i* if multiple vials and/or multiple injections are to be used from a single row.

Manually

The pattern will not be modified.

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 Standard Addition mode (it is necessary to set the *Display* and *Calculation* mode to *STDADD* in the calibration and method), where a calibration clone is created from the original calibration on the first row of the sequence, and then again on every *Unknown/Blank* that follows a *Standard*.

When multiple consecutive *Unknowns* follow the same *Standard*, they are treated as recalibration points for the same *Unknown* level in the current calibration. Whether the responses are averaged or replaced is determined by the *Recalibration* setting in the [Calibration Options](#) of the template calibration.

This mode 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. 59 . |
| Chromatogram | Displays the Chromatogram window described on pg. 156 . |
| Calibration | Displays the Calibration window described on pg. 313 . |
| Single Analysis | Displays the Single Analysis window described on pg. 108 . |
| Data Acquisition | Displays the Data Acquisition window described on pg. 366 . |
| Device Monitor | Displays the Device Monitor window described on pg. 128 . |
| Station Audit Trail <small>✓ Full version</small> | Displays the Audit Trail window described on pg. 411 . |
| Sequence Audit Trail... <small>✓ Full version</small> | Displays the Sequence Audit Trail window described on pg. 424 . |

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: 088-000888 |
| 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 | File | | Administrator | Instrument 1 | Files | Open Chromatogram C:\Clarity-08-04-00-026\DataFiles\DEMO1\... | 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 13:42:21 | 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: Instrument 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.cali - 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.cali - 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\Colbru... | 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.mdet.m... | 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. 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.

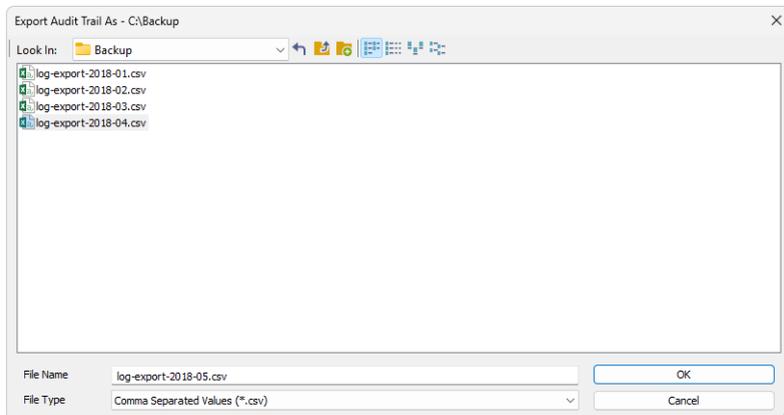


Fig. 214: Audit Trail - Export - Save As dialog

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*).

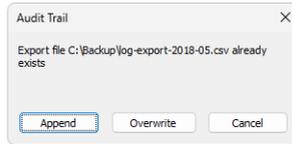


Fig. 215: Audit Trail System Message

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.

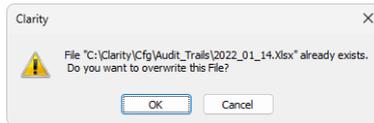


Fig. 216: Overwriting existing excel file.

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. 186). |
| 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. 193). |
| Hide Column(s) | Invoking the command hides all selected column(s) from display (for more details see the chapter Edit on pg. 186). |
| 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. 187). |

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. 424.

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

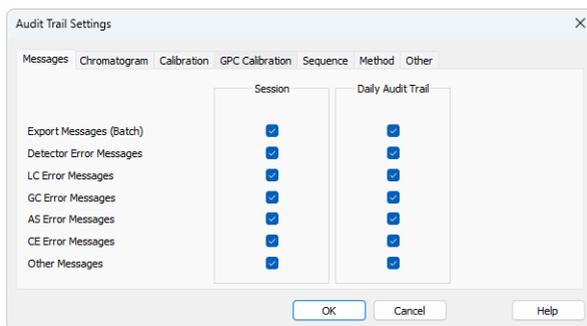


Fig. 217: Audit Trail Settings - Messages

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. 426).

Calibration

Selects which calibration file operations will be logged (for more details see the chapter **Properties...** on pg. 427).

Sequence

Selects which sequence operations will be logged (for more details see the chapter **Properties...** on pg. 428).

Method

Selects which method operations will be logged (for more details see the chapter **Properties...** on pg. 428).

Other

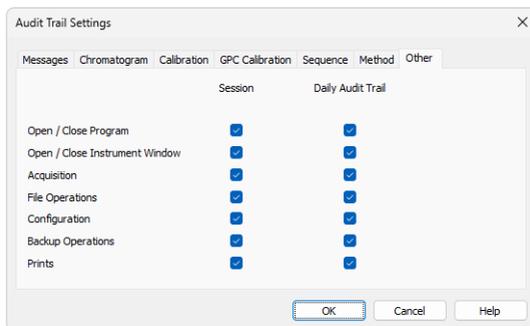


Fig. 218: Audit Trail Settings - Other

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. 59. |

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. 415). |
| 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. 186). |
| 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. 193). |
| Hide Column(s) | Invoking the command hides all selected column(s) from display (for more details see the chapter Edit on pg. 186). |
| 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. 187). |

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.

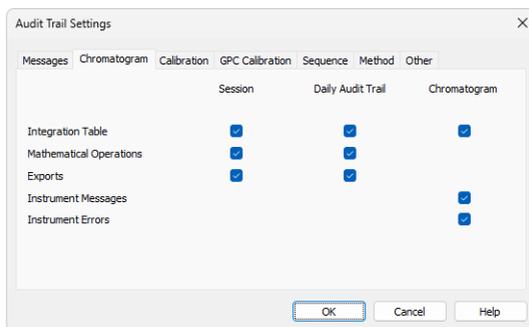


Fig. 219: Audit Trail Settings - Chromatogram

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.

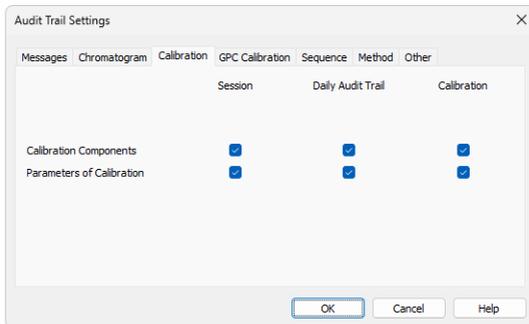


Fig. 220: Audit Trail Settings - Calibration

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.

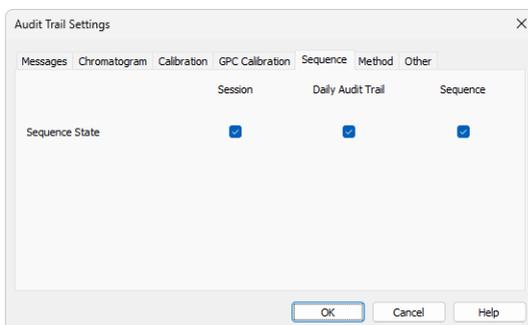


Fig. 221: Audit Trail Settings - Sequence

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.

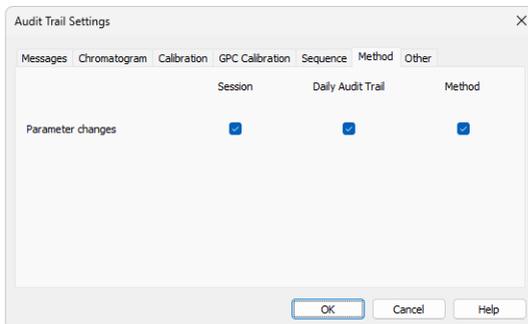


Fig. 222: Audit Trail Settings - Method

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.

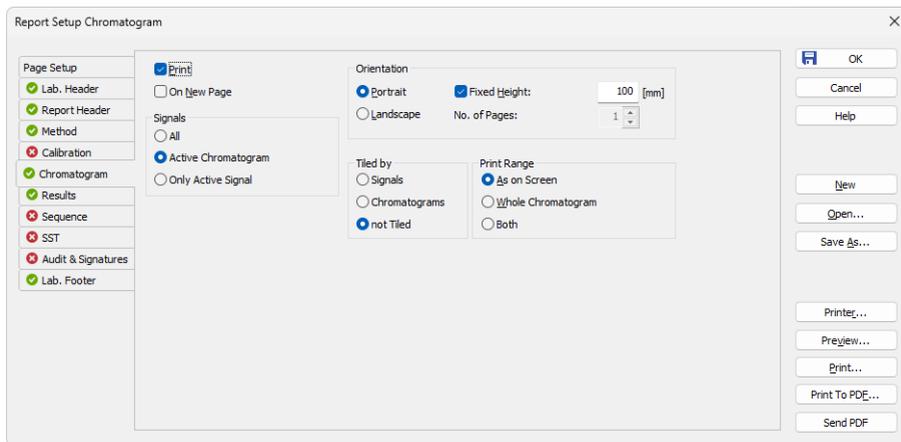


Fig. 223: Report Setup

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. 66. 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. 454).

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.

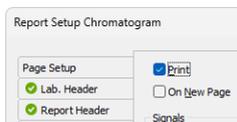
Then you can fill in the remaining information (recipient, text of the message, etc.) into the email message and send it.

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.

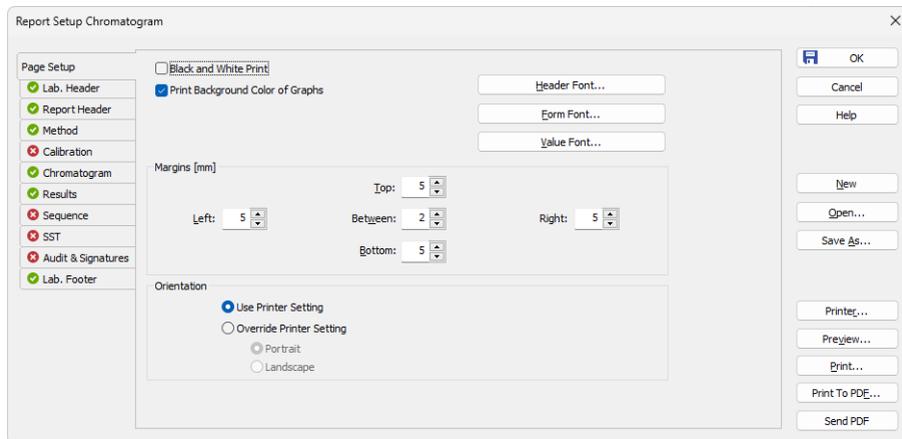


Fig. 224: Report Setup - Page Setup

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.

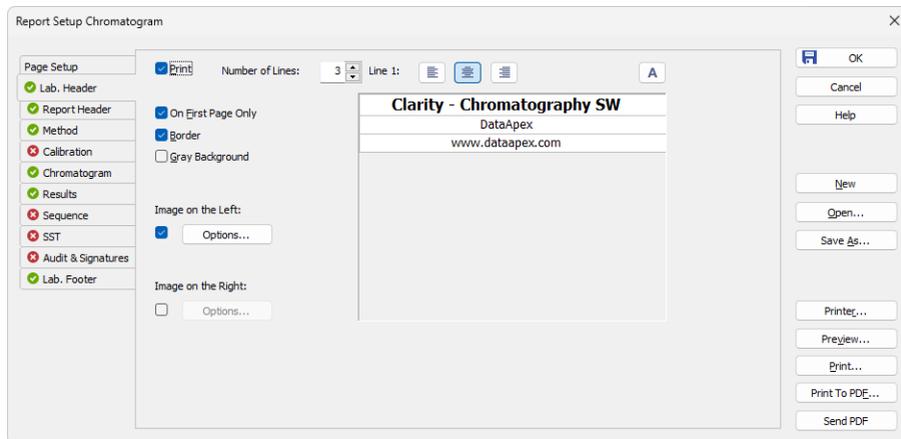


Fig. 225: Report Setup - Lab. Header

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>Current User</i> | %k | Inserts the name of the currently logged user. |
| <i>Print Date and Time in current Win format</i> | %R | Insert the date and time of printing in currently used windows format. |
| <i>Instrument Name</i> | %e | Inserts value of the <i>Instrument Name</i> . |
| <i>The percent sign %</i> | %% | Inserts percent 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.

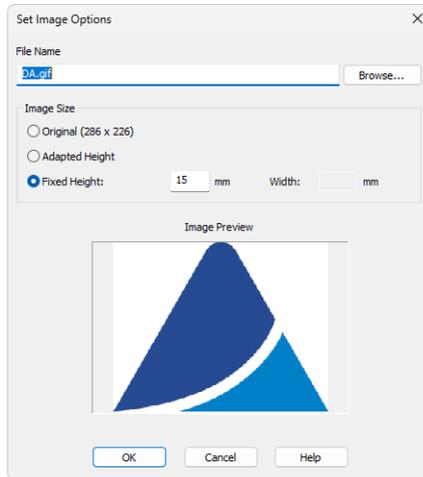


Fig. 226: Set Image Options

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 it's 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.

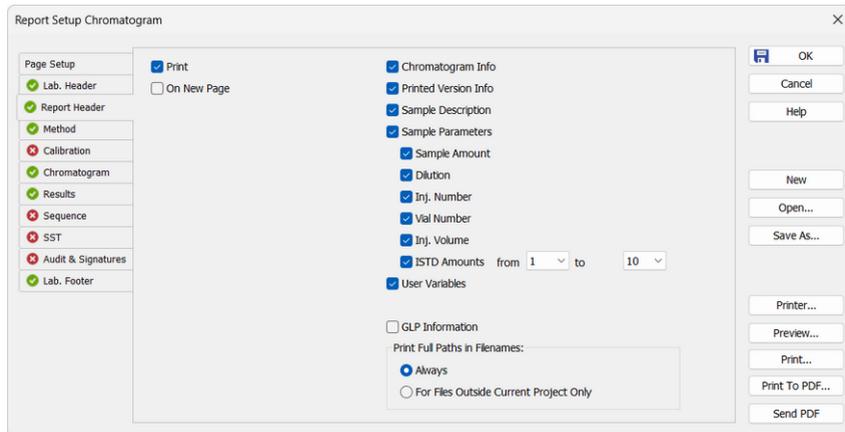


Fig. 227: Report Setup - Report Header

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:

Sample Amount - shows the Sample 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.

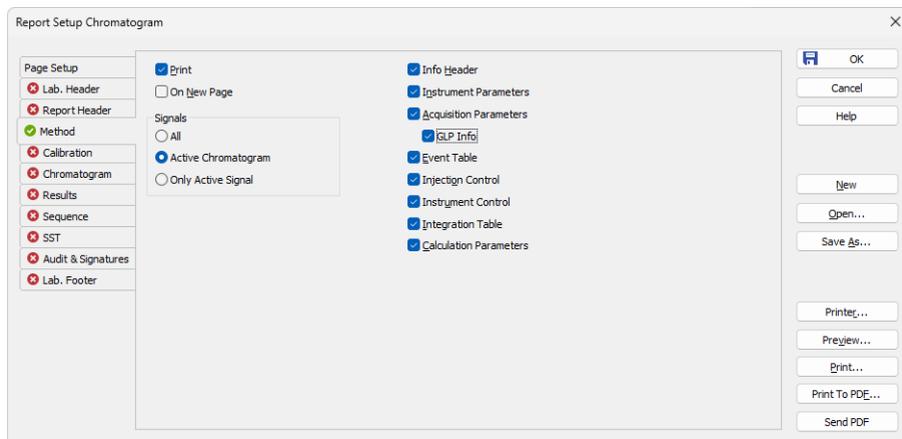


Fig. 228: Report Setup - Method

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](#) tab 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](#) tab 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](#) tab 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.

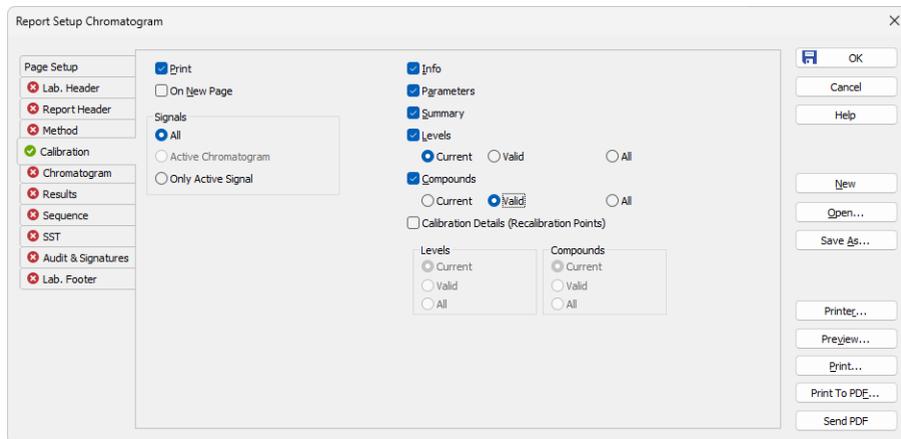


Fig. 229: Report Setup - Calibration

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 *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 off 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.

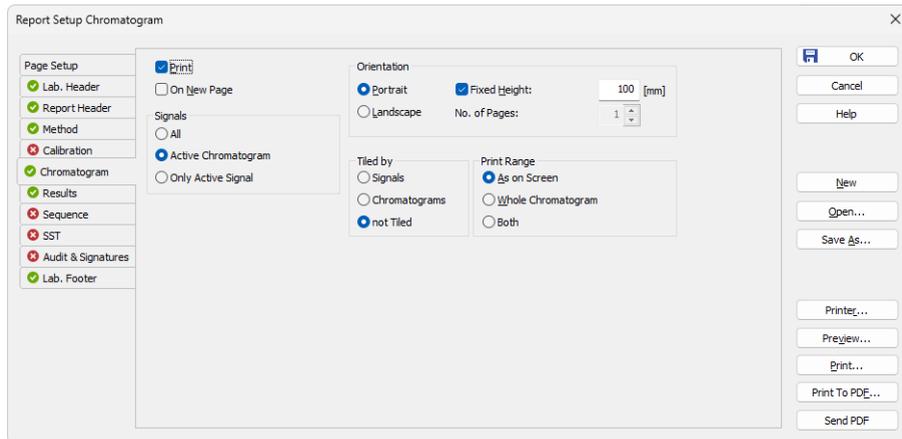


Fig. 230: Report Setup - Chromatogram

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.

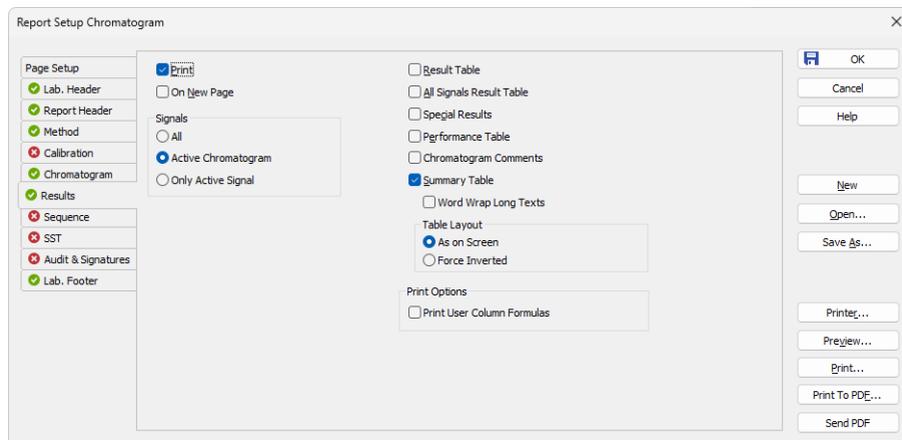


Fig. 231: Report Setup - Results

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: In the 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.

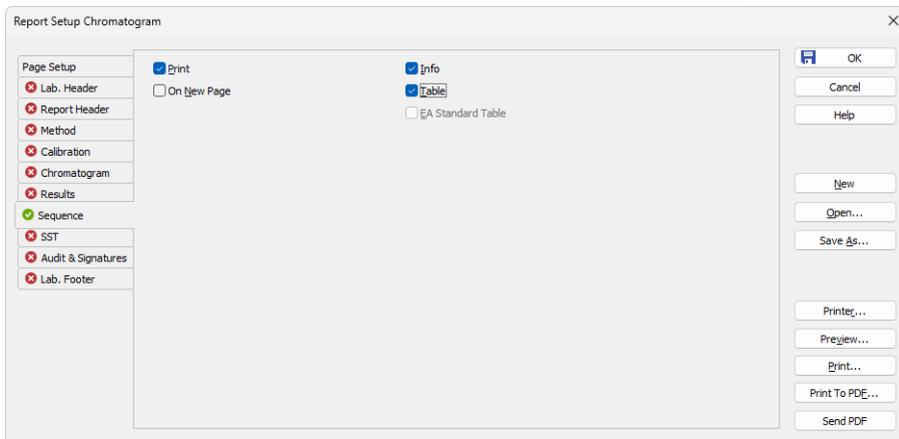


Fig. 232: Report Setup - Sequence

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. 382).

Table

Prints the sequence table.

8.10 Audit & Signatures ✓ Full version

Governs the print of local audit trails and electronic signatures.

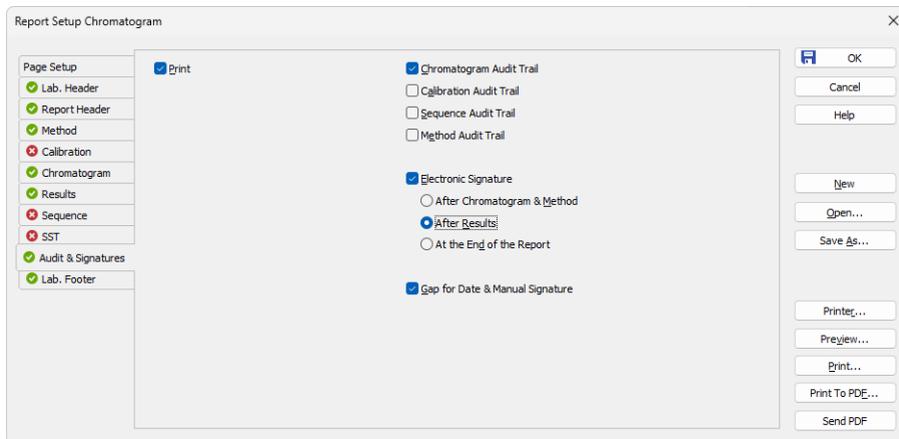


Fig. 233: Report Setup - Audit & Signatures

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.

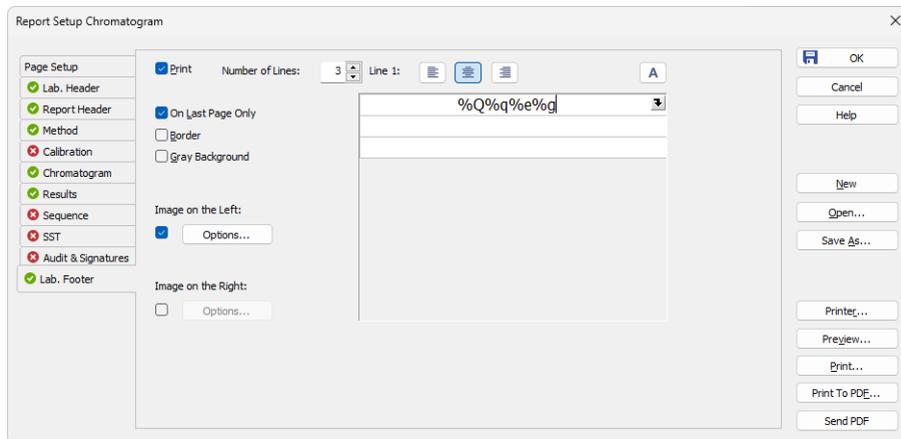


Fig. 234: Report Setup - Lab. Footer

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>Current User</i> | %k | Inserts the name of the currently logged user. |
| <i>Print Date and Time in current Win format</i> | %R | Insert the date and time of printing in currently used windows format. |
| <i>Instrument Name</i> | %e | Inserts value of the <i>Instrument Name</i> . |
| <i>The percent 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.

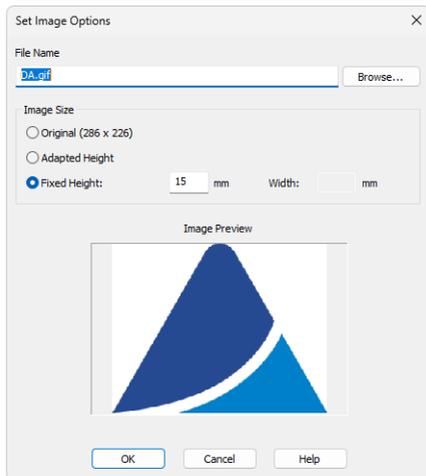


Fig. 235: Set Image Options

File Name

Displays the filename of the image including its path (relative to the **Clarity** root directory). **Clarity** supports various image file 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 this is a chromatogram plot showing Voltage [mV] vs Time [min] with several peaks labeled. At the bottom is a 'Result Table (ISTD - Data|PERS01)' with columns for Reten. Time, Response, Amount, Amount%, Peak Type, and Compound Name.

Chromatogram Info:

- File Name : C:\Clarity\DataFiles\DEMO1\Data\PERS01.prm
- Origin : 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 Data:

| Peak | Retention Time [min] | Approximate Voltage [mV] |
|------|----------------------|--------------------------|
| 1 | 1.19 | ~1 |
| 2 | 1.75 | ~1 |
| 3 | 2.30 ETHANOL | ~12 |
| 4 | 2.55 | ~1 |
| 5 | 2.857 T-BUTANOL | ~15 |

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.

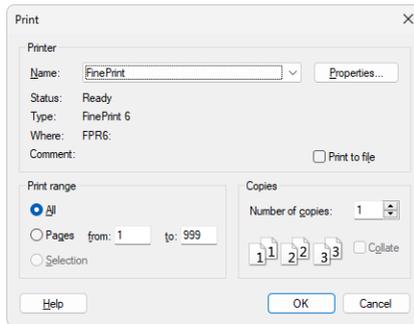


Fig. 237: Print

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:

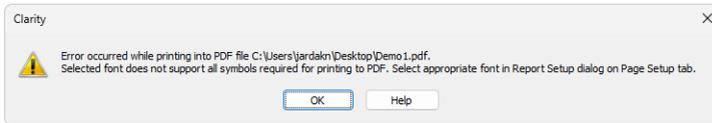


Fig. 238: Font with missing symbols

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

9.1.1 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.

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. To add device to the instrument drag always one device at once.

Cannot add selected (sub)device:

The message lists the reasons, why it is not possible to add selected device to the Instrument (for example the device and selected Instrument Type exclude each other, or the station does not have unlocked corresponding license, the device is already added to another Instrument, etc.).

Cannot create Detector/Pump/Autosampler...

This error message can occur if the device requires registration of an library, that was not successful. Please contact our support.

Cannot create RAW file

Cannot create raw file C:\Users\\AppData\Local\Temp\Clarity\\${ch1}temp.raw indicates some problems during creation of the chromatogram at the end of the analysis.

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 establish communication with XXXX SN xxx! XXXX SN xxx might not be turned on, connected, installed, configured or it might be malfunctioning or in use by another user.

In an attempt to open Instrument which has an uncommunicative device in configuration (e.g. the device is turned OFF). Retry if you think you resolved the problem (e.g., you turned the device ON), or cancel to continue to Instrument window that will be in Communication Error state - no measurement possible, but you can work with already measured chromatograms or prepare methods/sequences.

Cannot open file XXX. The file is already open on Instrument YYY.

If you attempt to open any file that is already opened on another instrument.

Cannot open USB communication for XY

For example Colibrick. Possible causes are if the A/D converter is connected over a USB hub or if there is a problem with DLL registration.

Changing project requires to restart instrument. (You will be prompted to save modified files.) Is this OK ?

If you have unsaved changes in any window of the Instrument and you also want to change a project.

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 (CLARITY\CFG).

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, or in the case you have made back up of Clarity.psw file, you can use it now, and do not have to set all the user accounts and settings again.

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. Used Clarity.cfg is empty so all the *System Configuration* settings and adding devices to the Instruments have to be done again.

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. If possible you can try to copy Clarity.cfg from installation media, or another installation of Clarity, and rewrite the corrupted file with it. Then you will have to manually reconfigure the *System Configuration* settings.

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 A/D converter during acquisition.

Error Occurred During Setup.

This message can happen during the configuration of a control module.

FAILED to send method to (sub)device

If the sending of the method is unsuccessful, e.g., device stops communicating with any of its parts.

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 anymore.

Method file XXX does not exist. Please select a valid method. For more information about warnings and errors on the other rows, point mouse cursor over the left side of "Status" Column for each row.

This happens when opening or checking a sequence which contains a name of a non-existent method.

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. Please contact our support.

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.

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. If you select Yes, the project *.prj file will be created, and Project can be used.

Project file <Project name> already exists but has no project directory! Do you want to create the project directory?

Project *.prj file with given name already exists, but there is no project folder with matching name. If you select Yes, the empty project folder with matching name will be created.

Project <Project name> already exists! Choose a different name.

Project with this name already exists. Select unique name for newly created project.

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/renaming or damaging the respective directory in the meantime.

The report style "*.sty" does not exist or is damaged. Default report style "Noname" will be used instead.

This message appears during the opening of any window while deleting/renaming 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 filter is applied to a too large interval.

Unable to lock instrument in unprotected mode!

When no user is created and you attempt to Lock an opened instrument.

XXX.met does not match current instrument configuration. To use this method for acquisition, it must be adapted and then saved. Do you want to adapt the method? If you click No method will be opened as read only.

If the instrument or method being opened does not correspond to the hardware which is currently present in the configuration.

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.

9.1.1.1 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.

9.1.2 Report error after Clarity crashed



Fig. 239: Send Report dialog

If **Clarity** encounters a serious problem and crashes, it will invoke a dialog during the crash that offers to report the problem to **DataApex**. Such reports help us locate the conditions leading to crashes and fix the faulty behavior accordingly.

However, in some cases, **Clarity** may crash without producing any message. In such cases, a 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. 54.

9.1.3 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 problems due to exhausted memory for the 32-bit Clarity process.

If an external control module process encounters a problem, the following message pops up. Communication error is invoked, and it is necessary to restart Clarity before further usage to prevent unanticipated behavior.

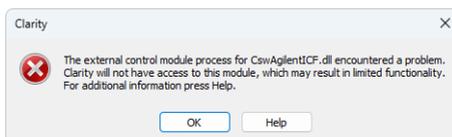


Fig. 240: External control module process error message

Until Clarity is restarted, it is not possible to enter the *System Configuration* dialog to prevent configuration corruption - the following message displays when trying to open the *System Configuration* dialog.

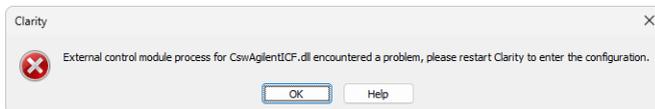


Fig. 241: Entering System Configuration disabled error message

9.1.4 Development version of Control Module

If Clarity detects a control module that is under development, it will display a yellow stripe in the *Instrument* window with the following text: *Development version of control modules: [module name]*.

Control modules under development have not yet passed DataApex quality assessment tests. Once tested and approved, they will be officially available in Clarity, and the yellow stripe will disappear.

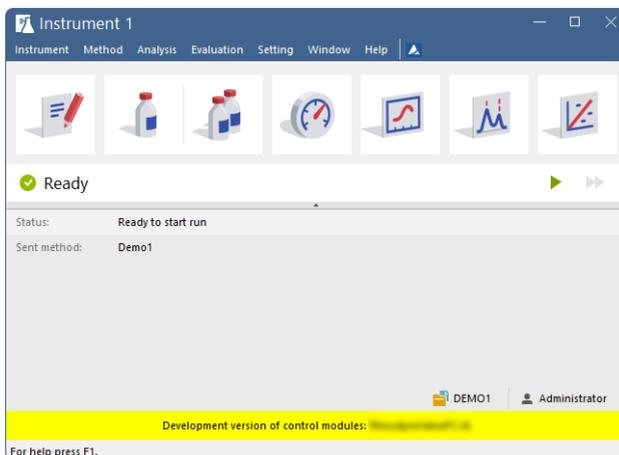


Fig. 242: Instrument window - Development version of control modules

9.1.5 Unauthorized Control Module

If a control module was not installed correctly, it is labeled as an unauthorized control module. DataApex is not liable for correct functionality of the given control module. Station with unauthorized control modules loses DataApex support.

In case Clarity detects that an unauthorized control module is configured on any Clarity Instrument, it will remove it from the configuration of the corresponding Instrument. The following message will appear just after Clarity start and this action will be logged in the *Audit Trail* as well.

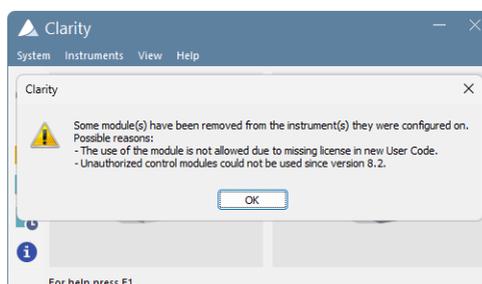


Fig. 243: Main window - Removal of unauthorized module from configuration

Once the unauthorized control module has been removed from [System Configuration](#) it cannot be assigned to an Instrument anymore.

If you installed Clarity according to our installation procedure, you will never experience the yellow stripe informing about unauthorized control modules.

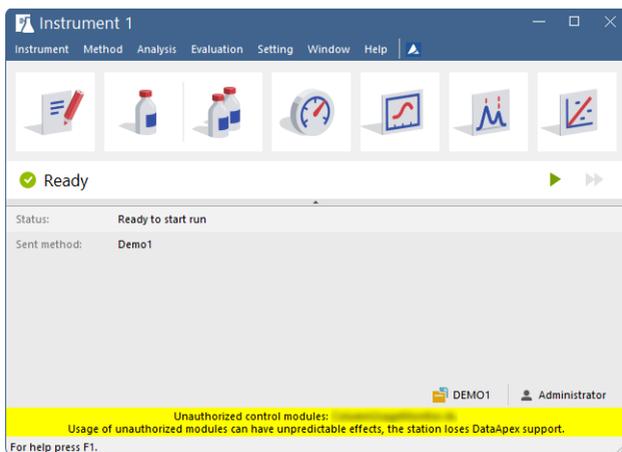


Fig. 244: Instrument window - Unauthorized control modules

Unauthorized UNI Ruby control modules can be configured on a Clarity Instrument via the UNI Ruby module accessible from the *Auxiliary* section of the "Available Control Modules" on page 13. It is important to acknowledge that any unauthorized control modules may be responsible for incorrect functionality (not Clarity itself).

9.2 How to get help

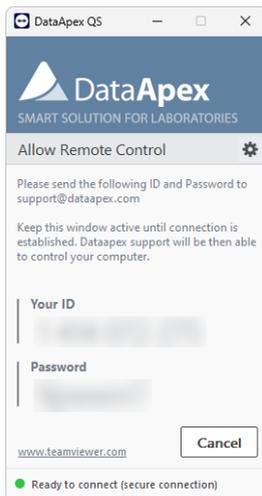
Invoke the help in **Clarity** and try to use fulltext search.

Consult the **Troubleshooting** chapter of the **User Guide** 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.

Solutions to problems connected to particular **hardware** can be found in the corresponding manuals.

As the last option when troubleshooting complicated issues, **DataApex** may provide remote support via **TeamViewer QuickSupport** to registered customers (paid service). To use this option, the user must first contact **DataApex Technical Support** (support@dataapex.com). The **TeamViewer QuickSupport** application can be downloaded by clicking *Help - TeamViewer QS* in the main *Clarity* window. The application is ready to be used directly after downloading.



10 Appendices

10.1 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

Access rights determine what actions users can perform in the system. For example, some users may have restricted permissions to change fundamental station settings, access certain instruments, or modify certain documents (e.g., methods).

Active calibration signal

When performing a multi-detector measurement, each calibration file can contain calibration curves for up to 32 signals, just like chromatograms. However, only one signal can be active and its data modified at any given time.

The active calibration signal, whether its table or curve, is identified by its name (or number if no standard chromatogram is opened), which is highlighted in the header of the Calibration Summary Table or in the calibration curve itself. Additionally, all signal-specific values are 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 displayed data and performed operations will only relate to this active chromatogram. The name of the active chromatogram is highlighted in the legend by bold letters.

Active chromatogram signal

When performing a multi-detector measurement, each chromatogram file may contain up to 32 detector 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 legend by bold letters.

Active detector

A detector selected in the *Select Detector* field, whose measurement and calculation parameters are displayed in the [Acquisition](#) or [Calculation](#) tabs in the [Method Setup](#) dialog. 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 is an 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 imports raw data, not the results.

Calibrated group

A group of peaks calibrated as a single component.

Calibration file (*.cal)

Contains calibration curves of all added compounds and further data, e.g., their amounts on different levels, for calibrated results.

Calibration standard

A chromatogram containing known amounts of compounds you want to evaluate 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

A version of the **Clarity** station that, does not allow the data acquisition, it is intended for data evaluation from another PC.

Configuration of the station

Holds the information about the number of Instruments, and the allocation of connected devices to each active instrument.

Desktop file (*.dsk)

A file used to store the user settings, such as User Options, size, location and appearance of all windows and panes, user columns.

Direct control of chromatograph (autosampler, pump)

An integrated additional module for selected devices (pumps, autosamplers etc.) enabling the direct control and monitoring of selected parameters. For example, directly controlled detectors (UV-VIS, PDA, etc.) gather digital data (or even the spectra) directly from the controlled instrument.

Electronic signature

The electronic signatures must fulfill the same function and prerequisites as the handwritten ones. 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.

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 set in the [Clarity](#) for each Instrument, where projects including all chromatographic data are located.

Integration Table

A part of the processing method that lists all operations affecting the chromatogram's peak integration. Integration is the process of determining peak areas and heights, essential for quantitative analysis. The table displays all modifications to the baseline or peaks applied to the chromatogram.

Locked file (READ ONLY)

A file that can only be read and not modified. The file may be *READ ONLY* for several reasons, including (but not exclusive to) chromatogram measured in *GLP mode* and opened outside of it, historic version of a chromatogram, or when a user account not having user rights to modify method/chromatogram/sequence etc.

Locked instrument

An Instrument with locked control. Lock mode can be activated using a command from the *Lock* submenu in the main [Clarity](#) window. An Instrument is unlocked by logging in as the same user who locked it, or anyone who has the Access Right *Take Control of Locked Instrument*.

Method file (*.met)

Defines the parameters of the acquisition and processing of the data. Its name is displayed in the **Information Table** of the [Instrument](#) window and its content is always copied to the newly created chromatogram.

Multi-detector configuration (measurement)

Setting of the station so that it measures and evaluates chromatograms with more than one detector's signal.

Printout

The layout of individual segments that should be printed (e.g., results, measurement conditions). The layout is defined by the report style.

Project directory

Directory used to store all files associated with the project (for example method, sequence, calibration files).

Project file (*.prj)

Identifies what project directory will be used, and holds the information about recently opened files.

Protected mode

A regime which enables only authorized users (users who have an account created in the [User Accounts](#) dialog) to work with the station and access data.

Raw data file - RAW

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 file (*.sty)

Defines what information will be included in a report and how it will be printed.

Sequence file (*.seq)

Defines a set of analyses to be performed automatically, storing all necessary parameters for each run, such as the measurement method, sample injection volume, and other analysis settings.

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 - see "Adjusting the size of panels".

System Suitability Test - SST

The Extension serves for statistic evaluation of the parameters from measured chromatograms. It can be used to validate the chromatographic system.

Status table

A table displayed in the [Instrument](#) window containing the names of system files, the status of the analysis currently in progress.

Tab

A tab is a section within a window or dialog that organizes different settings or options. Only one tab is visible at a time, and you can switch between them by clicking on their labels.

Toolbar

A toolbar is a set of icons that represent various commands. It's typically located at the top or side of the screen and can be customized by going to *View - Customize...* or by

right-clicking on the toolbar to open the context 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.

10.2 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 | |
| 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 | |
| Ctrl + ↓ | <i>Skip</i> | Skip the current sample | Sequence |
| 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 | |

11 Technical Specification

11.1 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.

11.2 Command line parameters

Command line parameters in Clarity allow for automation and remote control of various functions, including opening files, controlling instruments, managing calibrations, and running sequences.

11.2.1 Using Command Line Parameters

- Command line parameters can be used to start Clarity with predefined settings or to send commands to an already running instance.
- Parameters are processed in the order they are specified.
- Some parameters can also be defined in the OTHERS.INI configuration file, which overrides command line parameters.
- All used command line parameters are logged in the Audit Trail.
- Only one project file (.PRJ), one method file (.MET), and one sequence file (.SEQ) can be opened at a time per instrument; if multiple are specified, only the first one will be opened.
- Multiple chromatograms (.PRM) can be opened from a single command.
- Some parameters, like `cfg`, are ignored if Clarity is already running, and some like `user`, `password`, and `dsk` are ignored if an instrument is already open.
- Opening files may be blocked by certain conditions, such as an active sequence, an open modal dialog, or insufficient permissions to modify a project or method.
- Configuration files such as `.CFG`, `.SNO`, `.PSW`, and `.DSK` should be stored in the same directory to avoid incorrect behavior.
- The maximum command line length is 126 characters; exceeding this will result in a warning.
- All parameters (except file paths) are case-sensitive, unless stated otherwise.
- If spaces are needed in the command, enclose the value in quotation marks.

11.2.1.1 Example Usage

Correct syntax:

- *Clarity.exe command=value*

Incorrect syntax (spaces are not allowed):

- *Clarity.exe command = value*

To use file paths or values with spaces, enclose them in quotes:

- *Clarity.exe c="C:\Documents and Settings\Smith\Desktop\Ethanol in blood.met"*
- *Clarity.exe user="John Doe"*

11.2.2 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=PATH\FILENAME`

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 DATAAPEX.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. 135). 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. 135). 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

Exports the *Autostop Run Time* value from the method currently opened on the Instrument as ANSI text into the specified file.

description: 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

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.

description:

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

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.

description:

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.

The meaning of values are as follows:

possible values: 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

example: `clarity.exe i=3`

To work with two or more Instruments at once, you should use the MS Batch "START" command. "Examples" on page 500 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. 122). 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\<user name>\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` or
`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

In case the further command line parameters are wrong, **Clarity** will not try to open again.

description: 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 175.

syntax: `prm_export=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: None.

example: `clarity.exe prm_export="C:\Users\<user name>\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 175. 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\<user name>\AppData\Local\Temp\CLARITY\1.chr"`

prm_import_ex

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 175. 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.

description:

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

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.

description:

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.

example: `clarity.exe report_last_only`

resume_seq

description: 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.

syntax: `resume_seq=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 resume_seq=3` (will resume sequence measurement on Instruments 1 and 2)

run

description: 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.

syntax: `run=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 run=7` (will run single analysis on Instruments 1, 2 and 3)

run_seq

description: 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.

syntax: `run_seq=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 run_seq=7` (will run sequence measurement on Instruments 1, 2 and 3)

seq_export

description: Exports the active sequence into the specified *.TXT file.

syntax: `seq_export=PATH\FILENAME`

possible values: A valid path and filename.

implicit value: 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

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.

description:

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 500 section below the commands for more information.

seq_import_append

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.

description:

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 analysis 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)

stop_seq

description: Stops the sequence measurement after completing the current analysis on the specified Instrument.

syntax: `stop_seq=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 sequence after finishing current analysis 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.

clarity.exe u="John Doe"

example: **Clarity** will automatically log in the user account called "John Doe".

11.2.3 Examples

11.2.3.1 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
```

11.2.3.2 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"          cal_
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
```

11.2.3.3 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

11.3 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. 82).

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. 82).

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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